



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 07:16 AM EDT

PDB ID : 3O8L  
Title : Structure of phosphofructokinase from rabbit skeletal muscle  
Authors : Banaszak, K.; Chang, S.H.; Rypniewski, W.  
Deposited on : 2010-08-03  
Resolution : 3.20 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](mailto: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>.

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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 : 2.35  
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)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

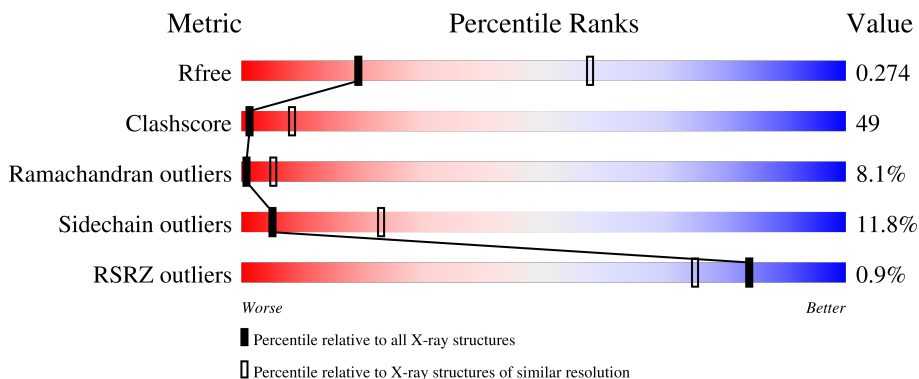
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	762	
1	B	762	

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
4	PO4	A	766	-	X	-	-
4	PO4	A	767	-	X	-	-
4	PO4	A	768	-	X	-	-
4	PO4	B	766	-	X	-	-
4	PO4	B	767	-	X	-	-
4	PO4	B	768	-	X	-	-

## 2 Entry composition [i](#)

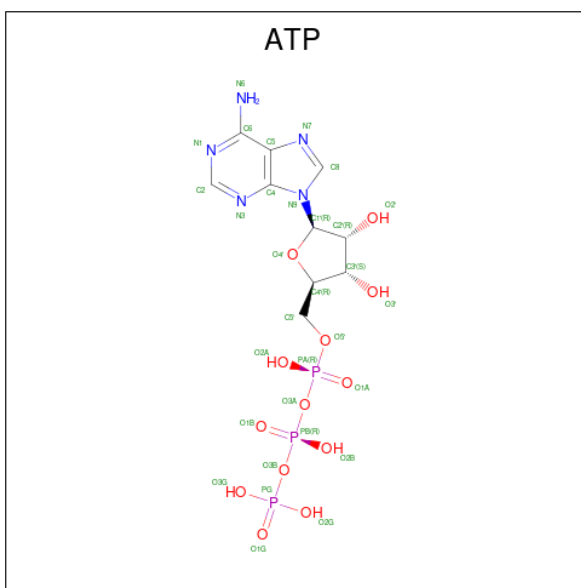
There are 4 unique types of molecules in this entry. The entry contains 11646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-phosphofructokinase, muscle type.

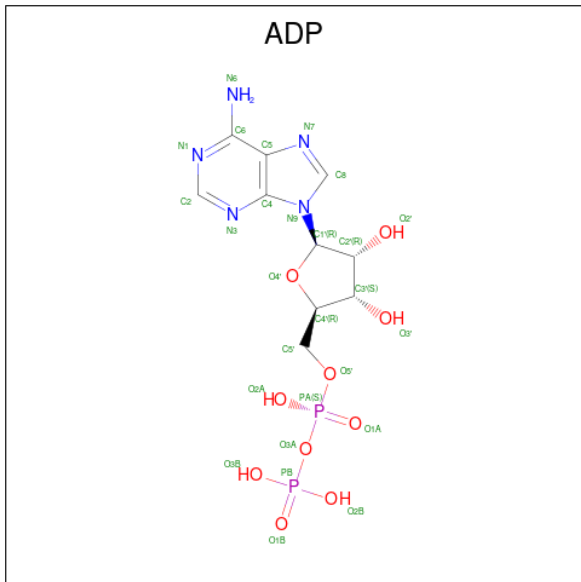
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	748	Total 5719	C 3583	N 1031	O 1068	S 37	406	0	0
1	B	748	Total 5719	C 3583	N 1031	O 1068	S 37	420	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



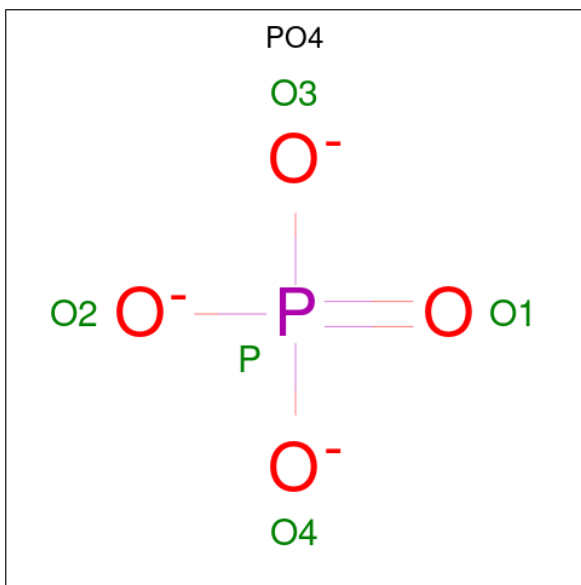
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

