



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:55 PM EDT

PDB ID : 1DDX
Title : CRYSTAL STRUCTURE OF A MIXTURE OF ARACHIDONIC ACID AND PROSTAGLANDIN BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2: PROSTAGLANDIN STRUCTURE
Authors : Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.
Deposited on : 1999-11-11
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

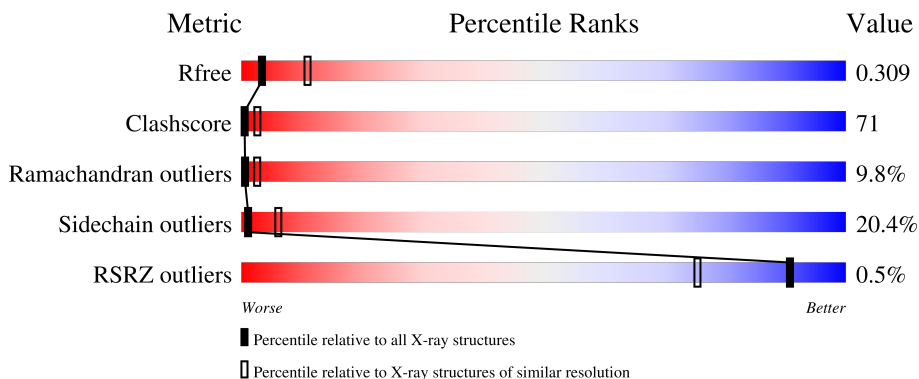
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	
1	B	552	
1	C	552	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36.2

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Mol	Chain	Length	Quality of chain
1	D	552	 18% 60% 20%
2	E	2	 100%
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	2	-	-	-	X
2	NAG	F	2	-	-	-	X
2	NAG	G	2	-	-	-	X
2	NAG	H	2	-	-	-	X
3	NAG	C	2681	-	-	-	X
4	BOG	A	702	-	-	-	X
4	BOG	C	2702	-	-	-	X
4	BOG	D	3702	-	-	-	X
5	PGX	A	701	-	-	X	X
5	PGX	B	1701	-	-	X	X
5	PGX	C	2701	-	-	X	X
5	PGX	D	3701	-	-	X	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18477 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4475	2885	750	815	25	0	0	0
1	B	552	4475	2885	750	815	25	0	0	0
1	C	552	4475	2885	750	815	25	0	0	0
1	D	552	4475	2885	750	815	25	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



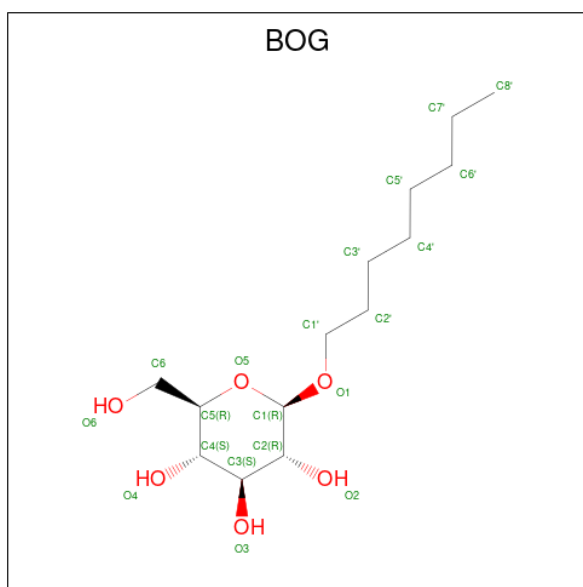
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0
2	G	2	28	16	2	10	0	0	0
2	H	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



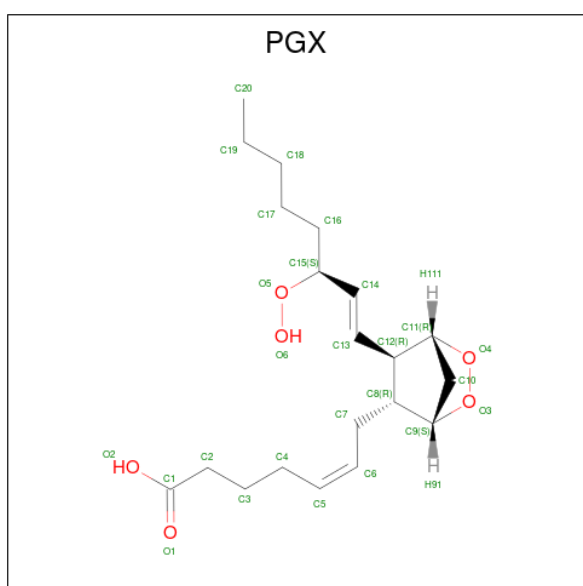
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	C	1	Total 14	C 8	N 1	O 5	0	0
3	C	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	B	1	Total C O 20 14 6	0	0
4	C	1	Total C O 20 14 6	0	0
4	D	1	Total C O 20 14 6	0	0

- Molecule 5 is 7-[6-(3-HYDROPEROXY-OCT-1-ENYL)-2,3-DIOXA-BICYCLO[2.2.1]HEPT-5-YL]-HEPT-5-ENOIC ACID (three-letter code: PGX) (formula: $C_{20}H_{32}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	20	5		
5	B	1	Total	C	O	0	0
			25	20	5		
5	C	1	Total	C	O	0	0
			25	20	5		
5	D	1	Total	C	O	0	0
			25	20	5		

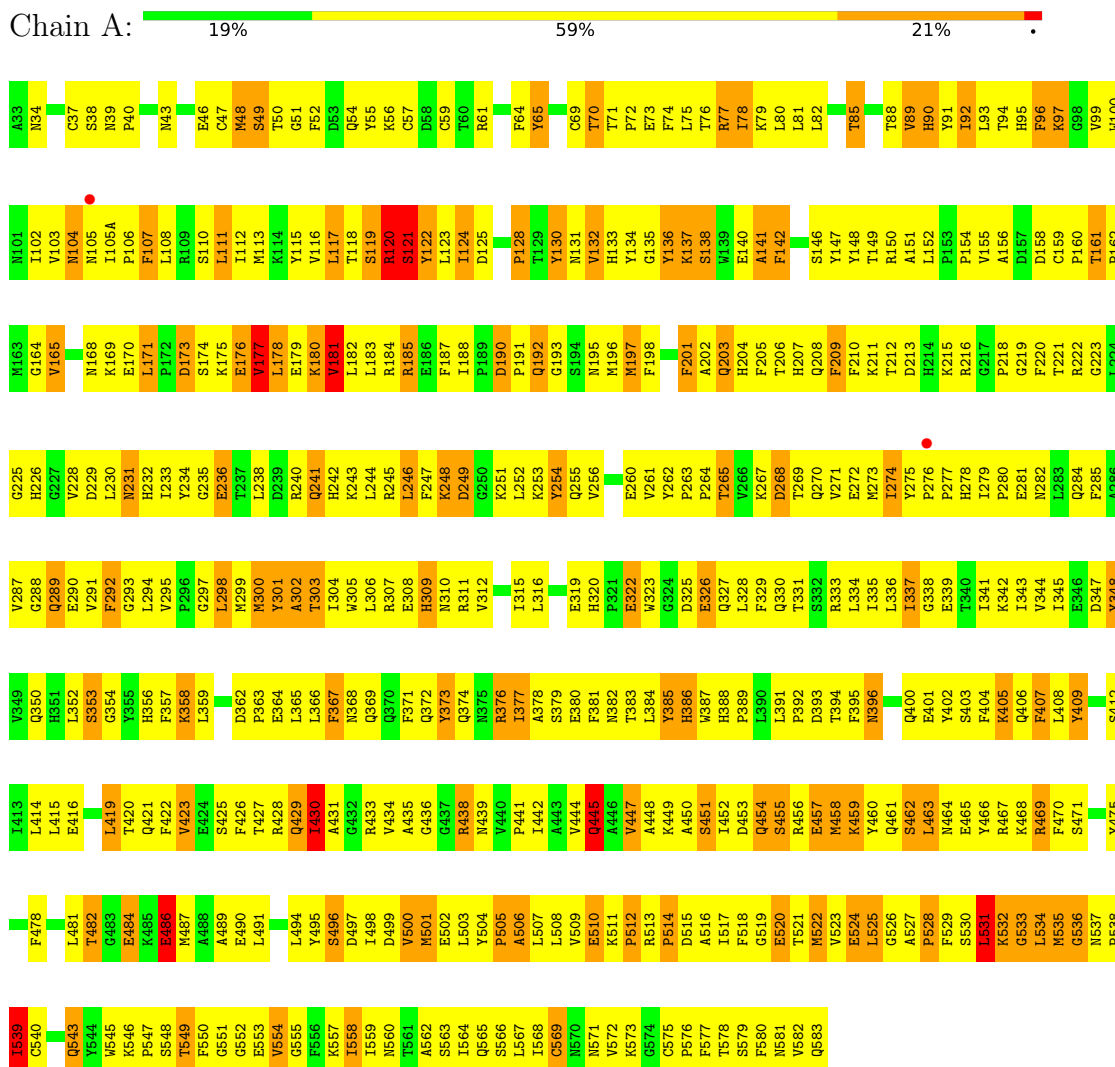
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	39	Total	O	0	0
			39	39		
6	C	46	Total	O	0	0
			46	46		
6	D	43	Total	O	0	0
			43	43		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)



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Q2289	S2353	G2483	Y2544	G3088	C3159	F3220	N3282	E3346	Y3409	F3470
E2290	G2354	E2484	W2545	V3089	P3160	T3221	L3283	D3347	S3412	S3471
W2291	F2295	K2485	K2546	W3101	T3161	R3222	L3284	Y3348	S3413	L3472
F2292	H2356	E2486	P2547	N3102	P3162	G3225	F3285	V3349	T3414	Y3475
G2293	F2357	M2487	S2548	V3103	M3163	H3226	A3286	H3350	L3415	E3480
L2294	K2358	M2488	T2549	V3104	G3164	H3227	V3287	L3351	L3416	L3481
V2295	L2359	E2489	F2550	N3105	V3165	G3228	G3289	L3352	E3417	E3481
		E2490	G2551	N3106	N3166	S3229	E3290	S3353	G3418	E3482
		L2491	E2552	F3107	K3169	R3230	E3291	G3354	L3419	L3483
		R2492	E2553	P3108	K3170	L3231	F3292	H3355	L3420	G3484
		A2493	W2554	L3108	E3171	H3232	G3293	F3357	Q3421	E3484
		L2494	L3109	L3108	P3172	H3233	G3294	K3358	F3422	E3485
		L2495	F2556	L3111	D3173	Y3234	V3295	L3359	V3423	E3486
		S2496	K2557	L3112	S3174	G3235		M3424	E3424	M3487
		R2497	I2558	M3113	K3175	E3236	L3298	S3425	S3425	G3490
		L2498	L2559	K3114	K3176	R3237	M3299	F3426	S3426	E3491
		Q2370	L2560	F3115	E3177	L3238	N3300	T3427	F3427	L3491
		R2371	N2561	W3116	V3178	D3239	Y3301	R3428	T3428	K3492
		F2372	G2562	L3117	L3178	D3240	A3302	Q3429	Q3429	A3493
		E2373	I2563	L3118	K3179	R3241	A3303	F3430	F3430	L3494
		M2310	O2564	T3119	K3180	Q3242	T3303	F3431	F3431	Y3495
		R2375	L2565	S3119	L3181	H3243	L3304	A3432	A3432	S3496
		R2376	S2566	K3120	L3182	K3244	W3305	Q3433	Q3433	D3497
		L2377	L2567	S3121	L3183	L3245	L3306	R3434	R3434	L3498
		I2378	L2568	Y3122	R3184	R3246	R3307	F3435	F3435	D3499
		A2378	C2569	L1223	R3185	F3247	E3308	A3436	A3436	V3500
		S2379	M2570	L1224	E3186	K3248	H3309	G3437	G3437	M3501
		E2380	Q2569	T3062	F3187	F3249	N3310	Q3438	Q3438	E3502
		F2381	W2571	G3063	L3188	R3249	R3311	R3439	R3439	E3503
		E2382	K2572	F3064	L3189	G3250	G3312	N3440	N3440	L3504
		T2383	K2573	Y3065	F3190	F3251	V3313	F3441	F3441	P3505
		T2384	P2576	G3066	D3191	L3252	L3315	T3442	T3442	P3506
		L2385	F2577	G3067	P3192	L3253	L3316	L3443	L3443	L3507
		H2386	L2578	C3069	Q3192	K3254	R3317	A3444	A3444	L3508
		W2387	S2579	T3070	K3193	Y3255	G3318	V3445	V3445	V3509
		E2395	S2580	T3071	S3194	Q3256	E3319	Q3446	Q3446	E3510
		R2388	N2581	P3072	N3195	V3256	E3319	A3447	A3447	K3511
		Q2327	W2582	E3073	M3196	I3257	E3322	A3448	A3448	P3512
		L2390	Q2583	F3074	M3197	L3258	W3323	K3449	K3449	P3514
		F2329	Q2583	F3075	F3198	E3260	G3324	A3450	A3450	D3515
		Q2330	T2331	L3076	A3199	V3261	F3325	A3451	A3451	A3516
		L2334	L2334	T3076	F3200	Y3262	D3326	I3452	I3452	I3517
		L2335	L2335	R3077	F3201	P3263	E3326	D3453	D3453	F3518
		L2336	Q2461	K3079	A3202	P3264	L3328	Q3454	Q3454	G3519
		L2337	S2462	L3080	Q3203	T3265	L3329	S3455	S3455	E3520
		G2338	S2462	L3081	H3204	Y3266	Q3330	S3456	S3456	T3521
		E2401	L2463	L3082	F3205	K3267	T3331	E3457	E3457	T3522
		E2399	L2463	T3085	F3196	D3268	L3334	M3458	M3458	M3522
		F2394	L2463	T3086	K3137	V3269	L3335	K3459	K3459	V3523
		F2395	N2464	T3087	K3137	E3272	L3336	Y3460	Y3460	E3524
		L2340	N2464	T3088	F3209	E3273	L3337	Q3461	Q3461	L3525
		F2404	E2465	T3089	K3210	M3274	L3338	S3462	S3462	G3526
		F2404	E2465	T3090	T3210	E3274	G3338	L3463	L3463	A3527
		K2405	R2466	T3091	T3212	Y3275	E3339	L3464	L3464	P3528
		Q2406	R2466	T3092	D3213	P3276	E3340	N3465	N3465	F3529
		Q2406	R2469	T3092	L3154	P3277	L3341	F3466	F3466	S3530
		L2344	L2534	T3092	L3155	H3278	L3342	Q3467	Q3467	L3531
		L2345	M2535	T3092	V3155	H3279	L3343	K3468	K3468	K3532
		L2346	G2536	T3092	A3156	I3279	L3344	L3469	L3469	G3533
		L2347	M2537	T3092	D3157	P3280	L3345			
		L2348	L2472	T3092	F3094	E3281	L3345			
		Y2349	Y2475	T3092	F3096	E3281	L3345			
		Q2350	L2481	T3092	F3096	E3281	L3345			
		L2352	T2482	T3092	K3097	E3281	L3345			

• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)



N3033	N3034	F3035	C3036	C3037	S3038	N3039	F3040	N3043	E3044	K3048	S3049	T3050	L2560	S2563	I2564	Q2565	E2502	G2437	R2438	L2503	Y2504	S2566	L2567	L2568	C2569	M2570	W2571	K2572	P2576	F2577	L2515	A2450	S2451	R2452	D2453	Q2454	S2455	R2456	M2522	F2523	E2524	L2525	G2526	A2527	F2529	M2530	E2465	S2466	R2467	L2533	L2534	M2535	S2471	R2469	F2470	L2408	G2536	M2537	L2472	S2412	E2413	L2414	H2351	E2416
G3088	V3089	W3101	N3102	V3103	N3104	N3105	N3106	L3107	L3108	L3111	L3112	M3113	F3114	W3115	V3116	L3117	L3118	S3119	K3120	S3121	Y3122	L1223	L3124	D3125	S3126	F3127	P3128	T3129	Y3130	N3131	V3132	H3133	E3073	Y3134	G3135	Y3136	T3076	R3077	W3139	K3078	E3140	A3141	F3142	S3143	S3146	Y3147	Y3148	T3149	R3150	A3151	L3152	Y3091	L3092	P3153	L3092	L3092	V3155	A3156	D3157	F3096	K3097	D3158		
C3159	P3160	T3161	P3162	M3163	G3164	V3165	N3168	K3169	E3170	L3171	P3172	D3173	S3174	K3175	E3176	V3177	L3178	E3179	K3180	L3181	L3182	L3183	R3184	R3185	E3186	F3187	L3188	R3189	D3190	P3191	Q3192	K3193	S3194	N3195	M3196	M3197	F3198	A3199	F3200	F3201	A3202	Q3203	H3204	F3205	T3206	H3207	Q3208	F3209	F3210	K3211	T3212	D3213	L3214	H3215	P3276	P3277	H3216	G3217	P3218	G3219				
F3220	T3221	R3222	G3225	H3226	G3227	V3228	S3229	R3230	L3231	L3232	D3233	Y3234	G3235	E3236	L3237	L3238	D3239	R3240	Q3241	H3242	K3243	L3244	R3245	L3246	F3247	K3248	R3249	G3250	F3251	L3252	K3253	Y3254	Q3255	V3256	I3257	E3260	V3261	Y3262	P3263	P3264	T3265	Y3266	K3267	D3268	T3269	Q3270	E3271	E3272	M3273	L3274	Y3275	L3276	H3277	P3278	L3279	P3280	E3281							
N3282	L3283	G3284	F3285	A3286	H3287	G3288	E3289	E3290	F3291	L3292	F3292	G3293	L3294	V3295	L3298	M3299	E3300	Y3301	A3302	T3303	L3304	W3305	L3306	R3307	E3308	H3309	N3310	R3311	G3312	L3315	L3316	R3317	G3318	E3319	E3322	W3323	G3324	D3325	E3326	P3327	L3328	F3329	Q3330	T3331	L3334	L3335	L3336	L3337	G3338	E3339	L3340	S3341	F3404	K3405	Q3406	L3343	L3344	L3345						
E3346	D3347	Y3348	V3349	K3350	H3351	L3352	G3353	S3354	E3355	L3356	D3362	P3363	E3364	L3365	L3366	F3367	N3368	Q3369	F3370	F3371	Q3372	Y3373	Q3374	N3375	R3376	I3377	A3378	S3379	E3380	F3381	V3382	N3383	T3384	Y3385	H3386	W3387	H3388	P3389	L3390	L3391	P3392	D3393	T3394	F3395	N3396	Q3400	E3401	Y3402	L3403	S3404	F3404	K3405	Q3406	L3407	K3408	R3409								
Y3409	S3412	T3413	L3414	L3415	E3416	H3417	G3418	L3481	L3482	L3483	F3426	T3427	R3428	Q3429	F3430	A3431	Q3432	R3433	F3434	A3435	G3436	M3437	N3438	N3439	F3440	P3441	L3442	A3443	V3444	Q3445	A3446	L3447	A3448	K3449	A3450	S3451	I3452	D3453	Q3454	S3455	R3456	T3457	M3458	K3459	Y3460	Q3461	S3462	L3463	N3464	F3464	Y3465	L3466	K3467	K3468	R3469									
F3470	S3471	L3472	Y3475	E3479	E3480	L3481	T3482	G3483	E3484	K3485	E3486	M3487	E3490	L3491	K3492	A3493	Y3495	D3497	I3498	D3499	V3500	M3501	E3502	L3503	Y3504	P3505	A3506	L3507	L3508	V3509	E3510	K3511	P3512	P3514	D3515	A3516	I3517	F3518	G3519	E3520	T3521	M3522	V3523	E3524	L3525	G3526	A3527	P3528	F3529	S3530	L3531	K3532	L3533											



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.24Å 134.80Å 122.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 36.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-3.00) 75.8 (36.19-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.00Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.267 , 0.324 0.254 , 0.309	Depositor DCC
R_{free} test set	4329 reflections (9.43%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.915	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18477	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGX, NAG, BOG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/4602	0.65	0/6239
1	B	0.45	0/4602	0.65	0/6239
1	C	0.45	0/4602	0.65	0/6239
1	D	0.46	0/4602	0.64	0/6239
All	All	0.45	0/18408	0.64	0/24956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4475	0	4373	650	0
1	B	4475	0	4373	653	0
1	C	4475	0	4373	663	0
1	D	4475	0	4373	668	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0
4	C	20	0	28	0	0
4	D	20	0	28	1	0
5	A	25	0	30	9	0
5	B	25	0	30	13	0
5	C	25	0	30	14	0
5	D	25	0	30	11	0
6	A	45	0	0	14	0
6	B	39	0	0	12	0
6	C	46	0	0	20	0
6	D	43	0	0	15	0
All	All	18477	0	17928	2579	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

All (2579) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3312:VAL:HA	1:D:3315:ILE:HD12	1.33	1.09
1:A:312:VAL:HA	1:A:315:ILE:HD12	1.33	1.08
1:B:1312:VAL:HA	1:B:1315:ILE:HD12	1.36	1.07
1:B:1301:TYR:HA	1:B:1304:ILE:HD12	1.37	1.07
1:A:99:VAL:HA	1:A:102:ILE:HD12	1.37	1.06
1:C:2273:MET:HE1	1:C:2287:VAL:HG22	1.36	1.05
1:C:2301:TYR:HA	1:C:2304:ILE:HD12	1.35	1.05
1:B:1099:VAL:HA	1:B:1102:ILE:HD12	1.38	1.05
1:D:3230:LEU:HB3	1:D:3233:ILE:HD12	1.39	1.04
1:D:3099:VAL:HA	1:D:3102:ILE:HD12	1.38	1.04
1:D:3301:TYR:HA	1:D:3304:ILE:HD12	1.35	1.03
1:C:2312:VAL:HA	1:C:2315:ILE:HD12	1.34	1.03
1:A:301:TYR:HA	1:A:304:ILE:HD12	1.37	1.02
1:B:1230:LEU:HB3	1:B:1233:ILE:HD12	1.39	1.01
1:C:2099:VAL:HA	1:C:2102:ILE:HD12	1.39	1.01
1:A:389:PRO:HG2	1:A:434:VAL:HG13	1.42	1.01
1:A:230:LEU:HB3	1:A:233:ILE:HD12	1.43	1.00
1:D:3273:MET:HE1	1:D:3287:VAL:HG22	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2208:GLN:HB3	1:C:2232:HIS:HD2	1.28	0.99
1:B:1208:GLN:HB3	1:B:1232:HIS:HD2	1.26	0.98
1:A:273:MET:HE1	1:A:287:VAL:HG22	1.46	0.98
1:D:3389:PRO:HG2	1:D:3434:VAL:HG13	1.44	0.97
1:A:208:GLN:HB3	1:A:232:HIS:HD2	1.29	0.96
1:B:1389:PRO:HG2	1:B:1434:VAL:HG13	1.48	0.96
1:B:1273:MET:HE1	1:B:1287:VAL:HG22	1.49	0.95
1:A:507:LEU:HD22	1:A:522:MET:HE3	1.49	0.94
1:C:2526:GLY:HA3	5:C:2701:PGX:H61	1.46	0.94
1:C:2385:TYR:HA	5:C:2701:PGX:O3	1.68	0.94
1:C:2308:GLU:HB2	1:C:2571:ASN:HD21	1.31	0.94
1:C:2507:LEU:HD22	1:C:2522:MET:HE3	1.50	0.94
1:D:3191:PRO:HD2	1:D:3433:ARG:HG3	1.50	0.94
1:D:3208:GLN:HB3	1:D:3232:HIS:HD2	1.32	0.94
1:A:308:GLU:HG3	1:A:336:LEU:HD11	1.49	0.93
1:B:1203:GLN:HG2	1:B:1298:LEU:HD11	1.49	0.93
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.50	0.93
1:B:1385:TYR:HA	5:B:1701:PGX:O3	1.68	0.93
1:A:308:GLU:HB2	1:A:571:ASN:HD21	1.31	0.93
1:B:1463:LEU:HD13	1:B:1506:ALA:HB3	1.48	0.92
1:B:1191:PRO:HD2	1:B:1433:ARG:HG3	1.51	0.92
1:C:2389:PRO:HG2	1:C:2434:VAL:HG13	1.50	0.92
1:A:463:LEU:HD13	1:A:506:ALA:HB3	1.50	0.92
1:B:1184:ARG:HD3	1:B:1187:PHE:HA	1.51	0.92
1:C:2463:LEU:HD13	1:C:2506:ALA:HB3	1.49	0.92
1:B:1245:ARG:HH22	1:B:1326:GLU:HG2	1.33	0.92
1:C:2191:PRO:HD2	1:C:2433:ARG:HG3	1.50	0.92
1:D:3463:LEU:HD13	1:D:3506:ALA:HB3	1.51	0.92
1:C:2230:LEU:HB3	1:C:2233:ILE:HD12	1.51	0.92
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.05	0.91
1:B:1308:GLU:HB2	1:B:1571:ASN:HD21	1.35	0.91
1:D:3308:GLU:HB2	1:D:3571:ASN:HD21	1.35	0.90
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.54	0.90
1:C:2308:GLU:HG3	1:C:2336:LEU:HD11	1.52	0.90
1:A:275:TYR:HE1	1:A:293:GLY:HA3	1.37	0.89
1:B:1308:GLU:HG3	1:B:1336:LEU:HD11	1.52	0.89
1:D:3308:GLU:HG3	1:D:3336:LEU:HD11	1.54	0.89
1:C:2184:ARG:HD3	1:C:2187:PHE:HA	1.55	0.89
1:C:2414:LEU:HA	1:C:2422:PHE:CE1	2.08	0.88
1:D:3203:GLN:HG2	1:D:3298:LEU:HD11	1.56	0.88
1:C:2203:GLN:HG2	1:C:2298:LEU:HD11	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3507:LEU:HD22	1:D:3522:MET:CE	2.03	0.87
1:C:2507:LEU:HD22	1:C:2522:MET:CE	2.04	0.87
1:D:3396:ASN:ND2	1:D:3401:GLU:HG2	1.89	0.87
1:B:1526:GLY:HA3	5:B:1701:PGX:H61	1.55	0.87
1:C:2391:LEU:HD23	1:C:2392:PRO:HD2	1.57	0.87
1:C:2502:GLU:HB2	1:C:2505:PRO:HG2	1.57	0.87
1:D:3414:LEU:HA	1:D:3422:PHE:CE1	2.10	0.87
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.39	0.86
1:A:502:GLU:HB2	1:A:505:PRO:HG2	1.57	0.86
1:B:1502:GLU:HB2	1:B:1505:PRO:HG2	1.56	0.86
1:A:526:GLY:HA3	5:A:701:PGX:H61	1.57	0.86
1:B:1507:LEU:HD22	1:B:1522:MET:CE	2.05	0.86
1:C:2275:TYR:HE1	1:C:2293:GLY:HA3	1.39	0.86
1:A:88:THR:HG22	1:A:92:ILE:HD11	1.58	0.86
1:A:350:GLN:HE22	1:A:358:LYS:HA	1.41	0.86
1:C:2245:ARG:HH22	1:C:2326:GLU:HG2	1.36	0.86
1:C:2350:GLN:HE22	1:C:2358:LYS:HA	1.39	0.86
1:D:3245:ARG:HH22	1:D:3326:GLU:HG2	1.40	0.86
1:D:3275:TYR:HE1	1:D:3293:GLY:HA3	1.41	0.86
1:D:3391:LEU:HD23	1:D:3392:PRO:HD2	1.58	0.86
1:D:3184:ARG:HD3	1:D:3187:PHE:HA	1.58	0.85
1:B:1275:TYR:HE1	1:B:1293:GLY:HA3	1.39	0.85
1:D:3088:THR:HG22	1:D:3092:ILE:HD11	1.58	0.85
1:C:2088:THR:HG22	1:C:2092:ILE:HD11	1.56	0.85
1:D:3507:LEU:HD22	1:D:3522:MET:HE3	1.56	0.85
1:B:1088:THR:HG22	1:B:1092:ILE:HD11	1.59	0.84
1:A:507:LEU:HD22	1:A:522:MET:CE	2.05	0.84
1:C:2103:VAL:HG22	1:C:2108:LEU:HB3	1.59	0.84
1:A:103:VAL:HG22	1:A:108:LEU:HB3	1.60	0.84
1:C:2419:LEU:O	1:C:2423:VAL:HG23	1.78	0.84
1:B:1350:GLN:HE22	1:B:1358:LYS:HA	1.42	0.84
1:A:184:ARG:HD3	1:A:187:PHE:HA	1.58	0.83
1:B:1414:LEU:HA	1:B:1422:PHE:CE1	2.13	0.83
1:C:2322:GLU:HG2	1:D:3052:PHE:N	1.94	0.83
1:B:1396:ASN:ND2	1:B:1401:GLU:HG2	1.92	0.83
1:D:3338:GLY:HA3	1:D:3559:ILE:HD13	1.60	0.83
1:C:2051:GLY:C	1:D:3322:GLU:HG2	1.98	0.82
1:D:3350:GLN:HE22	1:D:3358:LYS:HA	1.42	0.82
1:C:2396:ASN:ND2	1:C:2401:GLU:HG2	1.94	0.82
1:D:3502:GLU:HB2	1:D:3505:PRO:HG2	1.59	0.82
1:A:391:LEU:HD23	1:A:392:PRO:HD2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1507:LEU:HD22	1:B:1522:MET:HE3	1.61	0.82
1:D:3103:VAL:HG22	1:D:3108:LEU:HB3	1.62	0.82
1:B:1391:LEU:HD23	1:B:1392:PRO:HD2	1.61	0.82
1:D:3230:LEU:HG	1:D:3337:ILE:HG13	1.63	0.81
1:B:1208:GLN:HB3	1:B:1232:HIS:CD2	2.14	0.81
1:C:2387:TRP:CZ2	5:C:2701:PGX:H71	2.16	0.81
1:D:3526:GLY:HA3	5:D:3701:PGX:H61	1.62	0.81
1:A:396:ASN:ND2	1:A:401:GLU:HG2	1.95	0.81
1:A:197:MET:HE1	1:A:423:VAL:HA	1.63	0.80
1:A:216:ARG:HB3	1:A:220:PHE:CD1	2.17	0.80
1:D:3273:MET:SD	1:D:3290:GLU:HA	2.20	0.80
1:A:537:ASN:OD1	1:A:539:ILE:HG23	1.81	0.80
1:C:2534:LEU:HD22	5:C:2701:PGX:H182	1.62	0.80
1:A:275:TYR:CE1	1:A:293:GLY:HA3	2.16	0.80
1:B:1103:VAL:HG22	1:B:1108:LEU:HB3	1.64	0.80
1:A:338:GLY:HA3	1:A:559:ILE:HD13	1.62	0.80
1:C:2208:GLN:HB3	1:C:2232:HIS:CD2	2.14	0.80
1:C:2456:ARG:HA	6:C:4117:HOH:O	1.80	0.80
1:B:1338:GLY:HA3	1:B:1559:ILE:HD13	1.63	0.80
1:A:322:GLU:HG2	1:B:1052:PHE:N	1.96	0.79
1:B:1178:LEU:HA	1:B:1182:LEU:HD12	1.65	0.79
1:C:2578:THR:HG22	1:C:2579:SER:N	1.98	0.79
1:D:3208:GLN:HB3	1:D:3232:HIS:CD2	2.18	0.79
1:D:3578:THR:HG22	1:D:3579:SER:N	1.96	0.79
1:A:51:GLY:C	1:B:1322:GLU:HG2	2.03	0.79
1:D:3182:LEU:O	1:D:3438:ARG:HA	1.82	0.79
1:A:419:LEU:O	1:A:423:VAL:HG23	1.82	0.79
1:A:88:THR:O	1:A:91:TYR:HB3	1.83	0.79
1:C:2275:TYR:CE1	1:C:2293:GLY:HA3	2.18	0.78
1:A:161:THR:HG21	1:A:165:VAL:O	1.83	0.78
1:D:3275:TYR:CE1	1:D:3293:GLY:HA3	2.18	0.78
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.15	0.78
1:A:578:THR:HG22	1:A:579:SER:N	1.98	0.78
1:C:2273:MET:SD	1:C:2290:GLU:HA	2.24	0.78
1:D:3312:VAL:HA	1:D:3315:ILE:CD1	2.14	0.78
1:A:276:PRO:HD2	1:A:279:ILE:HG13	1.66	0.78
1:B:1275:TYR:CE1	1:B:1293:GLY:HA3	2.17	0.78
1:C:2387:TRP:HZ2	5:C:2701:PGX:H71	1.48	0.78
1:B:1088:THR:O	1:B:1091:TYR:HB3	1.84	0.78
1:A:414:LEU:HD11	1:A:419:LEU:HD22	1.66	0.77
1:B:1216:ARG:HB3	1:B:1220:PHE:CD1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2322:GLU:HG2	1:D:3051:GLY:C	2.03	0.77
1:B:1182:LEU:O	1:B:1438:ARG:HA	1.84	0.77
1:D:3161:THR:HG21	1:D:3165:VAL:O	1.83	0.77
1:D:3449:LYS:HA	1:D:3452:ILE:HD12	1.66	0.77
1:C:2449:LYS:HA	1:C:2452:ILE:HD12	1.65	0.77
1:D:3149:THR:O	1:D:3378:ALA:HA	1.84	0.77
1:A:185:ARG:HH21	1:A:438:ARG:NE	1.83	0.77
1:B:1553:GLU:OE1	1:B:1553:GLU:HA	1.83	0.77
1:D:3188:ILE:HD12	1:D:3439:ASN:HB2	1.66	0.77
1:D:3216:ARG:HB3	1:D:3220:PHE:CD1	2.20	0.77
1:D:3414:LEU:HD11	1:D:3419:LEU:HD22	1.67	0.77
1:C:2230:LEU:HG	1:C:2337:ILE:HG13	1.67	0.77
1:A:525:LEU:O	1:A:528:PRO:HD2	1.85	0.77
1:B:1197:MET:HE1	1:B:1423:VAL:HA	1.65	0.77
1:D:3273:MET:HG3	1:D:3285:PHE:O	1.85	0.77
1:D:3419:LEU:O	1:D:3423:VAL:HG23	1.85	0.77
1:B:1273:MET:SD	1:B:1290:GLU:HA	2.25	0.77
1:B:1504:TYR:HB3	1:B:1505:PRO:HD3	1.67	0.77
1:C:2052:PHE:N	1:D:3322:GLU:HG2	1.99	0.77
1:C:2273:MET:HG3	1:C:2285:PHE:O	1.85	0.77
1:C:2276:PRO:HD2	1:C:2279:ILE:HG13	1.65	0.77
1:B:1414:LEU:HD11	1:B:1419:LEU:HD22	1.66	0.76
1:C:2216:ARG:HB3	1:C:2220:PHE:CD1	2.19	0.76
1:D:3525:LEU:O	1:D:3528:PRO:HD2	1.84	0.76
1:C:2088:THR:O	1:C:2091:TYR:HB3	1.84	0.76
1:A:273:MET:HG3	1:A:285:PHE:O	1.84	0.76
1:B:1463:LEU:HD12	1:B:1503:LEU:HD12	1.67	0.76
1:B:1578:THR:HG22	1:B:1579:SER:N	2.01	0.76
1:C:2174:SER:OG	1:C:2449:LYS:HE2	1.85	0.76
1:D:3276:PRO:HD2	1:D:3279:ILE:HG13	1.67	0.76
1:D:3573:LYS:O	1:D:3576:PRO:HD3	1.85	0.76
1:C:2197:MET:HE1	1:C:2423:VAL:HA	1.67	0.76
1:D:3389:PRO:HB2	1:D:3434:VAL:HG22	1.68	0.76
1:A:403:SER:OG	1:A:406:GLN:HG3	1.86	0.76
1:B:1276:PRO:HD2	1:B:1279:ILE:HG13	1.68	0.76
1:C:2308:GLU:CB	1:C:2571:ASN:HD21	1.98	0.76
1:A:308:GLU:CB	1:A:571:ASN:HD21	1.99	0.76
1:C:2389:PRO:HB2	1:C:2434:VAL:HG22	1.68	0.76
1:B:1105(B):ILE:HG21	1:B:1108:LEU:HD12	1.68	0.76
1:B:1573:LYS:O	1:B:1576:PRO:HD3	1.86	0.76
1:D:3088:THR:O	1:D:3091:TYR:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ILE:HG13	1:A:431:ALA:N	2.00	0.75
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.68	0.75
1:D:3537:ASN:OD1	1:D:3539:ILE:HG23	1.87	0.75
1:B:1449:LYS:HA	1:B:1452:ILE:HD12	1.67	0.75
1:A:322:GLU:HG2	1:B:1051:GLY:C	2.06	0.75
1:C:2178:LEU:HA	1:C:2182:LEU:HD12	1.66	0.75
1:C:2244:LEU:O	1:C:2252:LEU:HD23	1.87	0.75
1:C:2497:ASP:HB3	1:C:2500:VAL:HG23	1.69	0.75
1:A:534:LEU:HD22	5:A:701:PGX:H182	1.68	0.75
1:B:1510:GLU:O	1:B:1512:PRO:HD3	1.85	0.75
1:C:2504:TYR:HB3	1:C:2505:PRO:HD3	1.67	0.75
1:C:2553:GLU:OE1	1:C:2553:GLU:HA	1.87	0.75
1:C:2281:GLU:HA	1:C:2284:GLN:HG3	1.69	0.75
1:C:2338:GLY:HA3	1:C:2559:ILE:HD13	1.67	0.75
1:C:2573:LYS:O	1:C:2576:PRO:HD3	1.86	0.75
1:B:1230:LEU:HG	1:B:1337:ILE:HG13	1.68	0.74
1:B:1430:ILE:HG13	1:B:1431:ALA:N	2.02	0.74
1:C:2182:LEU:O	1:C:2438:ARG:HA	1.87	0.74
1:C:2312:VAL:HA	1:C:2315:ILE:CD1	2.16	0.74
1:D:3430:ILE:HG13	1:D:3431:ALA:N	2.02	0.74
1:D:3185:ARG:HH21	1:D:3438:ARG:NE	1.86	0.74
1:A:553:GLU:OE1	1:A:553:GLU:HA	1.86	0.74
1:C:2161:THR:HG21	1:C:2165:VAL:O	1.87	0.74
1:D:3463:LEU:HD12	1:D:3503:LEU:HD12	1.69	0.74
1:D:3497:ASP:HB3	1:D:3500:VAL:HG23	1.68	0.74
1:A:273:MET:SD	1:A:290:GLU:HA	2.27	0.74
1:C:2442:ILE:O	1:C:2445:GLN:HB2	1.87	0.74
1:C:2463:LEU:HD12	1:C:2503:LEU:HD12	1.70	0.74
1:D:3402:TYR:HA	1:D:3406:GLN:OE1	1.87	0.74
1:C:2210:PHE:CE1	1:C:2382:ASN:HA	2.23	0.74
1:A:573:LYS:O	1:A:576:PRO:HD3	1.88	0.74
1:B:1161:THR:HG21	1:B:1165:VAL:O	1.88	0.74
1:A:402:TYR:HA	1:A:406:GLN:OE1	1.87	0.73
1:B:1402:TYR:HA	1:B:1406:GLN:OE1	1.88	0.73
1:D:3197:MET:HE1	1:D:3423:VAL:HA	1.70	0.73
1:A:510:GLU:O	1:A:512:PRO:HD3	1.87	0.73
1:C:2537:ASN:OD1	1:C:2539:ILE:HG23	1.87	0.73
1:C:2185:ARG:HH21	1:C:2438:ARG:NE	1.85	0.73
1:A:178:LEU:HA	1:A:182:LEU:HD12	1.70	0.73
1:B:1185:ARG:HH21	1:B:1438:ARG:NE	1.87	0.73
1:B:1273:MET:HG3	1:B:1285:PHE:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2510:GLU:O	1:C:2512:PRO:HD3	1.86	0.73
1:D:3190:ASP:OD1	1:D:3517:ILE:HB	1.88	0.73
1:A:52:PHE:N	1:B:1322:GLU:HG2	2.03	0.73
1:A:188:ILE:HD12	1:A:439:ASN:HB2	1.70	0.73
1:B:1442:ILE:O	1:B:1445:GLN:HB2	1.89	0.73
1:A:174:SER:OG	1:A:449:LYS:HE2	1.88	0.72
1:A:182:LEU:O	1:A:438:ARG:HA	1.89	0.72
1:D:3504:TYR:HB3	1:D:3505:PRO:HD3	1.70	0.72
1:B:1389:PRO:HB2	1:B:1434:VAL:HG22	1.71	0.72
1:B:1525:LEU:O	1:B:1528:PRO:HD2	1.89	0.72
1:B:1537:ASN:OD1	1:B:1539:ILE:HG23	1.89	0.72
1:D:3178:LEU:HA	1:D:3182:LEU:HD12	1.71	0.72
1:A:244:LEU:O	1:A:252:LEU:HD23	1.88	0.72
1:B:1387:TRP:CZ2	5:B:1701:PGX:H71	2.25	0.72
1:D:3510:GLU:O	1:D:3512:PRO:HD3	1.88	0.72
1:A:389:PRO:HB2	1:A:434:VAL:HG22	1.70	0.72
1:B:1312:VAL:HA	1:B:1315:ILE:CD1	2.16	0.72
1:D:3442:ILE:O	1:D:3445:GLN:HB2	1.88	0.72
1:C:2178:LEU:O	1:C:2182:LEU:HB2	1.90	0.72
1:C:2402:TYR:HA	1:C:2406:GLN:OE1	1.89	0.72
1:A:312:VAL:HA	1:A:315:ILE:CD1	2.15	0.72
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.72	0.72
1:B:1210:PHE:CE1	1:B:1382:ASN:HA	2.25	0.72
1:C:2188:ILE:HD12	1:C:2439:ASN:HB2	1.72	0.72
1:C:2525:LEU:O	1:C:2528:PRO:HD2	1.89	0.72
1:B:1178:LEU:O	1:B:1182:LEU:HB2	1.90	0.72
1:C:2414:LEU:HD11	1:C:2419:LEU:HD22	1.69	0.72
1:C:2430:ILE:HG13	1:C:2431:ALA:N	2.04	0.72
1:B:1149:THR:O	1:B:1378:ALA:HA	1.90	0.72
1:B:1534:LEU:HD22	5:B:1701:PGX:H182	1.71	0.72
1:C:2184:ARG:HB2	1:C:2439:ASN:C	2.10	0.72
1:D:3385:TYR:HA	5:D:3701:PGX:O4	1.89	0.72
1:A:449:LYS:HA	1:A:452:ILE:HD12	1.69	0.71
1:D:3311:ARG:HB2	6:D:4149:HOH:O	1.90	0.71
1:B:1308:GLU:CB	1:B:1571:ASN:HD21	2.02	0.71
1:A:442:ILE:O	1:A:445:GLN:HB2	1.90	0.71
1:B:1382:ASN:O	1:B:1385:TYR:HB3	1.91	0.71
1:B:1497:ASP:HB3	1:B:1500:VAL:HG23	1.72	0.71
1:C:2218:PRO:HD2	6:C:4099:HOH:O	1.91	0.71
1:D:3553:GLU:OE1	1:D:3553:GLU:HA	1.89	0.71
1:C:2527:ALA:HB3	1:C:2528:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1244:LEU:HD23	1:B:1271:VAL:HG21	1.71	0.70
1:A:232:HIS:O	1:A:288:GLY:HA3	1.90	0.70
1:A:454:GLN:HA	1:A:457:GLU:OE2	1.91	0.70
1:C:2335:ILE:HA	1:C:2559:ILE:HD11	1.72	0.70
1:D:3527:ALA:HB3	1:D:3528:PRO:HD3	1.73	0.70
1:A:190:ASP:OD1	1:A:517:ILE:HB	1.91	0.70
1:B:1403:SER:OG	1:B:1406:GLN:HG3	1.91	0.70
1:D:3387:TRP:CZ2	5:D:3701:PGX:H121	2.27	0.70
1:D:3501:MET:HE3	1:D:3505:PRO:HB2	1.73	0.70
1:A:404:PHE:HB2	1:A:405:LYS:HE3	1.74	0.70
1:B:1188:ILE:HD12	1:B:1439:ASN:HB2	1.72	0.70
1:B:1293:GLY:HA2	1:B:1299:MET:CE	2.22	0.70
1:D:3308:GLU:CB	1:D:3571:ASN:HD21	2.03	0.70
1:D:3563:SER:OG	1:D:3565:GLN:HB3	1.90	0.70
1:A:230:LEU:HG	1:A:337:ILE:HG13	1.73	0.70
1:B:1385:TYR:HB2	5:B:1701:PGX:H101	1.73	0.70
1:D:3138:SER:O	1:D:3141:ALA:HB3	1.92	0.70
1:C:2377:ILE:HA	6:C:4133:HOH:O	1.92	0.70
1:D:3454:GLN:HA	1:D:3457:GLU:OE2	1.92	0.70
1:A:385:TYR:O	1:A:387:TRP:N	2.25	0.69
1:C:2274:ILE:HG13	1:C:2290:GLU:O	1.92	0.69
1:B:1184:ARG:HB2	1:B:1439:ASN:C	2.12	0.69
1:C:2190:ASP:OD1	1:C:2517:ILE:HB	1.92	0.69
1:D:3178:LEU:O	1:D:3182:LEU:HB2	1.90	0.69
1:B:1281:GLU:HA	1:B:1284:GLN:HG3	1.74	0.69
1:B:1513:ARG:CZ	1:B:1520:GLU:HA	2.22	0.69
1:D:3513:ARG:CZ	1:D:3520:GLU:HA	2.22	0.69
1:B:1404:PHE:HB2	1:B:1405:LYS:HE3	1.72	0.69
1:C:2404:PHE:HB2	1:C:2405:LYS:HE3	1.74	0.69
1:A:335:ILE:HA	1:A:559:ILE:HD11	1.74	0.69
1:D:3350:GLN:NE2	1:D:3358:LYS:HA	2.08	0.69
1:A:281:GLU:HA	1:A:284:GLN:HG3	1.74	0.69
1:A:350:GLN:NE2	1:A:358:LYS:HA	2.08	0.69
1:A:524:GLU:OE2	1:A:524:GLU:HA	1.92	0.69
1:B:1275:TYR:CE2	1:B:1284:GLN:HA	2.28	0.69
1:C:2149:THR:O	1:C:2378:ALA:HA	1.92	0.69
1:C:2350:GLN:NE2	1:C:2358:LYS:HA	2.06	0.69
1:A:132:VAL:HG12	1:A:133:HIS:N	2.06	0.69
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.27	0.69
1:B:1206:THR:HG21	5:B:1701:PGX:H111	1.74	0.69
1:A:184:ARG:HB2	1:A:439:ASN:C	2.12	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ARG:CZ	1:A:520:GLU:HA	2.23	0.69
1:B:1244:LEU:O	1:B:1252:LEU:HD23	1.93	0.69
1:B:1414:LEU:HD11	1:B:1419:LEU:CD2	2.22	0.69
1:C:2226:HIS:ND1	1:C:2376:ARG:HD2	2.07	0.69
1:C:2148:TYR:HD1	1:C:2377:ILE:HG22	1.58	0.69
1:C:2322:GLU:OE1	1:D:3049:SER:HB2	1.93	0.69
1:D:3210:PHE:CE1	1:D:3382:ASN:HA	2.28	0.69
1:D:3281:GLU:HA	1:D:3284:GLN:HG3	1.75	0.68
1:D:3382:ASN:O	1:D:3385:TYR:HB3	1.93	0.68
1:B:1132:VAL:HG12	1:B:1133:HIS:N	2.07	0.68
1:D:3404:PHE:HB2	1:D:3405:LYS:HE3	1.73	0.68
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.76	0.68
1:B:1274:ILE:HG13	1:B:1290:GLU:O	1.94	0.68
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.74	0.68
1:B:1138:SER:O	1:B:1141:ALA:HB3	1.93	0.68
1:B:1203:GLN:CG	1:B:1298:LEU:HD11	2.22	0.68
1:C:2180:LYS:O	1:C:2181:VAL:HG13	1.93	0.68
1:A:293:GLY:HA2	1:A:299:MET:CE	2.24	0.68
1:A:463:LEU:HD12	1:A:503:LEU:HD12	1.75	0.68
1:C:2308:GLU:HB2	1:C:2571:ASN:ND2	2.07	0.68
1:C:2385:TYR:O	1:C:2387:TRP:N	2.27	0.68
1:A:149:THR:O	1:A:378:ALA:HA	1.94	0.68
1:A:178:LEU:O	1:A:182:LEU:HB2	1.94	0.68
1:C:2537:ASN:HB2	6:C:4123:HOH:O	1.93	0.68
1:D:3385:TYR:O	1:D:3387:TRP:N	2.26	0.68
1:B:1385:TYR:O	1:B:1387:TRP:N	2.26	0.68
1:D:3534:LEU:HD22	5:D:3701:PGX:H182	1.76	0.68
1:A:501:MET:HE3	1:A:505:PRO:HB2	1.75	0.67
1:B:1179:GLU:HA	1:B:1183:LEU:HD12	1.75	0.67
1:C:2403:SER:OG	1:C:2406:GLN:HG3	1.93	0.67
1:C:2513:ARG:CZ	1:C:2520:GLU:HA	2.24	0.67
1:C:2293:GLY:HA2	1:C:2299:MET:CE	2.24	0.67
1:D:3134:TYR:HD2	1:D:3136:TYR:CE1	2.12	0.67
1:C:2275:TYR:CE2	1:C:2284:GLN:HA	2.30	0.67
1:C:2563:SER:OG	1:C:2565:GLN:HB3	1.94	0.67
1:C:2463:LEU:HD13	1:C:2506:ALA:CB	2.23	0.67
1:A:148:TYR:HD1	1:A:377:ILE:HG22	1.59	0.67
1:B:1190:ASP:OD1	1:B:1517:ILE:HB	1.95	0.67
1:B:1563:SER:OG	1:B:1565:GLN:HB3	1.94	0.67
1:A:89:VAL:HA	1:A:92:ILE:HG13	1.75	0.67
1:B:1419:LEU:O	1:B:1423:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2244:LEU:HD23	1:C:2271:VAL:HG21	1.77	0.67
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.09	0.67
1:A:148:TYR:CD1	1:A:377:ILE:HG22	2.30	0.67
1:C:2382:ASN:O	1:C:2385:TYR:HB3	1.94	0.67
1:D:3179:GLU:HA	1:D:3183:LEU:HD12	1.75	0.67
1:A:381:PHE:CD1	1:A:529:PHE:HB3	2.30	0.66
1:D:3184:ARG:HB2	1:D:3439:ASN:C	2.15	0.66
1:A:308:GLU:HB2	1:A:571:ASN:ND2	2.08	0.66
1:B:1425:SER:O	1:B:1428:ARG:HG2	1.95	0.66
1:C:2148:TYR:CD1	1:C:2377:ILE:HG22	2.30	0.66
1:C:2150:ARG:HD3	6:C:4134:HOH:O	1.95	0.66
1:D:3567:LEU:HD12	1:D:3567:LEU:O	1.96	0.66
1:A:132:VAL:O	1:A:154:PRO:HG3	1.93	0.66
1:B:1381:PHE:CD1	1:B:1529:PHE:HB3	2.31	0.66
1:B:1463:LEU:HD13	1:B:1506:ALA:CB	2.23	0.66
1:D:3293:GLY:HA2	1:D:3299:MET:CE	2.24	0.66
1:B:1350:GLN:NE2	1:B:1358:LYS:HA	2.09	0.66
1:D:3148:TYR:HD1	1:D:3377:ILE:HG22	1.60	0.66
1:A:563:SER:OG	1:A:565:GLN:HB3	1.96	0.66
1:B:1454:GLN:HA	1:B:1457:GLU:OE2	1.95	0.66
1:D:3453:ASP:O	1:D:3456:ARG:HB2	1.96	0.66
1:B:1148:TYR:HD1	1:B:1377:ILE:HG22	1.60	0.66
1:A:263:PRO:HD3	1:A:303:THR:HG23	1.77	0.66
1:A:482:THR:HG22	6:A:4032:HOH:O	1.96	0.66
1:D:3428:ARG:HA	1:D:3582:VAL:HG23	1.78	0.66
1:D:3501:MET:CE	1:D:3505:PRO:HB2	2.26	0.66
1:B:1174:SER:OG	1:B:1449:LYS:HE2	1.94	0.66
1:C:2132:VAL:HG12	1:C:2133:HIS:N	2.10	0.66
1:C:2184:ARG:HB2	1:C:2439:ASN:HA	1.76	0.66
1:C:2425:SER:O	1:C:2428:ARG:HG2	1.94	0.66
1:D:3176:GLU:OE1	1:D:3180:LYS:HE2	1.96	0.66
1:D:3403:SER:OG	1:D:3406:GLN:HG3	1.95	0.66
1:B:1132:VAL:O	1:B:1154:PRO:HG3	1.95	0.66
1:C:2076:THR:O	1:C:2080:LEU:HG	1.96	0.66
1:D:3132:VAL:O	1:D:3154:PRO:HG3	1.95	0.66
1:D:3241:GLN:HG3	1:D:3242:HIS:N	2.11	0.66
1:A:179:GLU:HA	1:A:183:LEU:HD12	1.78	0.66
1:A:453:ASP:O	1:A:456:ARG:HB2	1.96	0.66
1:B:1148:TYR:CD1	1:B:1377:ILE:HG22	2.31	0.66
1:B:1205:PHE:O	1:B:1208:GLN:HG2	1.96	0.66
1:C:2280:PRO:HB2	1:C:2282:ASN:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3180:LYS:O	1:D:3181:VAL:HG13	1.96	0.66
1:D:3274:ILE:HG13	1:D:3290:GLU:O	1.94	0.66
1:C:2089:VAL:HA	1:C:2092:ILE:HG13	1.76	0.65
1:D:3174:SER:OG	1:D:3449:LYS:HE2	1.95	0.65
1:B:1527:ALA:HB3	1:B:1528:PRO:HD3	1.77	0.65
1:C:2381:PHE:CD1	1:C:2529:PHE:HB3	2.31	0.65
1:B:1335:ILE:HA	1:B:1559:ILE:HD11	1.78	0.65
1:B:1524:GLU:HA	1:B:1524:GLU:OE2	1.97	0.65
1:C:2179:GLU:HA	1:C:2183:LEU:HD12	1.78	0.65
1:C:2453:ASP:O	1:C:2456:ARG:HB2	1.96	0.65
1:C:2524:GLU:OE2	1:C:2524:GLU:HA	1.95	0.65
1:D:3148:TYR:CD1	1:D:3377:ILE:HG22	2.30	0.65
1:D:3335:ILE:HA	1:D:3559:ILE:HD11	1.78	0.65
1:A:456:ARG:HA	6:A:4021:HOH:O	1.96	0.65
1:B:1507:LEU:HD22	1:B:1522:MET:HE2	1.77	0.65
1:C:2203:GLN:CG	1:C:2298:LEU:HD11	2.26	0.65
1:C:2454:GLN:HA	1:C:2457:GLU:OE2	1.96	0.65
1:D:3089:VAL:HA	1:D:3092:ILE:HG13	1.78	0.65
1:D:3226:HIS:ND1	1:D:3376:ARG:HD2	2.12	0.65
1:C:2238:LEU:HD22	1:C:2242:HIS:NE2	2.11	0.65
1:C:2138:SER:O	1:C:2141:ALA:HB3	1.97	0.65
1:C:2176:GLU:OE1	1:C:2180:LYS:HE2	1.96	0.65
1:B:1206:THR:HA	1:B:1209:PHE:CZ	2.32	0.65
1:B:1532:LYS:O	1:B:1534:LEU:N	2.30	0.65
1:D:3381:PHE:CD1	1:D:3529:PHE:HB3	2.32	0.65
1:A:134:TYR:HD2	1:A:136:TYR:CE1	2.14	0.65
1:A:205:PHE:O	1:A:208:GLN:HG2	1.96	0.65
1:B:1232:HIS:O	1:B:1288:GLY:HA3	1.97	0.65
1:D:3208:GLN:HG3	1:D:3209:PHE:CD1	2.32	0.65
1:D:3306:LEU:HD23	1:D:3306:LEU:C	2.17	0.65
1:D:3414:LEU:HD11	1:D:3419:LEU:CD2	2.26	0.65
1:D:3578:THR:CG2	1:D:3579:SER:N	2.60	0.65
1:A:428:ARG:HA	1:A:582:VAL:HG23	1.79	0.65
1:C:2232:HIS:O	1:C:2288:GLY:HA3	1.97	0.65
1:C:2388:HIS:HB3	1:C:2444:VAL:HG11	1.79	0.65
1:C:2428:ARG:HA	1:C:2582:VAL:HG23	1.77	0.65
1:C:2567:LEU:O	1:C:2567:LEU:HD12	1.97	0.65
1:D:3085:THR:O	1:D:3089:VAL:HG23	1.97	0.65
1:D:3563:SER:HB2	6:D:4157:HOH:O	1.96	0.65
1:A:218:PRO:HD2	6:A:4003:HOH:O	1.97	0.64
1:B:1391:LEU:HD22	1:B:1404:PHE:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:HB3	1:A:444:VAL:HG11	1.79	0.64
1:D:3238:LEU:HD22	1:D:3242:HIS:NE2	2.12	0.64
1:A:238:LEU:HD22	1:A:242:HIS:NE2	2.12	0.64
1:D:3388:HIS:HB3	1:D:3444:VAL:HG11	1.80	0.64
1:A:97:LYS:HB2	1:A:356:HIS:CE1	2.32	0.64
1:A:203:GLN:CG	1:A:298:LEU:HD11	2.27	0.64
1:D:3206:THR:HA	1:D:3209:PHE:CZ	2.32	0.64
1:A:85:THR:O	1:A:89:VAL:HG23	1.98	0.64
1:A:389:PRO:CG	1:A:434:VAL:HG13	2.21	0.64
1:B:1176:GLU:OE1	1:B:1180:LYS:HE2	1.97	0.64
1:B:1295:VAL:HB	1:B:1298:LEU:HD22	1.79	0.64
1:C:2385:TYR:HA	5:C:2701:PGX:O4	1.97	0.64
1:A:414:LEU:HD11	1:A:419:LEU:CD2	2.27	0.64
1:B:1229:ASP:OD2	1:B:1231:ASN:HB3	1.98	0.64
1:C:2134:TYR:HD2	1:C:2136:TYR:CE1	2.15	0.64
1:D:3280:PRO:HB2	1:D:3282:ASN:OD1	1.98	0.64
1:A:425:SER:O	1:A:428:ARG:HG2	1.97	0.64
1:A:275:TYR:CE2	1:A:284:GLN:HA	2.33	0.64
1:C:2532:LYS:O	1:C:2534:LEU:N	2.31	0.64
1:D:3205:PHE:O	1:D:3208:GLN:HG2	1.98	0.64
1:D:3244:LEU:O	1:D:3252:LEU:HD23	1.97	0.64
1:D:3463:LEU:HD13	1:D:3506:ALA:CB	2.24	0.64
1:D:3524:GLU:HA	1:D:3524:GLU:OE2	1.96	0.64
1:A:138:SER:O	1:A:141:ALA:HB3	1.97	0.63
1:D:3130:TYR:HB3	1:D:3134:TYR:O	1.97	0.63
1:D:3191:PRO:CD	1:D:3433:ARG:HG3	2.27	0.63
1:B:1238:LEU:HD22	1:B:1242:HIS:NE2	2.13	0.63
1:C:2130:TYR:HB3	1:C:2134:TYR:O	1.98	0.63
1:C:2396:ASN:ND2	1:C:2396:ASN:N	2.45	0.63
1:B:1089:VAL:HA	1:B:1092:ILE:HG13	1.79	0.63
1:D:3057:CYS:HB3	1:D:3069:CYS:SG	2.38	0.63
1:D:3244:LEU:HD23	1:D:3271:VAL:HG21	1.79	0.63
1:A:245:ARG:NH2	1:A:326:GLU:HG2	2.12	0.63
1:A:274:ILE:HG13	1:A:290:GLU:O	1.97	0.63
1:B:1057:CYS:HB3	1:B:1069:CYS:SG	2.38	0.63
1:D:3132:VAL:HG12	1:D:3133:HIS:N	2.13	0.63
1:D:3578:THR:HG22	1:D:3579:SER:H	1.61	0.63
1:B:1184:ARG:HB2	1:B:1439:ASN:HA	1.80	0.63
1:C:2272:GLU:HA	6:C:4108:HOH:O	1.97	0.63
1:A:280:PRO:HB2	1:A:282:ASN:OD1	1.99	0.63
1:B:1203:GLN:HG2	1:B:1298:LEU:CD1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1567:LEU:HD12	1:B:1567:LEU:O	1.99	0.63
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.33	0.63
1:A:241:GLN:HG3	1:A:242:HIS:N	2.14	0.63
1:A:463:LEU:HD13	1:A:506:ALA:CB	2.25	0.63
1:C:2226:HIS:CE1	1:C:2376:ARG:HD2	2.34	0.63
1:A:306:LEU:C	1:A:306:LEU:HD23	2.18	0.63
1:A:532:LYS:O	1:A:534:LEU:N	2.31	0.63
1:B:1465:GLU:OE2	1:B:1465:GLU:HA	1.98	0.63
1:C:2132:VAL:O	1:C:2154:PRO:HG3	1.97	0.63
1:C:2502:GLU:HB3	6:C:4124:HOH:O	1.99	0.63
1:D:3203:GLN:CG	1:D:3298:LEU:HD11	2.27	0.63
1:A:208:GLN:HG3	1:A:209:PHE:CD1	2.34	0.63
1:A:391:LEU:HD22	1:A:404:PHE:CZ	2.34	0.63
1:A:465:GLU:HA	1:A:465:GLU:OE2	1.98	0.62
1:D:3308:GLU:O	1:D:3311:ARG:HB3	1.99	0.62
1:A:180:LYS:O	1:A:181:VAL:HG13	1.99	0.62
1:A:382:ASN:O	1:A:385:TYR:HB3	1.99	0.62
1:A:578:THR:CG2	1:A:579:SER:N	2.61	0.62
1:B:1245:ARG:NH2	1:B:1326:GLU:HG2	2.09	0.62
1:C:2578:THR:CG2	1:C:2579:SER:N	2.61	0.62
1:D:3507:LEU:HD22	1:D:3522:MET:HE2	1.80	0.62
1:A:118:THR:HA	1:A:121:SER:OG	2.00	0.62
1:B:1308:GLU:HB2	1:B:1571:ASN:ND2	2.11	0.62
1:B:1447:VAL:HG12	1:B:1448:ALA:N	2.13	0.62
1:D:3229:ASP:OD2	1:D:3231:ASN:HB3	1.99	0.62
1:D:3275:TYR:CE2	1:D:3284:GLN:HA	2.34	0.62
1:A:385:TYR:HA	5:A:701:PGX:O4	1.98	0.62
1:B:1510:GLU:OE1	1:B:1519:GLY:HA3	1.98	0.62
1:C:2391:LEU:HD22	1:C:2404:PHE:CZ	2.34	0.62
1:A:353:SER:HA	6:A:4023:HOH:O	2.00	0.62
1:B:1428:ARG:HA	1:B:1582:VAL:HG23	1.80	0.62
1:B:1442:ILE:N	1:B:1442:ILE:HD12	2.15	0.62
1:C:2085:THR:O	1:C:2089:VAL:HG23	2.00	0.62
1:D:3578:THR:CG2	1:D:3579:SER:H	2.13	0.62
1:C:2205:PHE:O	1:C:2208:GLN:HG2	1.99	0.62
1:D:3184:ARG:NH1	1:D:3441:PRO:HG3	2.13	0.62
1:B:1208:GLN:HG3	1:B:1209:PHE:CD1	2.35	0.62
1:D:3532:LYS:O	1:D:3534:LEU:N	2.33	0.62
1:A:327:GLN:NE2	1:B:1136:TYR:CD2	2.68	0.62
1:C:2208:GLN:HG3	1:C:2209:PHE:CD1	2.34	0.62
1:C:2229:ASP:OD2	1:C:2231:ASN:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2245:ARG:NH2	1:C:2326:GLU:HG2	2.11	0.62
1:D:3078:ILE:O	1:D:3082:LEU:HD12	2.00	0.62
1:D:3197:MET:CE	1:D:3423:VAL:HG13	2.29	0.62
1:D:3425:SER:O	1:D:3428:ARG:HG2	1.99	0.62
1:A:76:THR:O	1:A:80:LEU:HG	1.99	0.62
1:B:1134:TYR:HD2	1:B:1136:TYR:CE1	2.17	0.62
1:C:2131:ASN:ND2	1:C:2147:TYR:CD2	2.68	0.62
1:C:2193:GLY:O	1:C:2582:VAL:HG12	2.00	0.62
1:D:3184:ARG:HB2	1:D:3439:ASN:HA	1.82	0.62
1:A:136:TYR:HD2	1:B:1327:GLN:NE2	1.98	0.61
1:C:2465:GLU:HA	1:C:2465:GLU:OE2	2.00	0.61
1:D:3308:GLU:HB2	1:D:3571:ASN:ND2	2.12	0.61
1:A:113:MET:HE3	1:A:117:LEU:HD22	1.82	0.61
1:A:386:HIS:HB3	1:A:388:HIS:CE1	2.36	0.61
1:B:1072:PRO:HG2	1:B:1077:ARG:HE	1.64	0.61
1:A:206:THR:HA	1:A:209:PHE:CZ	2.35	0.61
1:A:229:ASP:OD2	1:A:231:ASN:HB3	2.00	0.61
1:C:2198:PHE:CE1	1:C:2352:LEU:HD13	2.35	0.61
1:D:3232:HIS:O	1:D:3288:GLY:HA3	2.01	0.61
1:D:3245:ARG:NH2	1:D:3326:GLU:HG2	2.14	0.61
1:D:3454:GLN:O	1:D:3457:GLU:HG3	2.00	0.61
1:B:1226:HIS:ND1	1:B:1376:ARG:HD2	2.15	0.61
1:B:1501:MET:HE3	1:B:1505:PRO:HB2	1.82	0.61
1:C:2210:PHE:O	1:C:2211:LYS:HG3	2.01	0.61
1:D:3263:PRO:HD3	1:D:3303:THR:HG23	1.82	0.61
1:B:1387:TRP:HZ2	5:B:1701:PGX:H71	1.65	0.61
1:C:2203:GLN:HG2	1:C:2298:LEU:CD1	2.30	0.61
1:C:2241:GLN:HG3	1:C:2242:HIS:N	2.14	0.61
1:A:295:VAL:HB	1:A:298:LEU:HD22	1.83	0.61
1:B:1191:PRO:CD	1:B:1433:ARG:HG3	2.29	0.61
1:A:130:TYR:HB3	1:A:134:TYR:O	2.00	0.61
1:A:136:TYR:CD2	1:B:1327:GLN:NE2	2.69	0.61
1:C:2306:LEU:HD23	1:C:2307:ARG:N	2.15	0.61
1:A:100:TRP:CD1	1:A:356:HIS:HB2	2.35	0.61
1:A:176:GLU:OE1	1:A:180:LYS:HE2	2.00	0.61
1:C:2074:PHE:HA	1:C:2077:ARG:HG3	1.83	0.61
1:D:3118:THR:HA	1:D:3121:SER:OG	2.01	0.61
1:D:3465:GLU:HA	1:D:3465:GLU:OE2	2.00	0.61
1:A:396:ASN:ND2	1:A:396:ASN:N	2.45	0.60
1:C:2118:THR:HA	1:C:2121:SER:OG	2.00	0.60
1:C:2327:GLN:NE2	1:D:3136:TYR:HD2	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2339:GLU:O	1:C:2342:LYS:HB3	2.00	0.60
1:C:2385:TYR:HB2	5:C:2701:PGX:H101	1.82	0.60
1:D:3095:HIS:HA	6:D:4153:HOH:O	2.01	0.60
1:D:3389:PRO:CG	1:D:3434:VAL:HG13	2.26	0.60
1:A:120:ARG:NH1	1:A:527:ALA:HB1	2.16	0.60
1:B:1076:THR:O	1:B:1080:LEU:HG	2.01	0.60
1:B:1120:ARG:NH1	1:B:1527:ALA:HB1	2.16	0.60
1:B:1171:LEU:HD12	1:B:1502:GLU:OE2	2.01	0.60
1:B:1454:GLN:O	1:B:1457:GLU:HG3	2.02	0.60
1:B:1197:MET:CE	1:B:1423:VAL:HG13	2.31	0.60
1:B:1210:PHE:O	1:B:1211:LYS:HG3	2.01	0.60
1:C:2113:MET:CA	1:C:2116:VAL:HG13	2.32	0.60
1:C:2184:ARG:HB2	1:C:2439:ASN:CA	2.31	0.60
1:C:2327:GLN:NE2	1:D:3136:TYR:CD2	2.70	0.60
1:C:2409:TYR:N	1:C:2409:TYR:CD2	2.69	0.60
1:C:2295:VAL:HB	1:C:2298:LEU:HD22	1.82	0.60
1:B:1118:THR:HA	1:B:1121:SER:OG	2.01	0.60
1:B:1501:MET:CE	1:B:1505:PRO:HB2	2.31	0.60
1:B:1562:ALA:HA	6:B:4092:HOH:O	2.01	0.60
1:B:1578:THR:CG2	1:B:1579:SER:N	2.64	0.60
1:D:3171:LEU:HD12	1:D:3502:GLU:OE2	2.01	0.60
1:D:3203:GLN:HG2	1:D:3298:LEU:CD1	2.29	0.60
1:D:3347:ASP:O	1:D:3348:TYR:C	2.40	0.60
1:D:3409:TYR:N	1:D:3409:TYR:CD2	2.68	0.60
1:C:2184:ARG:NH2	1:C:2441:PRO:HD3	2.17	0.60
1:C:2414:LEU:HD11	1:C:2419:LEU:CD2	2.31	0.60
1:D:3181:VAL:HG12	1:D:3487:MET:HG2	1.84	0.60
1:A:526:GLY:CA	5:A:701:PGX:H61	2.30	0.60
1:D:3295:VAL:HB	1:D:3298:LEU:HD22	1.83	0.60
1:A:184:ARG:HB2	1:A:439:ASN:CA	2.31	0.60
1:A:327:GLN:NE2	1:B:1136:TYR:HD2	2.00	0.60
1:B:1241:GLN:HG3	1:B:1242:HIS:N	2.15	0.60
1:C:2184:ARG:HA	1:C:2438:ARG:O	2.02	0.60
1:D:3072:PRO:HG2	1:D:3077:ARG:HE	1.65	0.60
1:A:203:GLN:HG2	1:A:298:LEU:CD1	2.30	0.60
1:B:1124:ILE:HD11	1:B:1528:PRO:HB2	1.84	0.60
1:A:409:TYR:N	1:A:409:TYR:CD2	2.69	0.60
1:B:1453:ASP:O	1:B:1456:ARG:HB2	2.01	0.60
1:A:180:LYS:HD2	1:A:490:GLU:OE1	2.02	0.59
1:B:1074:PHE:HA	1:B:1077:ARG:HG3	1.84	0.59
1:B:1180:LYS:O	1:B:1181:VAL:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2105(C):ILE:HG21	1:C:2108:LEU:HD12	1.84	0.59
1:C:2501:MET:HE3	1:C:2505:PRO:HB2	1.84	0.59
1:A:197:MET:CE	1:A:423:VAL:HG13	2.32	0.59
1:A:244:LEU:HD23	1:A:271:VAL:HG21	1.82	0.59
1:A:343:ILE:O	1:A:347:ASP:HB2	2.02	0.59
1:A:389:PRO:HG3	1:A:508:LEU:HD22	1.84	0.59
1:B:1089:VAL:HA	1:B:1092:ILE:CG1	2.32	0.59
1:B:1495:TYR:HE2	1:B:1502:GLU:HG3	1.67	0.59
1:B:1193:GLY:O	1:B:1582:VAL:HG12	2.02	0.59
1:C:2184:ARG:NH1	1:C:2441:PRO:HG3	2.18	0.59
1:A:78:ILE:O	1:A:82:LEU:HD12	2.01	0.59
1:B:1184:ARG:HD3	1:B:1187:PHE:CA	2.29	0.59
1:B:1267:LYS:HG2	1:B:1267:LYS:O	2.03	0.59
1:D:3136:TYR:O	1:D:3136:TYR:HD1	1.85	0.59
1:D:3504:TYR:HA	1:D:3507:LEU:HD12	1.84	0.59
1:A:276:PRO:O	1:A:279:ILE:HG12	2.02	0.59
1:A:501:MET:CE	1:A:505:PRO:HB2	2.32	0.59
1:B:1343:ILE:O	1:B:1347:ASP:HB2	2.01	0.59
1:C:2276:PRO:HD2	1:C:2279:ILE:CG1	2.32	0.59
1:C:2306:LEU:HD23	1:C:2306:LEU:C	2.23	0.59
1:D:3193:GLY:O	1:D:3582:VAL:HG12	2.02	0.59
1:B:1213:ASP:HB2	1:B:1222:ARG:HG3	1.85	0.59
1:D:3341:ILE:HG23	1:D:3534:LEU:HD12	1.85	0.59
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.84	0.59
1:D:3192:GLN:OE1	1:D:3517:ILE:HG22	2.02	0.59
1:D:3442:ILE:HD12	1:D:3442:ILE:N	2.18	0.59
1:A:57:CYS:HB3	1:A:69:CYS:SG	2.43	0.59
1:B:1130:TYR:HB3	1:B:1134:TYR:O	2.02	0.59
1:D:3076:THR:O	1:D:3080:LEU:HG	2.03	0.59
1:D:3447:VAL:HG12	1:D:3448:ALA:N	2.17	0.59
1:A:306:LEU:HD23	1:A:307:ARG:N	2.18	0.59
1:A:562:ALA:HA	6:A:4043:HOH:O	2.02	0.59
1:B:1388:HIS:HB3	1:B:1444:VAL:HG11	1.84	0.59
1:B:1554:VAL:HG12	1:B:1555:GLY:N	2.18	0.59
1:C:2276:PRO:O	1:C:2279:ILE:HG12	2.03	0.59
1:C:2578:THR:HG22	1:C:2579:SER:H	1.66	0.59
1:D:3184:ARG:NH2	1:D:3441:PRO:HD3	2.18	0.59
1:D:3391:LEU:HD22	1:D:3404:PHE:CZ	2.38	0.59
1:A:72:PRO:HG2	1:A:77:ARG:HE	1.67	0.58
1:A:347:ASP:O	1:A:348:TYR:C	2.40	0.58
1:C:2362:ASP:O	1:C:2365:LEU:HG	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2495:TYR:HE2	1:C:2502:GLU:HG3	1.67	0.58
1:D:3128:PRO:HG3	1:D:3376:ARG:HB2	1.85	0.58
1:D:3495:TYR:HE2	1:D:3502:GLU:HG3	1.68	0.58
1:A:74:PHE:HA	1:A:77:ARG:HG3	1.84	0.58
1:A:362:ASP:O	1:A:365:LEU:HG	2.03	0.58
1:D:3427:THR:HG21	1:D:3578:THR:HA	1.85	0.58
1:A:269:THR:OG1	1:A:271:VAL:HG23	2.02	0.58
1:A:276:PRO:HD2	1:A:279:ILE:CG1	2.34	0.58
1:A:387:TRP:CH2	5:A:701:PGX:H121	2.38	0.58
1:C:2097:LYS:HB2	1:C:2356:HIS:CE1	2.37	0.58
1:C:2347:ASP:O	1:C:2348:TYR:C	2.41	0.58
1:D:3097:LYS:HB2	1:D:3356:HIS:CE1	2.38	0.58
1:D:3205:PHE:HE2	5:D:3701:PGX:H171	1.68	0.58
1:A:191:PRO:HG3	1:A:433:ARG:NH1	2.18	0.58
1:A:554:VAL:HG12	1:A:555:GLY:N	2.18	0.58
1:B:1085:THR:O	1:B:1089:VAL:HG23	2.03	0.58
1:C:2120:ARG:NH1	1:C:2527:ALA:HB1	2.19	0.58
1:C:2171:LEU:HD12	1:C:2502:GLU:OE2	2.04	0.58
1:C:2507:LEU:HD21	1:C:2521:THR:HG22	1.85	0.58
1:A:184:ARG:NH1	1:A:441:PRO:HG3	2.19	0.58
1:A:341:ILE:HG23	1:A:534:LEU:HD12	1.86	0.58
1:A:389:PRO:HG2	1:A:434:VAL:CG1	2.26	0.58
1:B:1184:ARG:HB2	1:B:1439:ASN:CA	2.34	0.58
1:B:1255:GLN:HG2	1:B:1263:PRO:O	2.04	0.58
1:B:1306:LEU:HD23	1:B:1306:LEU:C	2.24	0.58
1:C:2414:LEU:HA	1:C:2422:PHE:HE1	1.67	0.58
1:D:3269:THR:OG1	1:D:3271:VAL:HG23	2.04	0.58
1:A:128:PRO:CG	1:A:376:ARG:NH1	2.67	0.58
1:A:193:GLY:O	1:A:582:VAL:HG12	2.03	0.58
1:B:1131:ASN:ND2	1:B:1147:TYR:CD2	2.72	0.58
1:B:1180:LYS:HD2	1:B:1490:GLU:OE1	2.04	0.58
1:C:2108:LEU:HD23	1:C:2111:LEU:CD2	2.34	0.58
1:C:2136:TYR:CD2	1:D:3327:GLN:NE2	2.72	0.58
1:C:2263:PRO:HD3	1:C:2303:THR:HG23	1.83	0.58
1:D:3113:MET:CA	1:D:3116:VAL:HG13	2.34	0.58
1:D:3226:HIS:CE1	1:D:3376:ARG:HD2	2.39	0.58
1:D:3554:VAL:HG12	1:D:3555:GLY:N	2.18	0.58
1:B:1192:GLN:OE1	1:B:1517:ILE:HG22	2.04	0.58
1:B:1322:GLU:HA	6:B:4068:HOH:O	2.03	0.58
1:C:2173:ASP:O	1:C:2177:VAL:HG23	2.03	0.58
1:D:3482:THR:C	1:D:3511:LYS:HB2	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD12	1:A:502:GLU:OE2	2.04	0.58
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.68	0.58
1:C:2150:ARG:HH22	1:C:2154:PRO:HA	1.69	0.58
1:D:3074:PHE:HA	1:D:3077:ARG:HG3	1.86	0.58
1:D:3507:LEU:CD2	1:D:3521:THR:HG22	2.33	0.58
1:B:1507:LEU:HD21	1:B:1521:THR:HG22	1.86	0.57
1:A:210:PHE:O	1:A:211:LYS:HG3	2.03	0.57
1:A:388:HIS:N	1:A:389:PRO:HD2	2.19	0.57
1:B:1244:LEU:CD2	1:B:1271:VAL:HG21	2.35	0.57
1:B:1276:PRO:HD2	1:B:1279:ILE:CG1	2.35	0.57
1:B:1396:ASN:ND2	1:B:1396:ASN:N	2.51	0.57
1:D:3113:MET:HE3	1:D:3117:LEU:HD22	1.86	0.57
1:D:3173:ASP:O	1:D:3177:VAL:HG23	2.03	0.57
1:A:414:LEU:HA	1:A:422:PHE:HE1	1.64	0.57
1:B:1293:GLY:HA2	1:B:1299:MET:HE3	1.87	0.57
1:B:1386:HIS:HB3	1:B:1388:HIS:CE1	2.39	0.57
1:C:2100:TRP:CD1	1:C:2356:HIS:HB2	2.39	0.57
1:A:113:MET:CA	1:A:116:VAL:HG13	2.34	0.57
1:B:1078:ILE:O	1:B:1082:LEU:HD12	2.04	0.57
1:B:1280:PRO:HB2	1:B:1282:ASN:OD1	2.04	0.57
1:D:3338:GLY:HA3	1:D:3559:ILE:CD1	2.31	0.57
1:D:3343:ILE:O	1:D:3347:ASP:HB2	2.05	0.57
1:A:267:LYS:O	1:A:267:LYS:HG2	2.03	0.57
1:C:2124:ILE:HD11	1:C:2528:PRO:HB2	1.85	0.57
1:C:2183:LEU:HD21	1:C:2445:GLN:HG3	1.86	0.57
1:A:94:THR:HG22	1:A:354:GLY:O	2.04	0.57
1:B:1097:LYS:HB2	1:B:1356:HIS:CE1	2.39	0.57
1:B:1427:THR:HG21	1:B:1578:THR:HA	1.85	0.57
1:C:2089:VAL:HA	1:C:2092:ILE:CG1	2.33	0.57
1:C:2201:PHE:O	1:C:2202:ALA:C	2.43	0.57
1:C:2206:THR:HA	1:C:2209:PHE:CZ	2.40	0.57
1:C:2386:HIS:HB3	1:C:2388:HIS:CE1	2.40	0.57
1:D:3205:PHE:CE2	1:D:3209:PHE:HZ	2.23	0.57
1:A:183:LEU:HD21	1:A:445:GLN:HG3	1.87	0.57
1:C:2072:PRO:HG2	1:C:2077:ARG:HE	1.70	0.57
1:C:2507:LEU:CD2	1:C:2521:THR:HG22	2.35	0.57
1:C:2578:THR:CG2	1:C:2579:SER:H	2.17	0.57
1:D:3191:PRO:HG3	1:D:3433:ARG:NH1	2.19	0.57
1:A:49:SER:HB2	1:B:1322:GLU:OE1	2.04	0.57
1:C:2530:SER:OG	5:C:2701:PGX:H162	2.05	0.57
1:D:3131:ASN:ND2	1:D:3147:TYR:CD2	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3507:LEU:HD21	1:D:3521:THR:HG22	1.87	0.57
1:A:578:THR:HG22	1:A:579:SER:H	1.68	0.57
1:B:1263:PRO:HD3	1:B:1303:THR:HG23	1.87	0.57
1:B:1308:GLU:O	1:B:1311:ARG:HB3	2.05	0.57
1:B:1464:ASN:OD1	1:B:1499:ASP:HA	2.05	0.57
1:C:2180:LYS:HD2	1:C:2490:GLU:OE1	2.04	0.57
1:C:2388:HIS:N	1:C:2389:PRO:HD2	2.19	0.57
1:D:3108:LEU:HD23	1:D:3111:LEU:CD2	2.35	0.57
1:D:3124:ILE:HD11	1:D:3528:PRO:HB2	1.87	0.57
1:D:3386:HIS:HB3	1:D:3388:HIS:CE1	2.39	0.57
1:A:504:TYR:HA	1:A:507:LEU:HD12	1.87	0.57
1:D:3188:ILE:HD12	1:D:3439:ASN:CB	2.34	0.57
1:D:3210:PHE:O	1:D:3211:LYS:HG3	2.05	0.57
1:D:3396:ASN:ND2	1:D:3396:ASN:N	2.51	0.57
1:D:3454:GLN:HA	1:D:3457:GLU:HG3	1.87	0.57
1:A:108:LEU:HD23	1:A:111:LEU:CD2	2.35	0.56
1:B:1173:ASP:O	1:B:1177:VAL:HG23	2.05	0.56
1:C:2234:TYR:CE1	1:C:2252:LEU:HD11	2.40	0.56
1:C:2554:VAL:HG12	1:C:2555:GLY:N	2.20	0.56
1:D:3184:ARG:HD3	1:D:3187:PHE:CA	2.34	0.56
1:D:3362:ASP:O	1:D:3365:LEU:HG	2.05	0.56
1:A:567:LEU:O	1:A:567:LEU:HD12	2.04	0.56
1:B:1108:LEU:HD23	1:B:1111:LEU:CD2	2.35	0.56
1:B:1347:ASP:O	1:B:1348:TYR:C	2.43	0.56
1:B:1537:ASN:HB2	6:B:4076:HOH:O	2.04	0.56
1:C:2078:ILE:O	1:C:2082:LEU:HD12	2.04	0.56
1:C:2094:THR:HG22	1:C:2354:GLY:O	2.05	0.56
1:C:2113:MET:HA	1:C:2116:VAL:HG13	1.87	0.56
1:C:2389:PRO:CB	1:C:2434:VAL:HG22	2.35	0.56
1:D:3120:ARG:NH1	1:D:3527:ALA:HB1	2.19	0.56
1:D:3235:GLY:HA3	1:D:3240:ARG:HG2	1.86	0.56
1:A:184:ARG:NH2	1:A:441:PRO:HD3	2.19	0.56
1:A:211:LYS:NZ	1:A:236:GLU:HG3	2.21	0.56
1:A:582:VAL:HG13	1:A:582:VAL:O	2.06	0.56
1:B:1211:LYS:NZ	1:B:1236:GLU:HG3	2.20	0.56
1:B:1265:THR:HG23	1:B:1268:ASP:OD2	2.05	0.56
1:B:1578:THR:HG22	1:B:1579:SER:H	1.69	0.56
1:C:2057:CYS:HB3	1:C:2069:CYS:SG	2.45	0.56
1:C:2113:MET:HE3	1:C:2117:LEU:HD22	1.87	0.56
1:C:2211:LYS:NZ	1:C:2236:GLU:HG3	2.20	0.56
1:C:2389:PRO:CG	1:C:2434:VAL:HG13	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2408:LEU:HD13	1:C:2409:TYR:CE2	2.41	0.56
1:D:3089:VAL:HA	1:D:3092:ILE:CG1	2.34	0.56
1:D:3276:PRO:O	1:D:3279:ILE:HG12	2.05	0.56
1:A:89:VAL:HA	1:A:92:ILE:CG1	2.35	0.56
1:B:1034:ASN:HB3	1:B:1037:CYS:SG	2.46	0.56
1:C:2305:TRP:O	1:C:2308:GLU:HB3	2.05	0.56
1:D:3281:GLU:HB3	6:D:4185:HOH:O	2.05	0.56
1:A:161:THR:HG23	1:A:165:VAL:HA	1.87	0.56
1:A:213:ASP:HB2	1:A:222:ARG:HG3	1.88	0.56
1:C:2192:GLN:OE1	1:C:2517:ILE:HG22	2.05	0.56
1:D:3293:GLY:HA2	1:D:3299:MET:HE3	1.87	0.56
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.73	0.56
1:A:447:VAL:HG12	1:A:448:ALA:N	2.20	0.56
1:B:1409:TYR:CD2	1:B:1409:TYR:N	2.70	0.56
1:B:1454:GLN:HA	1:B:1457:GLU:HG3	1.86	0.56
1:C:2389:PRO:HG3	1:C:2508:LEU:HD22	1.87	0.56
1:C:2507:LEU:HD22	1:C:2522:MET:HE2	1.87	0.56
1:B:1184:ARG:NH2	1:B:1441:PRO:HD3	2.20	0.56
1:B:1305:TRP:O	1:B:1308:GLU:HB3	2.06	0.56
1:D:3116:VAL:HA	1:D:3119:SER:OG	2.06	0.56
1:D:3238:LEU:HD23	1:D:3241:GLN:HG2	1.88	0.56
1:D:3331:THR:O	1:D:3335:ILE:HD12	2.05	0.56
1:D:3357:PHE:CE2	1:D:3359:LEU:HD23	2.41	0.56
1:A:184:ARG:HA	1:A:438:ARG:O	2.05	0.56
1:B:1226:HIS:CE1	1:B:1376:ARG:HD2	2.40	0.56
1:D:3113:MET:C	1:D:3116:VAL:HG13	2.25	0.56
1:D:3451:SER:HB2	1:D:3504:TYR:CE2	2.40	0.56
1:A:463:LEU:HG	1:A:463:LEU:O	2.04	0.56
1:B:1408:LEU:HD13	1:B:1409:TYR:CE2	2.40	0.56
1:D:3105(D):ILE:HG21	1:D:3108:LEU:HD12	1.86	0.56
1:D:3389:PRO:HG3	1:D:3508:LEU:HD22	1.87	0.56
1:A:128:PRO:HG3	1:A:376:ARG:HB2	1.87	0.56
1:A:128:PRO:HG2	1:A:376:ARG:NH1	2.20	0.56
1:A:362:ASP:OD1	1:A:364:GLU:HB2	2.06	0.56
1:B:1184:ARG:HA	1:B:1438:ARG:O	2.06	0.56
1:B:1362:ASP:O	1:B:1365:LEU:HG	2.05	0.56
1:B:1388:HIS:N	1:B:1389:PRO:HD2	2.21	0.56
1:B:1405:LYS:CD	1:B:1405:LYS:H	2.18	0.56
1:C:2128:PRO:CG	1:C:2376:ARG:NH1	2.68	0.56
1:C:2184:ARG:HD3	1:C:2187:PHE:CA	2.33	0.56
1:C:2265:THR:HG23	1:C:2268:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2329:PHE:HD2	1:C:2330:GLN:HG2	1.71	0.56
1:C:2454:GLN:HA	1:C:2457:GLU:HG3	1.88	0.56
1:C:2499:ASP:O	1:C:2501:MET:N	2.38	0.56
1:D:3161:THR:HG23	1:D:3165:VAL:HA	1.87	0.56
1:D:3364:GLU:HA	1:D:3367:PHE:CD1	2.41	0.56
1:A:454:GLN:HA	1:A:457:GLU:HG3	1.86	0.55
1:C:2267:LYS:O	1:C:2267:LYS:HG2	2.05	0.55
1:D:3428:ARG:O	1:D:3430:ILE:N	2.39	0.55
1:D:3582:VAL:HG13	1:D:3582:VAL:O	2.06	0.55
1:A:308:GLU:O	1:A:311:ARG:HB3	2.07	0.55
1:B:1113:MET:HE3	1:B:1117:LEU:HD22	1.89	0.55
1:B:1428:ARG:O	1:B:1430:ILE:N	2.38	0.55
1:D:3463:LEU:HB2	1:D:3503:LEU:HA	1.88	0.55
1:A:578:THR:CG2	1:A:579:SER:H	2.18	0.55
1:D:3185:ARG:HH21	1:D:3438:ARG:CD	2.20	0.55
1:D:3457:GLU:C	1:D:3459:LYS:H	2.10	0.55
1:A:372:GLN:HE22	1:B:1373:TYR:H	1.52	0.55
1:B:1116:VAL:HA	1:B:1119:SER:OG	2.07	0.55
1:C:2113:MET:HB2	1:C:2357:PHE:HZ	1.71	0.55
1:C:2343:ILE:O	1:C:2347:ASP:HB2	2.05	0.55
1:C:2501:MET:CE	1:C:2505:PRO:HB2	2.36	0.55
1:D:3389:PRO:CB	1:D:3434:VAL:HG22	2.36	0.55
1:A:104:ASN:ND2	1:A:358:LYS:HB2	2.20	0.55
1:B:1113:MET:C	1:B:1116:VAL:HG13	2.26	0.55
1:B:1238:LEU:HD23	1:B:1241:GLN:HG2	1.89	0.55
1:C:2191:PRO:HG3	1:C:2433:ARG:NH1	2.21	0.55
1:C:2442:ILE:HD12	1:C:2442:ILE:N	2.22	0.55
1:C:2447:VAL:HG12	1:C:2448:ALA:N	2.20	0.55
1:A:185:ARG:HH21	1:A:438:ARG:CZ	2.20	0.55
1:B:1184:ARG:CD	1:B:1187:PHE:HA	2.32	0.55
1:D:3113:MET:HE3	1:D:3116:VAL:HG22	1.87	0.55
1:B:1578:THR:CG2	1:B:1579:SER:H	2.20	0.55
1:C:2489:ALA:HB2	6:C:4140:HOH:O	2.05	0.55
1:D:3134:TYR:HD2	1:D:3136:TYR:HE1	1.54	0.55
1:D:3211:LYS:NZ	1:D:3236:GLU:HG3	2.21	0.55
1:D:3274:ILE:HG13	1:D:3290:GLU:C	2.27	0.55
1:D:3513:ARG:NH2	1:D:3520:GLU:HB2	2.22	0.55
1:B:1039:ASN:N	1:B:1040:PRO:CD	2.69	0.55
1:B:1113:MET:HB2	1:B:1357:PHE:HZ	1.72	0.55
1:C:2198:PHE:CZ	1:C:2352:LEU:HD13	2.42	0.55
1:C:2308:GLU:O	1:C:2311:ARG:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLN:O	1:A:457:GLU:HG3	2.07	0.55
1:C:2121:SER:O	1:C:2123:LEU:N	2.40	0.55
1:C:2128:PRO:HG3	1:C:2376:ARG:HB2	1.89	0.55
1:D:3339:GLU:O	1:D:3342:LYS:HB3	2.07	0.55
1:A:191:PRO:CD	1:A:433:ARG:HG3	2.30	0.55
1:A:507:LEU:HD22	1:A:522:MET:HE2	1.89	0.55
1:D:3184:ARG:HB2	1:D:3439:ASN:CA	2.37	0.55
1:D:3208:GLN:NE2	1:D:3232:HIS:NE2	2.55	0.55
1:D:3213:ASP:HB2	1:D:3222:ARG:HG3	1.88	0.55
1:D:3464:ASN:OD1	1:D:3499:ASP:HA	2.07	0.55
1:D:3566:SER:HA	1:D:3569:CYS:HB2	1.89	0.55
1:A:364:GLU:HA	1:A:367:PHE:CD1	2.42	0.54
1:A:387:TRP:CZ2	1:A:518:PHE:CZ	2.95	0.54
1:A:405:LYS:CD	1:A:405:LYS:H	2.18	0.54
1:A:435:ALA:HB3	1:A:512:PRO:HG3	1.88	0.54
1:B:1357:PHE:CE2	1:B:1359:LEU:HD23	2.42	0.54
1:B:1482:THR:C	1:B:1511:LYS:HB2	2.26	0.54
1:C:2387:TRP:CH2	5:C:2701:PGX:H121	2.42	0.54
1:A:308:GLU:HG3	1:A:336:LEU:CD1	2.32	0.54
1:A:387:TRP:CZ2	5:A:701:PGX:H121	2.41	0.54
1:A:451:SER:HB2	1:A:504:TYR:CE2	2.42	0.54
1:B:1582:VAL:O	1:B:1582:VAL:HG13	2.06	0.54
1:D:3305:TRP:O	1:D:3308:GLU:HB3	2.08	0.54
1:A:81:LEU:O	1:A:82:LEU:HG	2.07	0.54
1:A:184:ARG:HD3	1:A:187:PHE:CA	2.35	0.54
1:B:1380:GLU:HG3	1:B:1460:TYR:HE2	1.72	0.54
1:C:2208:GLN:NE2	1:C:2232:HIS:NE2	2.56	0.54
1:C:2514:PRO:O	1:C:2515:ASP:HB2	2.07	0.54
1:D:3100:TRP:CD1	1:D:3356:HIS:HB2	2.42	0.54
1:D:3255:GLN:HG2	1:D:3263:PRO:O	2.07	0.54
1:D:3265:THR:HG23	1:D:3268:ASP:OD2	2.07	0.54
1:A:150:ARG:HH22	1:A:154:PRO:HA	1.73	0.54
1:B:1113:MET:HE3	1:B:1116:VAL:HG22	1.89	0.54
1:B:1341:ILE:HG23	1:B:1534:LEU:HD12	1.89	0.54
1:B:1364:GLU:HA	1:B:1367:PHE:CD1	2.42	0.54
1:B:1463:LEU:HG	1:B:1463:LEU:O	2.08	0.54
1:B:1507:LEU:CD2	1:B:1521:THR:HG22	2.38	0.54
1:C:2185:ARG:HH21	1:C:2438:ARG:CZ	2.19	0.54
1:D:3121:SER:O	1:D:3123:LEU:N	2.41	0.54
1:A:173:ASP:O	1:A:177:VAL:HG23	2.07	0.54
1:B:1379:SER:O	1:B:1382:ASN:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1504:TYR:HA	1:B:1507:LEU:HD12	1.88	0.54
1:C:2253:LYS:O	1:C:2264:PRO:HG3	2.07	0.54
1:C:2547:PRO:HB3	1:C:2553:GLU:N	2.23	0.54
1:D:3389:PRO:HG2	1:D:3434:VAL:CG1	2.28	0.54
1:A:39:ASN:HD22	1:A:39:ASN:N	2.05	0.54
1:A:124:ILE:HD11	1:A:528:PRO:HB2	1.89	0.54
1:A:162:PRO:HG2	1:A:171:LEU:HD23	1.90	0.54
1:A:322:GLU:OE1	1:B:1049:SER:HB2	2.07	0.54
1:B:1274:ILE:HG13	1:B:1290:GLU:C	2.27	0.54
1:D:3352:LEU:HD21	1:D:3387:TRP:CH2	2.42	0.54
1:D:3408:LEU:HD13	1:D:3409:TYR:CE2	2.43	0.54
1:A:116:VAL:HA	1:A:119:SER:OG	2.08	0.54
1:B:1389:PRO:HG3	1:B:1508:LEU:HD22	1.90	0.54
1:C:2113:MET:C	1:C:2116:VAL:HG13	2.28	0.54
1:C:2352:LEU:HD21	1:C:2387:TRP:CH2	2.42	0.54
1:D:3267:LYS:O	1:D:3267:LYS:HG2	2.06	0.54
1:A:201:PHE:O	1:A:202:ALA:C	2.46	0.54
1:A:403:SER:N	1:A:406:GLN:OE1	2.41	0.54
1:A:407:PHE:HZ	1:A:426:PHE:HZ	1.54	0.54
1:B:1191:PRO:HG3	1:B:1433:ARG:NH1	2.23	0.54
1:B:1463:LEU:HB2	1:B:1503:LEU:HA	1.89	0.54
1:B:1482:THR:HG22	6:B:4081:HOH:O	2.07	0.54
1:C:2096:PHE:N	1:C:2096:PHE:CD1	2.75	0.54
1:C:2341:ILE:HG23	1:C:2534:LEU:HD12	1.89	0.54
1:D:3208:GLN:O	1:D:3211:LYS:HD3	2.08	0.54
1:A:357:PHE:CE2	1:A:359:LEU:HD23	2.43	0.54
1:C:2128:PRO:HG2	1:C:2376:ARG:NH1	2.23	0.54
1:C:2136:TYR:HD2	1:D:3327:GLN:NE2	2.05	0.54
1:C:2352:LEU:HD21	1:C:2387:TRP:HH2	1.72	0.54
1:D:3184:ARG:HH12	1:D:3441:PRO:HG3	1.72	0.54
1:A:457:GLU:C	1:A:459:LYS:H	2.11	0.54
1:A:568:ILE:HG23	1:A:572:VAL:HG21	1.90	0.54
1:B:1072:PRO:HG2	1:B:1077:ARG:NE	2.23	0.54
1:B:1113:MET:CA	1:B:1116:VAL:HG13	2.37	0.54
1:B:1201:PHE:O	1:B:1202:ALA:C	2.45	0.54
1:B:1306:LEU:HD23	1:B:1307:ARG:N	2.23	0.54
1:B:1482:THR:HB	1:B:1484:GLU:HG3	1.90	0.54
1:C:2104:ASN:ND2	1:C:2358:LYS:HB2	2.23	0.54
1:C:2152:LEU:HB2	1:C:2466:TYR:CE1	2.43	0.54
1:C:2191:PRO:CD	1:C:2433:ARG:HG3	2.29	0.54
1:C:2526:GLY:O	1:C:2530:SER:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2582:VAL:HG13	1:C:2582:VAL:O	2.08	0.54
1:D:3219:GLY:HA2	1:D:3458:MET:HE1	1.89	0.54
1:D:3396:ASN:HD22	1:D:3401:GLU:HG2	1.72	0.54
1:A:113:MET:C	1:A:116:VAL:HG13	2.28	0.53
1:A:113:MET:HA	1:A:116:VAL:HG13	1.90	0.53
1:A:463:LEU:HB2	1:A:503:LEU:HA	1.88	0.53
1:B:1161:THR:HG23	1:B:1165:VAL:HA	1.90	0.53
1:B:1573:LYS:HB2	6:B:4063:HOH:O	2.07	0.53
1:C:2048:MET:HA	6:C:4104:HOH:O	2.07	0.53
1:C:2113:MET:HE3	1:C:2116:VAL:HG22	1.90	0.53
1:C:2238:LEU:HD23	1:C:2241:GLN:HG2	1.90	0.53
1:C:2357:PHE:CE2	1:C:2359:LEU:HD23	2.42	0.53
1:C:2435:ALA:HB3	1:C:2512:PRO:HG3	1.90	0.53
1:D:3405:LYS:H	1:D:3405:LYS:CD	2.22	0.53
1:D:3467:ARG:NH1	1:D:3520:GLU:OE1	2.37	0.53
1:A:339:GLU:O	1:A:342:LYS:HB3	2.08	0.53
1:A:389:PRO:CB	1:A:434:VAL:HG22	2.37	0.53
1:A:454:GLN:O	1:A:457:GLU:N	2.41	0.53
1:B:1121:SER:O	1:B:1123:LEU:N	2.40	0.53
1:B:1184:ARG:NH1	1:B:1441:PRO:HG3	2.23	0.53
1:B:1208:GLN:NE2	1:B:1232:HIS:NE2	2.57	0.53
1:C:2099:VAL:HG12	1:C:2100:TRP:N	2.23	0.53
1:C:2142:PHE:CE2	1:D:3538:PRO:HG3	2.43	0.53
1:D:3482:THR:HB	1:D:3484:GLU:HG3	1.89	0.53
1:A:105(A):ILE:O	1:A:108:LEU:HB2	2.09	0.53
1:A:208:GLN:NE2	1:A:232:HIS:NE2	2.56	0.53
1:A:330:GLN:HE22	1:B:1140:GLU:HB2	1.73	0.53
1:A:498:ILE:O	1:A:501:MET:HB2	2.08	0.53
1:C:2088:THR:O	1:C:2092:ILE:HG12	2.08	0.53
1:C:2274:ILE:HG13	1:C:2290:GLU:C	2.27	0.53
1:C:2308:GLU:CA	1:C:2571:ASN:HD21	2.20	0.53
1:D:3201:PHE:O	1:D:3202:ALA:C	2.46	0.53
1:D:3276:PRO:HD2	1:D:3279:ILE:CG1	2.36	0.53
1:A:88:THR:O	1:A:92:ILE:HG12	2.08	0.53
1:A:232:HIS:O	1:A:288:GLY:CA	2.55	0.53
1:A:380:GLU:HG3	1:A:460:TYR:HE2	1.73	0.53
1:A:530:SER:HB2	5:A:701:PGX:H161	1.89	0.53
1:B:1128:PRO:HG3	1:B:1376:ARG:HB2	1.90	0.53
1:B:1188:ILE:HD12	1:B:1439:ASN:CB	2.38	0.53
1:B:1362:ASP:OD1	1:B:1364:GLU:HB2	2.08	0.53
1:B:1403:SER:N	1:B:1406:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1457:GLU:C	1:B:1459:LYS:H	2.11	0.53
1:C:2405:LYS:CD	1:C:2405:LYS:H	2.20	0.53
1:C:2457:GLU:C	1:C:2459:LYS:H	2.11	0.53
1:C:2463:LEU:HB2	1:C:2503:LEU:HA	1.90	0.53
1:D:3039:ASN:HD22	1:D:3039:ASN:N	2.06	0.53
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.08	0.53
1:D:3180:LYS:HD2	1:D:3490:GLU:OE1	2.08	0.53
1:D:3481:LEU:CD1	1:D:3510:GLU:HA	2.39	0.53
1:A:105(A):ILE:O	1:A:105(A):ILE:HG22	2.08	0.53
1:B:1105(B):ILE:CG2	1:B:1108:LEU:HD12	2.38	0.53
1:B:1254:TYR:C	1:B:1254:TYR:HD1	2.12	0.53
1:B:1329:PHE:HD2	1:B:1330:GLN:HG2	1.74	0.53
1:C:2039:ASN:N	1:C:2039:ASN:HD22	2.05	0.53
1:C:2116:VAL:HA	1:C:2119:SER:OG	2.09	0.53
1:D:3184:ARG:HA	1:D:3438:ARG:O	2.09	0.53
1:D:3388:HIS:N	1:D:3389:PRO:HD2	2.24	0.53
1:B:1388:HIS:O	1:B:1391:LEU:HB2	2.09	0.53
1:C:2188:ILE:HD12	1:C:2439:ASN:CB	2.39	0.53
1:C:2206:THR:HG21	5:C:2701:PGX:H111	1.90	0.53
1:C:2244:LEU:CD2	1:C:2271:VAL:HG21	2.38	0.53
1:D:3329:PHE:C	1:D:3329:PHE:CD2	2.82	0.53
1:D:3377:ILE:HG13	6:D:4180:HOH:O	2.08	0.53
1:A:64:PHE:HD2	1:A:70:THR:O	1.91	0.53
1:A:261:VAL:O	1:A:307:ARG:NH1	2.42	0.53
1:A:304:ILE:O	1:A:307:ARG:HB2	2.09	0.53
1:A:566:SER:HA	1:A:569:CYS:HB2	1.90	0.53
1:B:1385:TYR:HA	5:B:1701:PGX:O4	2.07	0.53
1:B:1389:PRO:HG2	1:B:1434:VAL:CG1	2.31	0.53
1:C:2255:GLN:HG2	1:C:2263:PRO:O	2.09	0.53
1:C:2380:GLU:HG3	1:C:2460:TYR:HE2	1.74	0.53
1:C:2464:ASN:OD1	1:C:2499:ASP:HA	2.08	0.53
1:C:2482:THR:HB	1:C:2484:GLU:HG3	1.90	0.53
1:D:3124:ILE:HD11	1:D:3529:PHE:N	2.24	0.53
1:D:3526:GLY:CA	5:D:3701:PGX:H61	2.35	0.53
1:A:120:ARG:HD2	1:A:527:ALA:HB1	1.91	0.53
1:A:152:LEU:HB2	1:A:466:TYR:CE1	2.44	0.53
1:A:188:ILE:HD12	1:A:439:ASN:CB	2.37	0.53
1:A:245:ARG:HH22	1:A:326:GLU:HA	1.74	0.53
1:A:507:LEU:HD21	1:A:521:THR:HG22	1.89	0.53
1:B:1198:PHE:CE1	1:B:1352:LEU:HD13	2.44	0.53
1:C:2108:LEU:O	1:C:2112:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2205:PHE:CE2	1:C:2209:PHE:HZ	2.27	0.53
1:C:2568:ILE:HG23	1:C:2572:VAL:HG21	1.89	0.53
1:D:3403:SER:N	1:D:3406:GLN:OE1	2.42	0.53
1:D:3407:PHE:HZ	1:D:3426:PHE:HZ	1.57	0.53
1:A:121:SER:O	1:A:123:LEU:N	2.41	0.53
1:A:205:PHE:CE2	1:A:209:PHE:HZ	2.26	0.53
1:A:225:GLY:HA3	1:A:229:ASP:OD1	2.07	0.53
1:C:2081:LEU:O	1:C:2082:LEU:HG	2.08	0.53
1:C:2155:VAL:HG23	1:C:2459:LYS:O	2.09	0.53
1:D:3387:TRP:CZ2	1:D:3518:PHE:CZ	2.97	0.53
1:D:3387:TRP:CH2	5:D:3701:PGX:H121	2.44	0.53
1:D:3414:LEU:HA	1:D:3422:PHE:HE1	1.71	0.53
1:A:113:MET:HB2	1:A:357:PHE:HZ	1.74	0.52
1:A:379:SER:O	1:A:382:ASN:HB3	2.08	0.52
1:A:507:LEU:CD2	1:A:521:THR:HG22	2.39	0.52
1:B:1105(B):ILE:HG22	1:B:1105(B):ILE:O	2.10	0.52
1:B:1162:PRO:HG2	1:B:1171:LEU:HD23	1.90	0.52
1:B:1254:TYR:C	1:B:1254:TYR:CD1	2.82	0.52
1:C:2161:THR:HG23	1:C:2165:VAL:HA	1.91	0.52
1:D:3104:ASN:ND2	1:D:3358:LYS:HB2	2.24	0.52
1:D:3128:PRO:CG	1:D:3376:ARG:NH1	2.72	0.52
1:D:3243:LYS:HA	6:D:4189:HOH:O	2.10	0.52
1:A:96:PHE:N	1:A:96:PHE:CD1	2.77	0.52
1:A:124:ILE:HD11	1:A:529:PHE:N	2.24	0.52
1:A:234:TYR:CE1	1:A:252:LEU:HD11	2.44	0.52
1:A:265:THR:HG23	1:A:268:ASP:OD2	2.08	0.52
1:B:1124:ILE:HD11	1:B:1529:PHE:N	2.25	0.52
1:B:1338:GLY:HA3	1:B:1559:ILE:CD1	2.35	0.52
1:B:1467:ARG:NH1	1:B:1520:GLU:OE1	2.41	0.52
1:C:2341:ILE:HD13	1:C:2534:LEU:HD12	1.91	0.52
1:D:3081:LEU:O	1:D:3082:LEU:HG	2.08	0.52
1:D:3254:TYR:HD1	1:D:3254:TYR:C	2.12	0.52
1:D:3352:LEU:HD21	1:D:3387:TRP:HH2	1.74	0.52
1:D:3454:GLN:O	1:D:3457:GLU:N	2.42	0.52
1:A:232:HIS:C	1:A:288:GLY:HA3	2.30	0.52
1:A:347:ASP:O	1:A:350:GLN:HB3	2.09	0.52
1:B:1096:PHE:N	1:B:1096:PHE:CD1	2.77	0.52
1:B:1182:LEU:C	1:B:1438:ARG:HA	2.29	0.52
1:B:1276:PRO:O	1:B:1279:ILE:HG12	2.08	0.52
1:B:1389:PRO:CG	1:B:1434:VAL:HG13	2.29	0.52
1:C:2454:GLN:O	1:C:2457:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3088:THR:O	1:D:3092:ILE:HG12	2.10	0.52
1:D:3244:LEU:CD2	1:D:3271:VAL:HG21	2.38	0.52
1:D:3435:ALA:HB3	1:D:3512:PRO:HG3	1.91	0.52
1:B:1435:ALA:HB3	1:B:1512:PRO:HG3	1.90	0.52
1:B:1500:VAL:O	1:B:1500:VAL:HG12	2.09	0.52
1:B:1538:PRO:O	1:B:1540:CYS:N	2.42	0.52
1:C:2120:ARG:HD2	1:C:2527:ALA:HB1	1.91	0.52
1:C:2197:MET:CE	1:C:2423:VAL:HG13	2.39	0.52
1:C:2308:GLU:HG3	1:C:2336:LEU:CD1	2.33	0.52
1:C:2362:ASP:OD1	1:C:2364:GLU:HB2	2.09	0.52
1:C:2403:SER:N	1:C:2406:GLN:OE1	2.43	0.52
1:C:2498:ILE:HG23	1:C:2499:ASP:N	2.24	0.52
1:D:3039:ASN:N	1:D:3040:PRO:CD	2.72	0.52
1:D:3495:TYR:CD2	1:D:3501:MET:HA	2.44	0.52
1:A:433:ARG:HD3	1:A:436:GLY:H	1.75	0.52
1:B:1389:PRO:CB	1:B:1434:VAL:HG22	2.38	0.52
1:B:1566:SER:HA	1:B:1569:CYS:HB2	1.91	0.52
1:C:2039:ASN:N	1:C:2040:PRO:CD	2.72	0.52
1:D:3128:PRO:HG2	1:D:3376:ARG:NH1	2.24	0.52
1:D:3162:PRO:HG2	1:D:3171:LEU:HD23	1.92	0.52
1:D:3206:THR:HA	1:D:3209:PHE:CE2	2.44	0.52
1:D:3254:TYR:C	1:D:3254:TYR:CD1	2.82	0.52
1:D:3463:LEU:O	1:D:3463:LEU:HG	2.10	0.52
1:A:39:ASN:N	1:A:40:PRO:CD	2.72	0.52
1:A:235:GLY:HA3	1:A:240:ARG:HG2	1.90	0.52
1:B:1185:ARG:HH21	1:B:1438:ARG:CZ	2.22	0.52
1:C:2407:PHE:HZ	1:C:2426:PHE:HZ	1.58	0.52
1:C:2463:LEU:HG	1:C:2463:LEU:O	2.08	0.52
1:D:3096:PHE:CD1	1:D:3096:PHE:N	2.78	0.52
1:D:3112:ILE:O	1:D:3115:TYR:N	2.43	0.52
1:D:3113:MET:CE	1:D:3117:LEU:HD22	2.40	0.52
1:D:3363:PRO:C	1:D:3365:LEU:H	2.13	0.52
1:D:3380:GLU:HG3	1:D:3460:TYR:HE2	1.74	0.52
1:A:246:LEU:HD23	1:A:251:LYS:HB2	1.91	0.52
1:B:1050:THR:HG21	1:B:1056:LYS:HB2	1.90	0.52
1:B:1202:ALA:CA	1:B:1348:TYR:HE1	2.23	0.52
1:B:1329:PHE:C	1:B:1329:PHE:CD2	2.82	0.52
1:B:1557:LYS:O	1:B:1558:ILE:C	2.47	0.52
1:D:3050:THR:HG21	1:D:3056:LYS:HB2	1.92	0.52
1:A:464:ASN:OD1	1:A:499:ASP:HA	2.09	0.52
1:A:482:THR:HG23	1:A:509:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLU:OE1	1:A:519:GLY:HA3	2.10	0.52
1:B:1234:TYR:CE1	1:B:1252:LEU:HD11	2.45	0.52
1:B:1304:ILE:O	1:B:1307:ARG:HB2	2.09	0.52
1:B:1352:LEU:HD21	1:B:1387:TRP:CH2	2.45	0.52
1:B:1467:ARG:NH1	1:B:1521:THR:OG1	2.42	0.52
1:C:2427:THR:HG21	1:C:2578:THR:HA	1.92	0.52
1:D:3241:GLN:OE1	1:D:3245:ARG:HD2	2.10	0.52
1:D:3379:SER:O	1:D:3382:ASN:HB3	2.10	0.52
1:A:140:GLU:HB2	1:B:1330:GLN:HE22	1.75	0.52
1:A:185:ARG:HH21	1:A:438:ARG:CD	2.22	0.52
1:A:255:GLN:HG2	1:A:263:PRO:O	2.09	0.52
1:A:377:ILE:HA	6:A:4037:HOH:O	2.10	0.52
1:C:2196:MET:CE	1:C:2431:ALA:HB2	2.40	0.52
1:C:2349:VAL:HG22	5:C:2701:PGX:O5	2.09	0.52
1:C:2364:GLU:HA	1:C:2367:PHE:CD1	2.44	0.52
1:D:3176:GLU:O	1:D:3177:VAL:C	2.48	0.52
1:A:305:TRP:O	1:A:308:GLU:HB3	2.10	0.52
1:A:308:GLU:CA	1:A:571:ASN:HD21	2.23	0.52
1:A:498:ILE:HG23	1:A:499:ASP:N	2.25	0.52
1:B:1206:THR:HA	1:B:1209:PHE:CE2	2.45	0.52
1:B:1253:LYS:O	1:B:1264:PRO:HG3	2.10	0.52
1:B:1433:ARG:HD3	1:B:1436:GLY:H	1.74	0.52
1:C:2184:ARG:CD	1:C:2187:PHE:HA	2.35	0.52
1:C:2202:ALA:CA	1:C:2348:TYR:HE1	2.23	0.52
1:C:2347:ASP:O	1:C:2350:GLN:HB3	2.09	0.52
1:D:3150:ARG:HH22	1:D:3154:PRO:HA	1.75	0.52
1:D:3306:LEU:HD23	1:D:3307:ARG:N	2.25	0.52
1:A:491:LEU:O	1:A:494:LEU:N	2.42	0.51
1:B:1232:HIS:C	1:B:1288:GLY:HA3	2.31	0.51
1:C:2330:GLN:HE22	1:D:3140:GLU:HB2	1.75	0.51
1:D:3072:PRO:HG2	1:D:3077:ARG:NE	2.24	0.51
1:D:3347:ASP:O	1:D:3350:GLN:N	2.43	0.51
1:A:427:THR:HG21	1:A:578:THR:HA	1.91	0.51
1:A:442:ILE:HD12	1:A:442:ILE:N	2.24	0.51
1:A:514:PRO:O	1:A:515:ASP:HB2	2.10	0.51
1:B:1099:VAL:HG12	1:B:1100:TRP:N	2.24	0.51
1:B:1463:LEU:HD12	1:B:1503:LEU:CD1	2.39	0.51
1:B:1577:PHE:C	1:B:1577:PHE:CD2	2.83	0.51
1:C:2179:GLU:O	1:C:2181:VAL:N	2.43	0.51
1:D:3225:GLY:HA3	1:D:3229:ASP:OD1	2.10	0.51
1:A:64:PHE:HA	1:A:71:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HG2	1:A:77:ARG:NE	2.25	0.51
1:A:261:VAL:H	1:A:307:ARG:NH2	2.07	0.51
1:A:467:ARG:NH1	1:A:521:THR:OG1	2.43	0.51
1:B:1128:PRO:CG	1:B:1376:ARG:NH1	2.74	0.51
1:C:2198:PHE:C	1:C:2198:PHE:CD2	2.83	0.51
1:C:2241:GLN:OE1	1:C:2245:ARG:HD2	2.10	0.51
1:C:2294:LEU:HB3	1:C:2409:TYR:CD2	2.45	0.51
1:C:2379:SER:O	1:C:2382:ASN:HB3	2.11	0.51
1:D:3185:ARG:NH2	6:D:4167:HOH:O	2.43	0.51
1:A:329:PHE:C	1:A:329:PHE:CD2	2.83	0.51
1:B:1152:LEU:HB2	1:B:1466:TYR:CE1	2.46	0.51
1:B:1209:PHE:HB3	1:B:1377:ILE:CD1	2.40	0.51
1:B:1270:GLN:N	1:B:1270:GLN:OE1	2.43	0.51
1:C:2509:VAL:O	1:C:2510:GLU:O	2.28	0.51
1:C:2577:PHE:C	1:C:2577:PHE:CD2	2.83	0.51
1:D:3197:MET:HE1	1:D:3423:VAL:HG13	1.92	0.51
1:A:50:THR:CG2	1:A:56:LYS:HB3	2.40	0.51
1:A:112:ILE:O	1:A:115:TYR:N	2.43	0.51
1:A:134:TYR:HD2	1:A:136:TYR:HE1	1.57	0.51
1:A:292:PHE:O	1:A:299:MET:HE2	2.10	0.51
1:A:526:GLY:O	1:A:530:SER:HB3	2.10	0.51
1:B:1156:ALA:O	1:B:1159:CYS:HB2	2.11	0.51
1:C:2185:ARG:NH2	6:C:4120:HOH:O	2.44	0.51
1:D:3183:LEU:HD21	1:D:3445:GLN:HG3	1.92	0.51
1:D:3568:ILE:HG23	1:D:3572:VAL:HG21	1.92	0.51
1:A:156:ALA:O	1:A:159:CYS:HB2	2.11	0.51
1:A:209:PHE:CD1	1:A:209:PHE:N	2.78	0.51
1:A:394:THR:HA	1:A:402:TYR:O	2.10	0.51
1:B:1120:ARG:HD2	1:B:1527:ALA:HB1	1.92	0.51
1:B:1339:GLU:O	1:B:1342:LYS:HB3	2.10	0.51
1:B:1396:ASN:HD22	1:B:1401:GLU:HG2	1.74	0.51
1:B:1568:ILE:HG23	1:B:1572:VAL:HG21	1.92	0.51
1:C:2394:THR:O	1:C:2429:GLN:NE2	2.40	0.51
1:D:3137:LYS:HD2	6:D:4174:HOH:O	2.10	0.51
1:D:3450:ALA:O	1:D:3452:ILE:N	2.43	0.51
1:A:513:ARG:NH2	1:A:520:GLU:HB2	2.26	0.51
1:B:1294:LEU:HB3	1:B:1409:TYR:CD2	2.45	0.51
1:B:1444:VAL:O	1:B:1444:VAL:CG1	2.59	0.51
1:C:2182:LEU:C	1:C:2438:ARG:HA	2.31	0.51
1:C:2433:ARG:HD3	1:C:2436:GLY:H	1.76	0.51
1:C:2482:THR:HG23	1:C:2509:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2547:PRO:O	1:C:2552:GLY:N	2.41	0.51
1:D:3050:THR:CG2	1:D:3056:LYS:HB3	2.41	0.51
1:D:3095:HIS:O	1:D:3097:LYS:N	2.43	0.51
1:D:3463:LEU:HD12	1:D:3503:LEU:CD1	2.38	0.51
1:D:3547:PRO:HB3	1:D:3553:GLU:N	2.25	0.51
1:A:253:LYS:O	1:A:264:PRO:HG3	2.10	0.51
1:A:363:PRO:C	1:A:365:LEU:H	2.14	0.51
1:A:547:PRO:HB3	1:A:553:GLU:N	2.26	0.51
1:B:1181:VAL:HG12	1:B:1487:MET:HG2	1.93	0.51
1:C:2113:MET:HA	1:C:2116:VAL:CG1	2.41	0.51
1:D:3156:ALA:O	1:D:3159:CYS:HB2	2.10	0.51
1:D:3347:ASP:O	1:D:3350:GLN:HB3	2.11	0.51
1:A:428:ARG:O	1:A:430:ILE:N	2.44	0.51
1:A:463:LEU:HD12	1:A:503:LEU:CD1	2.41	0.51
1:A:482:THR:HB	1:A:484:GLU:HG3	1.93	0.51
1:B:1208:GLN:O	1:B:1211:LYS:HD3	2.11	0.51
1:C:2185:ARG:HH21	1:C:2438:ARG:CD	2.23	0.51
1:C:2219:GLY:N	1:C:2458:MET:HE2	2.25	0.51
1:D:3113:MET:HA	1:D:3116:VAL:HG13	1.93	0.51
1:D:3202:ALA:CA	1:D:3348:TYR:HE1	2.23	0.51
1:D:3509:VAL:O	1:D:3510:GLU:O	2.29	0.51
1:B:1183:LEU:HD21	1:B:1445:GLN:HG3	1.93	0.51
1:B:1407:PHE:HZ	1:B:1426:PHE:HZ	1.58	0.51
1:C:2124:ILE:HD11	1:C:2529:PHE:N	2.26	0.51
1:C:2232:HIS:C	1:C:2288:GLY:HA3	2.31	0.51
1:C:2293:GLY:HA2	1:C:2299:MET:HE3	1.92	0.51
1:C:2566:SER:HA	1:C:2569:CYS:HB2	1.93	0.51
1:D:3121:SER:C	1:D:3123:LEU:H	2.15	0.51
1:D:3206:THR:HB	1:D:3210:PHE:CD2	2.46	0.51
1:D:3465:GLU:OE2	1:D:3468:LYS:CE	2.59	0.51
1:A:238:LEU:HD23	1:A:241:GLN:HG2	1.92	0.50
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.46	0.50
1:A:433:ARG:HH21	1:A:512:PRO:HB3	1.76	0.50
1:A:450:ALA:O	1:A:452:ILE:N	2.44	0.50
1:A:557:LYS:HA	1:A:560:ASN:HD22	1.76	0.50
1:B:1482:THR:HG23	1:B:1509:VAL:HG12	1.93	0.50
1:C:2064:PHE:HA	1:C:2071:THR:O	2.11	0.50
1:C:2387:TRP:CZ2	1:C:2518:PHE:CZ	2.99	0.50
1:C:2454:GLN:O	1:C:2457:GLU:N	2.43	0.50
1:C:2463:LEU:HD12	1:C:2503:LEU:CD1	2.40	0.50
1:D:3188:ILE:HB	1:D:3439:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3433:ARG:HD3	1:D:3436:GLY:H	1.75	0.50
1:D:3526:GLY:O	1:D:3530:SER:HB3	2.11	0.50
1:A:50:THR:HG21	1:A:56:LYS:HB2	1.92	0.50
1:A:247:PHE:HA	1:A:325:ASP:OD2	2.12	0.50
1:A:577:PHE:CD2	1:A:577:PHE:C	2.84	0.50
1:B:1243:LYS:HA	6:B:4095:HOH:O	2.12	0.50
1:C:2213:ASP:HB2	1:C:2222:ARG:HG3	1.94	0.50
1:A:179:GLU:O	1:A:181:VAL:N	2.44	0.50
1:B:1120:ARG:O	1:B:1122:TYR:N	2.44	0.50
1:B:1155:VAL:HG23	1:B:1459:LYS:O	2.11	0.50
1:B:1363:PRO:C	1:B:1365:LEU:H	2.14	0.50
1:B:1464:ASN:HD21	1:B:1475:TYR:H	1.59	0.50
1:B:1498:ILE:HG23	1:B:1499:ASP:N	2.26	0.50
1:C:2235:GLY:HA3	1:C:2240:ARG:HG2	1.92	0.50
1:C:2444:VAL:O	1:C:2444:VAL:CG1	2.60	0.50
1:D:3113:MET:HB2	1:D:3357:PHE:HZ	1.75	0.50
1:D:3482:THR:HG23	1:D:3509:VAL:HG12	1.93	0.50
1:A:329:PHE:HD2	1:A:330:GLN:HG2	1.76	0.50
1:C:2363:PRO:C	1:C:2365:LEU:H	2.12	0.50
1:D:3174:SER:O	1:D:3178:LEU:HB2	2.11	0.50
1:D:3514:PRO:O	1:D:3515:ASP:HB2	2.12	0.50
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.93	0.50
1:A:326:GLU:HB2	6:A:4005:HOH:O	2.10	0.50
1:B:1050:THR:CG2	1:B:1056:LYS:HB3	2.41	0.50
1:B:1150:ARG:HH22	1:B:1154:PRO:HA	1.76	0.50
1:C:2101:ASN:O	1:C:2105:ASN:ND2	2.44	0.50
1:C:2105(C):ILE:HB	1:C:2108:LEU:HB2	1.93	0.50
1:C:2121:SER:C	1:C:2123:LEU:H	2.15	0.50
1:C:2206:THR:HB	1:C:2210:PHE:CE2	2.46	0.50
1:C:2270:GLN:OE1	1:C:2270:GLN:N	2.45	0.50
1:C:2389:PRO:HG2	1:C:2434:VAL:CG1	2.32	0.50
1:D:3099:VAL:HG12	1:D:3100:TRP:N	2.27	0.50
1:B:1100:TRP:CD1	1:B:1356:HIS:HB2	2.47	0.50
1:B:1347:ASP:O	1:B:1350:GLN:HB3	2.11	0.50
1:B:1495:TYR:CD2	1:B:1501:MET:HA	2.46	0.50
1:C:2219:GLY:HA2	1:C:2458:MET:HE1	1.93	0.50
1:D:3300:MET:O	1:D:3304:ILE:HG13	2.12	0.50
1:D:3394:THR:HA	1:D:3402:TYR:O	2.10	0.50
1:D:3500:VAL:O	1:D:3500:VAL:HG12	2.11	0.50
1:A:228:VAL:HG23	6:A:4027:HOH:O	2.11	0.50
1:A:482:THR:C	1:A:511:LYS:HB2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LYS:HE3	1:B:1137:LYS:NZ	2.26	0.50
1:B:1245:ARG:HD2	1:B:1329:PHE:CE1	2.47	0.50
1:B:1394:THR:HA	1:B:1402:TYR:O	2.12	0.50
1:C:2202:ALA:HB2	1:C:2348:TYR:CE1	2.47	0.50
1:C:2396:ASN:N	1:C:2396:ASN:HD22	2.08	0.50
1:D:3132:VAL:HG23	6:D:4179:HOH:O	2.12	0.50
1:D:3232:HIS:C	1:D:3288:GLY:HA3	2.32	0.50
1:A:384:LEU:HB3	1:A:522:MET:CE	2.42	0.50
1:B:1088:THR:O	1:B:1092:ILE:HG12	2.12	0.50
1:B:1209:PHE:HB3	1:B:1377:ILE:HD11	1.93	0.50
1:B:1246:LEU:HD23	1:B:1251:LYS:HB2	1.94	0.50
1:C:2095:HIS:O	1:C:2097:LYS:N	2.45	0.50
1:C:2226:HIS:C	1:C:2377:ILE:HD12	2.31	0.50
1:C:2456:ARG:NE	1:C:2502:GLU:OE2	2.44	0.50
1:D:3134:TYR:CD2	1:D:3136:TYR:HE1	2.29	0.50
1:D:3308:GLU:CA	1:D:3571:ASN:HD21	2.24	0.50
1:D:3491:LEU:O	1:D:3494:LEU:N	2.45	0.50
1:A:99:VAL:HG12	1:A:100:TRP:N	2.27	0.50
1:A:148:TYR:HB2	1:A:219:GLY:O	2.12	0.50
1:A:182:LEU:C	1:A:438:ARG:HA	2.32	0.50
1:A:198:PHE:CE1	1:A:352:LEU:HD13	2.47	0.50
1:A:331:THR:O	1:A:335:ILE:HD12	2.11	0.50
1:B:1169:LYS:O	1:B:1170:GLU:HG3	2.12	0.50
1:B:1269:THR:OG1	1:B:1271:VAL:HG23	2.12	0.50
1:C:2254:TYR:C	1:C:2254:TYR:HD1	2.15	0.50
1:C:2428:ARG:O	1:C:2430:ILE:N	2.45	0.50
1:C:2449:LYS:CA	1:C:2452:ILE:HD12	2.36	0.50
1:C:2451:SER:HB2	1:C:2504:TYR:CE2	2.46	0.50
1:C:2464:ASN:ND2	1:C:2475:TYR:H	2.10	0.50
1:A:169:LYS:O	1:A:170:GLU:HG3	2.12	0.49
1:A:209:PHE:HB3	1:A:377:ILE:CD1	2.41	0.49