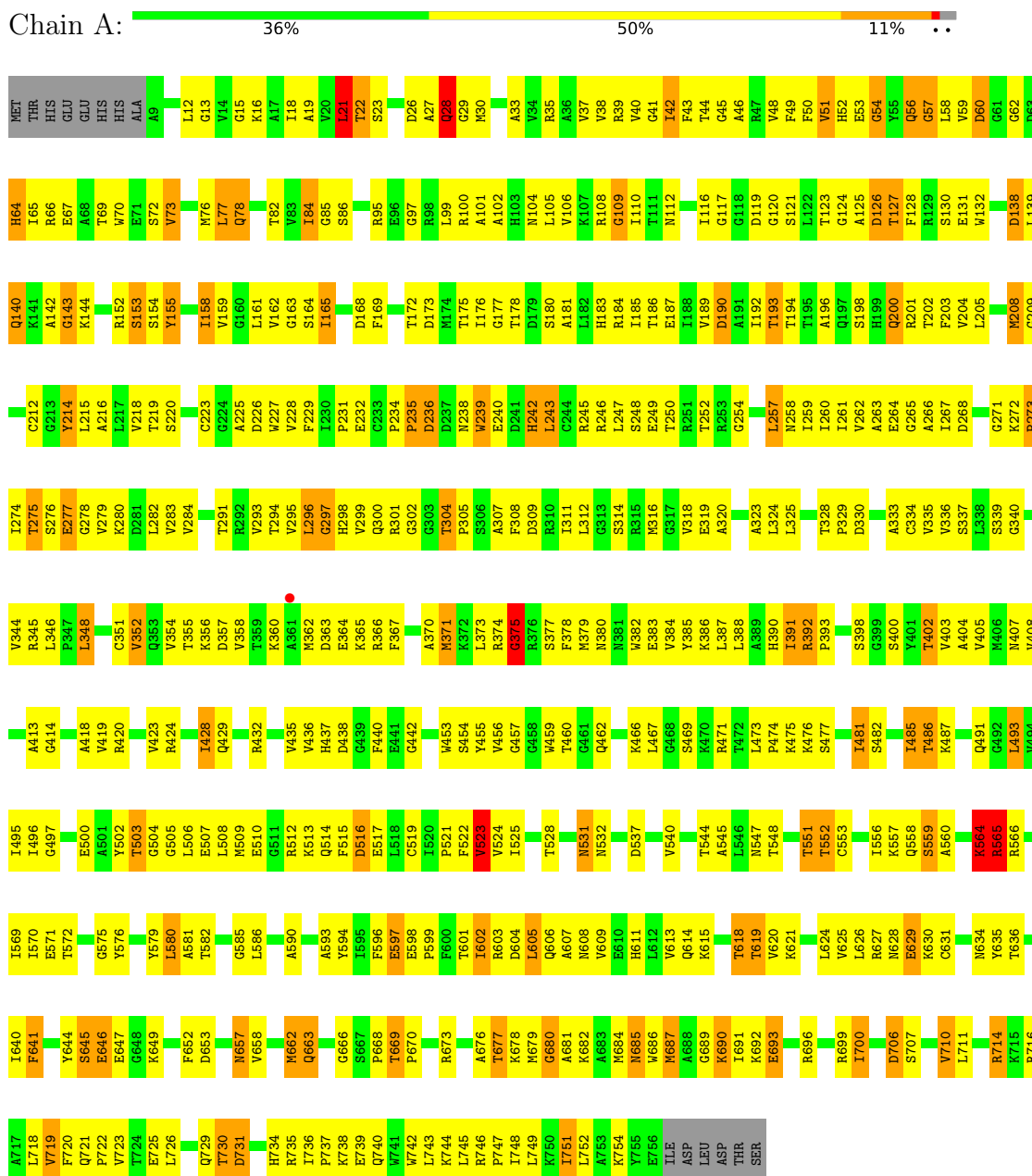


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	P 1	0	0
4	A	1	Total 5	O 4	P 1	0	0
4	A	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0

### 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: 6-phosphofructokinase, muscle type



● Molecule 1: 6-phosphofructokinase, muscle type



MET	THR	HIS	GLU	GLU	HIS	HIS	ALA	A9	R10	T11	L12	G13	V14	G15	K16	A17	I18	L21	T22	D26	A27	Q28	G29	M30	V34	R35	V38	R39	V40	G41	I42	F43	T44	R47	V51	Y55	Q56	G57	L58	V59	D60	G61	G62	D63	H64	I65	R66	G67	A68	T69	W70	E71				
S72	V73	S74	M75	L76	L77	Q78	T82	V83	I84	G89	F92	R95	R98	L99	R100	A101	M104	K107	R108	G109	I110	N111	M112	L113	I116	D119	G120	S121	L122	T123	G124	A125	D126	T127	F128	R129	W132	D138	K141	A142	G143	R144	I145	T146	A147	E148	E149									
S153	S154	Y155	L156	M157	I158	V159	G160	L161	I165	D166	F169	D173	M174	T175	I176	G177	D178	D179	S180	A181	L182	H183	G184	I185	T186	E187	I188	V189	D190	A191	I192	G193	T194	T195	S198	Q200	R201	F202	V203	V204	L205	K208	G209	R210	H211	G212	G213	Y214	L215	A216	L217	E148	E149			
T219	S220	L221	V228	F229	L230	L231	E232	C233	P234	P235	D236	D237	N238	D239	E240	D241	H242	L243	C244	R245	R246	L247	S248	E249	T250	R251	T252	R253	R256	L257	N258	T259	I260	L261	V262	A263	I267	D268	F273	L274	T275	E277	G278	V279	K280	D281	L282	V284	G288	V289	T291					
R293	V294	T295	L296	V299	Q300	R301	G302	G303	S306	A307	F308	D309	R310	I311	L312	G313	S314	S315	N316	G317	E319	A323	L324	T328	P329	P332	A333	C334	V335	V336	S337	L338	G339	G340	N341	Q342	A343	V344	R345	L346	P347	L348	K349	E350	C351	V352	G353	V354	T355	K356	D357	V358				
T359	K360	A361	K362	E364	K365	R366	F367	E369	A370	K371	K372	L373	R374	G375	R376	S377	F378	R379	N380	N381	V382	Y386	K386	L387	H390	P393	P396	K397	G399	S400	Y401	T402	V403	A404	N407	G409	A410	P411	A412	A413	G414	M415	N416	A417	A418	A419	R420	S421	T422	V423	R424					
I425	G426	L427	L428	Q429	G430	N431	R432	V433	L434	V435	V436	G439	F440	E441	G442	P443	A444	K445	G446	Q447	L448	E449	E450	A451	G452	W453	S454	V455	V456	W459	T460	G461	Q462	S465	K466	L467	K470	R471	T472	L473	P474	K475	K476	S477	T481	N484	L485	T486	R489	L490	Q491	G492				
L493	V494	L495	L496	E500	A501	Y502	T503	G504	G505	L506	L508	M509	E510	G511	R512	K513	Q514	F515	D516	E517	L518	C519	I520	P521	F522	V523	V524	V525	T528	V529	S530	N531	N532	G535	S536	D537	F538	S539	V540	D543	N547	T548	L549	C550	T551	T552	C553	D554	R555	L556	K557	Q558	S559			
A560	A561	G562	T563	K564	R565	R566	V567	F568	L569	M573	Y576	C577	G578	Y579	I581	G585	L586	G589	L595	F596	L600	E601	R603	D604	L605	Q606	P607	N608	V609	E610	H611	L612	L613	Q614	K615	M616	K617	T618	T619	V620	K621	R622	G623	L624	V625	L626	R627	N628	E629	K630	C631	M632				
E633	M634	Y635	T636	T637	D638	F639	I640	F641	M642	L643	V644	S645	E646	K649	G650	I651	F652	D653	K656	N657	L658	G659	G660	H661	M662	Q663	Q664	G665	G666	S667	P668	T669	P670	F671	D672	R673	N674	F675	A676	T677	K678	M679	G680	M684	N685	M686	M687	I691	L692	L693	R694	N695	R696	G698	R699	I700
N703	T704	D705	P706	S707	G708	C709	V710	L711	G712	M713	R714	K715	L718	V719	P722	V723	T724	E725	L726	Q727	N728	V729	T730	D731	H734	R735	I736	P737	K738	P739	Q740	W741	W742	L743	K744	L745	R746	P747	L748	L749	K750	I751	L752	A753	Y754	Y755	E756	I757	ASP	LEU	ASP	THR	SER			