1:A:408:LEU:HD13	1:A:409:TYR:CE2	2.46	0.49
1:B:1113:MET:O	1:B:1116:VAL:HG13	2.12	0.49
1:B:1198:PHE:HA	1:B:1580:PHE:CD2	2.46	0.49
1:C:2388:HIS:O	1:C:2391:LEU:HB2	2.11	0.49
1:D:3077:ARG:O	1:D:3081:LEU:HG	2.11	0.49
1:D:3465:GLU:OE2	1:D:3468:LYS:HE2	2.12	0.49
1:D:3577:PHE:C	1:D:3577:PHE:CD2	2.84	0.49
1:A:43:ASN:ND2	1:A:69:CYS:O	2.45	0.49
1:A:274:ILE:HG13	1:A:290:GLU:C	2.31	0.49
1:B:1064:PHE:HA	1:B:1071:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1108:LEU:O	1:B:1112:ILE:HG12	2.12	0.49
1:B:1151:ALA:HB2	1:B:1529:PHE:HZ	1.77	0.49
1:B:1174:SER:O	1:B:1178:LEU:HB2	2.11	0.49
1:C:2132:VAL:HG23	6:C:4132:HOH:O	2.11	0.49
1:C:2225:GLY:HA3	1:C:2229:ASP:OD1	2.12	0.49
1:C:2246:LEU:HD23	1:C:2251:LYS:HB2	1.94	0.49
1:C:2464:ASN:HD21	1:C:2475:TYR:H	1.58	0.49
1:D:3196:MET:CE	1:D:3431:ALA:HB2	2.42	0.49
1:A:121:SER:C	1:A:123:LEU:H	2.16	0.49
1:A:196:MET:CE	1:A:431:ALA:HB2	2.42	0.49
1:B:1081:LEU:O	1:B:1082:LEU:HG	2.12	0.49
1:B:1196:MET:CE	1:B:1431:ALA:HB2	2.42	0.49
1:B:1229:ASP:HA	1:B:1337:ILE:HD11	1.94	0.49
1:B:1308:GLU:CA	1:B:1571:ASN:HD21	2.24	0.49
1:B:1347:ASP:O	1:B:1350:GLN:N	2.45	0.49
1:C:2049:SER:HB2	1:D:3322:GLU:OE1	2.13	0.49
1:C:2287:VAL:HG23	1:C:2289:GLN:H	1.77	0.49
1:C:2394:THR:HA	1:C:2402:TYR:O	2.12	0.49
1:C:2499:ASP:C	1:C:2501:MET:H	2.15	0.49
1:D:3087:ASN:HB3	4:D:3702:BOG:H3	1.93	0.49
1:D:3557:LYS:HA	1:D:3560:ASN:HD22	1.77	0.49
1:A:190:ASP:HB2	1:A:517:ILE:HD12	1.94	0.49
1:A:545:TRP:CE3	1:A:545:TRP:HA	2.46	0.49
1:B:1039:ASN:N	1:B:1039:ASN:HD22	2.10	0.49
1:D:3064:PHE:HD2	1:D:3070:THR:O	1.96	0.49
1:D:3209:PHE:CD1	1:D:3209:PHE:N	2.79	0.49
1:D:3245:ARG:HH22	1:D:3326:GLU:HA	1.78	0.49
1:D:3464:ASN:HD21	1:D:3475:TYR:H	1.59	0.49
1:D:3523:VAL:HG12	1:D:3524:GLU:OE2	2.12	0.49
1:D:3545:TRP:HA	1:D:3545:TRP:CE3	2.47	0.49
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.52	0.49
1:A:241:GLN:OE1	1:A:245:ARG:HD2	2.11	0.49
1:A:352:LEU:HD21	1:A:387:TRP:HH2	1.78	0.49
1:B:1107:PHE:O	1:B:1111:LEU:HB3	2.12	0.49
1:B:1121:SER:C	1:B:1123:LEU:H	2.15	0.49
1:C:2050:THR:HG21	1:C:2056:LYS:HB2	1.94	0.49
1:C:2435:ALA:O	1:C:2510:GLU:O	2.30	0.49
1:C:2504:TYR:HA	1:C:2507:LEU:HD12	1.93	0.49
1:D:3276:PRO:HG3	1:D:3409:TYR:CD1	2.48	0.49
1:A:90:HIS:CD2	1:A:513:ARG:HG2	2.46	0.49
1:A:155:VAL:HG23	1:A:459:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ALA:O	1:A:303:THR:C	2.51	0.49
1:A:495:TYR:CD2	1:A:501:MET:HA	2.47	0.49
1:C:2128:PRO:HG3	1:C:2376:ARG:NH1	2.27	0.49
1:C:2150:ARG:NH2	1:C:2154:PRO:HA	2.27	0.49
1:C:2184:ARG:HH12	1:C:2441:PRO:HG3	1.77	0.49
1:D:3064:PHE:HA	1:D:3071:THR:O	2.12	0.49
1:D:3131:ASN:C	1:D:3131:ASN:OD1	2.50	0.49
1:D:3246:LEU:HD23	1:D:3251:LYS:HB2	1.93	0.49
1:D:3510:GLU:OE1	1:D:3519:GLY:HA3	2.13	0.49
1:A:244:LEU:CD2	1:A:271:VAL:HG21	2.42	0.49
1:B:1465:GLU:OE2	1:B:1468:LYS:CE	2.61	0.49
1:C:2156:ALA:O	1:C:2159:CYS:HB2	2.12	0.49
1:C:2162:PRO:HG2	1:C:2171:LEU:HD23	1.94	0.49
1:C:2209:PHE:HB3	1:C:2377:ILE:HD11	1.94	0.49
1:C:2254:TYR:C	1:C:2254:TYR:CD1	2.85	0.49
1:D:3557:LYS:O	1:D:3558:ILE:C	2.51	0.49
1:A:206:THR:HB	1:A:210:PHE:CD2	2.48	0.49
1:A:500:VAL:O	1:A:500:VAL:HG12	2.12	0.49
1:A:523:VAL:HG12	1:A:524:GLU:OE2	2.13	0.49
1:B:1206:THR:HB	1:B:1210:PHE:CD2	2.48	0.49
1:B:1241:GLN:OE1	1:B:1245:ARG:HD2	2.13	0.49
1:B:1456:ARG:NE	1:B:1502:GLU:OE2	2.45	0.49
1:B:1535:MET:O	1:B:1537:ASN:N	2.45	0.49
1:C:2120:ARG:O	1:C:2122:TYR:N	2.46	0.49
1:C:2195:ASN:OD1	1:C:2197:MET:HB2	2.13	0.49
1:C:2395:PHE:O	1:C:2402:TYR:HD2	1.95	0.49
1:C:2433:ARG:HH21	1:C:2512:PRO:HB3	1.78	0.49
1:C:2482:THR:C	1:C:2511:LYS:HB2	2.33	0.49
1:D:3096:PHE:O	1:D:3099:VAL:N	2.46	0.49
1:D:3113:MET:O	1:D:3116:VAL:HG13	2.12	0.49
1:D:3219:GLY:HA2	1:D:3458:MET:CE	2.43	0.49
1:D:3563:SER:O	1:D:3564:ILE:C	2.51	0.49
1:A:128:PRO:HG3	1:A:376:ARG:NH1	2.28	0.49
1:A:270:GLN:OE1	1:A:270:GLN:N	2.45	0.49
1:A:347:ASP:O	1:A:350:GLN:N	2.46	0.49
1:B:1202:ALA:HB2	1:B:1348:TYR:CE1	2.48	0.49
1:B:1205:PHE:CE2	5:B:1701:PGX:H171	2.48	0.49
1:B:1545:TRP:HA	1:B:1545:TRP:CE3	2.48	0.49
1:C:2072:PRO:HG2	1:C:2077:ARG:NE	2.27	0.49
1:C:2206:THR:HB	1:C:2210:PHE:CD2	2.48	0.49
1:C:2322:GLU:HB3	1:D:3052:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2347:ASP:O	1:C:2350:GLN:N	2.46	0.49
1:C:2450:ALA:O	1:C:2451:SER:C	2.51	0.49
1:D:3136:TYR:O	1:D:3136:TYR:CD1	2.66	0.49
1:A:95:HIS:O	1:A:97:LYS:N	2.46	0.49
1:B:1195:ASN:OD1	1:B:1197:MET:HB2	2.13	0.49
1:B:1339:GLU:OE2	1:B:1558:ILE:CG2	2.61	0.49
1:B:1513:ARG:NH2	1:B:1520:GLU:HB2	2.28	0.49
1:B:1523:VAL:HG12	1:B:1524:GLU:OE2	2.13	0.49
1:C:2107:PHE:O	1:C:2111:LEU:HB3	2.13	0.49
1:C:2209:PHE:HB3	1:C:2377:ILE:CD1	2.43	0.49
1:C:2467:ARG:NH1	1:C:2521:THR:OG1	2.44	0.49
1:D:3253:LYS:O	1:D:3264:PRO:HG3	2.12	0.49
1:A:219:GLY:N	1:A:458:MET:HE2	2.28	0.48
1:A:403:SER:HB2	1:A:405:LYS:HZ2	1.78	0.48
1:A:464:ASN:HD21	1:A:475:TYR:H	1.60	0.48
1:A:513:ARG:HB2	1:A:516:ALA:HB3	1.95	0.48
1:B:1449:LYS:CA	1:B:1452:ILE:HD12	2.40	0.48
1:B:1507:LEU:HD22	1:B:1522:MET:HB2	1.95	0.48
1:B:1530:SER:OG	5:B:1701:PGX:H162	2.13	0.48
1:B:1547:PRO:HB3	1:B:1553:GLU:N	2.28	0.48
1:C:2112:ILE:O	1:C:2115:TYR:N	2.46	0.48
1:C:2151:ALA:HB2	1:C:2529:PHE:HZ	1.78	0.48
1:C:2301:TYR:O	1:C:2302:ALA:C	2.49	0.48
1:C:2450:ALA:O	1:C:2452:ILE:N	2.46	0.48
1:D:3151:ALA:HB2	1:D:3529:PHE:HZ	1.78	0.48
1:D:3198:PHE:CE1	1:D:3352:LEU:HD13	2.48	0.48
1:D:3537:ASN:HB2	6:D:4170:HOH:O	2.13	0.48
1:A:371:PHE:HZ	1:A:536:GLY:N	2.11	0.48
1:B:1038:SER:C	1:B:1040:PRO:HD3	2.34	0.48
1:B:1064:PHE:HD2	1:B:1070:THR:O	1.96	0.48
1:B:1352:LEU:HD21	1:B:1387:TRP:HH2	1.76	0.48
1:C:2495:TYR:CD2	1:C:2501:MET:HA	2.48	0.48
1:D:3198:PHE:HA	1:D:3580:PHE:CD2	2.48	0.48
1:D:3294:LEU:HB3	1:D:3409:TYR:CD2	2.47	0.48
1:D:3362:ASP:OD1	1:D:3364:GLU:HB2	2.13	0.48
1:C:2187:PHE:HB2	1:C:2393:ASP:OD1	2.12	0.48
1:C:2467:ARG:NH1	1:C:2520:GLU:OE1	2.42	0.48
1:C:2545:TRP:CE3	1:C:2545:TRP:HA	2.47	0.48
1:D:3403:SER:OG	1:D:3405:LYS:HD2	2.13	0.48
1:A:103:VAL:C	1:A:105:ASN:H	2.16	0.48
1:A:176:GLU:O	1:A:177:VAL:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ILE:O	1:A:568:ILE:HD12	2.14	0.48
1:B:1176:GLU:O	1:B:1177:VAL:C	2.51	0.48
1:B:1235:GLY:HA3	1:B:1240:ARG:HG2	1.94	0.48
1:B:1331:THR:O	1:B:1335:ILE:HD12	2.13	0.48
1:B:1344:VAL:HG12	1:B:1345:ILE:N	2.27	0.48
1:B:1535:MET:C	1:B:1537:ASN:H	2.16	0.48
1:C:2140:GLU:HB2	1:D:3330:GLN:HE22	1.78	0.48
1:C:2316:LEU:O	1:C:2319:GLU:N	2.47	0.48
1:C:2495:TYR:CE2	1:C:2502:GLU:HG3	2.48	0.48
1:D:3130:TYR:CE2	1:D:3135:GLY:O	2.66	0.48
1:D:3169:LYS:O	1:D:3170:GLU:HG3	2.13	0.48
1:D:3198:PHE:C	1:D:3198:PHE:CD2	2.87	0.48
1:B:1394:THR:O	1:B:1429:GLN:NE2	2.44	0.48
1:B:1454:GLN:O	1:B:1457:GLU:N	2.46	0.48
1:D:3152:LEU:HB2	1:D:3466:TYR:CE1	2.47	0.48
1:D:3182:LEU:C	1:D:3438:ARG:HA	2.32	0.48
1:A:116:VAL:HG22	1:A:117:LEU:N	2.27	0.48
1:A:120:ARG:O	1:A:122:TYR:N	2.47	0.48
1:A:254:TYR:HD1	1:A:254:TYR:C	2.17	0.48
1:A:464:ASN:ND2	1:A:475:TYR:H	2.12	0.48
1:A:538:PRO:HG2	1:B:1139:TRP:HZ3	1.78	0.48
1:B:1190:ASP:HB2	1:B:1517:ILE:HD12	1.95	0.48
1:B:1387:TRP:CZ2	1:B:1518:PHE:CZ	3.01	0.48
1:B:1523:VAL:HG11	6:B:4064:HOH:O	2.12	0.48
1:C:2077:ARG:O	1:C:2081:LEU:HG	2.14	0.48
1:C:2131:ASN:C	1:C:2131:ASN:OD1	2.52	0.48
1:C:2315:ILE:HD13	1:C:2558:ILE:HD11	1.95	0.48
1:C:2316:LEU:CD1	1:C:2331:THR:HB	2.44	0.48
1:C:2389:PRO:HB2	1:C:2433:ARG:O	2.13	0.48
1:D:3034:ASN:HB3	1:D:3037:CYS:SG	2.53	0.48
1:D:3090:HIS:CD2	1:D:3513:ARG:HG2	2.49	0.48
1:D:3113:MET:HA	1:D:3116:VAL:CG1	2.44	0.48
1:D:3187:PHE:HB2	1:D:3393:ASP:OD1	2.13	0.48
1:D:3371:PHE:CE1	1:D:3532:LYS:HE2	2.49	0.48
1:D:3450:ALA:O	1:D:3451:SER:C	2.52	0.48
1:D:3538:PRO:O	1:D:3540:CYS:N	2.46	0.48
1:A:206:THR:HB	1:A:210:PHE:CE2	2.48	0.48
1:A:396:ASN:N	1:A:396:ASN:HD22	2.10	0.48
1:B:1090:HIS:CD2	1:B:1513:ARG:HG2	2.49	0.48
1:B:1092:ILE:HG12	1:B:1092:ILE:H	1.36	0.48
1:B:1131:ASN:C	1:B:1131:ASN:OD1	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1206:THR:HB	1:B:1210:PHE:CE2	2.49	0.48
1:B:1232:HIS:O	1:B:1288:GLY:CA	2.61	0.48
1:B:1303:THR:O	1:B:1307:ARG:HG3	2.14	0.48
1:B:1467:ARG:O	1:B:1472:LEU:HB2	2.13	0.48
1:C:2137:LYS:NZ	1:D:3546:LYS:HE3	2.28	0.48
1:C:2463:LEU:CD1	1:C:2503:LEU:HA	2.44	0.48
1:D:3120:ARG:O	1:D:3122:TYR:N	2.46	0.48
1:D:3120:ARG:HD2	1:D:3527:ALA:HB1	1.95	0.48
1:D:3185:ARG:HH21	1:D:3438:ARG:CZ	2.27	0.48
1:D:3513:ARG:HB2	1:D:3516:ALA:HB3	1.96	0.48
1:A:185:ARG:NH2	6:A:4024:HOH:O	2.45	0.48
1:A:229:ASP:OD2	1:A:229:ASP:C	2.51	0.48
1:A:388:HIS:O	1:A:391:LEU:HB2	2.14	0.48
1:A:524:GLU:OE2	1:A:524:GLU:CA	2.60	0.48
1:B:1113:MET:CE	1:B:1117:LEU:HD22	2.43	0.48
1:B:1196:MET:CE	1:B:1196:MET:HA	2.44	0.48
1:C:2050:THR:CG2	1:C:2056:LYS:HB3	2.44	0.48
1:D:3148:TYR:HB2	1:D:3219:GLY:O	2.12	0.48
1:D:3206:THR:HB	1:D:3210:PHE:CE2	2.48	0.48
1:D:3234:TYR:CE1	1:D:3252:LEU:HD11	2.48	0.48
1:D:3247:PHE:HA	1:D:3325:ASP:OD2	2.13	0.48
1:D:3344:VAL:HG12	1:D:3345:ILE:N	2.28	0.48
1:D:3388:HIS:O	1:D:3391:LEU:HB2	2.13	0.48
1:D:3498:ILE:HG23	1:D:3499:ASP:N	2.29	0.48
1:D:3521:THR:HG22	1:D:3522:MET:N	2.29	0.48
1:B:1187:PHE:HB2	1:B:1393:ASP:OD1	2.14	0.48
1:B:1451:SER:HB2	1:B:1504:TYR:CE2	2.49	0.48
1:C:2196:MET:CE	1:C:2196:MET:HA	2.44	0.48
1:C:2384:LEU:HB3	1:C:2522:MET:HE2	1.96	0.48
1:C:2428:ARG:HB3	6:C:4126:HOH:O	2.13	0.48
1:D:3209:PHE:HB3	1:D:3377:ILE:CD1	2.43	0.48
1:A:191:PRO:HG2	1:A:515:ASP:O	2.13	0.48
1:A:192:GLN:OE1	1:A:517:ILE:HG22	2.14	0.48
1:A:209:PHE:HB3	1:A:377:ILE:HD11	1.96	0.48
1:A:373:TYR:H	1:B:1372:GLN:HE22	1.62	0.48
1:B:1272:GLU:HA	6:B:4061:HOH:O	2.13	0.48
1:B:1308:GLU:HG3	1:B:1336:LEU:CD1	2.35	0.48
1:C:2134:TYR:HD2	1:C:2136:TYR:HE1	1.59	0.48
1:A:462:SER:CB	1:A:465:GLU:HG2	2.43	0.47
1:A:462:SER:HB3	1:A:465:GLU:HG2	1.96	0.47
1:B:1197:MET:O	1:B:1198:PHE:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1301:TYR:O	1:B:1302:ALA:C	2.52	0.47
1:B:1499:ASP:O	1:B:1501:MET:N	2.47	0.47
1:C:2329:PHE:C	1:C:2329:PHE:CD2	2.87	0.47
1:C:2381:PHE:HB2	1:C:2529:PHE:CD1	2.49	0.47
1:D:3387:TRP:HZ2	5:D:3701:PGX:H71	1.79	0.47
1:A:208:GLN:O	1:A:211:LYS:HD3	2.14	0.47
1:A:254:TYR:C	1:A:254:TYR:CD1	2.87	0.47
1:A:287:VAL:HG23	1:A:289:GLN:H	1.78	0.47
1:B:1056:LYS:HG3	1:B:1057:CYS:N	2.29	0.47
1:B:1108:LEU:HA	1:B:1111:LEU:HD23	1.95	0.47
1:B:1116:VAL:HG22	1:B:1117:LEU:N	2.30	0.47
1:B:1185:ARG:HH21	1:B:1438:ARG:CD	2.26	0.47
1:C:2155:VAL:HG12	1:C:2159:CYS:SG	2.54	0.47
1:C:2304:ILE:O	1:C:2307:ARG:HB2	2.14	0.47
1:D:3080:LEU:C	1:D:3082:LEU:H	2.18	0.47
1:D:3463:LEU:CD1	1:D:3503:LEU:HA	2.44	0.47
1:A:198:PHE:CD2	1:A:198:PHE:C	2.87	0.47
1:A:202:ALA:CA	1:A:348:TYR:HE1	2.27	0.47
1:B:1197:MET:HE1	1:B:1423:VAL:HG13	1.96	0.47
1:B:1404:PHE:H	1:B:1405:LYS:HZ2	1.61	0.47
1:C:2208:GLN:O	1:C:2211:LYS:HD3	2.14	0.47
1:D:3179:GLU:O	1:D:3181:VAL:N	2.47	0.47
1:A:108:LEU:O	1:A:112:ILE:HG12	2.15	0.47
1:A:113:MET:HA	1:A:116:VAL:CG1	2.43	0.47
1:A:198:PHE:HA	1:A:580:PHE:CD2	2.50	0.47
1:A:303:THR:O	1:A:307:ARG:HG3	2.15	0.47
1:A:338:GLY:HA3	1:A:559:ILE:CD1	2.39	0.47
1:B:1128:PRO:HG2	1:B:1376:ARG:NH1	2.30	0.47
1:B:1150:ARG:NH2	1:B:1154:PRO:HA	2.29	0.47
1:B:1295:VAL:CB	1:B:1298:LEU:HD22	2.43	0.47
1:B:1309:HIS:HD2	1:B:1310:ASN:OD1	1.97	0.47
1:B:1316:LEU:CD1	1:B:1331:THR:HB	2.45	0.47
1:C:2183:LEU:HD21	1:C:2445:GLN:CG	2.44	0.47
1:C:2463:LEU:HB3	6:C:4112:HOH:O	2.15	0.47
1:A:205:PHE:HE2	5:A:701:PGX:H171	1.78	0.47
1:A:481:LEU:CD1	1:A:510:GLU:HA	2.44	0.47
1:A:499:ASP:C	1:A:501:MET:H	2.18	0.47
1:B:1287:VAL:HG23	1:B:1289:GLN:H	1.80	0.47
1:B:1463:LEU:CD1	1:B:1503:LEU:HA	2.44	0.47
1:C:2080:LEU:C	1:C:2082:LEU:H	2.17	0.47
1:C:2090:HIS:CD2	1:C:2513:ARG:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2169:LYS:O	1:C:2170:GLU:HG3	2.13	0.47
1:C:2403:SER:OG	1:C:2405:LYS:HD2	2.13	0.47
1:D:3245:ARG:O	1:D:3253:LYS:HG3	2.15	0.47
1:D:3435:ALA:O	1:D:3510:GLU:O	2.32	0.47
1:A:120:ARG:HH11	1:A:527:ALA:HB1	1.80	0.47
1:A:150:ARG:NH2	1:A:154:PRO:HA	2.29	0.47
1:A:175:LYS:O	1:A:179:GLU:HG3	2.14	0.47
1:B:1190:ASP:OD2	1:B:1193:GLY:N	2.48	0.47
1:B:1273:MET:CE	1:B:1287:VAL:H	2.28	0.47
1:B:1450:ALA:O	1:B:1454:GLN:HG3	2.15	0.47
1:B:1532:LYS:C	1:B:1534:LEU:N	2.68	0.47
1:B:1564:ILE:O	1:B:1568:ILE:HD12	2.15	0.47
1:C:2178:LEU:HD22	1:C:2183:LEU:CD1	2.45	0.47
1:C:2191:PRO:HG2	1:C:2515:ASP:O	2.15	0.47
1:C:2387:TRP:CZ2	5:C:2701:PGX:C7	2.95	0.47
1:D:3487:MET:O	1:D:3490:GLU:HB3	2.13	0.47
1:A:50:THR:HG21	1:A:56:LYS:CB	2.45	0.47
1:A:458:MET:O	1:A:459:LYS:C	2.53	0.47
1:B:1050:THR:HG21	1:B:1056:LYS:CB	2.44	0.47
1:B:1108:LEU:HD23	1:B:1111:LEU:HD23	1.97	0.47
1:B:1142:PHE:O	1:B:1376:ARG:NH2	2.36	0.47
1:B:1183:LEU:HD22	1:B:1442:ILE:HG13	1.96	0.47
1:B:1247:PHE:HA	1:B:1325:ASP:OD2	2.15	0.47
1:B:1276:PRO:HB2	1:B:1278:HIS:CE1	2.49	0.47
1:B:1302:ALA:O	1:B:1303:THR:C	2.51	0.47
1:C:2181:VAL:HG12	1:C:2487:MET:HG2	1.97	0.47
1:C:2232:HIS:O	1:C:2288:GLY:CA	2.61	0.47
1:C:2396:ASN:HD22	1:C:2401:GLU:HG2	1.79	0.47
1:C:2481:LEU:CD1	1:C:2510:GLU:HA	2.45	0.47
1:C:2491:LEU:O	1:C:2494:LEU:N	2.47	0.47
1:C:2532:LYS:C	1:C:2534:LEU:N	2.68	0.47
1:C:2543:GLN:H	1:C:2543:GLN:CD	2.18	0.47
1:C:2546:LYS:HE3	1:D:3137:LYS:NZ	2.29	0.47
1:C:2557:LYS:O	1:C:2558:ILE:C	2.51	0.47
1:D:3096:PHE:O	1:D:3098:GLY:N	2.47	0.47
1:D:3183:LEU:HD21	1:D:3445:GLN:CG	2.45	0.47
1:D:3219:GLY:N	1:D:3458:MET:HE2	2.29	0.47
1:D:3304:ILE:HG22	1:D:3571:ASN:HD22	1.79	0.47
1:A:107:PHE:O	1:A:111:LEU:HB3	2.15	0.47
1:A:134:TYR:CD2	1:A:136:TYR:HE1	2.33	0.47
1:B:1086:PRO:HG2	6:B:4096:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:ARG:HH12	1:B:1272:GLU:HB2	1.80	0.47
1:C:2056:LYS:HE2	6:C:4097:HOH:O	2.14	0.47
1:C:2573:LYS:HB2	6:C:4110:HOH:O	2.14	0.47
1:D:3150:ARG:NH2	1:D:3154:PRO:HA	2.30	0.47
1:D:3209:PHE:HB3	1:D:3377:ILE:HD11	1.96	0.47
1:D:3449:LYS:CA	1:D:3452:ILE:HD12	2.39	0.47
1:D:3481:LEU:HD12	1:D:3481:LEU:O	2.14	0.47
1:A:206:THR:HA	1:A:209:PHE:CE2	2.50	0.47
1:A:316:LEU:CD1	1:A:331:THR:HB	2.45	0.47
1:A:433:ARG:HH21	1:A:512:PRO:CB	2.28	0.47
1:B:1076:THR:O	1:B:1079:LYS:HB2	2.14	0.47
1:B:1316:LEU:O	1:B:1319:GLU:N	2.48	0.47
1:B:1372:GLN:O	1:B:1374:GLN:N	2.47	0.47
1:B:1389:PRO:HG2	1:B:1434:VAL:HG22	1.97	0.47
1:B:1403:SER:OG	1:B:1405:LYS:HD2	2.15	0.47
1:B:1509:VAL:O	1:B:1510:GLU:O	2.31	0.47
1:B:1514:PRO:O	1:B:1515:ASP:HB2	2.14	0.47
1:C:2132:VAL:HG21	1:C:2219:GLY:HA3	1.97	0.47
1:D:3095:HIS:O	1:D:3100:TRP:CD1	2.68	0.47
1:D:3215:LYS:H	1:D:3215:LYS:HG2	1.51	0.47
1:D:3270:GLN:OE1	1:D:3270:GLN:N	2.47	0.47
1:D:3308:GLU:HG3	1:D:3336:LEU:CD1	2.35	0.47
1:D:3467:ARG:NH1	1:D:3521:THR:OG1	2.47	0.47
1:A:184:ARG:CD	1:A:187:PHE:HA	2.38	0.47
1:A:229:ASP:HA	1:A:337:ILE:HD11	1.97	0.47
1:A:429:GLN:O	1:A:429:GLN:HG2	2.14	0.47
1:A:509:VAL:O	1:A:510:GLU:O	2.32	0.47
1:A:547:PRO:O	1:A:552:GLY:N	2.43	0.47
1:C:2105(C):ILE:O	1:C:2108:LEU:HB2	2.15	0.47
1:C:2261:VAL:H	1:C:2307:ARG:NH2	2.13	0.47
1:C:2403:SER:HB2	1:C:2405:LYS:HZ2	1.80	0.47
1:C:2510:GLU:OE1	1:C:2519:GLY:HA3	2.15	0.47
1:D:3108:LEU:HD23	1:D:3111:LEU:HD23	1.97	0.47
1:D:3116:VAL:HG22	1:D:3117:LEU:N	2.30	0.47
1:D:3229:ASP:OD2	1:D:3229:ASP:C	2.53	0.47
1:A:386:HIS:HB2	1:A:504:TYR:CE1	2.50	0.46
1:A:465:GLU:OE2	1:A:468:LYS:CE	2.63	0.46
1:B:1219:GLY:N	1:B:1458:MET:HE2	2.29	0.46
1:B:1225:GLY:HA3	1:B:1229:ASP:OD1	2.15	0.46
1:B:1444:VAL:O	1:B:1444:VAL:HG12	2.15	0.46
1:C:2113:MET:CE	1:C:2117:LEU:HD22	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2176:GLU:O	1:C:2179:GLU:N	2.48	0.46
1:C:2209:PHE:CD1	1:C:2209:PHE:N	2.79	0.46
1:C:2295:VAL:CB	1:C:2298:LEU:HD22	2.46	0.46
1:A:219:GLY:HA2	1:A:458:MET:HE1	1.96	0.46
1:A:444:VAL:O	1:A:444:VAL:CG1	2.62	0.46
1:A:538:PRO:HG2	1:B:1139:TRP:CZ3	2.50	0.46
1:B:1134:TYR:HD2	1:B:1136:TYR:HE1	1.61	0.46
1:B:1205:PHE:CE2	1:B:1209:PHE:HZ	2.33	0.46
1:B:1386:HIS:HD2	1:B:1451:SER:HB3	1.79	0.46
1:C:2302:ALA:O	1:C:2303:THR:C	2.53	0.46
1:C:2303:THR:O	1:C:2307:ARG:HG3	2.15	0.46
1:C:2450:ALA:O	1:C:2454:GLN:HG3	2.15	0.46
1:D:3107:PHE:O	1:D:3111:LEU:HB3	2.15	0.46
1:D:3535:MET:C	1:D:3537:ASN:H	2.19	0.46
1:D:3543:GLN:CD	1:D:3543:GLN:H	2.18	0.46
1:A:80:LEU:C	1:A:82:LEU:H	2.18	0.46
1:A:137:LYS:HZ1	1:B:1546:LYS:HE3	1.80	0.46
1:A:183:LEU:HD21	1:A:445:GLN:CG	2.45	0.46
1:B:1124:ILE:H	1:B:1124:ILE:HG12	1.59	0.46
1:B:1526:GLY:O	1:B:1530:SER:HB3	2.15	0.46
1:C:2103:VAL:C	1:C:2105:ASN:H	2.19	0.46
1:C:2344:VAL:HG12	1:C:2345:ILE:N	2.30	0.46
1:D:3303:THR:O	1:D:3307:ARG:HG3	2.16	0.46
1:D:3403:SER:HB2	1:D:3405:LYS:HZ2	1.80	0.46
1:D:3553:GLU:OE1	1:D:3553:GLU:CA	2.63	0.46
1:A:456:ARG:NE	1:A:502:GLU:OE2	2.48	0.46
1:B:1300:MET:O	1:B:1304:ILE:HG13	2.14	0.46
1:B:1435:ALA:HB2	1:B:1518:PHE:HA	1.97	0.46
1:C:2187:PHE:CD1	1:C:2187:PHE:C	2.89	0.46
1:C:2433:ARG:HH21	1:C:2512:PRO:CB	2.29	0.46
1:C:2513:ARG:NH2	1:C:2520:GLU:HB2	2.31	0.46
1:D:3190:ASP:OD2	1:D:3193:GLY:N	2.49	0.46
1:D:3304:ILE:O	1:D:3307:ARG:HB2	2.16	0.46
1:D:3567:LEU:HD12	1:D:3567:LEU:C	2.35	0.46
1:A:274:ILE:HD12	1:A:291:VAL:HA	1.96	0.46
1:A:295:VAL:CB	1:A:298:LEU:HD22	2.44	0.46
1:A:341:ILE:HD13	1:A:534:LEU:HD12	1.97	0.46
1:A:381:PHE:CD1	1:A:529:PHE:CB	2.97	0.46
1:B:1077:ARG:O	1:B:1081:LEU:HG	2.15	0.46
1:B:1389:PRO:HB2	1:B:1433:ARG:O	2.15	0.46
1:B:1414:LEU:HA	1:B:1422:PHE:HE1	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1481:LEU:CD1	1:B:1510:GLU:HA	2.46	0.46
1:C:2056:LYS:HG3	1:C:2057:CYS:N	2.30	0.46
1:C:2429:GLN:O	1:C:2429:GLN:HG2	2.15	0.46
1:C:2547:PRO:C	1:C:2552:GLY:HA2	2.36	0.46
1:C:2583:GLN:CD	1:C:2583:GLN:N	2.69	0.46
1:D:3174:SER:N	6:D:4188:HOH:O	2.48	0.46
1:D:3232:HIS:O	1:D:3288:GLY:CA	2.63	0.46
1:D:3245:ARG:HD2	1:D:3329:PHE:CE1	2.50	0.46
1:D:3435:ALA:HB2	1:D:3518:PHE:HA	1.96	0.46
1:A:113:MET:HE3	1:A:116:VAL:HG22	1.97	0.46
1:A:176:GLU:O	1:A:179:GLU:N	2.49	0.46
1:A:384:LEU:HB3	1:A:522:MET:HE2	1.97	0.46
1:A:499:ASP:O	1:A:501:MET:N	2.49	0.46
1:B:1095:HIS:O	1:B:1097:LYS:N	2.49	0.46
1:B:1198:PHE:C	1:B:1198:PHE:CD2	2.89	0.46
1:C:2174:SER:O	1:C:2178:LEU:HB2	2.16	0.46
1:C:2197:MET:O	1:C:2198:PHE:C	2.54	0.46
1:C:2514:PRO:O	1:C:2515:ASP:CB	2.63	0.46
1:D:3261:VAL:O	1:D:3307:ARG:NH1	2.49	0.46
1:D:3276:PRO:HB2	1:D:3278:HIS:CE1	2.50	0.46
1:D:3301:TYR:O	1:D:3302:ALA:C	2.54	0.46
1:D:3405:LYS:HE3	1:D:3405:LYS:H	1.81	0.46
1:D:3513:ARG:O	1:D:3515:ASP:N	2.49	0.46
1:A:124:ILE:HD11	1:A:528:PRO:C	2.36	0.46
1:A:456:ARG:NH1	6:A:4045:HOH:O	2.48	0.46
1:A:489:ALA:HB2	6:A:4044:HOH:O	2.14	0.46
1:A:513:ARG:O	1:A:515:ASP:N	2.48	0.46
1:B:1137:LYS:N	6:B:4080:HOH:O	2.49	0.46
1:B:1179:GLU:O	1:B:1181:VAL:N	2.48	0.46
1:B:1395:PHE:O	1:B:1402:TYR:HD2	1.99	0.46
1:C:2105(C):ILE:CB	1:C:2108:LEU:HD12	2.46	0.46
1:C:2116:VAL:HG22	1:C:2117:LEU:N	2.31	0.46
1:C:2176:GLU:O	1:C:2177:VAL:C	2.54	0.46
1:C:2219:GLY:HA2	1:C:2458:MET:CE	2.46	0.46
1:C:2490:GLU:O	1:C:2493:ALA:HB3	2.16	0.46
1:D:3162:PRO:HB2	1:D:3171:LEU:CD2	2.46	0.46
1:A:61:ARG:NH2	1:B:1545:TRP:O	2.48	0.46
1:A:383:THR:O	1:A:385:TYR:N	2.49	0.46
1:B:1391:LEU:HD13	1:B:1404:PHE:HE2	1.80	0.46
1:B:1499:ASP:C	1:B:1501:MET:H	2.18	0.46
1:C:2105(C):ILE:CG2	1:C:2108:LEU:HD12	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2381:PHE:CD1	1:C:2529:PHE:CB	2.99	0.46
1:C:2513:ARG:HB2	1:C:2516:ALA:HB3	1.98	0.46
1:D:3175:LYS:O	1:D:3178:LEU:HB3	2.16	0.46
1:D:3261:VAL:H	1:D:3307:ARG:NH2	2.14	0.46
1:B:1116:VAL:O	1:B:1119:SER:OG	2.34	0.46
1:B:1323:TRP:CE3	1:B:1327:GLN:HG2	2.51	0.46
1:C:2065:TYR:CD2	1:C:2065:TYR:N	2.84	0.46
1:C:2273:MET:CE	1:C:2287:VAL:H	2.28	0.46
1:D:3076:THR:O	1:D:3079:LYS:HB2	2.16	0.46
1:D:3078:ILE:HD13	1:D:3078:ILE:N	2.30	0.46
1:D:3089:VAL:O	1:D:3092:ILE:HG12	2.16	0.46
1:D:3274:ILE:HD12	1:D:3291:VAL:HA	1.98	0.46
1:D:3532:LYS:C	1:D:3534:LEU:N	2.69	0.46
1:A:405:LYS:HE3	1:A:405:LYS:H	1.81	0.46
1:A:463:LEU:CD1	1:A:503:LEU:HA	2.46	0.46
1:B:1113:MET:HA	1:B:1116:VAL:HG13	1.96	0.46
1:B:1120:ARG:HH11	1:B:1527:ALA:HB1	1.80	0.46
1:B:1245:ARG:HH22	1:B:1326:GLU:HA	1.81	0.46
1:B:1567:LEU:HD12	1:B:1567:LEU:C	2.37	0.46
1:C:2064:PHE:HD2	1:C:2070:THR:O	1.99	0.46
1:C:2504:TYR:O	1:C:2507:LEU:HB2	2.16	0.46
1:C:2546:LYS:HE3	1:D:3137:LYS:HZ1	1.80	0.46
1:D:3059:CYS:HB3	1:D:3064:PHE:O	2.16	0.46
1:D:3195:ASN:OD1	1:D:3197:MET:HB2	2.15	0.46
1:D:3287:VAL:HG23	1:D:3289:GLN:H	1.80	0.46
1:D:3421:GLN:O	1:D:3422:PHE:C	2.54	0.46
1:A:131:ASN:C	1:A:131:ASN:OD1	2.53	0.45
1:A:532:LYS:C	1:A:534:LEU:N	2.68	0.45
1:B:1308:GLU:OE2	1:B:1308:GLU:HA	2.16	0.45
1:B:1543:GLN:CD	1:B:1543:GLN:H	2.19	0.45
1:C:2183:LEU:HD22	1:C:2442:ILE:HG13	1.98	0.45
1:C:2273:MET:CE	1:C:2287:VAL:HG22	2.26	0.45
1:C:2276:PRO:HG3	1:C:2409:TYR:CD1	2.51	0.45
1:C:2464:ASN:HD21	1:C:2475:TYR:N	2.14	0.45
1:C:2549:THR:HG23	1:D:3137:LYS:HD3	1.98	0.45
1:D:3187:PHE:CD1	1:D:3187:PHE:C	2.90	0.45
1:D:3190:ASP:HB2	1:D:3517:ILE:HD12	1.97	0.45
1:D:3309:HIS:HD2	1:D:3310:ASN:OD1	1.98	0.45
1:D:3315:ILE:HD13	1:D:3558:ILE:HD11	1.97	0.45
1:A:89:VAL:O	1:A:90:HIS:C	2.54	0.45
1:A:187:PHE:HB2	1:A:393:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:VAL:HA	1:A:260:GLU:O	2.17	0.45
1:A:371:PHE:CE1	1:A:532:LYS:HE2	2.51	0.45
1:B:1151:ALA:HB2	1:B:1529:PHE:CZ	2.51	0.45
1:B:1380:GLU:HG3	1:B:1460:TYR:CE2	2.50	0.45
1:C:2247:PHE:HA	1:C:2325:ASP:OD2	2.15	0.45
1:D:3043:ASN:ND2	1:D:3069:CYS:O	2.49	0.45
1:A:148:TYR:HD2	1:A:219:GLY:O	1.98	0.45
1:A:240:ARG:HH12	1:A:272:GLU:HB2	1.81	0.45
1:A:357:PHE:HE2	1:A:359:LEU:HD23	1.81	0.45
1:B:1105(B):ILE:HG21	1:B:1108:LEU:CD1	2.42	0.45
1:B:1495:TYR:CE2	1:B:1502:GLU:HG3	2.48	0.45
1:C:2043:ASN:ND2	1:C:2069:CYS:O	2.49	0.45
1:C:2089:VAL:O	1:C:2090:HIS:C	2.53	0.45
1:C:2331:THR:O	1:C:2335:ILE:HD12	2.16	0.45
1:D:3173:ASP:OD2	1:D:3175:LYS:N	2.49	0.45
1:D:3191:PRO:HG2	1:D:3515:ASP:O	2.16	0.45
1:D:3230:LEU:CG	1:D:3337:ILE:HG13	2.41	0.45
1:D:3301:TYR:O	1:D:3304:ILE:HB	2.16	0.45
1:D:3381:PHE:O	5:D:3701:PGX:H101	2.17	0.45
1:A:65:TYR:N	1:A:65:TYR:CD2	2.84	0.45
1:A:184:ARG:CB	1:A:439:ASN:HA	2.44	0.45
1:A:184:ARG:HH12	1:A:441:PRO:HG3	1.80	0.45
1:A:196:MET:CE	1:A:196:MET:HA	2.47	0.45
1:A:347:ASP:OD2	1:A:564:ILE:HG22	2.17	0.45
1:B:1065:TYR:CD2	1:B:1065:TYR:N	2.84	0.45
1:B:1148:TYR:HB2	1:B:1219:GLY:O	2.17	0.45
1:B:1455:SER:HA	1:B:1460:TYR:CD1	2.51	0.45
1:B:1464:ASN:ND2	1:B:1475:TYR:H	2.14	0.45
1:C:2108:LEU:HA	1:C:2111:LEU:HD23	1.98	0.45
1:C:2142:PHE:O	1:C:2376:ARG:NH2	2.37	0.45
1:C:2387:TRP:HZ2	5:C:2701:PGX:C7	2.24	0.45
1:C:2395:PHE:CD1	1:C:2407:PHE:CD2	3.04	0.45
1:C:2534:LEU:HD13	1:C:2534:LEU:HA	1.87	0.45
1:D:3380:GLU:HG3	1:D:3460:TYR:CE2	2.52	0.45
1:D:3386:HIS:HB2	1:D:3504:TYR:CE1	2.50	0.45
1:D:3404:PHE:H	1:D:3405:LYS:HZ2	1.63	0.45
1:A:538:PRO:HG3	1:B:1142:PHE:CE2	2.51	0.45
1:B:1080:LEU:C	1:B:1082:LEU:H	2.19	0.45
1:B:1191:PRO:HG2	1:B:1515:ASP:O	2.17	0.45
1:B:1209:PHE:CD1	1:B:1209:PHE:N	2.79	0.45
1:B:1216:ARG:HB3	1:B:1220:PHE:HD1	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1405:LYS:HE3	1:B:1405:LYS:H	1.82	0.45
1:C:2137:LYS:HZ1	1:D:3546:LYS:HE3	1.81	0.45
1:C:2148:TYR:HB2	1:C:2219:GLY:O	2.16	0.45
1:C:2215:LYS:H	1:C:2215:LYS:HG2	1.50	0.45
1:C:2245:ARG:HH22	1:C:2326:GLU:HA	1.82	0.45
1:C:2371:PHE:HZ	1:C:2536:GLY:N	2.14	0.45
1:C:2380:GLU:HG3	1:C:2460:TYR:CE2	2.51	0.45
1:C:2523:VAL:HG12	1:C:2524:GLU:OE2	2.16	0.45
1:D:3050:THR:HG21	1:D:3056:LYS:CB	2.46	0.45
1:D:3095:HIS:O	1:D:3100:TRP:HD1	1.99	0.45
1:D:3176:GLU:O	1:D:3179:GLU:N	2.50	0.45
1:D:3389:PRO:HB2	1:D:3433:ARG:O	2.16	0.45
1:D:3464:ASN:ND2	1:D:3475:TYR:H	2.14	0.45
1:A:190:ASP:OD1	1:A:192:GLN:HG3	2.16	0.45
1:A:218:PRO:C	1:A:458:MET:CE	2.85	0.45
1:A:246:LEU:HB3	1:A:251:LYS:O	2.16	0.45
1:A:389:PRO:HB2	1:A:433:ARG:O	2.17	0.45
1:A:435:ALA:O	1:A:510:GLU:O	2.34	0.45
1:A:465:GLU:OE2	1:A:468:LYS:HE2	2.17	0.45
1:A:530:SER:OG	5:A:701:PGX:H162	2.17	0.45
1:A:564:ILE:O	1:A:568:ILE:CD1	2.65	0.45
1:B:1095:HIS:O	1:B:1100:TRP:CD1	2.70	0.45
1:B:1128:PRO:HG3	1:B:1376:ARG:NH1	2.30	0.45
1:C:2168:ASN:C	1:C:2170:GLU:N	2.70	0.45
1:C:2190:ASP:OD1	1:C:2192:GLN:HG3	2.17	0.45
1:C:2198:PHE:HA	1:C:2580:PHE:CD2	2.52	0.45
1:C:2363:PRO:C	1:C:2365:LEU:N	2.70	0.45
1:C:2498:ILE:O	1:C:2501:MET:HB2	2.16	0.45
1:D:3065:TYR:N	1:D:3065:TYR:CD2	2.85	0.45
1:D:3151:ALA:HB2	1:D:3529:PHE:CZ	2.51	0.45
1:D:3198:PHE:CZ	1:D:3352:LEU:HD13	2.51	0.45
1:D:3302:ALA:O	1:D:3303:THR:C	2.53	0.45
1:D:3369:GLN:O	1:D:3371:PHE:N	2.49	0.45
1:D:3535:MET:O	1:D:3537:ASN:N	2.49	0.45
1:A:174:SER:O	1:A:178:LEU:HB2	2.17	0.45
1:A:276:PRO:HB2	1:A:278:HIS:CE1	2.51	0.45
1:B:1176:GLU:O	1:B:1179:GLU:N	2.50	0.45
1:B:1198:PHE:CZ	1:B:1352:LEU:HD13	2.51	0.45
1:B:1276:PRO:HG3	1:B:1409:TYR:CD1	2.52	0.45
1:C:2383:THR:O	1:C:2385:TYR:N	2.49	0.45
1:C:2523:VAL:HG12	1:C:2524:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2535:MET:O	1:C:2537:ASN:N	2.50	0.45
1:C:2568:ILE:HG23	1:C:2572:VAL:CG2	2.46	0.45
1:A:197:MET:HE1	1:A:423:VAL:HG13	1.99	0.45
1:B:1168:ASN:C	1:B:1170:GLU:N	2.70	0.45
1:B:1173:ASP:C	1:B:1173:ASP:OD2	2.55	0.45
1:B:1274:ILE:HD12	1:B:1291:VAL:HG23	1.98	0.45
1:B:1504:TYR:O	1:B:1507:LEU:HB2	2.17	0.45
1:C:2190:ASP:OD2	1:C:2193:GLY:N	2.50	0.45
1:C:2347:ASP:O	1:C:2348:TYR:O	2.35	0.45
1:C:2455:SER:HA	1:C:2460:TYR:CD1	2.51	0.45
1:C:2513:ARG:O	1:C:2515:ASP:N	2.50	0.45
1:C:2538:PRO:O	1:C:2540:CYS:N	2.49	0.45
1:D:3155:VAL:HG23	1:D:3459:LYS:O	2.17	0.45
1:D:3161:THR:O	1:D:3164:GLY:N	2.48	0.45
1:D:3229:ASP:HA	1:D:3337:ILE:HD11	1.98	0.45
1:D:3386:HIS:HD2	1:D:3451:SER:HB3	1.81	0.45
1:D:3404:PHE:N	1:D:3404:PHE:CD1	2.85	0.45
1:D:3433:ARG:HH21	1:D:3512:PRO:HB3	1.81	0.45
1:D:3563:SER:C	1:D:3565:GLN:N	2.69	0.45
1:A:294:LEU:HB3	1:A:409:TYR:CD2	2.52	0.45
1:A:381:PHE:HB2	1:A:529:PHE:CD1	2.51	0.45
1:B:1175:LYS:O	1:B:1178:LEU:HB3	2.16	0.45
5:B:1701:PGX:H202	6:B:4074:HOH:O	2.17	0.45
1:C:2059:CYS:HB3	1:C:2064:PHE:O	2.16	0.45
1:C:2190:ASP:HB2	1:C:2517:ILE:HD12	1.97	0.45
1:C:2357:PHE:HE2	1:C:2359:LEU:HD23	1.81	0.45
1:D:3034:ASN:HA	1:D:3035:PRO:HD2	1.86	0.45
1:D:3197:MET:O	1:D:3198:PHE:C	2.55	0.45
1:D:3201:PHE:O	1:D:3204:HIS:N	2.50	0.45
1:D:3415:LEU:HD23	1:D:3415:LEU:HA	1.82	0.45
1:A:107:PHE:H	1:A:107:PHE:HD2	1.65	0.45
1:A:535:MET:C	1:A:537:ASN:H	2.20	0.45
1:B:1201:PHE:O	1:B:1204:HIS:N	2.50	0.45
1:B:1465:GLU:OE2	1:B:1468:LYS:HE2	2.17	0.45
1:C:2184:ARG:CB	1:C:2439:ASN:HA	2.44	0.45
1:C:2261:VAL:O	1:C:2307:ARG:NH1	2.50	0.45
1:C:2276:PRO:HB2	1:C:2278:HIS:CE1	2.52	0.45
1:C:2487:MET:O	1:C:2490:GLU:HB3	2.17	0.45
1:D:3103:VAL:C	1:D:3105:ASN:H	2.21	0.45
1:D:3162:PRO:HB2	1:D:3171:LEU:HD21	1.99	0.45
1:D:3295:VAL:CB	1:D:3298:LEU:HD22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3481:LEU:HD12	1:D:3510:GLU:HA	1.98	0.45
1:D:3507:LEU:HD22	1:D:3522:MET:HB2	1.98	0.45
1:A:195:ASN:OD1	1:A:197:MET:HB2	2.17	0.44
1:A:300:MET:O	1:A:304:ILE:HG13	2.16	0.44
1:A:404:PHE:N	1:A:404:PHE:CD1	2.85	0.44
1:A:449:LYS:CA	1:A:452:ILE:HD12	2.41	0.44
1:B:1229:ASP:OD2	1:B:1229:ASP:C	2.55	0.44
1:C:2099:VAL:HA	1:C:2102:ILE:CD1	2.28	0.44
1:D:3530:SER:HB2	5:D:3701:PGX:H161	1.99	0.44
1:D:3532:LYS:C	1:D:3534:LEU:H	2.21	0.44
1:A:183:LEU:HD22	1:A:442:ILE:HG13	1.98	0.44
1:A:383:THR:C	1:A:385:TYR:N	2.71	0.44
1:A:405:LYS:H	1:A:405:LYS:CE	2.30	0.44
1:A:454:GLN:O	1:A:455:SER:C	2.55	0.44
1:B:1188:ILE:HB	1:B:1439:ASN:ND2	2.33	0.44
1:B:1226:HIS:C	1:B:1377:ILE:HD12	2.38	0.44
1:B:1381:PHE:HB2	1:B:1529:PHE:CD1	2.52	0.44
1:B:1458:MET:O	1:B:1459:LYS:C	2.56	0.44
1:C:2566:SER:O	1:C:2567:LEU:C	2.56	0.44
1:D:3065:TYR:HB2	1:D:3066:GLY:H	1.64	0.44
1:D:3381:PHE:CD1	1:D:3529:PHE:CB	2.99	0.44
1:A:108:LEU:HD23	1:A:111:LEU:HD23	1.99	0.44
1:A:113:MET:CE	1:A:117:LEU:HD22	2.47	0.44
1:A:168:ASN:C	1:A:170:GLU:N	2.69	0.44
1:A:219:GLY:HA2	1:A:458:MET:CE	2.46	0.44
1:A:462:SER:O	1:A:465:GLU:HB2	2.16	0.44
1:B:1162:PRO:HB2	1:B:1171:LEU:CD2	2.47	0.44
1:B:1369:GLN:O	1:B:1371:PHE:N	2.50	0.44
1:B:1405:LYS:H	1:B:1405:LYS:CE	2.30	0.44
1:B:1513:ARG:HB2	1:B:1516:ALA:HB3	1.99	0.44
1:C:2389:PRO:HG2	1:C:2434:VAL:HG22	1.98	0.44
1:C:2507:LEU:HD22	1:C:2522:MET:HB2	2.00	0.44
1:D:3246:LEU:HB3	1:D:3251:LYS:O	2.17	0.44
1:D:3329:PHE:HD2	1:D:3330:GLN:HG2	1.82	0.44
1:A:37:CYS:O	1:A:39:ASN:ND2	2.50	0.44
1:A:136:TYR:O	1:A:136:TYR:HD1	2.01	0.44
1:A:538:PRO:O	1:A:540:CYS:N	2.51	0.44
1:B:1095:HIS:O	1:B:1100:TRP:HD1	2.00	0.44
1:B:1205:PHE:HE2	5:B:1701:PGX:H171	1.82	0.44
1:B:1273:MET:HE2	1:B:1285:PHE:O	2.18	0.44
1:B:1381:PHE:CD1	1:B:1529:PHE:CB	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1389:PRO:HB2	1:B:1434:VAL:HA	2.00	0.44
1:B:1487:MET:O	1:B:1490:GLU:HB3	2.18	0.44
1:C:2050:THR:HG21	1:C:2056:LYS:CB	2.47	0.44
1:C:2112:ILE:O	1:C:2115:TYR:HB3	2.17	0.44
1:C:2339:GLU:OE2	1:C:2558:ILE:CG2	2.66	0.44
1:D:3308:GLU:HA	1:D:3308:GLU:OE2	2.17	0.44
1:D:3352:LEU:HG	1:D:3518:PHE:HE2	1.83	0.44
1:D:3371:PHE:HZ	1:D:3536:GLY:N	2.15	0.44
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.53	0.44
1:A:395:PHE:O	1:A:402:TYR:HD2	2.00	0.44
1:A:548:SER:O	1:A:550:PHE:N	2.50	0.44
1:B:1187:PHE:CD1	1:B:1187:PHE:C	2.90	0.44
1:B:1490:GLU:O	1:B:1493:ALA:HB3	2.17	0.44
1:C:2405:LYS:HE3	1:C:2405:LYS:H	1.83	0.44
1:C:2524:GLU:OE2	1:C:2524:GLU:CA	2.62	0.44
1:C:2532:LYS:C	1:C:2534:LEU:H	2.20	0.44
1:D:3196:MET:HG2	1:D:3429:GLN:HG2	2.00	0.44
1:D:3202:ALA:HB2	1:D:3348:TYR:CE1	2.52	0.44
1:D:3316:LEU:CD1	1:D:3331:THR:HB	2.47	0.44
1:D:3513:ARG:HH21	1:D:3520:GLU:HB2	1.83	0.44
1:A:295:VAL:HB	1:A:298:LEU:HB2	1.99	0.44
1:A:315:ILE:HD13	1:A:558:ILE:HD11	1.99	0.44
1:A:339:GLU:OE2	1:A:558:ILE:CG2	2.66	0.44
1:A:435:ALA:HB2	1:A:518:PHE:HA	1.99	0.44
1:A:450:ALA:O	1:A:451:SER:C	2.55	0.44
1:B:1107:PHE:H	1:B:1107:PHE:HD2	1.64	0.44
1:B:1173:ASP:OD2	1:B:1175:LYS:N	2.51	0.44
1:B:1371:PHE:HZ	1:B:1536:GLY:N	2.15	0.44
1:B:1436:GLY:HA2	1:B:1512:PRO:HG2	2.00	0.44
1:B:1462:SER:HB3	1:B:1465:GLU:HG2	1.99	0.44
1:B:1513:ARG:O	1:B:1515:ASP:N	2.50	0.44
1:C:2103:VAL:O	1:C:2105:ASN:N	2.51	0.44
1:C:2134:TYR:CD2	1:C:2136:TYR:HE1	2.35	0.44
1:C:2206:THR:HA	1:C:2209:PHE:CE2	2.52	0.44
1:C:2369:GLN:O	1:C:2371:PHE:N	2.50	0.44
1:D:3056:LYS:HA	6:D:4150:HOH:O	2.17	0.44
1:D:3198:PHE:HB2	1:D:3580:PHE:HB3	1.99	0.44
1:A:150:ARG:HD2	1:A:380:GLU:OE1	2.17	0.44
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.52	0.44
1:A:470:PHE:CD2	1:A:470:PHE:N	2.85	0.44
1:A:521:THR:HG22	1:A:522:MET:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ILE:HG23	1:A:572:VAL:CG2	2.47	0.44
1:A:583:GLN:CD	1:A:583:GLN:N	2.70	0.44
1:B:1136:TYR:HD1	1:B:1136:TYR:O	2.00	0.44
1:B:1175:LYS:O	1:B:1179:GLU:HG3	2.18	0.44
1:B:1261:VAL:O	1:B:1307:ARG:NH1	2.51	0.44
1:B:1386:HIS:HB2	1:B:1504:TYR:CE1	2.52	0.44
1:B:1461:GLN:H	1:B:1466:TYR:HE2	1.65	0.44
1:B:1548:SER:O	1:B:1550:PHE:N	2.50	0.44
1:C:2124:ILE:H	1:C:2124:ILE:HG12	1.61	0.44
1:C:2373:TYR:H	1:D:3372:GLN:HE22	1.65	0.44
1:C:2454:GLN:O	1:C:2455:SER:C	2.54	0.44
1:D:3108:LEU:HA	1:D:3111:LEU:HD23	1.99	0.44
1:D:3173:ASP:OD2	1:D:3173:ASP:C	2.55	0.44
1:D:3352:LEU:HD12	1:D:3352:LEU:HA	1.81	0.44
1:D:3396:ASN:N	1:D:3396:ASN:HD22	2.16	0.44
1:A:59:CYS:HB3	1:A:64:PHE:O	2.18	0.44
1:A:112:ILE:O	1:A:115:TYR:HB3	2.17	0.44
1:A:507:LEU:HD22	1:A:522:MET:HB2	1.99	0.44
1:B:1113:MET:HA	1:B:1116:VAL:CG1	2.47	0.44
1:B:1178:LEU:HD22	1:B:1183:LEU:CD1	2.48	0.44
1:B:1482:THR:CG2	1:B:1509:VAL:HG12	2.48	0.44
1:C:2161:THR:O	1:C:2164:GLY:N	2.46	0.44
1:C:2269:THR:OG1	1:C:2271:VAL:HG23	2.17	0.44
1:C:2352:LEU:HG	1:C:2518:PHE:HE2	1.83	0.44
1:D:3292:PHE:O	1:D:3299:MET:HE2	2.18	0.44
1:D:3363:PRO:C	1:D:3365:LEU:N	2.70	0.44
1:D:3444:VAL:O	1:D:3444:VAL:CG1	2.65	0.44
1:D:3444:VAL:O	1:D:3445:GLN:C	2.56	0.44
1:A:77:ARG:O	1:A:81:LEU:HG	2.18	0.44
1:A:137:LYS:NZ	1:B:1546:LYS:HE3	2.32	0.44
1:A:532:LYS:C	1:A:534:LEU:H	2.21	0.44
1:A:535:MET:O	1:A:537:ASN:N	2.51	0.44
1:B:1435:ALA:O	1:B:1510:GLU:O	2.36	0.44
1:C:2274:ILE:HD11	1:C:2290:GLU:HG3	2.00	0.44
1:C:2323:TRP:CE3	1:C:2327:GLN:HG2	2.52	0.44
1:C:2482:THR:HG22	6:C:4128:HOH:O	2.17	0.44
1:C:2567:LEU:HD12	1:C:2567:LEU:C	2.37	0.44
1:D:3105(D):ILE:CG2	1:D:3108:LEU:HD12	2.48	0.44
1:D:3405:LYS:H	1:D:3405:LYS:CE	2.30	0.44
1:A:112:ILE:HB	1:A:357:PHE:CE1	2.53	0.43
1:A:187:PHE:CD1	1:A:187:PHE:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:HB3	1:B:1052:PHE:CD2	2.52	0.43
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.81	0.43
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.85	0.43
1:A:467:ARG:NH1	1:A:520:GLU:OE1	2.44	0.43
1:A:543:GLN:O	1:B:1137:LYS:HE2	2.18	0.43
1:B:1160:PRO:HD2	1:B:1164:GLY:O	2.18	0.43
1:B:1292:PHE:O	1:B:1299:MET:HE2	2.18	0.43
1:B:1363:PRO:C	1:B:1365:LEU:N	2.72	0.43
1:B:1429:GLN:O	1:B:1429:GLN:HG2	2.18	0.43
1:C:2105(C):ILE:O	1:C:2108:LEU:N	2.50	0.43
1:C:2112:ILE:HB	1:C:2357:PHE:CE1	2.53	0.43
1:D:3178:LEU:HD22	1:D:3183:LEU:CD1	2.48	0.43
1:D:3182:LEU:O	1:D:3438:ARG:CA	2.61	0.43
1:D:3184:ARG:CB	1:D:3439:ASN:HA	2.48	0.43
1:D:3381:PHE:HB2	1:D:3529:PHE:CD1	2.53	0.43
1:D:3499:ASP:O	1:D:3501:MET:N	2.51	0.43
1:D:3524:GLU:OE2	1:D:3524:GLU:CA	2.65	0.43
1:D:3583:GLN:N	1:D:3583:GLN:CD	2.72	0.43
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.83	0.43
1:A:248:LYS:N	1:A:325:ASP:OD1	2.51	0.43
1:A:461:GLN:H	1:A:466:TYR:HE2	1.65	0.43
1:A:546:LYS:HE3	1:B:1137:LYS:HZ1	1.82	0.43
1:B:1112:ILE:O	1:B:1116:VAL:HG13	2.18	0.43
1:B:1304:ILE:HG22	1:B:1571:ASN:HD22	1.82	0.43
1:B:1442:ILE:N	1:B:1442:ILE:CD1	2.81	0.43
1:B:1524:GLU:OE2	1:B:1524:GLU:CA	2.65	0.43
1:C:2052:PHE:CD2	1:D:3322:GLU:HB3	2.53	0.43
1:C:2252:LEU:HD12	1:C:2309:HIS:CG	2.53	0.43
1:C:2503:LEU:O	1:C:2504:TYR:C	2.55	0.43
1:C:2557:LYS:HA	1:C:2560:ASN:HD22	1.82	0.43
1:D:3461:GLN:H	1:D:3466:TYR:HE2	1.66	0.43
1:D:3495:TYR:CE2	1:D:3502:GLU:HG3	2.51	0.43
1:D:3532:LYS:HB3	1:D:3533:GLY:H	1.70	0.43
1:A:495:TYR:CE2	1:A:502:GLU:HG3	2.50	0.43
1:A:557:LYS:O	1:A:558:ILE:C	2.56	0.43
1:B:1112:ILE:O	1:B:1115:TYR:HB3	2.18	0.43
1:B:1190:ASP:OD1	1:B:1192:GLN:HG3	2.18	0.43
1:B:1219:GLY:HA2	1:B:1458:MET:CE	2.49	0.43
1:B:1229:ASP:OD2	1:B:1231:ASN:N	2.51	0.43
1:B:1352:LEU:HD12	1:B:1352:LEU:HA	1.79	0.43
1:B:1563:SER:C	1:B:1565:GLN:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2124:ILE:HG22	1:C:2125:ASP:N	2.33	0.43
1:C:2175:LYS:O	1:C:2179:GLU:HG3	2.19	0.43
1:C:2371:PHE:CE1	1:C:2532:LYS:HE2	2.53	0.43
1:D:3126:SER:HA	1:D:3127:PRO:C	2.39	0.43
1:D:3148:TYR:HD2	1:D:3219:GLY:O	2.01	0.43
1:D:3339:GLU:OE2	1:D:3558:ILE:CG2	2.66	0.43
1:D:3482:THR:CA	1:D:3511:LYS:HB2	2.48	0.43
1:D:3509:VAL:O	1:D:3510:GLU:C	2.56	0.43
1:D:3525:LEU:C	1:D:3528:PRO:HD2	2.38	0.43
1:D:3528:PRO:O	1:D:3529:PHE:C	2.56	0.43
1:A:161:THR:O	1:A:164:GLY:N	2.50	0.43
1:A:173:ASP:OD2	1:A:173:ASP:C	2.57	0.43
1:A:188:ILE:HB	1:A:439:ASN:ND2	2.34	0.43
1:B:1104:ASN:ND2	1:B:1358:LYS:HB2	2.33	0.43
1:B:1507:LEU:CD2	1:B:1522:MET:HB2	2.47	0.43
1:C:2304:ILE:HG22	1:C:2567:LEU:HD11	2.01	0.43
1:C:2327:GLN:HB2	1:D:3136:TYR:HE2	1.83	0.43
1:C:2463:LEU:HD12	1:C:2503:LEU:HA	2.00	0.43
1:D:3185:ARG:HH21	1:D:3438:ARG:HD3	1.81	0.43
1:D:3249:ASP:HA	1:D:3328:LEU:CD1	2.48	0.43
1:D:3298:LEU:HD12	1:D:3298:LEU:HA	1.76	0.43
1:D:3547:PRO:O	1:D:3552:GLY:N	2.48	0.43
1:A:107:PHE:CD2	1:A:107:PHE:N	2.86	0.43
1:A:216:ARG:HB3	1:A:220:PHE:HD1	1.73	0.43
1:A:249:ASP:HA	1:A:328:LEU:CD1	2.48	0.43
1:A:276:PRO:HG3	1:A:409:TYR:CD1	2.53	0.43
1:A:308:GLU:HA	1:A:308:GLU:OE2	2.18	0.43
1:A:363:PRO:C	1:A:365:LEU:N	2.71	0.43
1:A:380:GLU:HG3	1:A:460:TYR:CE2	2.52	0.43
1:A:389:PRO:HG2	1:A:434:VAL:HG22	2.01	0.43
1:A:455:SER:HA	1:A:460:TYR:CD1	2.53	0.43
1:B:1183:LEU:HD21	1:B:1445:GLN:CG	2.48	0.43
1:B:1241:GLN:OE1	1:B:1329:PHE:CZ	2.72	0.43
1:B:1252:LEU:HD12	1:B:1309:HIS:CG	2.53	0.43
1:B:1287:VAL:O	1:B:1288:GLY:C	2.56	0.43
1:B:1463:LEU:HD12	1:B:1503:LEU:HA	2.00	0.43
1:B:1532:LYS:C	1:B:1534:LEU:H	2.22	0.43
1:C:2034:ASN:HB3	1:C:2037:CYS:SG	2.58	0.43
1:C:2240:ARG:HH12	1:C:2272:GLU:HB2	1.83	0.43
1:C:2427:THR:HG23	1:C:2578:THR:HG23	2.00	0.43
1:C:2465:GLU:OE2	1:C:2468:LYS:CE	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:4113:HOH:O	1:D:3140:GLU:HB2	2.18	0.43
1:D:3124:ILE:HD11	1:D:3528:PRO:C	2.39	0.43
1:D:3130:TYR:CD2	1:D:3135:GLY:O	2.72	0.43
1:D:3315:ILE:H	1:D:3315:ILE:HG13	1.52	0.43
1:D:3455:SER:HA	1:D:3460:TYR:CD1	2.53	0.43
1:D:3490:GLU:O	1:D:3493:ALA:HB3	2.18	0.43
1:A:396:ASN:HD22	1:A:401:GLU:HG2	1.78	0.43
1:B:1134:TYR:CD2	1:B:1136:TYR:HE1	2.37	0.43
1:B:1150:ARG:HD2	1:B:1380:GLU:OE1	2.17	0.43
1:B:1482:THR:CA	1:B:1511:LYS:HB2	2.48	0.43
1:B:1564:ILE:O	1:B:1568:ILE:CD1	2.66	0.43
1:C:2320:HIS:C	1:C:2322:GLU:H	2.21	0.43
1:C:2341:ILE:HD12	1:C:2534:LEU:O	2.18	0.43
1:C:2462:SER:CB	1:C:2465:GLU:HG2	2.48	0.43
1:D:3124:ILE:H	1:D:3124:ILE:HG12	1.57	0.43
1:D:3240:ARG:HH12	1:D:3272:GLU:HB2	1.83	0.43
1:D:3368:ASN:OD1	1:D:3368:ASN:N	2.51	0.43
1:D:3566:SER:O	1:D:3567:LEU:C	2.56	0.43
1:A:301:TYR:O	1:A:302:ALA:C	2.56	0.43
1:B:1130:TYR:CE2	1:B:1135:GLY:O	2.72	0.43
1:B:1155:VAL:HG12	1:B:1159:CYS:SG	2.58	0.43
1:B:1230:LEU:CG	1:B:1337:ILE:HG13	2.46	0.43
1:B:1320:HIS:CD2	1:B:1323:TRP:CE2	3.06	0.43
1:C:2444:VAL:O	1:C:2444:VAL:HG12	2.18	0.43
1:D:3089:VAL:O	1:D:3090:HIS:C	2.56	0.43
1:D:3112:ILE:HB	1:D:3357:PHE:CE1	2.54	0.43
1:D:3168:ASN:C	1:D:3170:GLU:N	2.72	0.43
1:D:3456:ARG:NE	1:D:3502:GLU:OE2	2.51	0.43
1:D:3469:ARG:HA	1:D:3469:ARG:HD2	1.77	0.43
1:D:3564:ILE:O	1:D:3568:ILE:HD12	2.18	0.43
1:B:1065:TYR:HB2	1:B:1066:GLY:H	1.61	0.43
1:B:1089:VAL:O	1:B:1092:ILE:HG12	2.19	0.43
1:B:1096:PHE:O	1:B:1098:GLY:N	2.52	0.43
1:B:1124:ILE:HG22	1:B:1125:ASP:N	2.33	0.43
1:B:1184:ARG:HH12	1:B:1441:PRO:HG3	1.82	0.43
1:B:1481:LEU:HD12	1:B:1481:LEU:O	2.19	0.43
1:B:1498:ILE:O	1:B:1501:MET:HB2	2.18	0.43
1:B:1566:SER:HA	1:B:1569:CYS:CB	2.48	0.43
1:B:1577:PHE:CG	1:B:1578:THR:N	2.87	0.43
1:C:2108:LEU:HD23	1:C:2111:LEU:HD23	1.99	0.43
1:C:2231:ASN:OD1	1:C:2231:ASN:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2320:HIS:C	1:C:2322:GLU:N	2.72	0.43
1:C:2383:THR:C	1:C:2385:TYR:N	2.70	0.43
1:C:2535:MET:C	1:C:2537:ASN:H	2.21	0.43
1:C:2546:LYS:HA	6:C:4145:HOH:O	2.19	0.43
1:C:2563:SER:O	1:C:2564:ILE:C	2.57	0.43
1:C:2564:ILE:O	1:C:2568:ILE:CD1	2.66	0.43
1:D:3274:ILE:HD11	1:D:3290:GLU:HG3	2.00	0.43
1:D:3434:VAL:HG13	1:D:3508:LEU:CD2	2.49	0.43
1:D:3462:SER:CB	1:D:3465:GLU:HG2	2.48	0.43
1:D:3531:LEU:HD12	1:D:3531:LEU:HA	1.82	0.43
1:A:38:SER:C	1:A:40:PRO:HD3	2.39	0.43
1:A:151:ALA:HB2	1:A:529:PHE:HZ	1.82	0.43
1:A:274:ILE:HD12	1:A:291:VAL:CA	2.49	0.43
1:A:301:TYR:O	1:A:304:ILE:HB	2.18	0.43
1:A:327:GLN:CG	1:B:1136:TYR:CE2	3.02	0.43
1:A:403:SER:H	1:A:406:GLN:HB2	1.84	0.43
1:B:1341:ILE:HD13	1:B:1534:LEU:HD12	2.00	0.43
1:C:2078:ILE:HD13	1:C:2078:ILE:N	2.33	0.43
1:C:2139:TRP:CZ3	1:D:3538:PRO:HG2	2.53	0.43
1:C:2243:LYS:O	1:C:2253:LYS:HE3	2.18	0.43
1:C:2301:TYR:O	1:C:2302:ALA:O	2.36	0.43
1:C:2386:HIS:HB2	1:C:2504:TYR:CE1	2.54	0.43
1:D:3372:GLN:O	1:D:3374:GLN:N	2.50	0.43
1:A:130:TYR:CE2	1:A:135:GLY:O	2.72	0.43
1:B:1078:ILE:HD13	1:B:1078:ILE:N	2.34	0.43
1:B:1315:ILE:HD13	1:B:1558:ILE:HD11	1.99	0.43
1:C:2099:VAL:CA	1:C:2102:ILE:HD12	2.28	0.43
1:C:2173:ASP:OD2	1:C:2175:LYS:N	2.51	0.43
1:D:3038:SER:C	1:D:3040:PRO:HD3	2.38	0.43
1:D:3124:ILE:HG22	1:D:3125:ASP:N	2.34	0.43
1:D:3442:ILE:N	1:D:3442:ILE:CD1	2.81	0.43
1:D:3566:SER:HA	1:D:3569:CYS:CB	2.48	0.43
1:A:76:THR:O	1:A:79:LYS:HB2	2.19	0.42
1:A:185:ARG:NH2	1:A:438:ARG:NE	2.61	0.42
1:A:245:ARG:NH2	1:A:326:GLU:HA	2.33	0.42
1:A:262:TYR:HA	1:A:303:THR:HG23	2.00	0.42
1:A:427:THR:HG22	1:A:427:THR:O	2.19	0.42
1:A:427:THR:HG23	1:A:578:THR:HG23	2.01	0.42
1:B:1059:CYS:HB3	1:B:1064:PHE:O	2.18	0.42
1:B:1273:MET:HE1	1:B:1287:VAL:H	1.83	0.42
1:B:1301:TYR:O	1:B:1304:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1467:ARG:NH2	1:B:1520:GLU:OE1	2.49	0.42
1:B:1475:TYR:CD2	1:B:1480:GLU:HG2	2.54	0.42
1:C:2405:LYS:H	1:C:2405:LYS:CE	2.31	0.42
1:D:3112:ILE:O	1:D:3115:TYR:HB3	2.19	0.42
1:D:3226:HIS:C	1:D:3377:ILE:HD12	2.39	0.42
1:D:3267:LYS:HB3	6:D:4185:HOH:O	2.17	0.42
1:A:142:PHE:O	1:A:376:ARG:NH2	2.40	0.42
1:A:202:ALA:HB2	1:A:348:TYR:CE1	2.55	0.42
1:A:229:ASP:OD2	1:A:231:ASN:N	2.50	0.42
1:A:243:LYS:O	1:A:253:LYS:HE3	2.19	0.42
1:A:507:LEU:CD2	1:A:522:MET:HB2	2.49	0.42
1:A:531:LEU:HD12	1:A:531:LEU:HA	1.80	0.42
1:B:1073:GLU:O	1:B:1077:ARG:HG2	2.19	0.42
1:B:1427:THR:CG2	1:B:1578:THR:HA	2.48	0.42
1:C:2246:LEU:HG	1:C:2248:LYS:HB2	2.01	0.42
1:C:2280:PRO:HG2	1:C:2283:LEU:HG	2.01	0.42
1:C:2322:GLU:HA	6:C:4115:HOH:O	2.19	0.42
1:C:2462:SER:O	1:C:2465:GLU:HB2	2.19	0.42
1:D:3094:THR:HG22	1:D:3354:GLY:O	2.18	0.42
1:D:3150:ARG:HD2	1:D:3380:GLU:OE1	2.19	0.42
1:D:3160:PRO:HD2	1:D:3164:GLY:O	2.19	0.42
1:A:197:MET:O	1:A:198:PHE:C	2.56	0.42
1:A:201:PHE:N	1:A:301:TYR:HE2	2.17	0.42
1:A:302:ALA:O	1:A:304:ILE:N	2.52	0.42
1:A:309:HIS:HD2	1:A:310:ASN:OD1	2.02	0.42
1:A:380:GLU:N	1:A:460:TYR:OH	2.52	0.42
1:A:481:LEU:HD12	1:A:481:LEU:O	2.19	0.42
1:B:1184:ARG:CB	1:B:1439:ASN:HA	2.47	0.42
1:B:1275:TYR:CE2	1:B:1284:GLN:CA	3.00	0.42
1:B:1563:SER:O	1:B:1564:ILE:C	2.57	0.42
1:C:2073:GLU:O	1:C:2077:ARG:HG2	2.19	0.42
1:C:2274:ILE:HD12	1:C:2291:VAL:HA	2.01	0.42
1:C:2308:GLU:HA	1:C:2308:GLU:OE2	2.19	0.42
1:C:2404:PHE:H	1:C:2404:PHE:HD1	1.67	0.42
1:C:2435:ALA:HB2	1:C:2518:PHE:HA	2.00	0.42
1:C:2547:PRO:CB	1:C:2552:GLY:HA2	2.48	0.42
1:D:3107:PHE:CD2	1:D:3107:PHE:N	2.87	0.42
1:D:3181:VAL:HG12	1:D:3487:MET:CG	2.50	0.42
1:A:113:MET:O	1:A:116:VAL:HG13	2.20	0.42
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.77	0.42
1:A:534:LEU:HD13	1:A:534:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:VAL:O	1:B:1090:HIS:C	2.57	0.42
1:B:1196:MET:HG2	1:B:1429:GLN:O	2.19	0.42
1:B:1261:VAL:H	1:B:1307:ARG:NH2	2.17	0.42
1:B:1444:VAL:O	1:B:1445:GLN:C	2.58	0.42
1:C:2245:ARG:HD2	1:C:2329:PHE:CE1	2.54	0.42
1:C:2458:MET:O	1:C:2459:LYS:C	2.56	0.42
1:C:2548:SER:O	1:C:2550:PHE:N	2.53	0.42
1:D:3202:ALA:HA	1:D:3348:TYR:HE1	1.83	0.42
1:D:3323:TRP:CE3	1:D:3327:GLN:HG2	2.54	0.42
1:D:3395:PHE:O	1:D:3402:TYR:HD2	2.02	0.42
1:D:3530:SER:C	1:D:3532:LYS:H	2.23	0.42
1:A:56:LYS:HA	6:A:4007:HOH:O	2.18	0.42
1:A:124:ILE:HG22	1:A:125:ASP:N	2.34	0.42
1:A:173:ASP:OD2	1:A:175:LYS:N	2.53	0.42
1:B:1094:THR:HG22	1:B:1354:GLY:O	2.20	0.42
1:B:1099:VAL:O	1:B:1102:ILE:HB	2.19	0.42
1:B:1162:PRO:HB2	1:B:1171:LEU:HD21	2.01	0.42
1:B:1190:ASP:OD2	1:B:1192:GLN:HB2	2.18	0.42
1:B:1421:GLN:O	1:B:1422:PHE:C	2.58	0.42
1:C:2095:HIS:O	1:C:2100:TRP:HD1	2.02	0.42
1:C:2500:VAL:O	1:C:2500:VAL:HG12	2.19	0.42
1:C:2531:LEU:HD12	1:C:2531:LEU:HA	1.80	0.42
1:D:3128:PRO:HG3	1:D:3376:ARG:NH1	2.34	0.42
1:D:3155:VAL:HG12	1:D:3159:CYS:SG	2.59	0.42
1:D:3357:PHE:HE2	1:D:3359:LEU:HD23	1.81	0.42
1:D:3568:ILE:HG23	1:D:3572:VAL:CG2	2.48	0.42
1:A:344:VAL:HG12	1:A:345:ILE:N	2.34	0.42
1:A:404:PHE:N	1:A:404:PHE:HD1	2.18	0.42
1:A:404:PHE:H	1:A:405:LYS:HZ2	1.67	0.42
1:B:1105(B):ILE:O	1:B:1108:LEU:HB2	2.19	0.42
1:B:1124:ILE:HD11	1:B:1528:PRO:C	2.40	0.42
1:B:1182:LEU:O	1:B:1438:ARG:CA	2.62	0.42
1:B:1205:PHE:CZ	1:B:1344:VAL:HG21	2.54	0.42
1:B:1245:ARG:O	1:B:1253:LYS:HG3	2.19	0.42
1:B:1396:ASN:N	1:B:1396:ASN:HD22	2.17	0.42
1:C:2150:ARG:HD2	1:C:2380:GLU:OE1	2.19	0.42
1:C:2390:LEU:HD21	1:C:2517:ILE:HD11	2.01	0.42
1:C:2462:SER:HB3	1:C:2465:GLU:HG2	2.02	0.42
1:C:2481:LEU:HD12	1:C:2510:GLU:HA	2.02	0.42
1:C:2521:THR:HG22	1:C:2522:MET:N	2.33	0.42
1:D:3184:ARG:CD	1:D:3187:PHE:HA	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3185:ARG:HE	1:D:3438:ARG:HD3	1.85	0.42
1:D:3211:LYS:O	1:D:3212:THR:C	2.58	0.42
1:D:3458:MET:O	1:D:3459:LYS:C	2.58	0.42
1:D:3467:ARG:NH2	1:D:3520:GLU:OE1	2.52	0.42
1:D:3470:PHE:CD2	1:D:3470:PHE:N	2.87	0.42
1:A:92:ILE:HG12	1:A:92:ILE:H	1.34	0.42
1:A:95:HIS:O	1:A:100:TRP:CD1	2.73	0.42
1:A:151:ALA:HB2	1:A:529:PHE:CZ	2.55	0.42
1:A:155:VAL:HG12	1:A:159:CYS:SG	2.59	0.42
1:A:320:HIS:C	1:A:322:GLU:H	2.22	0.42
1:A:404:PHE:HD1	1:A:404:PHE:H	1.67	0.42
1:A:482:THR:CG2	1:A:509:VAL:HG12	2.49	0.42
1:B:1198:PHE:HB2	1:B:1580:PHE:HB3	2.00	0.42
1:B:1230:LEU:HD11	1:B:1337:ILE:HA	2.02	0.42
1:B:1531:LEU:HD12	1:B:1531:LEU:HA	1.79	0.42
1:C:2391:LEU:HD13	1:C:2404:PHE:HE2	1.84	0.42
1:C:2467:ARG:O	1:C:2472:LEU:HB2	2.19	0.42
1:C:2564:ILE:O	1:C:2568:ILE:HD12	2.19	0.42
1:D:3467:ARG:O	1:D:3472:LEU:HB2	2.19	0.42
1:D:3503:LEU:O	1:D:3504:TYR:C	2.58	0.42
1:B:1099:VAL:CA	1:B:1102:ILE:HD12	2.29	0.42
1:B:1112:ILE:HB	1:B:1357:PHE:CE1	2.55	0.42
1:B:1274:ILE:HD12	1:B:1291:VAL:HA	2.01	0.42
1:B:1404:PHE:N	1:B:1404:PHE:CD1	2.88	0.42
1:C:2302:ALA:O	1:C:2304:ILE:N	2.52	0.42
1:C:2348:TYR:HD2	1:C:2349:VAL:N	2.18	0.42
1:C:2528:PRO:O	1:C:2529:PHE:C	2.58	0.42
1:C:2532:LYS:HB3	1:C:2533:GLY:H	1.68	0.42
1:C:2564:ILE:HG23	1:C:2565:GLN:N	2.35	0.42
1:D:3141:ALA:O	1:D:3143:SER:N	2.53	0.42
1:D:3530:SER:O	1:D:3532:LYS:N	2.52	0.42
1:A:503:LEU:O	1:A:504:TYR:C	2.56	0.42
1:A:523:VAL:HG12	1:A:524:GLU:N	2.33	0.42
1:A:532:LYS:O	1:A:535:MET:N	2.53	0.42
1:A:563:SER:C	1:A:565:GLN:N	2.72	0.42
1:B:1389:PRO:CB	1:B:1434:VAL:HA	2.49	0.42
1:B:1568:ILE:HG23	1:B:1572:VAL:CG2	2.50	0.42
1:C:2110:SER:O	1:C:2111:LEU:C	2.57	0.42
1:C:2113:MET:O	1:C:2117:LEU:HD22	2.20	0.42
1:C:2197:MET:HG3	1:C:2578:THR:HG21	2.01	0.42
1:C:2211:LYS:O	1:C:2212:THR:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2230:LEU:CG	1:C:2337:ILE:HG13	2.44	0.42
1:D:3074:PHE:O	1:D:3077:ARG:N	2.53	0.42
1:D:3256:VAL:HA	1:D:3260:GLU:O	2.20	0.42
1:D:3295:VAL:HB	1:D:3298:LEU:HB2	2.02	0.42
1:D:3384:LEU:HB2	5:D:3701:PGX:O3	2.19	0.42
1:D:3404:PHE:N	1:D:3404:PHE:HD1	2.17	0.42
1:D:3433:ARG:HH21	1:D:3512:PRO:CB	2.33	0.42
1:D:3564:ILE:HG22	6:D:4157:HOH:O	2.19	0.42
1:D:3577:PHE:CG	1:D:3578:THR:N	2.87	0.42
1:A:48:MET:HE1	1:B:1551:GLY:O	2.19	0.42
1:A:103:VAL:C	1:A:105:ASN:N	2.73	0.42
1:A:116:VAL:CG2	1:A:117:LEU:N	2.82	0.42
1:A:160:PRO:HD2	1:A:164:GLY:O	2.20	0.42
1:A:185:ARG:HH21	1:A:438:ARG:HD3	1.85	0.42
1:A:226:HIS:C	1:A:377:ILE:HD12	2.40	0.42
1:A:234:TYR:HB2	1:A:333:ARG:NH1	2.35	0.42
1:A:315:ILE:H	1:A:315:ILE:HG13	1.56	0.42
1:A:350:GLN:NE2	1:A:359:LEU:H	2.18	0.42
1:A:478:PHE:O	1:A:482:THR:OG1	2.37	0.42
1:A:487:MET:O	1:A:490:GLU:HB3	2.20	0.42
1:B:1126:SER:HA	1:B:1127:PRO:C	2.38	0.42
1:B:1384:LEU:HB3	1:B:1522:MET:CE	2.50	0.42
1:B:1450:ALA:O	1:B:1451:SER:C	2.57	0.42
1:B:1528:PRO:O	1:B:1529:PHE:C	2.58	0.42
1:B:1530:SER:C	1:B:1532:LYS:H	2.23	0.42
1:C:2404:PHE:CD1	1:C:2404:PHE:N	2.85	0.42
1:C:2507:LEU:CD2	1:C:2522:MET:HB2	2.50	0.42
1:C:2538:PRO:HG2	1:D:3139:TRP:HZ3	1.85	0.42
1:C:2553:GLU:OE1	1:C:2553:GLU:CA	2.62	0.42
1:D:3105(D):ILE:CB	1:D:3108:LEU:HD12	2.49	0.42
1:D:3231:ASN:O	1:D:3235:GLY:N	2.52	0.42
1:D:3295:VAL:HG12	1:D:3298:LEU:H	1.85	0.42
1:D:3318:GLN:OE1	1:D:3318:GLN:HA	2.19	0.42
1:D:3357:PHE:CD2	1:D:3359:LEU:HD23	2.55	0.42
1:D:3427:THR:HG23	1:D:3578:THR:HG23	2.02	0.42
1:D:3481:LEU:O	1:D:3511:LYS:N	2.53	0.42
1:A:454:GLN:O	1:A:456:ARG:N	2.52	0.41
1:B:1141:ALA:O	1:B:1143:SER:N	2.52	0.41
1:B:1371:PHE:CE1	1:B:1532:LYS:HE2	2.55	0.41
1:B:1465:GLU:OE2	1:B:1465:GLU:CA	2.68	0.41
1:C:2038:SER:C	1:C:2040:PRO:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2173:ASP:OD2	1:C:2173:ASP:C	2.58	0.41
1:C:2249:ASP:HA	1:C:2328:LEU:CD1	2.50	0.41
1:C:2262:TYR:HA	1:C:2303:THR:HG23	2.02	0.41
1:C:2530:SER:O	1:C:2532:LYS:N	2.52	0.41
1:D:3073:GLU:O	1:D:3076:THR:HB	2.20	0.41
1:D:3092:ILE:HG12	1:D:3092:ILE:H	1.36	0.41
1:D:3099:VAL:O	1:D:3102:ILE:HB	2.20	0.41
1:D:3229:ASP:OD2	1:D:3231:ASN:N	2.53	0.41
1:D:3345:ILE:CG1	1:D:3534:LEU:HG	2.50	0.41
1:D:3548:SER:O	1:D:3550:PHE:N	2.53	0.41
1:A:403:SER:OG	1:A:405:LYS:HD2	2.20	0.41
1:A:444:VAL:O	1:A:444:VAL:HG12	2.20	0.41
1:B:1099:VAL:HA	1:B:1102:ILE:CD1	2.29	0.41
1:B:1368:ASN:OD1	1:B:1368:ASN:N	2.53	0.41
1:B:1535:MET:O	1:B:1540:CYS:HB2	2.20	0.41
1:B:1557:LYS:HA	1:B:1560:ASN:HD22	1.85	0.41
1:C:2064:PHE:CE2	1:C:2072:PRO:HB3	2.54	0.41
1:C:2404:PHE:H	1:C:2405:LYS:HZ2	1.66	0.41
1:D:3274:ILE:HD12	1:D:3291:VAL:CA	2.49	0.41
1:A:372:GLN:O	1:A:374:GLN:N	2.51	0.41
1:A:531:LEU:O	1:A:535:MET:HB2	2.21	0.41
1:B:1136:TYR:HB2	6:B:4080:HOH:O	2.20	0.41
1:B:1202:ALA:HA	1:B:1348:TYR:HE1	1.85	0.41
1:B:1275:TYR:HE2	1:B:1284:GLN:CA	2.34	0.41
1:B:1301:TYR:O	1:B:1302:ALA:O	2.38	0.41
1:C:2184:ARG:NE	1:C:2439:ASN:OD1	2.48	0.41
1:C:2350:GLN:NE2	1:C:2359:LEU:H	2.17	0.41
1:C:2404:PHE:HD1	1:C:2404:PHE:N	2.18	0.41
1:C:2504:TYR:HB3	1:C:2505:PRO:CD	2.45	0.41
1:D:3316:LEU:O	1:D:3319:GLU:N	2.52	0.41
1:A:74:PHE:O	1:A:75:LEU:C	2.59	0.41
1:A:108:LEU:HA	1:A:111:LEU:HD23	2.02	0.41
1:A:274:ILE:HD11	1:A:290:GLU:HG3	2.03	0.41
1:A:295:VAL:HG12	1:A:297:GLY:H	1.85	0.41
1:A:352:LEU:HG	1:A:518:PHE:HE2	1.86	0.41
1:A:386:HIS:HD2	1:A:451:SER:HB3	1.85	0.41
1:A:394:THR:O	1:A:429:GLN:NE2	2.47	0.41
1:A:509:VAL:O	1:A:510:GLU:C	2.59	0.41
1:A:532:LYS:HB3	1:A:533:GLY:H	1.70	0.41
1:B:1347:ASP:OD2	1:B:1564:ILE:HG22	2.20	0.41
1:B:1403:SER:HB2	1:B:1405:LYS:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:THR:HG23	1:B:1578:THR:HG23	2.02	0.41
1:B:1517:ILE:O	1:B:1517:ILE:HG13	2.20	0.41
1:B:1523:VAL:HG12	1:B:1524:GLU:N	2.36	0.41
1:B:1532:LYS:O	1:B:1535:MET:N	2.53	0.41
1:C:2074:PHE:O	1:C:2077:ARG:N	2.53	0.41
1:C:2096:PHE:O	1:C:2098:GLY:N	2.53	0.41
1:C:2120:ARG:HH11	1:C:2527:ALA:HB1	1.83	0.41
1:C:2151:ALA:HB2	1:C:2529:PHE:CZ	2.53	0.41
1:C:2275:TYR:CE2	1:C:2284:GLN:CA	3.03	0.41
1:C:2275:TYR:HE2	1:C:2284:GLN:HA	1.84	0.41
1:D:3059:CYS:HA	1:D:3062:THR:HG21	2.01	0.41
1:D:3383:THR:C	1:D:3385:TYR:N	2.74	0.41
1:D:3404:PHE:H	1:D:3404:PHE:HD1	1.68	0.41
1:A:50:THR:CG2	1:A:56:LYS:CB	2.98	0.41
1:A:73:GLU:O	1:A:77:ARG:HG2	2.20	0.41
1:A:103:VAL:O	1:A:105:ASN:N	2.53	0.41
1:B:1246:LEU:HG	1:B:1248:LYS:HB2	2.02	0.41
1:B:1295:VAL:HG12	1:B:1298:LEU:H	1.85	0.41
1:B:1308:GLU:OE2	1:B:1311:ARG:HD3	2.21	0.41
1:B:1383:THR:O	1:B:1385:TYR:N	2.54	0.41
1:B:1464:ASN:HD21	1:B:1475:TYR:N	2.19	0.41
1:B:1530:SER:O	1:B:1532:LYS:N	2.53	0.41
1:B:1583:GLN:CD	1:B:1583:GLN:N	2.74	0.41
1:C:2139:TRP:HZ3	1:D:3538:PRO:HG2	1.86	0.41
1:C:2185:ARG:HH21	1:C:2438:ARG:HD3	1.85	0.41
1:C:2309:HIS:HD2	1:C:2310:ASN:OD1	2.03	0.41
1:C:2384:LEU:HB3	1:C:2522:MET:CE	2.50	0.41
1:C:2389:PRO:CB	1:C:2434:VAL:HA	2.51	0.41
1:D:3148:TYR:CZ	1:D:3221:THR:HB	2.55	0.41
1:D:3196:MET:CE	1:D:3196:MET:HA	2.51	0.41
1:D:3274:ILE:HD12	1:D:3291:VAL:HG23	2.01	0.41
1:D:3380:GLU:N	1:D:3460:TYR:OH	2.53	0.41
1:D:3394:THR:O	1:D:3429:GLN:NE2	2.46	0.41
1:A:39:ASN:N	1:A:39:ASN:ND2	2.68	0.41
1:A:327:GLN:HG3	1:B:1136:TYR:CE2	2.55	0.41
1:B:1096:PHE:O	1:B:1097:LYS:C	2.58	0.41
1:B:1383:THR:C	1:B:1385:TYR:N	2.72	0.41
1:B:1434:VAL:HG13	1:B:1508:LEU:CD2	2.50	0.41
1:C:2156:ALA:C	1:C:2158:ASP:N	2.73	0.41
1:C:2186:GLU:N	6:C:4100:HOH:O	2.52	0.41
1:C:2295:VAL:HB	1:C:2298:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2389:PRO:HB2	1:C:2434:VAL:HA	2.03	0.41
1:C:2530:SER:C	1:C:2532:LYS:H	2.23	0.41
1:D:3056:LYS:HG3	1:D:3057:CYS:N	2.36	0.41
1:D:3112:ILE:O	1:D:3116:VAL:HG13	2.21	0.41
1:D:3123:LEU:O	1:D:3469:ARG:NH2	2.54	0.41
1:D:3377:ILE:HA	6:D:4180:HOH:O	2.20	0.41
1:D:3450:ALA:O	1:D:3454:GLN:HG3	2.21	0.41
1:D:3507:LEU:CD2	1:D:3522:MET:HB2	2.51	0.41
1:A:95:HIS:O	1:A:100:TRP:HD1	2.02	0.41
1:A:137:LYS:HD3	1:B:1549:THR:HG23	2.02	0.41
1:A:178:LEU:HD22	1:A:183:LEU:CD1	2.50	0.41
1:A:197:MET:HG3	1:A:578:THR:HG21	2.03	0.41
1:A:514:PRO:O	1:A:515:ASP:CB	2.66	0.41
1:A:551:GLY:O	1:B:1048:MET:HE1	2.21	0.41
1:B:1481:LEU:O	1:B:1511:LYS:N	2.53	0.41
1:B:1535:MET:C	1:B:1537:ASN:N	2.74	0.41
1:C:2454:GLN:O	1:C:2456:ARG:N	2.53	0.41
1:D:3096:PHE:O	1:D:3097:LYS:C	2.59	0.41
1:D:3105(D):ILE:CG2	1:D:3108:LEU:HB2	2.51	0.41
1:D:3190:ASP:OD1	1:D:3192:GLN:HG3	2.20	0.41
1:A:184:ARG:NH2	1:A:391:LEU:O	2.48	0.41
1:A:366:LEU:C	1:A:368:ASN:H	2.24	0.41
1:A:516:ALA:HB1	6:A:4048:HOH:O	2.21	0.41
1:B:1309:HIS:O	1:B:1312:VAL:N	2.53	0.41
1:B:1487:MET:O	1:B:1488:ALA:C	2.59	0.41
1:B:1522:MET:O	1:B:1522:MET:HG3	2.21	0.41
1:C:2065:TYR:N	1:C:2071:THR:O	2.49	0.41
1:C:2185:ARG:HE	1:C:2438:ARG:HD3	1.86	0.41
1:C:2229:ASP:OD2	1:C:2229:ASP:C	2.58	0.41
1:C:2372:GLN:O	1:C:2374:GLN:N	2.50	0.41
1:C:2415:LEU:HD23	1:C:2415:LEU:HA	1.83	0.41
1:D:3218:PRO:C	1:D:3458:MET:CE	2.88	0.41
1:D:3243:LYS:O	1:D:3253:LYS:HE3	2.21	0.41
1:D:3462:SER:HB3	1:D:3465:GLU:HG2	2.03	0.41
1:D:3486:GLU:HB3	1:D:3487:MET:H	1.73	0.41
1:D:3514:PRO:O	1:D:3515:ASP:CB	2.69	0.41
1:D:3535:MET:O	1:D:3540:CYS:HB2	2.21	0.41
1:A:56:LYS:HG3	1:A:57:CYS:N	2.35	0.41
1:A:117:LEU:HD13	1:A:117:LEU:HA	1.81	0.41
1:A:132:VAL:HG23	6:A:4038:HOH:O	2.21	0.41
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASN:OD1	1:A:368:ASN:N	2.54	0.41
1:A:464:ASN:HD21	1:A:475:TYR:N	2.18	0.41
1:A:530:SER:C	1:A:532:LYS:H	2.24	0.41
1:A:553:GLU:OE1	1:A:553:GLU:CA	2.60	0.41
1:B:1110:SER:O	1:B:1111:LEU:C	2.59	0.41
1:B:1132:VAL:HG21	1:B:1219:GLY:HA3	2.03	0.41
1:B:1503:LEU:O	1:B:1504:TYR:C	2.59	0.41
1:C:2039:ASN:N	1:C:2039:ASN:ND2	2.69	0.41
1:C:2089:VAL:O	1:C:2092:ILE:HG12	2.21	0.41
1:C:2096:PHE:O	1:C:2099:VAL:N	2.54	0.41
1:C:2162:PRO:HB2	1:C:2171:LEU:CD2	2.51	0.41
1:C:2185:ARG:NH2	1:C:2438:ARG:NE	2.63	0.41
1:C:2218:PRO:C	1:C:2458:MET:CE	2.89	0.41
1:C:2341:ILE:HD13	1:C:2534:LEU:CD1	2.50	0.41
1:C:2347:ASP:OD2	1:C:2564:ILE:HG22	2.21	0.41
1:C:2366:LEU:HA	1:C:2369:GLN:CG	2.51	0.41
1:C:2449:LYS:HA	1:C:2452:ILE:CD1	2.44	0.41
1:C:2482:THR:CG2	1:C:2509:VAL:HG12	2.51	0.41
1:C:2509:VAL:O	1:C:2510:GLU:C	2.59	0.41
1:D:3103:VAL:C	1:D:3105:ASN:N	2.75	0.41
1:D:3124:ILE:HG22	1:D:3125:ASP:H	1.85	0.41
1:D:3152:LEU:HD12	1:D:3466:TYR:CD1	2.56	0.41
1:D:3175:LYS:O	1:D:3179:GLU:HG3	2.21	0.41
1:D:3429:GLN:HG2	1:D:3429:GLN:O	2.20	0.41
1:D:3479:GLU:O	1:D:3483:GLY:N	2.49	0.41
1:D:3499:ASP:C	1:D:3501:MET:H	2.23	0.41
1:D:3504:TYR:O	1:D:3507:LEU:HB2	2.20	0.41
1:A:428:ARG:O	1:A:582:VAL:HG21	2.21	0.41
1:A:486:GLU:HB3	1:A:487:MET:H	1.70	0.41
1:A:563:SER:O	1:A:564:ILE:C	2.59	0.41
1:B:1249:ASP:HA	1:B:1328:LEU:CD1	2.50	0.41
1:B:1273:MET:CE	1:B:1287:VAL:HG22	2.34	0.41
1:B:1470:PHE:CD2	1:B:1470:PHE:N	2.88	0.41
1:B:1509:VAL:O	1:B:1510:GLU:C	2.59	0.41
1:C:2216:ARG:HB3	1:C:2220:PHE:HD1	1.76	0.41
1:C:2256:VAL:HA	1:C:2260:GLU:O	2.21	0.41
1:C:2287:VAL:O	1:C:2288:GLY:C	2.58	0.41
1:C:2295:VAL:HG12	1:C:2298:LEU:H	1.86	0.41
1:C:2465:GLU:OE2	1:C:2468:LYS:HE2	2.21	0.41
1:D:3073:GLU:O	1:D:3077:ARG:HG2	2.21	0.41
1:D:3105(D):ILE:HG22	1:D:3108:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3252:LEU:HD12	1:D:3309:HIS:CG	2.56	0.41
1:D:3280:PRO:HG2	1:D:3283:LEU:HG	2.03	0.41
1:D:3444:VAL:O	1:D:3444:VAL:HG12	2.21	0.41
1:A:105(A):ILE:O	1:A:108:LEU:N	2.55	0.40
1:A:110:SER:O	1:A:111:LEU:C	2.60	0.40
1:A:113:MET:O	1:A:116:VAL:HG22	2.21	0.40
1:A:162:PRO:HB2	1:A:171:LEU:CD2	2.51	0.40
1:A:268:ASP:OD1	1:A:268:ASP:N	2.54	0.40
1:A:295:VAL:HG12	1:A:298:LEU:H	1.86	0.40
1:A:421:GLN:O	1:A:422:PHE:C	2.59	0.40
1:A:530:SER:O	1:A:532:LYS:N	2.54	0.40
1:B:1268:ASP:OD1	1:B:1268:ASP:N	2.53	0.40
1:C:2076:THR:O	1:C:2079:LYS:HB2	2.21	0.40
1:C:2128:PRO:HG3	1:C:2376:ARG:HH11	1.86	0.40
1:C:2300:MET:O	1:C:2304:ILE:HG13	2.21	0.40
1:C:2498:ILE:CG2	1:C:2499:ASP:N	2.83	0.40
1:C:2534:LEU:HD22	5:C:2701:PGX:C18	2.43	0.40
1:D:3205:PHE:CZ	1:D:3344:VAL:HG21	2.56	0.40
1:D:3436:GLY:HA2	1:D:3512:PRO:HG2	2.02	0.40
1:D:3475:TYR:CD1	1:D:3481:LEU:HB2	2.56	0.40
1:A:132:VAL:HG21	1:A:219:GLY:HA3	2.03	0.40
1:A:341:ILE:HD13	1:A:534:LEU:CD1	2.51	0.40
1:A:383:THR:O	1:A:384:LEU:C	2.59	0.40
1:A:389:PRO:HB2	1:A:434:VAL:HA	2.02	0.40
1:A:454:GLN:CA	1:A:457:GLU:HG3	2.51	0.40
1:B:1209:PHE:CZ	5:B:1701:PGX:H192	2.56	0.40
1:B:1302:ALA:O	1:B:1304:ILE:N	2.54	0.40
1:B:1320:HIS:CD2	1:B:1323:TRP:CZ2	3.09	0.40
1:B:1388:HIS:NE2	1:B:1447:VAL:CG1	2.85	0.40
1:B:1407:PHE:HD1	1:B:1413:ILE:HD13	1.87	0.40
1:C:2148:TYR:HD2	1:C:2219:GLY:O	2.04	0.40
1:C:2280:PRO:HG2	1:C:2283:LEU:CG	2.52	0.40
1:C:2470:PHE:CD2	1:C:2470:PHE:N	2.88	0.40
1:C:2503:LEU:HG	1:C:2507:LEU:CD1	2.51	0.40
1:C:2563:SER:C	1:C:2565:GLN:N	2.72	0.40
1:D:3103:VAL:HG12	1:D:3104:ASN:N	2.37	0.40
1:D:3402:TYR:OH	1:D:3417:HIS:CE1	2.74	0.40
1:A:65:TYR:N	1:A:71:THR:O	2.52	0.40
1:A:204:HIS:CD2	1:A:292:PHE:CE2	3.09	0.40
1:A:369:GLN:O	1:A:371:PHE:N	2.54	0.40
1:A:481:LEU:O	1:A:511:LYS:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1245:ARG:NH2	1:B:1326:GLU:HA	2.37	0.40
1:B:1274:ILE:HD11	1:B:1290:GLU:HG3	2.04	0.40
1:B:1433:ARG:HH21	1:B:1512:PRO:CB	2.35	0.40
1:C:2085:THR:O	1:C:2088:THR:HB	2.21	0.40
1:C:2093:LEU:HB3	1:C:2355:TYR:CD1	2.56	0.40
1:C:2162:PRO:HB2	1:C:2171:LEU:HD21	2.04	0.40
1:C:2308:GLU:OE2	1:C:2311:ARG:HD3	2.21	0.40
1:C:2336:LEU:O	1:C:2337:ILE:C	2.59	0.40
1:C:2428:ARG:O	1:C:2582:VAL:HG21	2.22	0.40
1:C:2481:LEU:HD12	1:C:2481:LEU:O	2.21	0.40
1:D:3050:THR:CG2	1:D:3056:LYS:CB	2.99	0.40
1:D:3095:HIS:C	1:D:3097:LYS:N	2.74	0.40
1:D:3427:THR:CG2	1:D:3578:THR:HA	2.50	0.40
1:D:3498:ILE:O	1:D:3501:MET:HB2	2.21	0.40
1:A:47:CYS:SG	1:A:55:TYR:HD1	2.44	0.40
1:A:75:LEU:HD12	1:A:75:LEU:O	2.21	0.40
1:A:223:GLY:HA2	1:A:236:GLU:OE1	2.21	0.40
1:A:273:MET:CE	1:A:287:VAL:H	2.34	0.40
1:A:274:ILE:HD12	1:A:291:VAL:HG23	2.04	0.40
1:A:304:ILE:HG22	1:A:571:ASN:HD22	1.86	0.40
1:B:1112:ILE:O	1:B:1115:TYR:N	2.54	0.40
1:B:1262:TYR:HA	1:B:1303:THR:HG23	2.02	0.40
1:B:1295:VAL:O	1:B:1297:GLY:N	2.55	0.40
1:B:1357:PHE:CD2	1:B:1359:LEU:HD23	2.56	0.40
1:B:1437:GLY:O	1:B:1438:ARG:C	2.59	0.40
1:B:1450:ALA:O	1:B:1452:ILE:N	2.54	0.40
1:B:1514:PRO:O	1:B:1515:ASP:CB	2.70	0.40
1:C:2124:ILE:HD11	1:C:2528:PRO:C	2.41	0.40
1:C:2301:TYR:O	1:C:2304:ILE:HB	2.21	0.40
1:C:2454:GLN:C	1:C:2456:ARG:N	2.74	0.40
1:D:3132:VAL:HG21	1:D:3219:GLY:HA3	2.03	0.40
1:D:3198:PHE:O	1:D:3199:ALA:C	2.60	0.40
1:D:3201:PHE:N	1:D:3301:TYR:HE2	2.19	0.40
1:D:3383:THR:O	1:D:3385:TYR:N	2.54	0.40
1:D:3464:ASN:HD21	1:D:3475:TYR:N	2.19	0.40
1:A:99:VAL:O	1:A:102:ILE:HB	2.21	0.40
1:A:142:PHE:CE2	1:B:1538:PRO:HG3	2.56	0.40
1:A:231:ASN:O	1:A:235:GLY:N	2.55	0.40
1:A:245:ARG:O	1:A:253:LYS:HG3	2.21	0.40
1:A:295:VAL:O	1:A:298:LEU:N	2.55	0.40
1:A:454:GLN:C	1:A:456:ARG:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HD12	1:A:510:GLU:HA	2.03	0.40
1:A:498:ILE:CG2	1:A:499:ASP:N	2.84	0.40
1:A:525:LEU:C	1:A:528:PRO:HD2	2.41	0.40
1:B:1034:ASN:HA	1:B:1035:PRO:HD2	1.86	0.40
1:B:1211:LYS:O	1:B:1212:THR:C	2.59	0.40
1:B:1348:TYR:HD2	1:B:1349:VAL:N	2.20	0.40
1:B:1531:LEU:O	1:B:1535:MET:HB2	2.21	0.40
1:C:2112:ILE:O	1:C:2116:VAL:HG13	2.21	0.40
1:C:2320:HIS:CD2	1:C:2323:TRP:CE2	3.10	0.40
1:C:2461:GLN:H	1:C:2466:TYR:HE2	1.67	0.40
1:C:2535:MET:O	1:C:2540:CYS:HB2	2.22	0.40
1:C:2538:PRO:HG2	1:D:3139:TRP:CZ3	2.57	0.40
1:D:3036:CYS:O	1:D:3037:CYS:C	2.60	0.40
1:D:3136:TYR:CD1	1:D:3136:TYR:C	2.94	0.40
1:D:3216:ARG:HB3	1:D:3220:PHE:HD1	1.79	0.40
1:D:3273:MET:CE	1:D:3287:VAL:H	2.34	0.40
1:D:3428:ARG:O	1:D:3582:VAL:HG21	2.22	0.40
1:D:3475:TYR:CD2	1:D:3480:GLU:HG2	2.56	0.40
1:D:3564:ILE:HG13	1:D:3568:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/552 (100%)	374 (68%)	124 (22%)	52 (10%)	0	3
1	B	550/552 (100%)	379 (69%)	119 (22%)	52 (10%)	0	3
1	C	550/552 (100%)	372 (68%)	120 (22%)	58 (10%)	0	2
1	D	550/552 (100%)	376 (68%)	121 (22%)	53 (10%)	0	3
All	All	2200/2208 (100%)	1501 (68%)	484 (22%)	215 (10%)	0	2

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	A	176	GLU
1	A	180	LYS
1	A	348	TYR
1	A	386	HIS
1	A	400	GLN
1	A	429	GLN
1	A	486	GLU
1	A	510	GLU
1	A	514	PRO
1	B	1121	SER
1	B	1122	TYR
1	B	1176	GLU
1	B	1180	LYS
1	B	1348	TYR
1	B	1386	HIS
1	B	1400	GLN
1	B	1429	GLN
1	B	1486	GLU
1	B	1510	GLU
1	C	2121	SER
1	C	2122	TYR
1	C	2176	GLU
1	C	2180	LYS
1	C	2181	VAL
1	C	2348	TYR
1	C	2386	HIS
1	C	2400	GLN
1	C	2429	GLN
1	C	2486	GLU
1	C	2500	VAL
1	C	2510	GLU
1	C	2514	PRO
1	D	3121	SER
1	D	3122	TYR
1	D	3176	GLU
1	D	3180	LYS
1	D	3348	TYR
1	D	3386	HIS
1	D	3400	GLN
1	D	3429	GLN

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Mol	Chain	Res	Type
1	D	3486	GLU
1	D	3510	GLU
1	A	96	PHE
1	A	120	ARG
1	A	141	ALA
1	A	142	PHE
1	A	177	VAL
1	A	181	VAL
1	A	292	PHE
1	A	500	VAL
1	A	533	GLY
1	A	536	GLY
1	A	539	ILE
1	A	549	THR
1	B	1096	PHE
1	B	1120	ARG
1	B	1141	ALA
1	B	1142	PHE
1	B	1181	VAL
1	B	1292	PHE
1	B	1302	ALA
1	B	1423	VAL
1	B	1458	MET
1	B	1500	VAL
1	B	1514	PRO
1	B	1533	GLY
1	B	1536	GLY
1	B	1539	ILE
1	B	1549	THR
1	C	2096	PHE
1	C	2120	ARG
1	C	2141	ALA
1	C	2142	PHE
1	C	2177	VAL
1	C	2292	PHE
1	C	2302	ALA
1	C	2459	LYS
1	C	2512	PRO
1	C	2533	GLY
1	C	2539	ILE
1	D	3096	PHE
1	D	3097	LYS