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.68Å 163.68Å 356.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.00 – 3.20 45.54 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.00-3.20) 100.0 (45.54-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 3.19Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.238 , 0.302 0.212 , 0.274	Depositor DCC
$R_{free}$ test set	2362 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.9	Xtrriage
Anisotropy	0.290	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 113.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11646	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, ATP, ADP

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	0.59	0/5819	0.83	3/7859 (0.0%)
1	B	0.61	0/5819	0.80	1/7859 (0.0%)
All	All	0.60	0/11638	0.81	4/15718 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	GLY	N-CA-C	-6.49	96.87	113.10
1	A	523	VAL	CB-CA-C	-6.48	99.09	111.40
1	A	21	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	375	GLY	N-CA-C	5.07	125.78	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TYR	Sidechain

## 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	5719	0	5742	482	0
1	B	5719	0	5742	564	0
2	A	62	0	24	5	0
2	B	62	0	24	1	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	15	0	0	1	0
4	B	15	0	0	1	0
All	All	11646	0	11556	1037	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 49.

All (1037) 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:A:634:ASN:HD22	1:B:646:GLU:HG2	0.99	1.09
1:A:646:GLU:HG2	1:B:634:ASN:HD22	1.22	1.03
1:A:296:LEU:H	1:A:296:LEU:HD12	1.23	1.02
1:A:751:ILE:HD13	1:A:752:LEU:N	1.75	1.00
1:B:609:VAL:HG22	1:B:644:TYR:CE2	1.95	0.99
1:B:283:VAL:HG21	1:B:291:THR:HG21	1.45	0.98
1:A:634:ASN:ND2	1:B:646:GLU:HG2	1.79	0.98
1:B:35:ARG:HH11	1:B:77:LEU:HD13	1.25	0.96
1:A:391:ILE:HD12	1:A:392:ARG:H	1.29	0.96
1:A:28:GLN:H	1:A:28:GLN:HE21	1.11	0.96
1:A:257:LEU:HD12	1:A:259:ILE:HD11	1.46	0.95
1:B:514:GLN:H	1:B:514:GLN:HE21	1.12	0.91
1:A:334:CYS:SG	1:A:345:ARG:HB3	2.10	0.91
1:B:221:LEU:HD23	1:B:674:ASN:ND2	1.85	0.91
1:A:392:ARG:HB3	1:A:393:PRO:CA	2.01	0.90
1:B:39:ARG:HD2	1:B:70:TRP:CZ2	2.06	0.90
1:A:259:ILE:HG22	1:A:261:ILE:CD1	2.01	0.90
1:B:734:HIS:O	1:B:736:ILE:HG23	1.72	0.90
1:B:159:VAL:HG23	1:B:324:LEU:HD23	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:HB3	1:A:393:PRO:HA	1.53	0.89
1:A:257:LEU:H	1:A:257:LEU:HD23	1.38	0.89
1:B:296:LEU:HD12	1:B:296:LEU:H	1.36	0.88
1:B:549:ILE:HD12	1:B:659:LEU:HD13	1.56	0.88
1:B:509:MET:SD	1:B:512:ARG:NH1	2.48	0.87
1:A:491:GLN:HB3	1:A:700:ILE:HD11	1.55	0.87
1:B:664:GLN:C	1:B:666:GLY:H	1.73	0.87
1:A:44:THR:HG21	1:A:325:LEU:HD11	1.56	0.86
1:A:18:ILE:HG22	1:A:112:ASN:HB2	1.57	0.86
1:B:520:ILE:HG22	1:B:700:ILE:HD11	1.56	0.86
1:B:416:ASN:OD1	1:B:466:LYS:HB2	1.74	0.86
1:B:275:THR:HG23	1:B:278:GLY:HA3	1.58	0.85
1:B:419:VAL:O	1:B:423:VAL:HG23	1.77	0.85
1:A:66:ARG:HA	1:A:66:ARG:NE	1.90	0.84
1:A:280:LYS:HG2	1:A:291:THR:CG2	2.07	0.84
1:A:392:ARG:CB	1:A:393:PRO:HA	2.06	0.84
1:B:221:LEU:HD23	1:B:674:ASN:HD22	1.37	0.84
1:B:120:GLY:O	1:B:123:THR:HG22	1.77	0.84
1:A:245:ARG:O	1:A:249:GLU:HG3	1.77	0.83
1:B:184:ARG:NH1	1:B:303:GLY:HA3	1.94	0.83
1:A:58:LEU:HG	1:A:101:ALA:HB1	1.59	0.83
1:B:348:LEU:O	1:B:352:VAL:HG23	1.77	0.82
1:A:165:ILE:O	1:A:215:LEU:HD11	1.78	0.82
1:B:595:ILE:HD13	1:B:595:ILE:H	1.43	0.81