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Mol	Chain	Res	Type
1	D	3141	ALA
1	D	3142	PHE
1	D	3177	VAL
1	D	3181	VAL
1	D	3292	PHE
1	D	3500	VAL
1	D	3514	PRO
1	D	3533	GLY
1	D	3539	ILE
1	A	97	LYS
1	A	106	PRO
1	A	302	ALA
1	A	367	PHE
1	A	451	SER
1	A	458	MET
1	A	459	LYS
1	A	512	PRO
1	B	1097	LYS
1	B	1106	PRO
1	B	1177	VAL
1	B	1373	TYR
1	B	1512	PRO
1	C	2097	LYS
1	C	2104	ASN
1	C	2106	PRO
1	C	2303	THR
1	C	2367	PHE
1	C	2423	VAL
1	C	2458	MET
1	C	2531	LEU
1	C	2536	GLY
1	C	2549	THR
1	D	3120	ARG
1	D	3302	ALA
1	D	3423	VAL
1	D	3451	SER
1	D	3458	MET
1	D	3459	LYS
1	D	3512	PRO
1	D	3536	GLY
1	D	3549	THR
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	303	THR
1	A	373	TYR
1	A	423	VAL
1	A	447	VAL
1	A	506	ALA
1	B	1201	PHE
1	B	1303	THR
1	B	1309	HIS
1	B	1317	LYS
1	B	1367	PHE
1	B	1370	GLN
1	B	1445	GLN
1	B	1459	LYS
1	B	1531	LEU
1	B	1558	ILE
1	C	2370	GLN
1	C	2451	SER
1	C	2496	SER
1	D	3106	PRO
1	D	3201	PHE
1	D	3367	PHE
1	D	3445	GLN
1	D	3454	GLN
1	D	3528	PRO
1	D	3531	LEU
1	D	3558	ILE
1	A	201	PHE
1	A	309	HIS
1	A	445	GLN
1	A	454	GLN
1	A	496	SER
1	A	528	PRO
1	A	531	LEU
1	B	1212	THR
1	B	1284	GLN
1	B	1447	VAL
1	B	1454	GLN
1	B	1496	SER
1	B	1528	PRO
1	C	2037	CYS
1	C	2194	SER
1	C	2201	PHE

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Mol	Chain	Res	Type
1	C	2212	THR
1	C	2309	HIS
1	C	2373	TYR
1	C	2384	LEU
1	C	2445	GLN
1	C	2454	GLN
1	C	2528	PRO
1	D	3228	VAL
1	D	3303	THR
1	D	3309	HIS
1	D	3370	GLN
1	D	3373	TYR
1	D	3447	VAL
1	D	3496	SER
1	D	3554	VAL
1	A	212	THR
1	A	277	PRO
1	A	554	VAL
1	A	558	ILE
1	B	1132	VAL
1	B	1277	PRO
1	B	1554	VAL
1	C	2364	GLU
1	C	2447	VAL
1	C	2506	ALA
1	C	2558	ILE
1	C	2565	GLN
1	D	3277	PRO
1	D	3565	GLN
1	A	132	VAL
1	C	2128	PRO
1	C	2277	PRO
1	C	2554	VAL
1	B	1128	PRO
1	B	1430	ILE
1	C	2132	VAL
1	D	3132	VAL
1	A	430	ILE
1	A	505	PRO
1	B	1538	PRO
1	C	2505	PRO
1	D	3128	PRO

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Mol	Chain	Res	Type
1	D	3430	ILE
1	A	128	PRO
1	C	2538	PRO
1	D	3505	PRO
1	D	3538	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/493 (100%)	391 (79%)	102 (21%)	1	6
1	B	493/493 (100%)	391 (79%)	102 (21%)	1	6
1	C	493/493 (100%)	393 (80%)	100 (20%)	1	6
1	D	493/493 (100%)	394 (80%)	99 (20%)	1	6
All	All	1972/1972 (100%)	1569 (80%)	403 (20%)	1	6

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	48	MET
1	A	49	SER
1	A	54	GLN
1	A	65	TYR
1	A	70	THR
1	A	77	ARG
1	A	78	ILE
1	A	85	THR
1	A	89	VAL
1	A	90	HIS
1	A	92	ILE
1	A	93	LEU
1	A	107	PHE
1	A	111	LEU
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	119	SER
1	A	120	ARG
1	A	121	SER
1	A	124	ILE
1	A	130	TYR
1	A	136	TYR
1	A	137	LYS
1	A	138	SER
1	A	146	SER
1	A	158	ASP
1	A	161	THR
1	A	165	VAL
1	A	171	LEU
1	A	173	ASP
1	A	177	VAL
1	A	178	LEU
1	A	181	VAL
1	A	185	ARG
1	A	190	ASP
1	A	192	GLN
1	A	197	MET
1	A	203	GLN
1	A	207	HIS
1	A	209	PHE
1	A	215	LYS
1	A	221	THR
1	A	231	ASN
1	A	236	GLU
1	A	241	GLN
1	A	246	LEU
1	A	248	LYS
1	A	249	ASP
1	A	254	TYR
1	A	265	THR
1	A	268	ASP
1	A	274	ILE
1	A	289	GLN
1	A	298	LEU
1	A	300	MET
1	A	301	TYR
1	A	319	GLU
1	A	322	GLU

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Mol	Chain	Res	Type
1	A	326	GLU
1	A	334	LEU
1	A	337	ILE
1	A	353	SER
1	A	358	LYS
1	A	376	ARG
1	A	377	ILE
1	A	385	TYR
1	A	396	ASN
1	A	405	LYS
1	A	407	PHE
1	A	409	TYR
1	A	412	SER
1	A	416	GLU
1	A	419	LEU
1	A	420	THR
1	A	430	ILE
1	A	438	ARG
1	A	445	GLN
1	A	455	SER
1	A	457	GLU
1	A	462	SER
1	A	463	LEU
1	A	469	ARG
1	A	471	SER
1	A	482	THR
1	A	484	GLU
1	A	486	GLU
1	A	496	SER
1	A	501	MET
1	A	520	GLU
1	A	522	MET
1	A	524	GLU
1	A	525	LEU
1	A	531	LEU
1	A	532	LYS
1	A	534	LEU
1	A	535	MET
1	A	539	ILE
1	A	543	GLN
1	A	549	THR
1	A	569	CYS

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Mol	Chain	Res	Type
1	A	575	CYS
1	A	581	ASN
1	B	1046	GLU
1	B	1048	MET
1	B	1049	SER
1	B	1054	GLN
1	B	1065	TYR
1	B	1070	THR
1	B	1077	ARG
1	B	1078	ILE
1	B	1085	THR
1	B	1089	VAL
1	B	1090	HIS
1	B	1092	ILE
1	B	1093	LEU
1	B	1107	PHE
1	B	1111	LEU
1	B	1117	LEU
1	B	1119	SER
1	B	1120	ARG
1	B	1121	SER
1	B	1124	ILE
1	B	1130	TYR
1	B	1136	TYR
1	B	1137	LYS
1	B	1138	SER
1	B	1146	SER
1	B	1158	ASP
1	B	1161	THR
1	B	1165	VAL
1	B	1171	LEU
1	B	1173	ASP
1	B	1177	VAL
1	B	1178	LEU
1	B	1181	VAL
1	B	1185	ARG
1	B	1190	ASP
1	B	1192	GLN
1	B	1197	MET
1	B	1203	GLN
1	B	1207	HIS
1	B	1209	PHE

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Mol	Chain	Res	Type
1	B	1215	LYS
1	B	1221	THR
1	B	1231	ASN
1	B	1236	GLU
1	B	1241	GLN
1	B	1246	LEU
1	B	1248	LYS
1	B	1249	ASP
1	B	1252	LEU
1	B	1254	TYR
1	B	1257	ILE
1	B	1265	THR
1	B	1268	ASP
1	B	1274	ILE
1	B	1298	LEU
1	B	1300	MET
1	B	1301	TYR
1	B	1319	GLU
1	B	1322	GLU
1	B	1326	GLU
1	B	1334	LEU
1	B	1337	ILE
1	B	1353	SER
1	B	1358	LYS
1	B	1376	ARG
1	B	1377	ILE
1	B	1385	TYR
1	B	1396	ASN
1	B	1405	LYS
1	B	1407	PHE
1	B	1409	TYR
1	B	1412	SER
1	B	1416	GLU
1	B	1419	LEU
1	B	1420	THR
1	B	1422	PHE
1	B	1430	ILE
1	B	1438	ARG
1	B	1445	GLN
1	B	1455	SER
1	B	1457	GLU
1	B	1462	SER