1:A:646:GLU:HG2	1:B:634:ASN:HB2	1.62	0.81
1:B:35:ARG:HH12	1:B:77:LEU:HD22	1.42	0.81
1:B:618:THR:HG22	1:B:619:THR:N	1.95	0.81
1:A:40:VAL:HG21	1:A:318:VAL:HG22	1.61	0.81
1:A:296:LEU:H	1:A:296:LEU:CD1	1.94	0.81
1:B:514:GLN:HE21	1:B:514:GLN:N	1.78	0.81
1:A:391:ILE:HD11	2:A:765:ATP:O2G	1.79	0.81
1:B:208:MET:HB2	1:B:300:GLN:OE1	1.81	0.80
1:B:663:GLN:C	1:B:665:GLY:H	1.84	0.80
1:B:382:TRP:CZ2	1:B:386:LYS:HD2	2.16	0.80
1:B:641:PHE:CD2	1:B:656:LYS:HD3	2.17	0.80
1:A:491:GLN:HB3	1:A:700:ILE:CD1	2.10	0.80
1:A:243:LEU:HD12	1:A:243:LEU:O	1.82	0.80
1:A:364:GLU:O	1:A:366:ARG:N	2.15	0.80
1:A:391:ILE:HD11	2:A:765:ATP:PG	2.22	0.80
1:B:419:VAL:HG11	1:B:467:LEU:HD11	1.62	0.80
1:A:646:GLU:HG2	1:B:634:ASN:ND2	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:HD11	1:B:333:ALA:HB2	1.65	0.79
1:B:687:MET:HE3	1:B:687:MET:O	1.81	0.79
1:B:41:GLY:O	1:B:44:THR:HG22	1.81	0.79
1:B:35:ARG:NH1	1:B:77:LEU:HD13	1.96	0.79
1:A:646:GLU:CG	1:B:634:ASN:HB2	2.13	0.78
1:B:440:PHE:O	1:B:443:PRO:HD2	1.83	0.78
1:A:246:ARG:O	1:A:250:THR:HG22	1.84	0.78
1:A:268:ASP:HB3	1:A:274:ILE:HD11	1.65	0.78
1:B:509:MET:O	1:B:512:ARG:HB2	1.83	0.78
1:A:259:ILE:HG22	1:A:261:ILE:HD12	1.66	0.78
1:A:354:VAL:HA	1:A:357:ASP:OD2	1.83	0.78
1:A:280:LYS:HG2	1:A:291:THR:HG22	1.64	0.77
1:B:436:VAL:HG22	1:B:448:ILE:HD12	1.64	0.77
1:A:696:ARG:HG3	1:A:696:ARG:HH11	1.50	0.77
1:A:208:MET:HB2	1:A:300:GLN:OE1	1.84	0.77
1:B:658:VAL:HG12	1:B:658:VAL:O	1.83	0.77
1:A:172:THR:OG1	1:A:337:SER:HB2	1.83	0.76
1:A:380:ASN:O	1:A:384:VAL:HG23	1.85	0.76
1:B:350:GLU:O	1:B:354:VAL:HG23	1.85	0.76
1:B:441:GLU:OE2	1:B:472:THR:HG21	1.83	0.76
1:A:335:VAL:HG23	1:A:348:LEU:HG	1.67	0.76
1:B:470:LYS:HE2	1:B:471:ARG:H	1.50	0.76
1:A:312:LEU:O	1:A:316:MET:HG2	1.84	0.76
1:B:412:ALA:O	1:B:415:MET:HG3	1.86	0.76
1:B:664:GLN:C	1:B:666:GLY:N	2.38	0.76
1:A:391:ILE:HD12	1:A:392:ARG:N	2.01	0.76
1:B:257:LEU:HD12	1:B:259:ILE:HD11	1.68	0.76
1:A:120:GLY:O	1:A:123:THR:HG22	1.84	0.76
1:B:443:PRO:O	1:B:484:ASN:ND2	2.18	0.75
1:A:516:ASP:O	1:A:519:CYS:HB2	1.87	0.75
1:A:348:LEU:O	1:A:352:VAL:HG23	1.86	0.75
1:A:33:ALA:O	1:A:37:VAL:HG23	1.87	0.74
1:B:420:ARG:HH11	1:B:460:THR:HB	1.52	0.74
1:A:296:LEU:HD12	1:A:296:LEU:N	1.99	0.74
1:B:418:ALA:HB2	1:B:676:ALA:HB1	1.68	0.74
1:A:734:HIS:O	1:A:736:ILE:HG23	1.86	0.74
1:A:601:THR:HG22	1:A:604:ASP:OD2	1.87	0.74
1:A:590:ALA:HB2	1:A:624:LEU:HD23	1.69	0.74
1:A:551:THR:HG22	1:A:552:THR:N	2.00	0.74
1:B:618:THR:HG22	1:B:619:THR:H	1.52	0.74
1:B:642:ASN:HD22	1:B:642:ASN:N	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:THR:HG23	1:B:72:SER:HB3	1.70	0.73
1:A:192:ILE:HG22	1:A:193:THR:N	2.02	0.73
1:B:459:TRP:HD1	1:B:459:TRP:H	1.34	0.73
1:B:40:VAL:HG22	1:B:751:ILE:HD11	1.71	0.72
1:A:120:GLY:HA2	1:A:123:THR:HG22	1.70	0.72
1:A:668:PRO:HG2	1:A:673:ARG:HE	1.54	0.72
1:A:548:THR:O	1:A:552:THR:HG23	1.88	0.72
1:B:124:GLY:HA2	1:B:127:THR:HG22	1.70	0.72
1:A:275:THR:HG23	1:A:278:GLY:HA3	1.72	0.72
1:B:316:MET:HE3	1:B:337:SER:HA	1.72	0.72
1:A:82:THR:HG21	1:A:86:SER:HB2	1.72	0.72
1:A:605:LEU:HD11	1:A:640:ILE:HD12	1.72	0.72
1:A:609:VAL:C	1:A:611:HIS:H	1.93	0.72
1:B:296:LEU:H	1:B:296:LEU:CD1	2.03	0.72
1:B:39:ARG:HD2	1:B:70:TRP:CE2	2.24	0.71
1:B:656:LYS:HG3	1:B:656:LYS:O	1.87	0.71
1:A:58:LEU:HD11	1:A:105:LEU:HD21	1.70	0.71
1:B:275:THR:O	1:B:279:VAL:HG23	1.90	0.71
1:A:220:SER:HB3	1:A:225:ALA:HB3	1.72	0.71