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Mol	Chain	Res	Type
1	B	1463	LEU
1	B	1469	ARG
1	B	1471	SER
1	B	1482	THR
1	B	1484	GLU
1	B	1486	GLU
1	B	1496	SER
1	B	1501	MET
1	B	1520	GLU
1	B	1522	MET
1	B	1524	GLU
1	B	1525	LEU
1	B	1531	LEU
1	B	1532	LYS
1	B	1534	LEU
1	B	1535	MET
1	B	1539	ILE
1	B	1543	GLN
1	B	1549	THR
1	B	1581	ASN
1	C	2046	GLU
1	C	2048	MET
1	C	2049	SER
1	C	2054	GLN
1	C	2065	TYR
1	C	2070	THR
1	C	2077	ARG
1	C	2078	ILE
1	C	2085	THR
1	C	2089	VAL
1	C	2090	HIS
1	C	2092	ILE
1	C	2093	LEU
1	C	2107	PHE
1	C	2111	LEU
1	C	2117	LEU
1	C	2119	SER
1	C	2120	ARG
1	C	2121	SER
1	C	2124	ILE
1	C	2130	TYR
1	C	2136	TYR

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Mol	Chain	Res	Type
1	C	2137	LYS
1	C	2138	SER
1	C	2146	SER
1	C	2158	ASP
1	C	2161	THR
1	C	2165	VAL
1	C	2171	LEU
1	C	2173	ASP
1	C	2177	VAL
1	C	2178	LEU
1	C	2181	VAL
1	C	2185	ARG
1	C	2190	ASP
1	C	2192	GLN
1	C	2197	MET
1	C	2203	GLN
1	C	2207	HIS
1	C	2209	PHE
1	C	2215	LYS
1	C	2221	THR
1	C	2231	ASN
1	C	2236	GLU
1	C	2241	GLN
1	C	2246	LEU
1	C	2248	LYS
1	C	2249	ASP
1	C	2254	TYR
1	C	2257	ILE
1	C	2265	THR
1	C	2274	ILE
1	C	2289	GLN
1	C	2298	LEU
1	C	2300	MET
1	C	2319	GLU
1	C	2322	GLU
1	C	2326	GLU
1	C	2334	LEU
1	C	2337	ILE
1	C	2353	SER
1	C	2358	LYS
1	C	2376	ARG
1	C	2377	ILE

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Mol	Chain	Res	Type
1	C	2385	TYR
1	C	2396	ASN
1	C	2405	LYS
1	C	2407	PHE
1	C	2409	TYR
1	C	2412	SER
1	C	2416	GLU
1	C	2419	LEU
1	C	2420	THR
1	C	2430	ILE
1	C	2438	ARG
1	C	2445	GLN
1	C	2455	SER
1	C	2457	GLU
1	C	2462	SER
1	C	2463	LEU
1	C	2469	ARG
1	C	2471	SER
1	C	2482	THR
1	C	2484	GLU
1	C	2486	GLU
1	C	2496	SER
1	C	2501	MET
1	C	2520	GLU
1	C	2522	MET
1	C	2524	GLU
1	C	2525	LEU
1	C	2531	LEU
1	C	2532	LYS
1	C	2534	LEU
1	C	2535	MET
1	C	2539	ILE
1	C	2543	GLN
1	C	2549	THR
1	C	2569	CYS
1	C	2581	ASN
1	D	3046	GLU
1	D	3048	MET
1	D	3049	SER
1	D	3054	GLN
1	D	3065	TYR
1	D	3070	THR

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Mol	Chain	Res	Type
1	D	3077	ARG
1	D	3078	ILE
1	D	3085	THR
1	D	3089	VAL
1	D	3090	HIS
1	D	3092	ILE
1	D	3093	LEU
1	D	3107	PHE
1	D	3111	LEU
1	D	3117	LEU
1	D	3119	SER
1	D	3120	ARG
1	D	3121	SER
1	D	3124	ILE
1	D	3130	TYR
1	D	3136	TYR
1	D	3137	LYS
1	D	3138	SER
1	D	3146	SER
1	D	3158	ASP
1	D	3161	THR
1	D	3165	VAL
1	D	3171	LEU
1	D	3173	ASP
1	D	3178	LEU
1	D	3181	VAL
1	D	3185	ARG
1	D	3190	ASP
1	D	3192	GLN
1	D	3197	MET
1	D	3203	GLN
1	D	3207	HIS
1	D	3209	PHE
1	D	3215	LYS
1	D	3221	THR
1	D	3231	ASN
1	D	3236	GLU
1	D	3241	GLN
1	D	3246	LEU
1	D	3249	ASP
1	D	3254	TYR
1	D	3257	ILE

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Mol	Chain	Res	Type
1	D	3265	THR
1	D	3274	ILE
1	D	3289	GLN
1	D	3298	LEU
1	D	3300	MET
1	D	3301	TYR
1	D	3319	GLU
1	D	3322	GLU
1	D	3326	GLU
1	D	3334	LEU
1	D	3337	ILE
1	D	3353	SER
1	D	3358	LYS
1	D	3376	ARG
1	D	3377	ILE
1	D	3385	TYR
1	D	3396	ASN
1	D	3405	LYS
1	D	3407	PHE
1	D	3409	TYR
1	D	3412	SER
1	D	3416	GLU
1	D	3419	LEU
1	D	3420	THR
1	D	3430	ILE
1	D	3438	ARG
1	D	3445	GLN
1	D	3455	SER
1	D	3457	GLU
1	D	3462	SER
1	D	3463	LEU
1	D	3469	ARG
1	D	3471	SER
1	D	3482	THR
1	D	3484	GLU
1	D	3486	GLU
1	D	3496	SER
1	D	3501	MET
1	D	3520	GLU
1	D	3522	MET
1	D	3524	GLU
1	D	3525	LEU

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Mol	Chain	Res	Type
1	D	3531	LEU
1	D	3532	LYS
1	D	3534	LEU
1	D	3535	MET
1	D	3539	ILE
1	D	3543	GLN
1	D	3549	THR
1	D	3569	CYS
1	D	3581	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	207	HIS
1	A	208	GLN
1	A	320	HIS
1	A	327	GLN
1	A	350	GLN
1	A	372	GLN
1	A	374	GLN
1	A	388	HIS
1	A	396	ASN
1	A	411	ASN
1	A	417	HIS
1	A	560	ASN
1	A	565	GLN
1	A	571	ASN
1	A	581	ASN
1	B	1204	HIS
1	B	1208	GLN
1	B	1320	HIS
1	B	1327	GLN
1	B	1350	GLN
1	B	1356	HIS
1	B	1372	GLN
1	B	1374	GLN
1	B	1396	ASN
1	B	1411	ASN
1	B	1560	ASN
1	B	1565	GLN
1	B	1571	ASN

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Mol	Chain	Res	Type
1	B	1581	ASN
1	C	2043	ASN
1	C	2208	GLN
1	C	2320	HIS
1	C	2327	GLN
1	C	2350	GLN
1	C	2396	ASN
1	C	2411	ASN
1	C	2417	HIS
1	C	2464	ASN
1	C	2560	ASN
1	C	2565	GLN
1	C	2571	ASN
1	C	2581	ASN
1	D	3204	HIS
1	D	3208	GLN
1	D	3320	HIS
1	D	3327	GLN
1	D	3350	GLN
1	D	3372	GLN
1	D	3374	GLN
1	D	3388	HIS
1	D	3396	ASN
1	D	3411	ASN
1	D	3417	HIS
1	D	3464	ASN
1	D	3560	ASN
1	D	3565	GLN
1	D	3571	ASN
1	D	3581	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates i

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	0.68	0	17,19,21	0.66	0
2	NAG	E	2	2	14,14,15	0.78	0	17,19,21	0.50	0
2	NAG	F	1	1,2	14,14,15	0.88	0	17,19,21	0.72	0
2	NAG	F	2	2	14,14,15	0.91	0	17,19,21	0.52	0
2	NAG	G	1	1,2	14,14,15	0.66	0	17,19,21	0.68	0
2	NAG	G	2	2	14,14,15	0.78	0	17,19,21	0.50	0
2	NAG	H	1	1,2	14,14,15	0.75	0	17,19,21	0.67	0
2	NAG	H	2	2	14,14,15	0.82	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

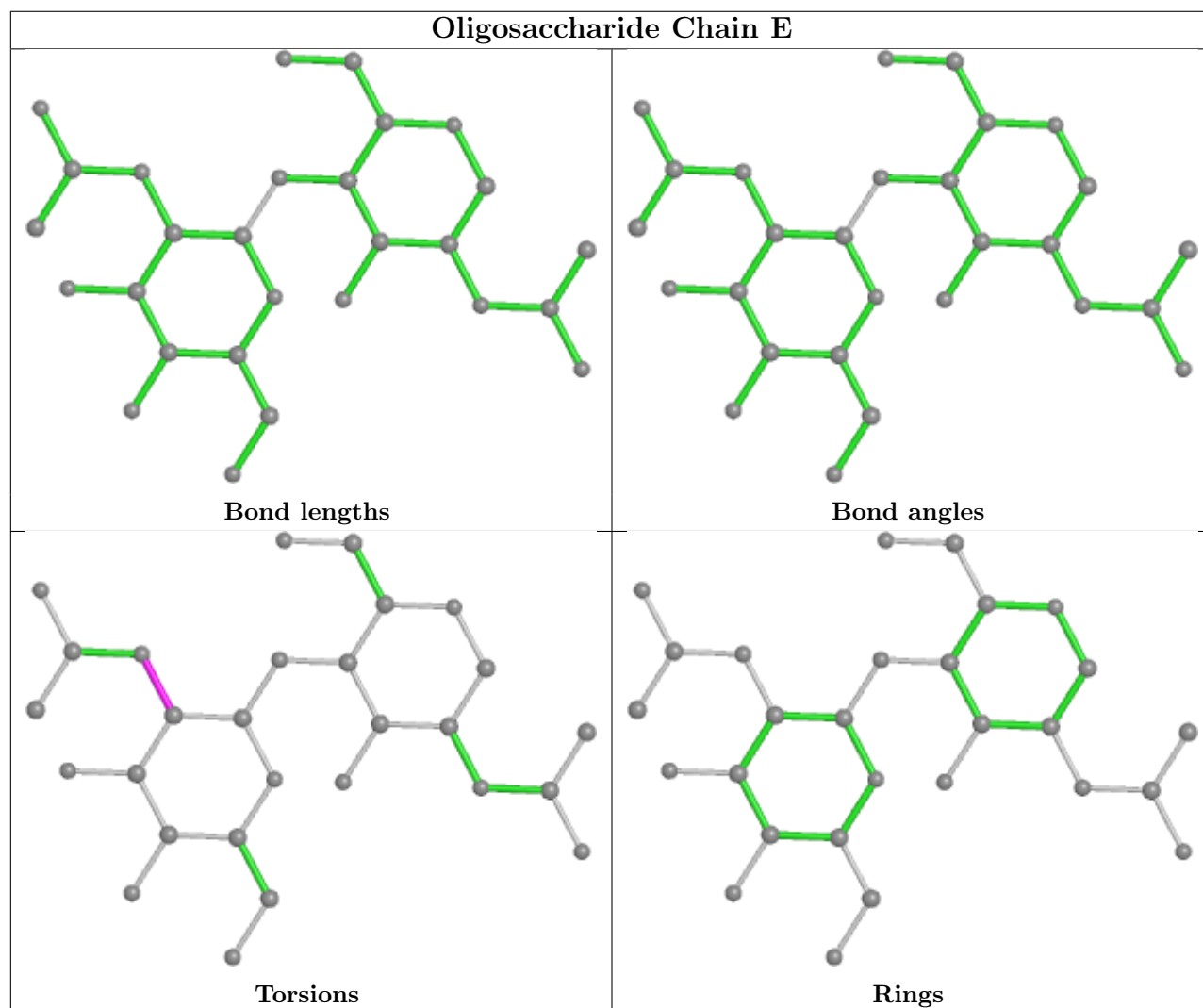
All (4) torsion outliers are listed below:

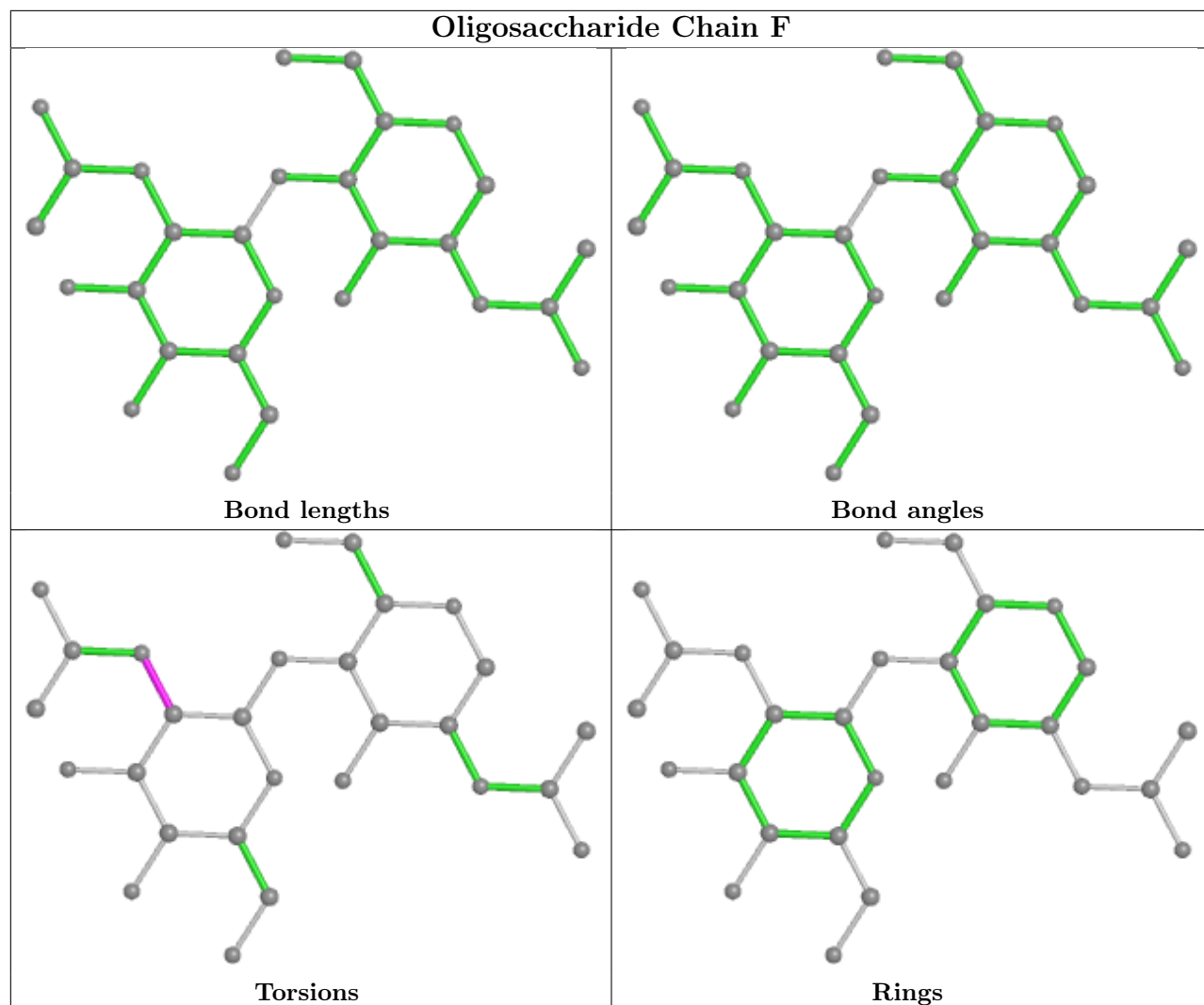
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7

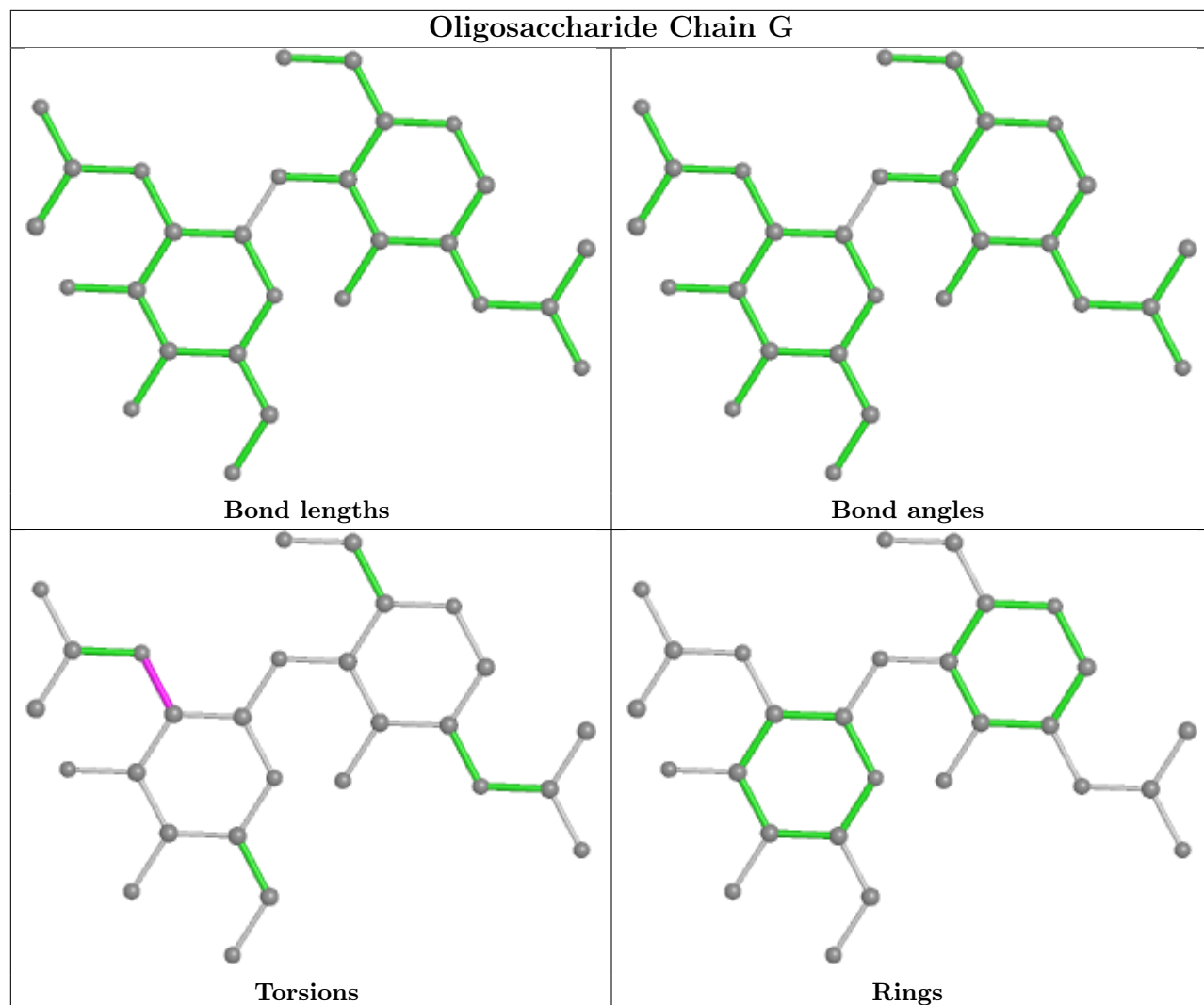
There are no ring outliers.

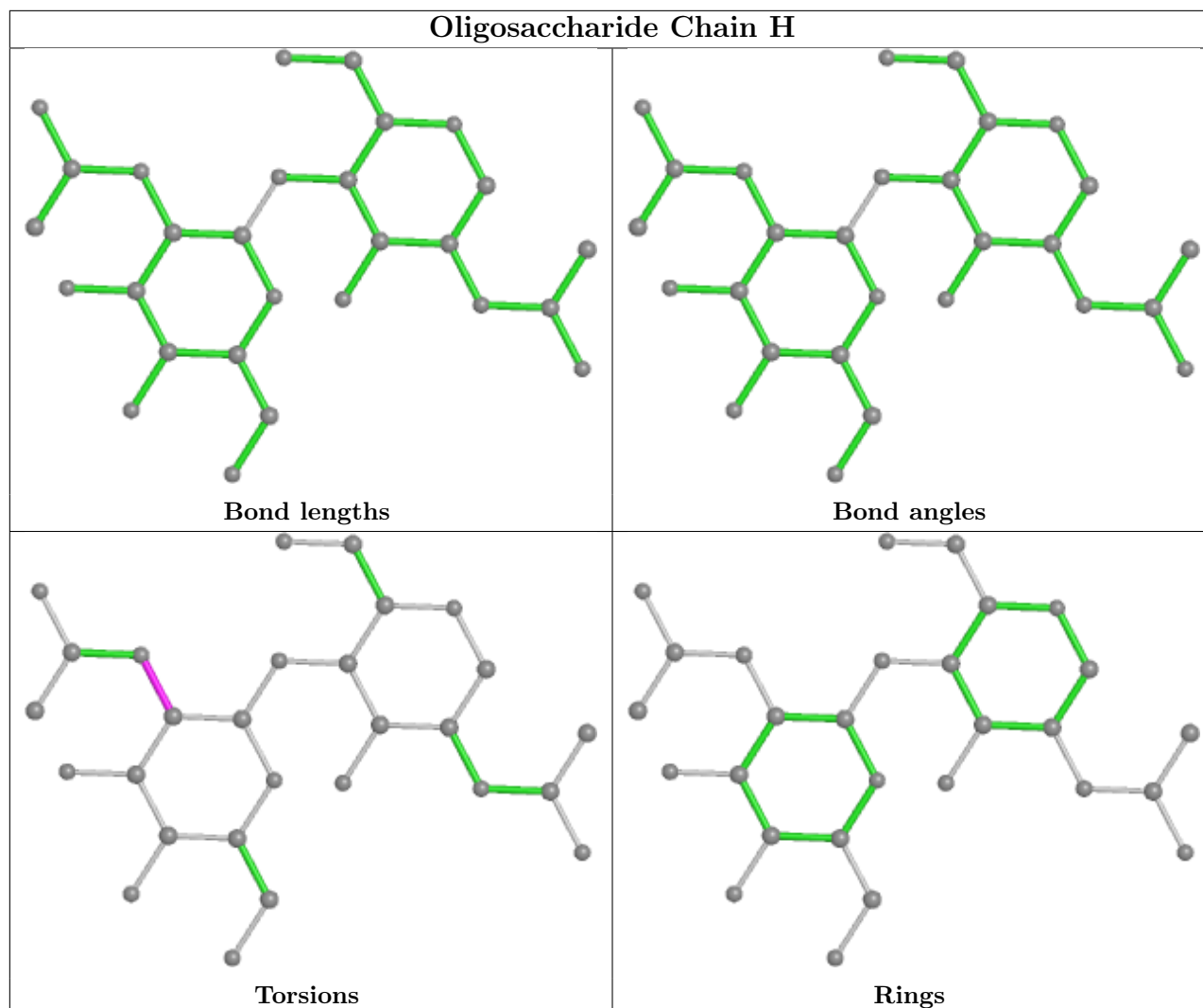
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	3671	1	14,14,15	0.60	0	17,19,21	0.97	1 (5%)
5	PGX	A	701	-	24,26,27	1.48	2 (8%)	24,33,34	1.49	1 (4%)
3	NAG	C	2671	1	14,14,15	0.70	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	3681	1	14,14,15	0.61	0	17,19,21	0.49	0
4	BOG	A	702	-	20,20,20	0.90	2 (10%)	25,25,25	0.61	0
4	BOG	B	1702	-	20,20,20	0.87	2 (10%)	25,25,25	0.62	0
3	NAG	B	1671	1	14,14,15	0.56	0	17,19,21	0.87	1 (5%)
3	NAG	B	1681	1	14,14,15	0.67	0	17,19,21	0.62	0
3	NAG	A	671	1	14,14,15	0.69	0	17,19,21	1.09	2 (11%)
4	BOG	D	3702	-	20,20,20	0.89	2 (10%)	25,25,25	0.59	0
4	BOG	C	2702	-	20,20,20	0.97	2 (10%)	25,25,25	0.60	0
3	NAG	C	2681	1	14,14,15	0.70	0	17,19,21	0.60	0
5	PGX	B	1701	-	24,26,27	1.49	2 (8%)	24,33,34	1.48	1 (4%)
5	PGX	D	3701	-	24,26,27	1.47	2 (8%)	24,33,34	1.49	1 (4%)
5	PGX	C	2701	-	24,26,27	1.44	1 (4%)	24,33,34	1.47	1 (4%)
3	NAG	A	681	1	14,14,15	0.69	0	17,19,21	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	3671	1	-	2/6/23/26	0/1/1/1
5	PGX	A	701	-	-	11/19/40/42	0/2/2/2
3	NAG	C	2671	1	-	2/6/23/26	0/1/1/1
3	NAG	D	3681	1	-	2/6/23/26	0/1/1/1
4	BOG	A	702	-	-	2/11/31/31	0/1/1/1
4	BOG	B	1702	-	-	2/11/31/31	0/1/1/1
3	NAG	B	1671	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1681	1	-	2/6/23/26	0/1/1/1
3	NAG	A	671	1	-	2/6/23/26	0/1/1/1
4	BOG	D	3702	-	-	2/11/31/31	0/1/1/1
4	BOG	C	2702	-	-	2/11/31/31	0/1/1/1
3	NAG	C	2681	1	-	2/6/23/26	0/1/1/1
5	PGX	B	1701	-	-	11/19/40/42	0/2/2/2
5	PGX	D	3701	-	-	11/19/40/42	0/2/2/2
5	PGX	C	2701	-	-	11/19/40/42	0/2/2/2
3	NAG	A	681	1	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1701	PGX	O4-O3	-5.54	1.24	1.46
5	D	3701	PGX	O4-O3	-5.50	1.24	1.46
5	C	2701	PGX	O4-O3	-5.50	1.24	1.46
5	A	701	PGX	O4-O3	-5.42	1.24	1.46
4	C	2702	BOG	O1-C1	2.84	1.45	1.40
4	A	702	BOG	O1-C1	2.28	1.44	1.40
4	D	3702	BOG	O1-C1	2.28	1.44	1.40
5	A	701	PGX	C8-C9	2.24	1.57	1.53
4	B	1702	BOG	O5-C1	2.22	1.47	1.41
4	B	1702	BOG	O1-C1	2.20	1.43	1.40
4	A	702	BOG	O5-C1	2.15	1.47	1.41
5	D	3701	PGX	C8-C9	2.12	1.57	1.53
4	C	2702	BOG	O5-C1	2.08	1.47	1.41
5	B	1701	PGX	C8-C9	2.03	1.57	1.53
4	D	3702	BOG	O5-C1	2.02	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3701	PGX	C11-C10-C9	-6.25	85.67	103.73
5	A	701	PGX	C11-C10-C9	-6.19	85.86	103.73
5	B	1701	PGX	C11-C10-C9	-6.16	85.95	103.73
5	C	2701	PGX	C11-C10-C9	-6.15	85.99	103.73
3	A	671	NAG	C2-N2-C7	-2.68	119.09	122.90
3	C	2671	NAG	C2-N2-C7	-2.38	119.51	122.90
3	D	3671	NAG	C1-O5-C5	2.35	115.38	112.19
3	A	671	NAG	C1-O5-C5	2.29	115.30	112.19
3	B	1671	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	PGX	C6-C7-C8-C12
5	A	701	PGX	C8-C12-C13-C14
5	A	701	PGX	C11-C12-C13-C14
5	A	701	PGX	C14-C15-C16-C17
5	A	701	PGX	O5-C15-C16-C17
5	B	1701	PGX	C6-C7-C8-C12
5	B	1701	PGX	C8-C12-C13-C14
5	B	1701	PGX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	B	1701	PGX	C14-C15-C16-C17
5	B	1701	PGX	O5-C15-C16-C17
5	C	2701	PGX	C6-C7-C8-C12
5	C	2701	PGX	C8-C12-C13-C14
5	C	2701	PGX	C11-C12-C13-C14
5	C	2701	PGX	C14-C15-C16-C17
5	C	2701	PGX	O5-C15-C16-C17
5	D	3701	PGX	C6-C7-C8-C12
5	D	3701	PGX	C8-C12-C13-C14
5	D	3701	PGX	C11-C12-C13-C14
5	D	3701	PGX	C14-C15-C16-C17
5	D	3701	PGX	O5-C15-C16-C17
3	C	2671	NAG	O5-C5-C6-O6
3	A	671	NAG	O5-C5-C6-O6
3	B	1671	NAG	O5-C5-C6-O6
4	B	1702	BOG	C4-C5-C6-O6
4	D	3702	BOG	C4-C5-C6-O6
3	C	2671	NAG	C4-C5-C6-O6
3	A	671	NAG	C4-C5-C6-O6
3	B	1671	NAG	C4-C5-C6-O6
4	A	702	BOG	C4-C5-C6-O6
3	D	3671	NAG	O5-C5-C6-O6
4	B	1702	BOG	O5-C5-C6-O6
5	A	701	PGX	C1-C2-C3-C4
5	B	1701	PGX	C1-C2-C3-C4
5	C	2701	PGX	C1-C2-C3-C4
5	D	3701	PGX	C1-C2-C3-C4
4	D	3702	BOG	O5-C5-C6-O6
3	D	3671	NAG	C4-C5-C6-O6
4	C	2702	BOG	C4-C5-C6-O6
4	A	702	BOG	O5-C5-C6-O6
4	C	2702	BOG	O5-C5-C6-O6
3	C	2681	NAG	C4-C5-C6-O6
5	A	701	PGX	C6-C7-C8-C9
5	B	1701	PGX	C6-C7-C8-C9
5	C	2701	PGX	C6-C7-C8-C9
5	D	3701	PGX	C6-C7-C8-C9
5	A	701	PGX	C13-C14-C15-C16
5	C	2701	PGX	C13-C14-C15-C16
5	D	3701	PGX	C13-C14-C15-C16
3	C	2681	NAG	O5-C5-C6-O6
3	A	681	NAG	C4-C5-C6-O6

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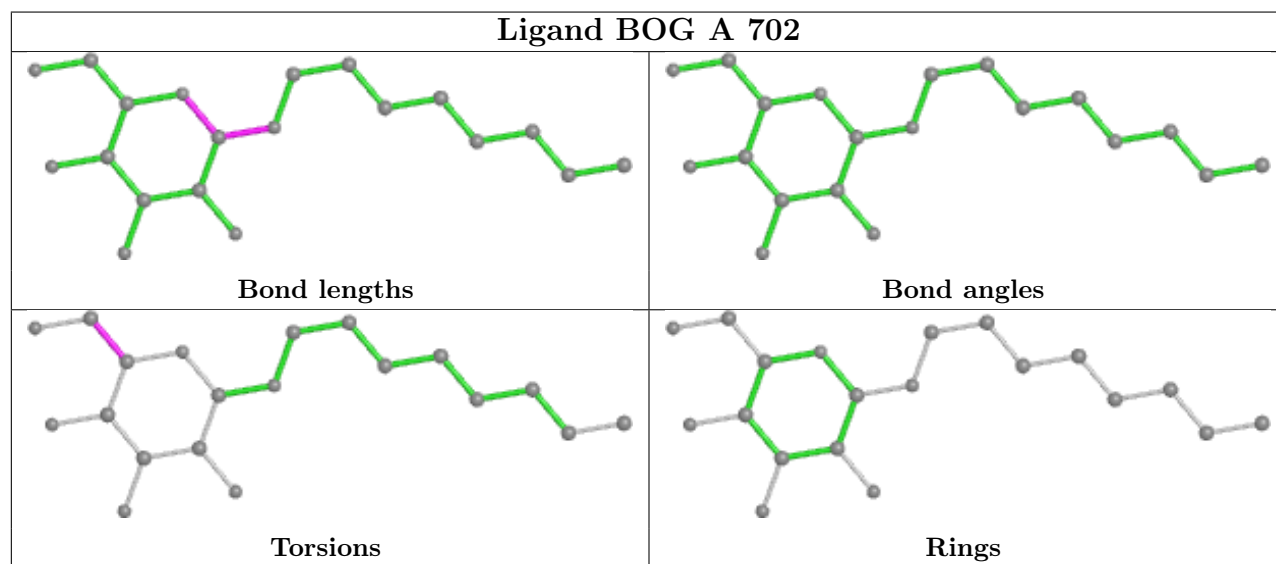
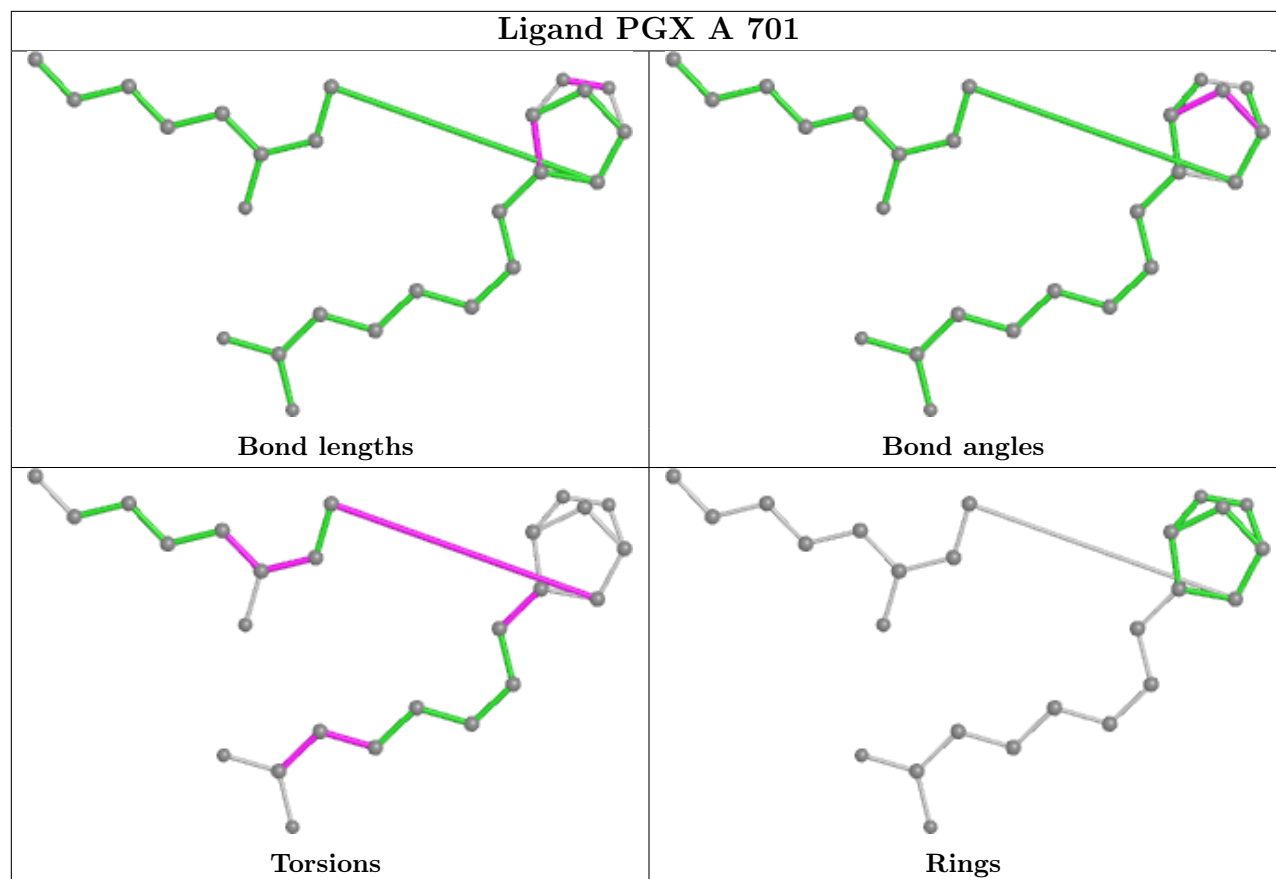
Mol	Chain	Res	Type	Atoms
3	B	1681	NAG	C4-C5-C6-O6
3	A	681	NAG	O5-C5-C6-O6
3	D	3681	NAG	C4-C5-C6-O6
5	A	701	PGX	C13-C14-C15-O5
5	B	1701	PGX	C13-C14-C15-O5
5	C	2701	PGX	C13-C14-C15-O5
5	D	3701	PGX	C13-C14-C15-O5
5	B	1701	PGX	C13-C14-C15-C16
3	B	1681	NAG	O5-C5-C6-O6
5	D	3701	PGX	O1-C1-C2-C3
5	A	701	PGX	O1-C1-C2-C3
5	B	1701	PGX	O1-C1-C2-C3
5	C	2701	PGX	O1-C1-C2-C3
5	A	701	PGX	O2-C1-C2-C3
5	B	1701	PGX	O2-C1-C2-C3
5	C	2701	PGX	O2-C1-C2-C3
3	D	3681	NAG	O5-C5-C6-O6
5	D	3701	PGX	O2-C1-C2-C3

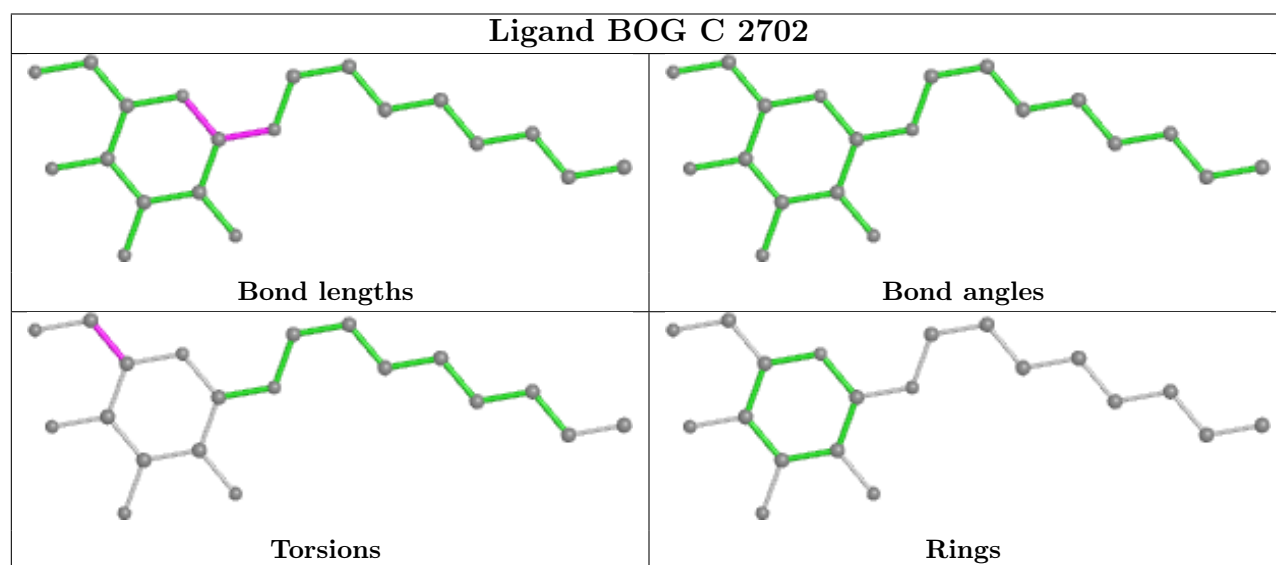
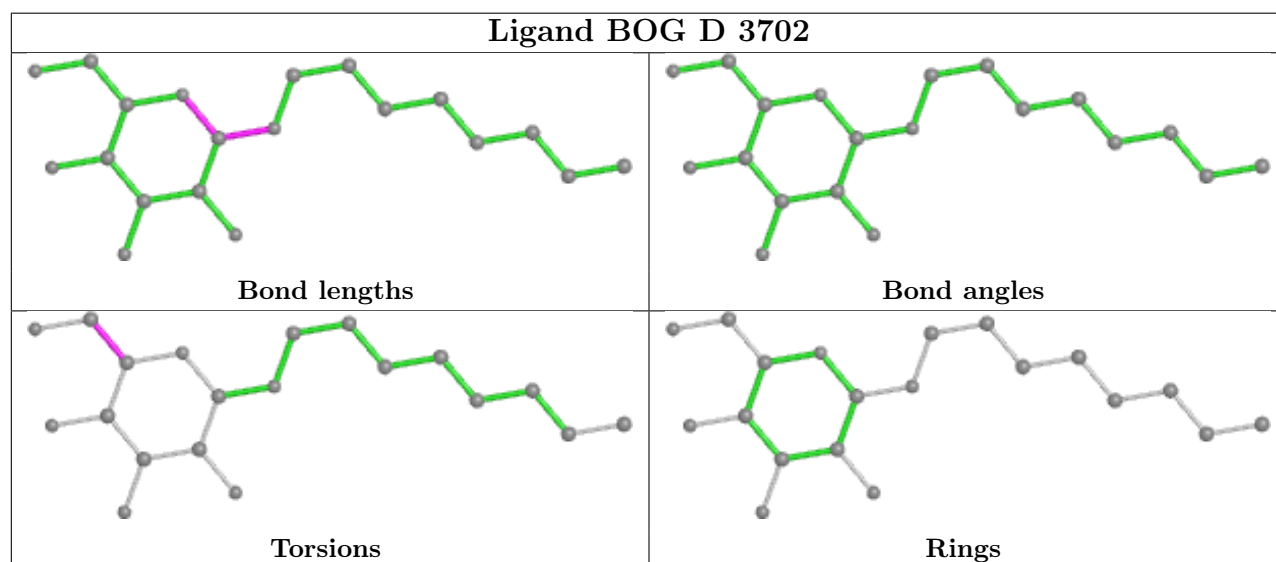
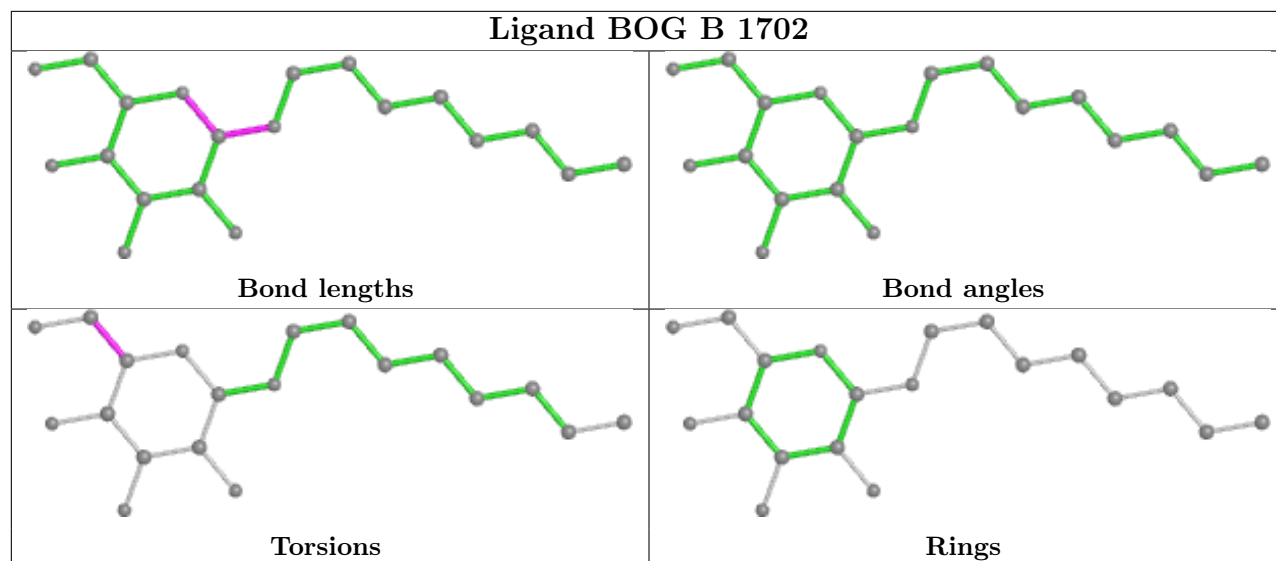
There are no ring outliers.