1:B:47:ARG:HD2	1:B:67:GLU:OE1	1.90	0.71
1:B:744:LYS:O	1:B:747:PRO:HD2	1.89	0.71
1:B:215:LEU:O	1:B:219:THR:CG2	2.38	0.71
1:B:281:ASP:O	1:B:284:VAL:N	2.24	0.71
1:B:595:ILE:HD12	1:B:746:ARG:NH1	2.05	0.71
1:A:387:LEU:HD23	1:A:428:ILE:HD13	1.71	0.71
1:B:679:MET:HE1	1:B:718:LEU:HD11	1.71	0.71
1:B:159:VAL:HG23	1:B:324:LEU:CD2	2.20	0.71
1:B:283:VAL:HG23	1:B:284:VAL:N	2.05	0.71
1:B:528:THR:HG23	1:B:531:ASN:H	1.56	0.70
1:B:95:ARG:HA	1:B:98:ARG:HD2	1.72	0.70
1:B:663:GLN:O	1:B:665:GLY:N	2.24	0.70
1:A:679:MET:HE3	1:A:718:LEU:HD11	1.73	0.70
1:B:231:PRO:O	1:B:233:CYS:N	2.25	0.70
1:A:297:GLY:O	1:A:299:VAL:HG13	1.91	0.69
1:B:205:LEU:HD22	1:B:296:LEU:HD11	1.73	0.69
1:B:232:GLU:HG2	1:B:374:ARG:HG2	1.74	0.69
1:A:190:ASP:O	1:A:193:THR:HG22	1.92	0.69
1:B:69:THR:CG2	1:B:72:SER:HB3	2.22	0.69
1:A:275:THR:OG1	1:A:277:GLU:HG2	1.92	0.69
1:B:38:VAL:O	1:B:42:ILE:HG12	1.94	0.68
1:A:392:ARG:CB	1:A:393:PRO:CA	2.66	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLY:O	1:B:335:VAL:HG13	1.93	0.68
1:B:605:LEU:HD21	1:B:640:ILE:HD13	1.74	0.68
1:B:328:THR:HB	1:B:329:PRO:CD	2.23	0.68
1:B:679:MET:CE	1:B:718:LEU:HD11	2.22	0.68
1:A:521:PRO:HB3	1:A:707:SER:HB2	1.76	0.68
1:A:69:THR:HG23	1:A:72:SER:H	1.57	0.68
1:A:280:LYS:HG3	1:A:293:VAL:HG23	1.76	0.68
1:B:205:LEU:HD23	1:B:294:THR:HB	1.74	0.68
1:B:247:LEU:HD23	1:B:258:ASN:ND2	2.08	0.68
1:B:35:ARG:NH1	1:B:77:LEU:HD22	2.08	0.68
1:B:61:GLY:O	1:B:63:ASP:N	2.26	0.68
1:B:158:ILE:HD11	1:B:333:ALA:CB	2.22	0.68
1:B:731:ASP:OD1	1:B:731:ASP:O	2.12	0.68
1:B:551:THR:HG22	1:B:552:THR:N	2.08	0.68
1:A:257:LEU:HD12	1:A:259:ILE:CD1	2.23	0.67
1:B:481:ILE:O	1:B:485:ILE:HG23	1.95	0.67
1:A:364:GLU:C	1:A:366:ARG:H	1.97	0.67
1:B:435:VAL:CG1	1:B:467:LEU:HD21	2.24	0.67
1:A:268:ASP:HB3	1:A:274:ILE:CD1	2.24	0.67
1:B:281:ASP:O	1:B:283:VAL:N	2.27	0.67
1:B:493:LEU:HD23	1:B:495:ILE:HD11	1.77	0.67
1:A:27:ALA:O	1:A:30:MET:HG3	1.94	0.67
1:B:531:ASN:HD21	1:B:538:PHE:HA	1.59	0.67
1:A:51:VAL:HG12	1:A:51:VAL:O	1.95	0.66
1:A:259:ILE:HG22	1:A:261:ILE:HD11	1.76	0.66
1:A:262:VAL:HG12	1:A:263:ALA:O	1.95	0.66
1:B:456:VAL:O	1:B:459:TRP:CD1	2.49	0.66
1:B:459:TRP:CD2	1:B:466:LYS:NZ	2.63	0.66
1:B:609:VAL:HG13	1:B:644:TYR:CD2	2.30	0.66
1:B:247:LEU:CD2	1:B:258:ASN:HD22	2.08	0.66
1:A:726:LEU:O	1:A:730:THR:HG22	1.95	0.66
1:A:258:ASN:C	1:A:259:ILE:HD12	2.16	0.66
1:A:711:LEU:HD11	1:A:718:LEU:HG	1.78	0.66
1:B:722:PRO:HG2	1:B:725:GLU:HB2	1.77	0.66
1:A:481:ILE:HG12	1:A:482:SER:N	2.10	0.66
1:B:595:ILE:HD13	1:B:595:ILE:N	2.11	0.66
1:A:601:THR:O	1:A:604:ASP:N	2.27	0.65
1:A:619:THR:HG23	1:A:620:VAL:H	1.61	0.65
1:B:502:TYR:OH	1:B:730:THR:HG21	1.96	0.65
1:B:65:ILE:HG22	1:B:65:ILE:O	1.95	0.65
1:B:510:GLU:O	1:B:512:ARG:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:O	1:A:299:VAL:N	2.30	0.65
1:B:402:THR:HG21	1:B:432:ARG:NH2	2.12	0.65
1:A:312:LEU:HD11	1:A:316:MET:HE2	1.79	0.65
1:A:420:ARG:HA	1:A:456:VAL:HG11	1.78	0.65
1:B:247:LEU:HA	1:B:250:THR:HG22	1.79	0.65
1:A:528:THR:HG23	1:A:531:ASN:H	1.61	0.65
1:B:473:LEU:HD21	1:B:503:THR:HG22	1.78	0.65
1:A:228:VAL:HG12	1:A:229:PHE:N	2.12	0.65
1:B:419:VAL:HG21	1:B:467:LEU:HD12	1.79	0.65
1:B:495:ILE:HG22	1:B:501:ALA:HB1	1.79	0.65
1:A:419:VAL:O	1:A:423:VAL:HG23	1.97	0.65
1:B:39:ARG:CD	1:B:70:TRP:CE2	2.79	0.65
1:B:345:ARG:O	1:B:346:LEU:HD23	1.96	0.65
1:B:512:ARG:HH22	1:B:707:SER:HB2	1.60	0.65
1:B:514:GLN:H	1:B:514:GLN:NE2	1.90	0.65
1:A:66:ARG:HH21	1:A:108:ARG:NH2	1.95	0.64
1:A:333:ALA:HB1	1:A:348:LEU:HD12	1.78	0.64
1:A:387:LEU:HD22	1:A:428:ILE:HG21	1.79	0.64
1:A:646:GLU:CG	1:B:634:ASN:HD22	2.04	0.64
1:B:296:LEU:HD12	1:B:296:LEU:N	2.11	0.64
1:A:159:VAL:HG23	1:A:324:LEU:CD2	2.28	0.64
1:A:296:LEU:O	1:A:297:GLY:O	2.14	0.64
1:A:39:ARG:HD2	1:A:70:TRP:CE2	2.32	0.64
1:A:586:LEU:HD12	1:A:586:LEU:O	1.96	0.64
1:A:123:THR:O	1:A:127:THR:HG22	1.96	0.64
1:B:21:LEU:O	1:B:21:LEU:HD23	1.97	0.64
1:B:112:ASN:OD1	1:B:157:ASN:HB2	1.98	0.64
1:B:247:LEU:HA	1:B:250:THR:CG2	2.28	0.64
1:B:387:LEU:CD2	1:B:428:ILE:HD13	2.27	0.64
1:B:726:LEU:HD23	1:B:729:GLN:OE1	1.97	0.64
1:A:475:LYS:O	1:A:477:SER:N	2.31	0.63
1:B:110:ILE:HD12	1:B:110:ILE:H	1.62	0.63
1:B:567:VAL:HG22	1:B:616:MET:HE1	1.80	0.63
1:B:577:CYS:HA	1:B:597:GLU:OE2	1.97	0.63
1:A:569:ILE:HD12	1:A:641:PHE:HA	1.79	0.63
1:B:686:TRP:HZ2	1:B:709:CYS:HG	1.46	0.63
1:A:159:VAL:HG23	1:A:324:LEU:HD23	1.79	0.63
1:B:585:GLY:HA2	1:B:626:LEU:HD12	1.80	0.63
1:B:228:VAL:HG12	1:B:229:PHE:N	2.13	0.63
1:B:9:ALA:HB1	1:B:11:THR:HG22	1.80	0.63
1:B:334:CYS:HA	1:B:346:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ARG:HG3	1:B:456:VAL:HB	1.81	0.63
1:B:612:LEU:O	1:B:616:MET:HG2	1.99	0.63
1:A:280:LYS:O	1:A:284:VAL:HG23	1.99	0.63
1:B:481:ILE:O	1:B:481:ILE:HD12	1.99	0.63
1:A:102:ALA:O	1:A:106:VAL:HG23	1.99	0.63
1:A:609:VAL:C	1:A:611:HIS:N	2.51	0.63
1:B:232:GLU:O	1:B:371:MET:HG2	1.98	0.63
1:B:182:LEU:HD11	1:B:218:VAL:HG11	1.80	0.63
1:B:193:THR:HG23	1:B:194:THR:N	2.13	0.63
1:B:428:ILE:HG13	1:B:453:TRP:HZ3	1.62	0.63
1:B:724:THR:HA	1:B:727:GLN:HE21	1.63	0.62
1:A:503:THR:HG22	1:A:504:GLY:N	2.15	0.62
1:B:624:LEU:HD12	1:B:625:VAL:N	2.14	0.62
1:A:22:THR:HG21	1:A:82:THR:OG1	1.99	0.62
1:B:101:ALA:HA	1:B:104:ASN:HD22	1.64	0.62
1:B:249:GLU:HA	1:B:252:THR:HG22	1.82	0.62
1:B:481:ILE:HD12	1:B:481:ILE:C	2.18	0.62
1:B:436:VAL:HG22	1:B:448:ILE:CD1	2.29	0.62
1:A:35:ARG:HD3	1:A:77:LEU:HD13	1.82	0.62
1:A:731:ASP:OD1	1:A:731:ASP:C	2.37	0.62
1:A:56:GLN:O	1:A:59:VAL:N	2.32	0.62
1:A:202:THR:HG22	1:A:202:THR:O	2.00	0.61
1:A:496:ILE:CD1	1:A:525:ILE:HD12	2.30	0.61
1:B:605:LEU:HD11	1:B:640:ILE:HD12	1.82	0.61
1:B:669:THR:O	1:B:673:ARG:HG3	2.00	0.61
1:A:49:PHE:CD1	1:A:110:ILE:HD11	2.34	0.61
1:A:565:ARG:HG2	1:A:565:ARG:HH21	1.65	0.61
1:B:376:ARG:HH21	1:B:376:ARG:HB3	1.65	0.61
1:A:185:ILE:HD11	1:A:215:LEU:HD23	1.82	0.61
1:B:514:GLN:N	1:B:514:GLN:NE2	2.46	0.61
1:B:634:ASN:O	1:B:636:THR:HG23	2.01	0.61
1:A:50:PHE:CE2	1:A:84:ILE:HD11	2.36	0.61
1:A:259:ILE:CG2	1:A:261:ILE:HD11	2.31	0.61
1:A:19:ALA:HA	1:A:49:PHE:O	2.01	0.61
1:B:283:VAL:HG23	1:B:284:VAL:H	1.65	0.61
1:B:481:ILE:HD11	1:B:518:LEU:HD21	1.82	0.61
1:B:485:ILE:HG12	1:B:517:GLU:HB3	1.82	0.61
1:B:126:ASP:HB2	1:B:348:LEU:HD22	1.81	0.61
1:B:316:MET:HE1	1:B:338:LEU:HB2	1.82	0.61
1:A:35:ARG:HH12	1:A:752:LEU:HD13	1.66	0.60
1:B:228:VAL:HG12	1:B:229:PHE:H	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:PRO:HB2	1:B:673:ARG:HG2	1.83	0.60
1:A:722:PRO:HG2	1:A:725:GLU:HG3	1.82	0.60
1:B:601:THR:O	1:B:603:ARG:N	2.34	0.60
1:A:308:PHE:CZ	1:A:312:LEU:HD22	2.36	0.60
1:B:307:ALA:H	1:B:547:ASN:HD21	1.47	0.60
1:B:495:ILE:CG2	1:B:501:ALA:HB1	2.32	0.60
1:A:609:VAL:O	1:A:611:HIS:N	2.30	0.60
1:B:627:ARG:NH2	1:B:636:THR:HA	2.17	0.60
1:B:604:ASP:O	1:B:607:ALA:N	2.33	0.60
1:A:52:HIS:HA	1:A:84:ILE:O	2.02	0.60