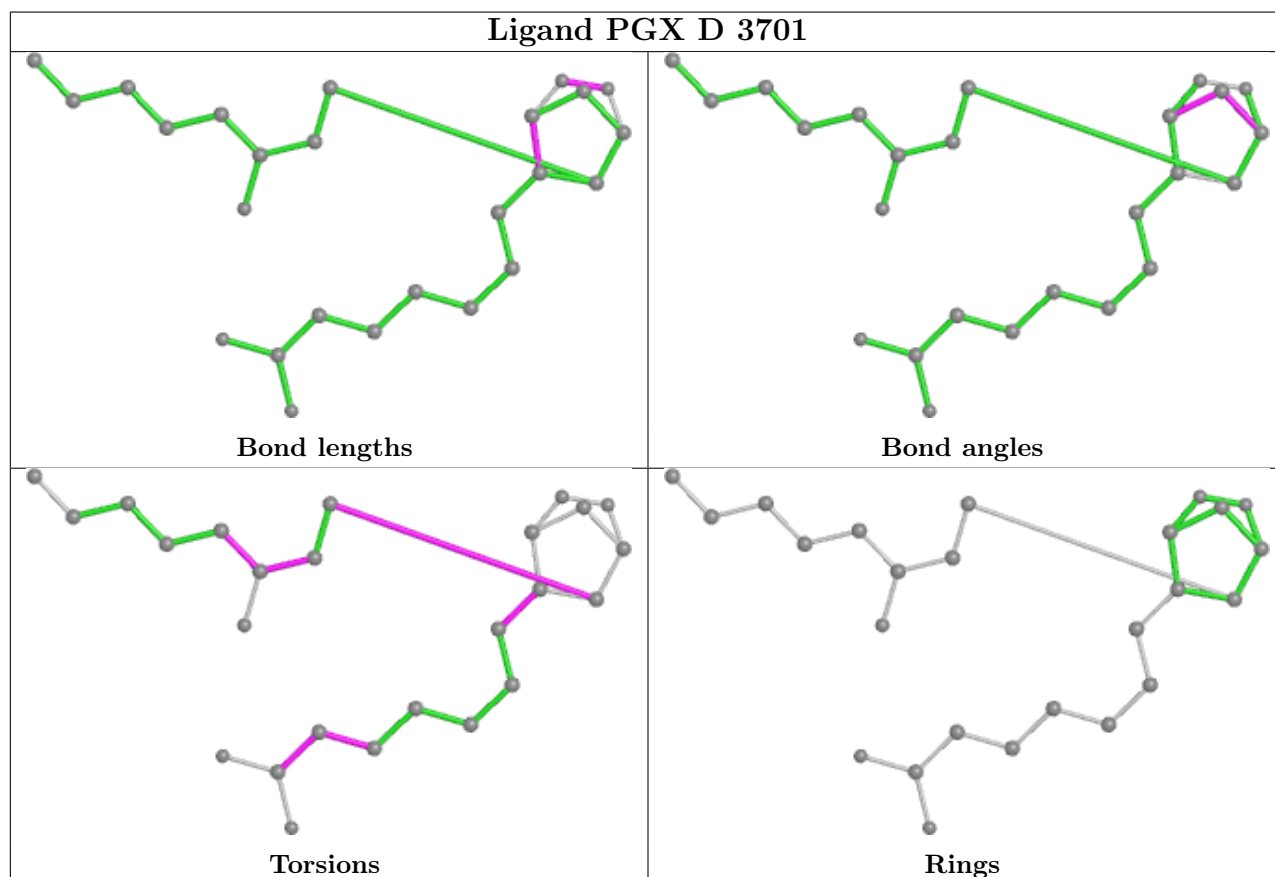
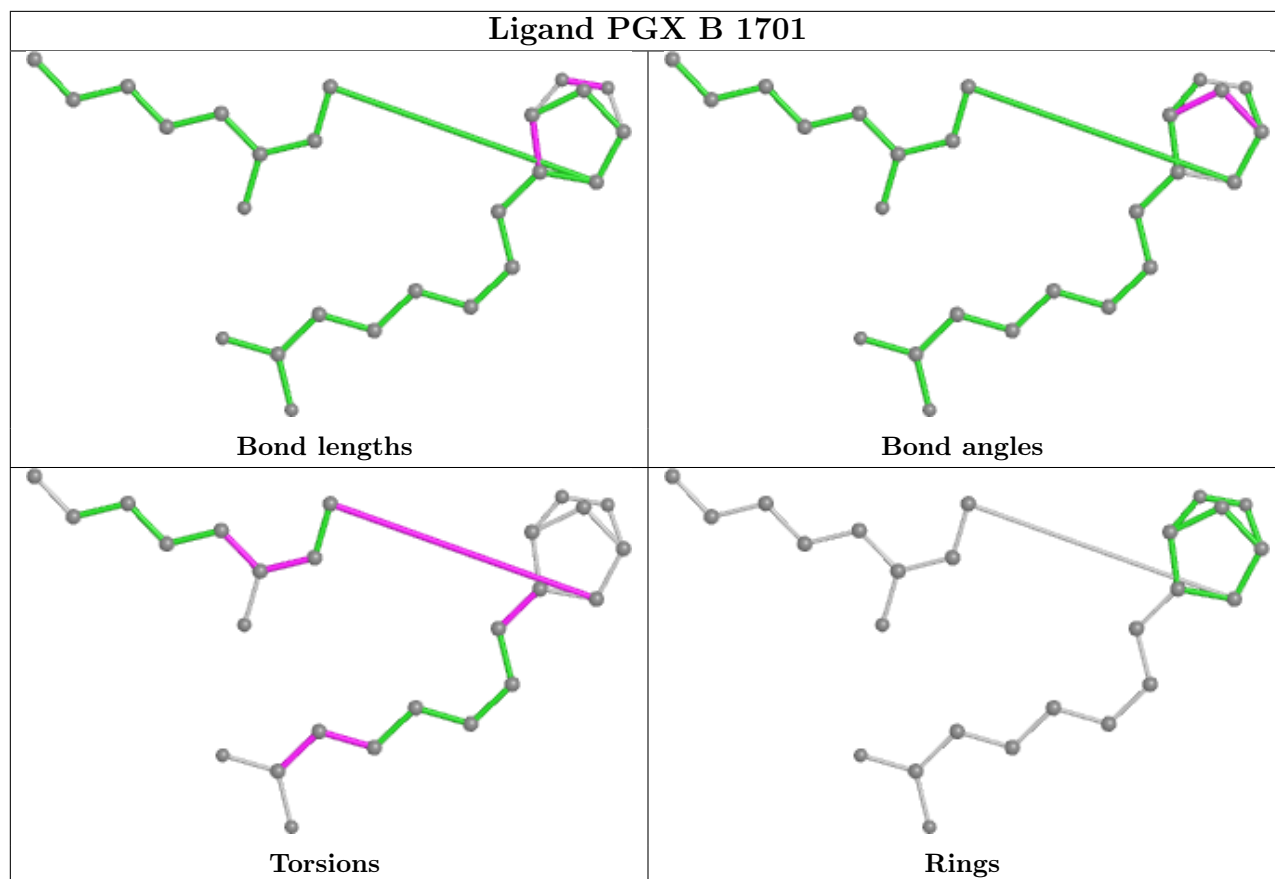
5 monomers are involved in 48 short contacts:

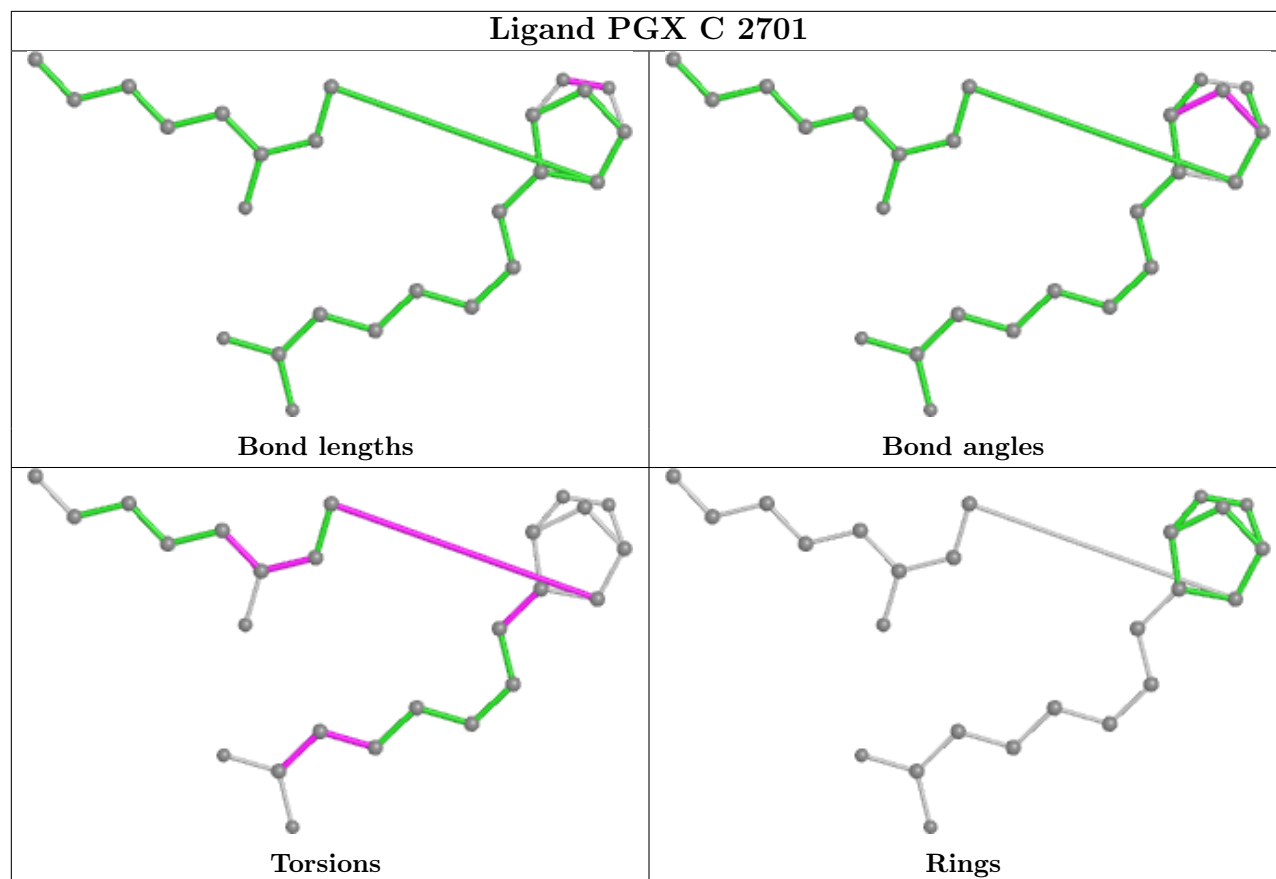
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	PGX	9	0
4	D	3702	BOG	1	0
5	B	1701	PGX	13	0
5	D	3701	PGX	11	0
5	C	2701	PGX	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/552 (100%)	-0.19	2 (0%) 92 79	2, 25, 52, 71	0
1	B	552/552 (100%)	-0.13	5 (0%) 84 63	3, 25, 51, 70	0
1	C	552/552 (100%)	-0.20	2 (0%) 92 79	2, 25, 51, 70	0
1	D	552/552 (100%)	-0.14	3 (0%) 91 75	3, 25, 51, 70	0
All	All	2208/2208 (100%)	-0.17	12 (0%) 91 75	2, 25, 51, 71	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ASN	3.1
1	B	1103	VAL	3.1
1	D	3105(D)	ILE	3.1
1	C	2083	LYS	2.9
1	B	1102	ILE	2.9
1	B	1105	ASN	2.7
1	D	3583	GLN	2.4
1	B	1095	HIS	2.2
1	A	276	PRO	2.1
1	B	1105(B)	ILE	2.1
1	C	2357	PHE	2.1
1	D	3496	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

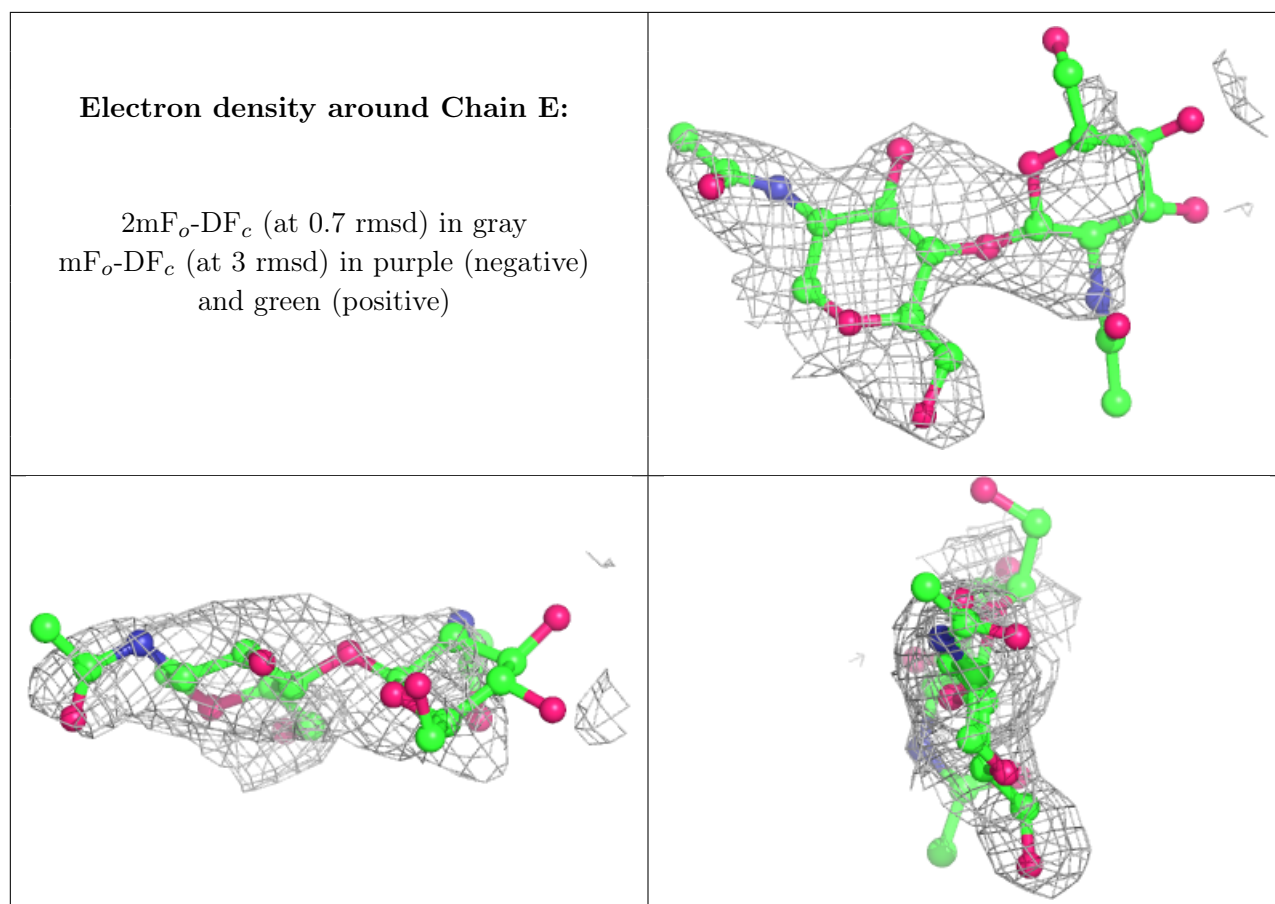
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

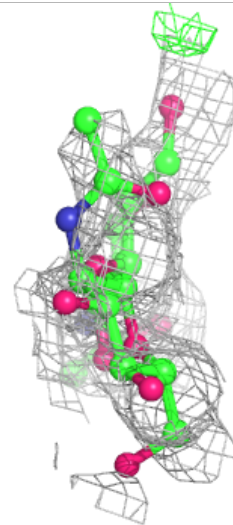
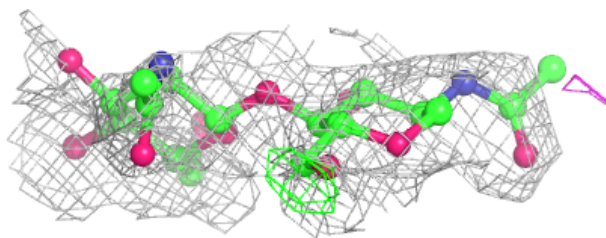
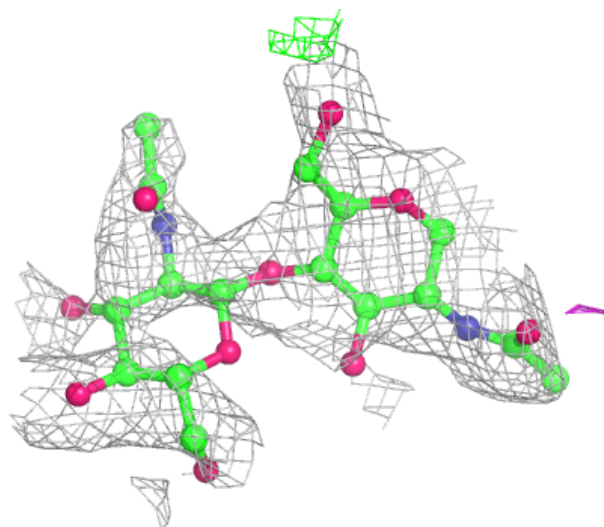
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.55	0.47	78,81,84,84	0
2	NAG	H	2	14/15	0.56	0.48	77,80,85,86	0
2	NAG	G	2	14/15	0.60	0.50	78,81,85,85	0
2	NAG	E	2	14/15	0.68	0.63	77,81,84,84	0
2	NAG	F	1	14/15	0.79	0.34	52,60,67,74	0
2	NAG	E	1	14/15	0.83	0.38	52,59,65,72	0
2	NAG	H	1	14/15	0.84	0.36	51,62,66,71	0
2	NAG	G	1	14/15	0.86	0.24	51,59,64,72	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



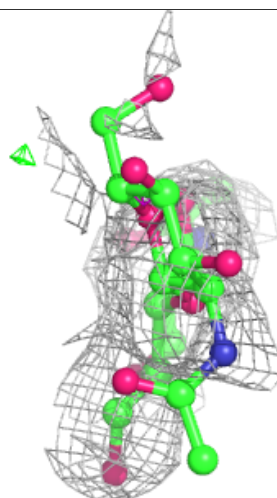
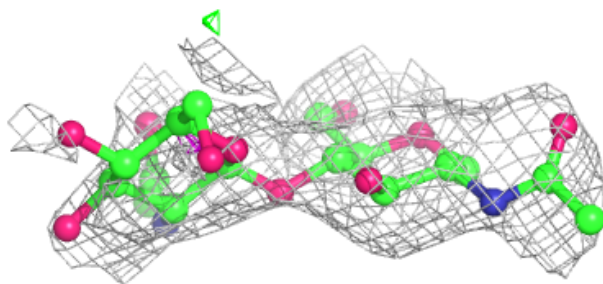
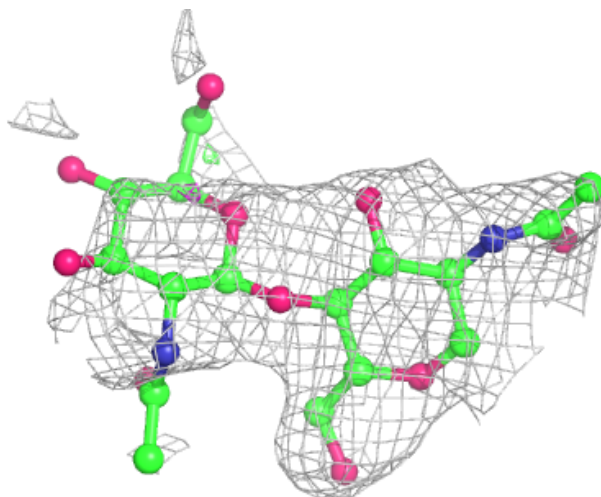
Electron density around Chain F:

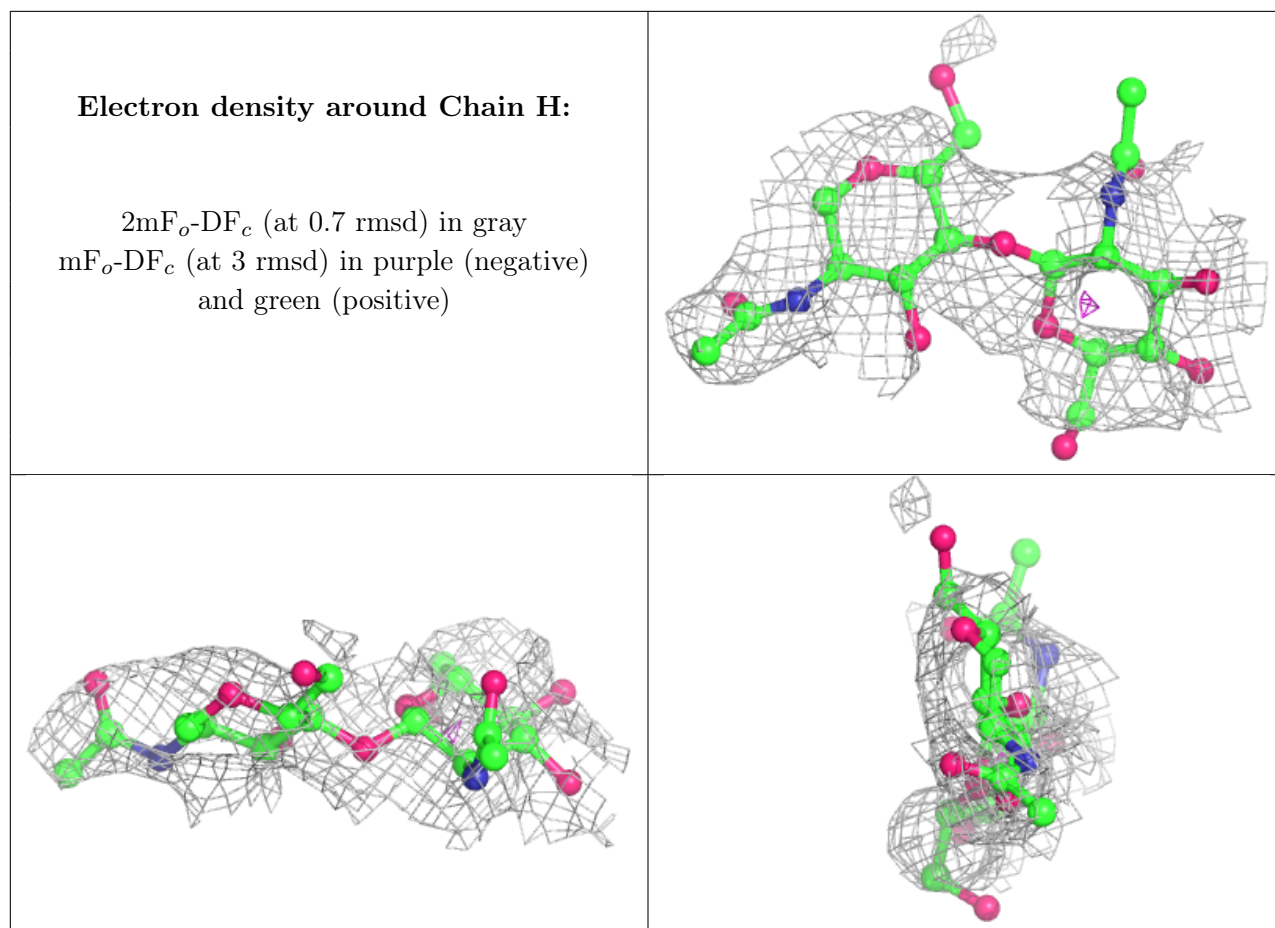
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

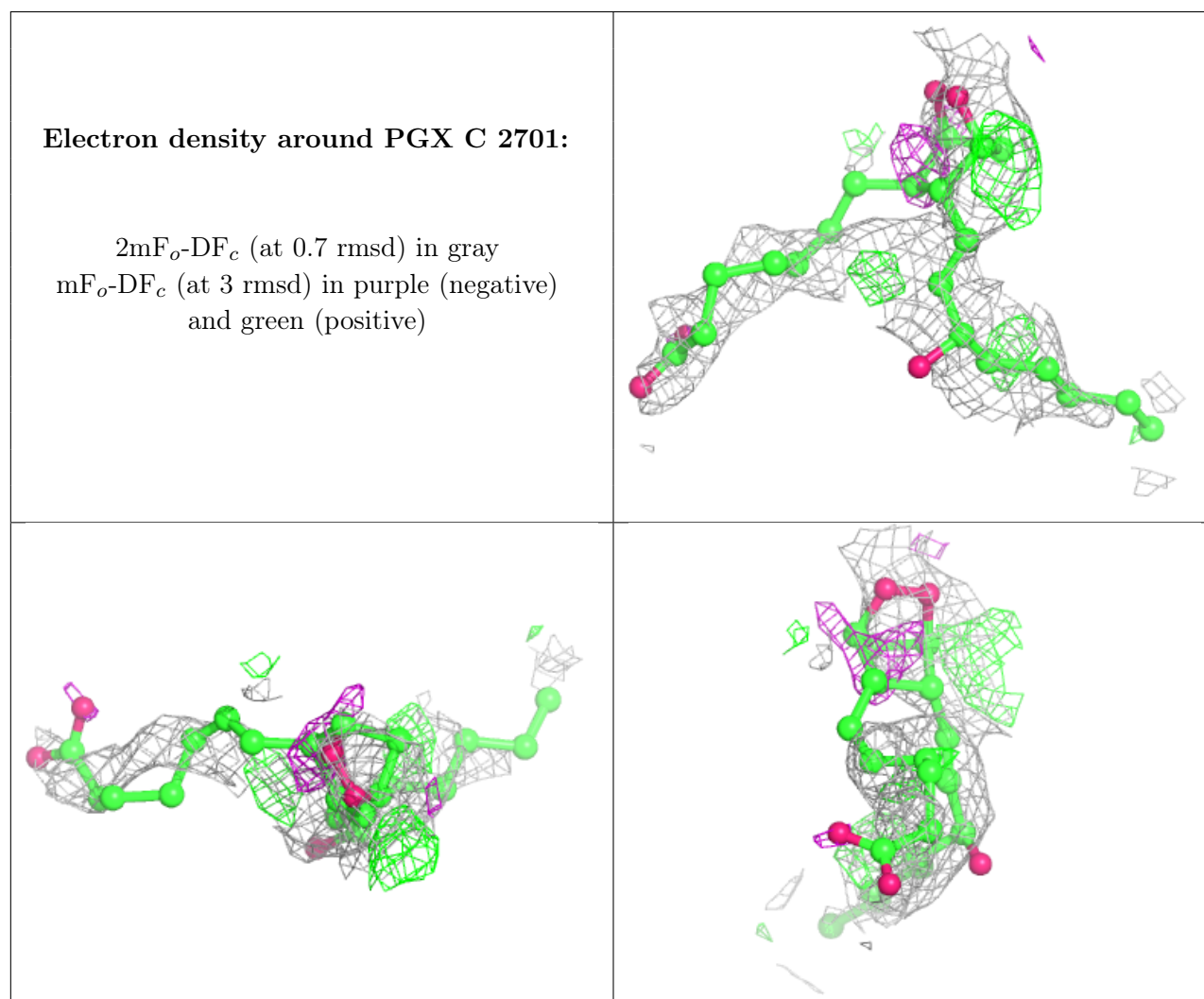
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2681	14/15	0.53	0.54	66,69,73,73	0
5	PGX	C	2701	25/26	0.63	0.53	75,79,84,84	0
5	PGX	B	1701	25/26	0.67	0.49	72,78,84,85	0
3	NAG	A	681	14/15	0.70	0.40	67,70,73,74	0
5	PGX	D	3701	25/26	0.71	0.43	74,78,86,87	0
5	PGX	A	701	25/26	0.72	0.48	73,78,86,87	0
3	NAG	B	1681	14/15	0.75	0.38	66,71,73,75	0
4	BOG	D	3702	20/20	0.75	0.42	46,53,59,62	0
4	BOG	C	2702	20/20	0.76	0.48	56,60,64,66	0
4	BOG	A	702	20/20	0.76	0.55	54,58,62,65	0
4	BOG	B	1702	20/20	0.79	0.39	50,54,59,59	0
3	NAG	D	3681	14/15	0.84	0.28	66,70,72,73	0

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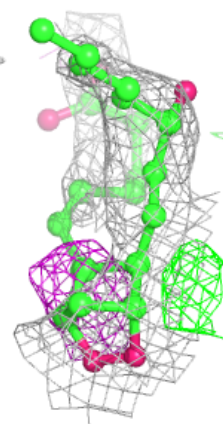
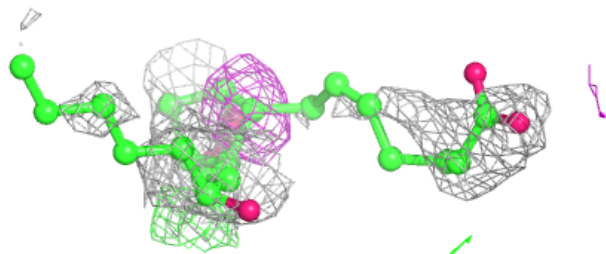
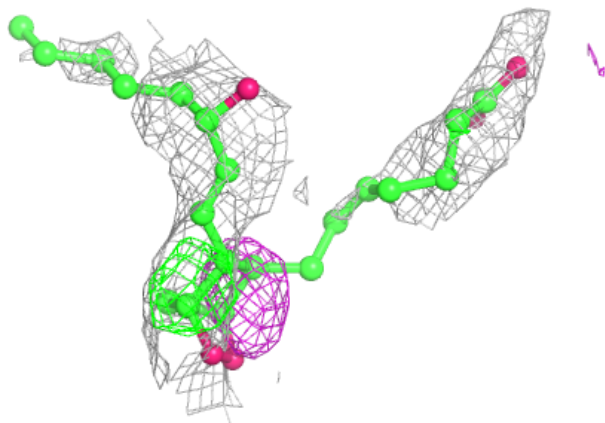
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	C	2671	14/15	0.86	0.18	7,10,25,28	0
3	NAG	A	671	14/15	0.89	0.18	2,9,25,27	0
3	NAG	B	1671	14/15	0.89	0.18	5,10,25,26	0
3	NAG	D	3671	14/15	0.91	0.14	2,9,23,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



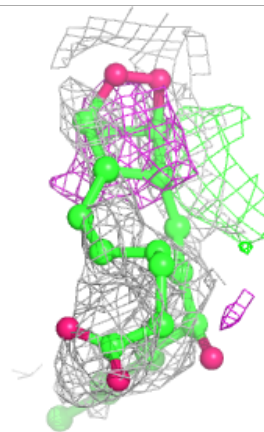
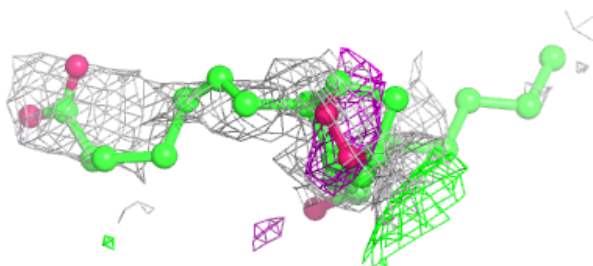
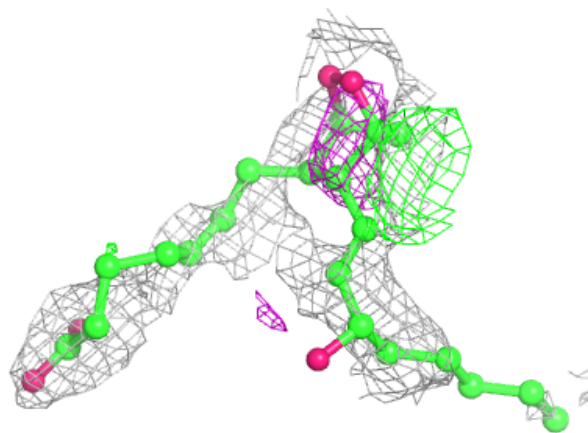
Electron density around PGX B 1701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



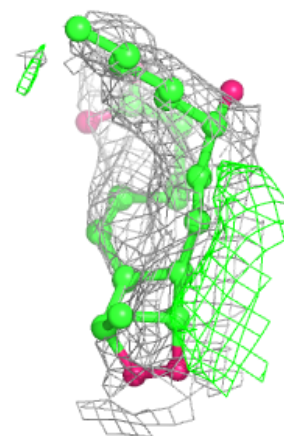
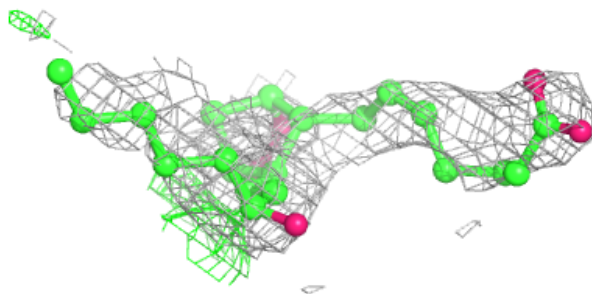
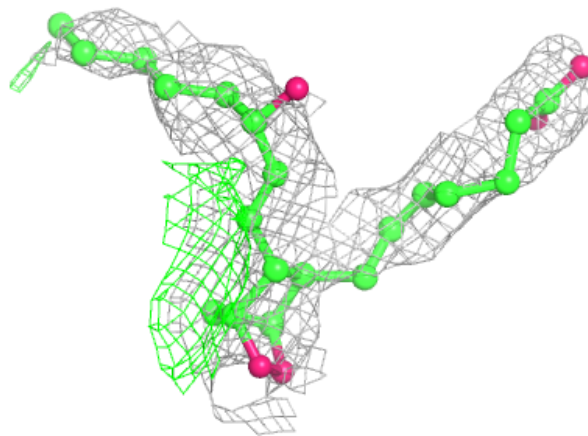
Electron density around PGX D 3701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



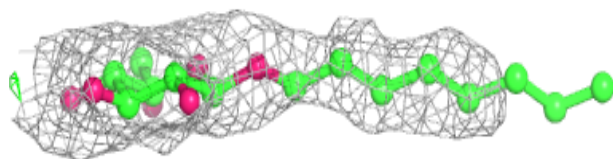
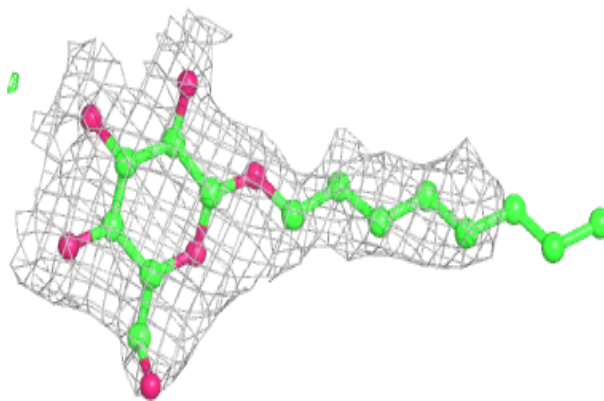
Electron density around PGX A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

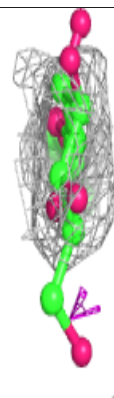
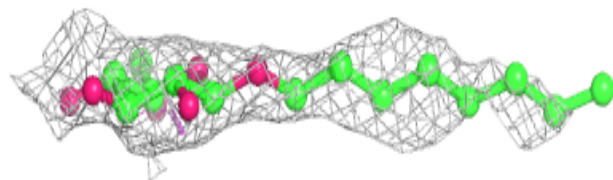
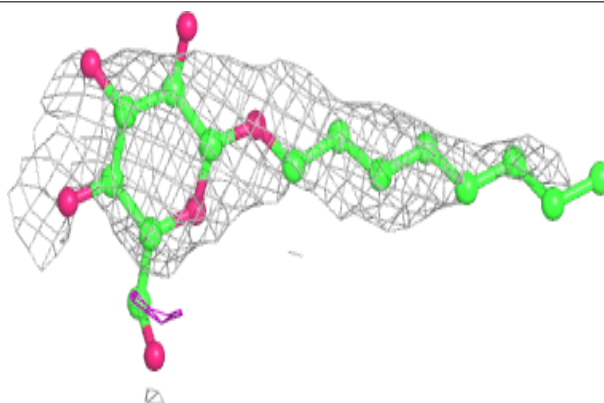


Electron density around BOG D 3702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

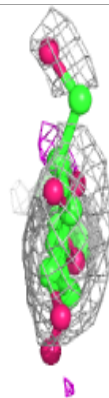
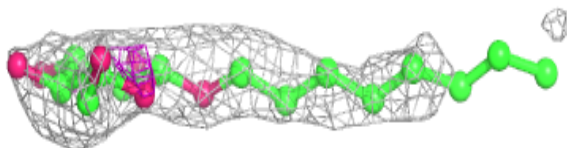
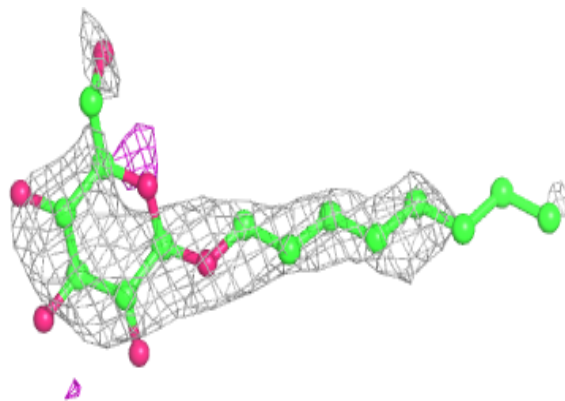
**Electron density around BOG C 2702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

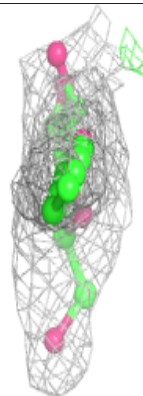
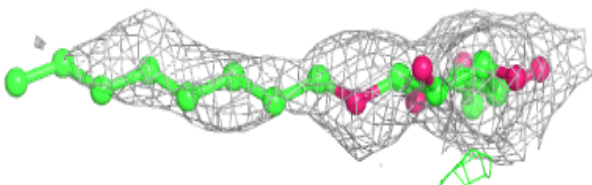
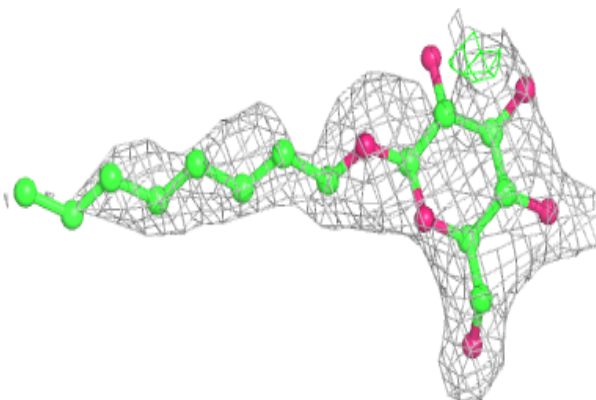


Electron density around BOG A 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BOG B 1702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.