1:B:333:ALA:HB1	1:B:348:LEU:HD12	1.84	0.60
1:A:99:LEU:HD12	1:A:100:ARG:N	2.17	0.60
1:A:183:HIS:O	1:A:187:GLU:HG3	2.01	0.60
1:A:28:GLN:H	1:A:28:GLN:NE2	1.93	0.59
1:A:590:ALA:HA	1:A:624:LEU:HB3	1.83	0.59
1:A:120:GLY:CA	1:A:123:THR:HG22	2.32	0.59
1:A:280:LYS:HG2	1:A:291:THR:HG21	1.83	0.59
1:B:18:ILE:HD12	1:B:324:LEU:HD12	1.84	0.59
1:B:185:ILE:HD12	1:B:219:THR:HB	1.85	0.59
1:B:425:ILE:O	1:B:429:GLN:HG3	2.02	0.59
1:B:456:VAL:HA	1:B:459:TRP:NE1	2.17	0.59
1:A:78:GLN:N	1:A:78:GLN:OE1	2.35	0.59
1:B:185:ILE:O	1:B:189:VAL:HG23	2.00	0.59
1:B:459:TRP:CD1	1:B:459:TRP:N	2.64	0.59
1:B:687:MET:HE1	1:B:691:ILE:HD11	1.83	0.59
1:A:66:ARG:HA	1:A:66:ARG:CZ	2.32	0.59
1:A:593:ALA:HA	1:A:626:LEU:O	2.02	0.59
1:B:416:ASN:HB3	1:B:459:TRP:HB3	1.84	0.59
1:B:660:GLY:C	1:B:662:MET:H	2.06	0.59
1:B:675:PHE:HA	1:B:678:LYS:HE2	1.85	0.59
2:A:763:ATP:O2A	2:A:763:ATP:O2B	2.21	0.59
1:B:404:ALA:HB2	1:B:490:ILE:HD12	1.84	0.59
1:B:532:ASN:O	1:B:737:PRO:HD3	2.02	0.59
1:B:595:ILE:HD12	1:B:746:ARG:HH12	1.65	0.59
1:B:166:ASP:OD1	1:B:209:GLY:HA2	2.02	0.58
1:B:700:ILE:HG13	1:B:700:ILE:O	2.02	0.58
1:B:314:SER:O	1:B:318:VAL:HG23	2.03	0.58
1:B:481:ILE:HD11	1:B:518:LEU:CD2	2.33	0.58
1:A:459:TRP:HA	1:A:462:GLN:HG3	1.85	0.58
1:B:306:SER:O	1:B:310:ARG:HG3	2.04	0.58
1:A:267:ILE:HA	1:A:273:PRO:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:MET:HG3	1:B:718:LEU:HD12	1.83	0.58
1:A:726:LEU:HD23	1:A:729:GLN:OE1	2.03	0.58
1:B:416:ASN:OD1	1:B:466:LYS:CB	2.49	0.58
1:B:535:GLY:O	1:B:712:GLY:HA3	2.03	0.58
1:A:398:SER:C	1:A:400:SER:H	2.07	0.58
1:B:663:GLN:C	1:B:665:GLY:N	2.51	0.58
1:B:215:LEU:O	1:B:219:THR:HG22	2.03	0.58
1:A:751:ILE:HD13	1:A:751:ILE:C	2.23	0.57
1:B:216:ALA:O	1:B:219:THR:HG23	2.04	0.57
1:A:646:GLU:HG2	1:B:634:ASN:CB	2.32	0.57
1:B:319:GLU:OE2	1:B:345:ARG:NE	2.37	0.57
1:A:153:SER:O	1:A:155:TYR:N	2.26	0.57
1:A:268:ASP:CB	1:A:274:ILE:HD11	2.34	0.57
1:A:524:VAL:CG1	1:A:710:VAL:HG22	2.34	0.57
1:B:9:ALA:C	1:B:11:THR:H	2.06	0.57
1:B:39:ARG:HG3	1:B:39:ARG:HH11	1.69	0.57
1:B:369:GLU:O	1:B:373:LEU:HB2	2.03	0.57
1:A:15:GLY:O	1:A:16:LYS:HG2	2.05	0.57
1:B:158:ILE:HD13	1:B:158:ILE:H	1.70	0.57
1:B:323:ALA:HA	1:B:345:ARG:HH12	1.70	0.57
1:A:116:ILE:HG12	1:A:161:LEU:HD13	1.86	0.57
1:A:243:LEU:HD12	1:A:247:LEU:HD12	1.87	0.57
1:A:95:ARG:C	1:A:97:GLY:H	2.07	0.57
1:B:40:VAL:HG21	1:B:318:VAL:HG13	1.85	0.57
1:B:435:VAL:HB	1:B:467:LEU:HD21	1.87	0.57
1:A:42:ILE:HD13	1:A:48:VAL:HG23	1.87	0.57
1:A:371:MET:SD	1:A:378:PHE:CE2	2.98	0.56
1:B:611:HIS:CE1	1:B:754:LYS:HB3	2.40	0.56
1:A:50:PHE:O	1:A:51:VAL:HG23	2.05	0.56
1:B:387:LEU:HD22	1:B:428:ILE:HD13	1.86	0.56
1:A:219:THR:O	1:A:223:CYS:SG	2.57	0.56
1:A:312:LEU:HD11	1:A:316:MET:CE	2.35	0.56
1:A:564:LYS:HE2	1:A:564:LYS:HA	1.86	0.56
1:A:523:VAL:HG22	1:A:686:TRP:CZ3	2.39	0.56
1:B:485:ILE:HD12	1:B:485:ILE:O	2.05	0.56
1:A:682:LYS:HG2	1:A:718:LEU:HD23	1.87	0.56
1:B:169:PHE:CE2	1:B:351:CYS:HB3	2.40	0.56
1:B:609:VAL:HG13	1:B:644:TYR:HD2	1.70	0.56
1:B:642:ASN:N	1:B:642:ASN:ND2	2.53	0.56
1:B:669:THR:HB	1:B:670:PRO:HD2	1.86	0.56
1:A:714:ARG:HE	1:A:714:ARG:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:CD2	1:B:674:ASN:HD22	2.15	0.56
1:A:352:VAL:HA	1:A:355:THR:HG22	1.86	0.56
1:B:247:LEU:HD23	1:B:258:ASN:HD22	1.70	0.56
1:A:471:ARG:HB3	1:A:500:GLU:HG3	1.87	0.56
1:A:532:ASN:O	1:A:737:PRO:HD3	2.05	0.56
1:B:556:ILE:HG22	1:B:568:PHE:CD2	2.40	0.56
1:B:543:ASP:HB3	1:B:672:ASP:OD2	2.06	0.56
1:B:275:THR:HG23	1:B:278:GLY:CA	2.32	0.56
1:B:257:LEU:O	1:B:257:LEU:HG	2.06	0.55
1:B:292:ARG:O	1:B:293:VAL:HG23	2.06	0.55
1:B:372:LYS:HA	1:B:379:MET:HE1	1.88	0.55
1:A:26:ASP:O	1:A:301:ARG:NH1	2.39	0.55
1:A:177:GLY:N	1:A:309:ASP:OD1	2.37	0.55
1:B:235:PRO:HD2	1:B:267:ILE:O	2.07	0.55
1:B:281:ASP:O	1:B:282:LEU:C	2.43	0.55
1:B:611:HIS:HE1	1:B:754:LYS:HB3	1.70	0.55
1:A:686:TRP:CZ3	1:A:687:MET:HG2	2.41	0.55
1:B:124:GLY:CA	1:B:127:THR:HG22	2.37	0.55
1:B:190:ASP:O	1:B:194:THR:HG23	2.07	0.55
1:B:745:LEU:O	1:B:748:ILE:HG12	2.06	0.55
1:A:153:SER:C	1:A:155:TYR:H	2.08	0.55
1:A:391:ILE:HD12	1:A:391:ILE:H	1.71	0.55
1:A:408:VAL:O	1:A:497:GLY:HA3	2.06	0.55
1:A:101:ALA:HA	1:A:104:ASN:HD22	1.71	0.55
1:B:708:GLY:O	1:B:723:VAL:HG22	2.05	0.55
1:A:168:ASP:OD2	1:A:169:PHE:N	2.39	0.55
1:A:335:VAL:CG2	1:A:348:LEU:HG	2.37	0.55
1:A:605:LEU:HD21	1:A:640:ILE:HD13	1.88	0.55
1:B:299:VAL:HG23	1:B:300:GLN:N	2.22	0.55
1:A:294:THR:HG22	1:A:295:VAL:N	2.22	0.55
1:A:696:ARG:HG3	1:A:696:ARG:NH1	2.21	0.55
1:B:535:GLY:O	1:B:714:ARG:HD2	2.06	0.55
1:B:537:ASP:HB3	1:B:741:TRP:NE1	2.20	0.55
1:B:562:GLY:C	1:B:564:LYS:H	2.08	0.55
1:A:402:THR:HB	1:A:432:ARG:HB3	1.89	0.55
1:A:569:ILE:HG12	1:A:625:VAL:HB	1.88	0.55
1:A:627:ARG:NH2	1:A:636:THR:HA	2.21	0.55
1:A:646:GLU:HG3	1:B:634:ASN:HB2	1.86	0.55
1:A:726:LEU:O	1:A:730:THR:CG2	2.54	0.55
1:B:160:GLY:O	1:B:335:VAL:HA	2.07	0.55
1:B:240:GLU:N	1:B:240:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLU:OE2	1:B:472:THR:CG2	2.54	0.55
1:A:387:LEU:CD2	1:A:428:ILE:HG21	2.37	0.54
1:B:18:ILE:HD12	1:B:324:LEU:CD1	2.38	0.54
1:B:485:ILE:HD12	1:B:485:ILE:C	2.28	0.54
1:B:641:PHE:CG	1:B:656:LYS:HD3	2.42	0.54
1:A:275:THR:HG23	1:A:278:GLY:CA	2.37	0.54
1:A:275:THR:O	1:A:279:VAL:HG23	2.07	0.54
1:B:402:THR:HG23	1:B:491:GLN:HE21	1.72	0.54
1:A:551:THR:CG2	1:A:552:THR:N	2.68	0.54
1:B:471:ARG:HB2	1:B:500:GLU:HG2	1.90	0.54
1:A:271:GLY:O	1:A:273:PRO:HD3	2.07	0.54
1:B:289:TYR:C	1:B:291:THR:H	2.11	0.54
1:B:565:ARG:HG3	1:B:565:ARG:HH11	1.73	0.54
1:A:231:PRO:O	1:A:234:PRO:HD3	2.07	0.54
1:A:271:GLY:O	1:A:273:PRO:CD	2.55	0.54
1:A:513:LYS:HB2	1:A:514:GLN:NE2	2.23	0.54
1:A:679:MET:O	1:A:681:ALA:N	2.40	0.54
1:B:193:THR:C	1:B:195:THR:H	2.11	0.54
1:B:523:VAL:HG22	1:B:686:TRP:CZ3	2.42	0.54
1:B:551:THR:O	1:B:552:THR:C	2.46	0.54
1:A:204:VAL:HG12	1:A:204:VAL:O	2.07	0.54
1:A:340:GLY:HA2	1:A:716:ARG:HA	1.90	0.54
1:A:403:VAL:HG12	1:A:404:ALA:N	2.23	0.54
1:B:609:VAL:HA	1:B:644:TYR:HE2	1.72	0.54
1:A:53:GLU:O	1:A:54:GLY:O	2.26	0.54
1:B:119:ASP:OD1	1:B:120:GLY:N	2.38	0.54
1:B:267:ILE:HA	1:B:273:PRO:HA	1.88	0.54
1:A:29:GLY:HA3	1:A:176:ILE:CG2	2.38	0.54
1:A:721:GLN:NE2	1:A:726:LEU:HD21	2.23	0.54
1:B:376:ARG:CB	1:B:376:ARG:NH2	2.70	0.54
1:B:420:ARG:HH11	1:B:460:THR:CB	2.20	0.54
1:B:21:LEU:HD23	1:B:21:LEU:C	2.28	0.54
1:B:175:THR:O	1:B:178:THR:HG22	2.08	0.54
1:B:364:GLU:O	1:B:366:ARG:N	2.41	0.54
1:B:382:TRP:CE2	1:B:386:LYS:HD2	2.43	0.54
1:B:605:LEU:HG	1:B:643:LEU:HD23	1.90	0.54
1:A:722:PRO:HG2	1:A:725:GLU:CG	2.37	0.53
1:B:726:LEU:O	1:B:729:GLN:HB2	2.08	0.53
1:B:11:THR:O	1:B:13:GLY:N	2.42	0.53
1:B:409:GLY:HA2	1:B:471:ARG:HB3	1.89	0.53
1:A:436:VAL:HG13	1:A:442:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HA	1:A:73:VAL:HG11	1.89	0.53
1:A:375:GLY:HA2	1:A:379:MET:CE	2.39	0.53
1:A:435:VAL:HG13	1:A:467:LEU:CD2	2.39	0.53
1:B:21:LEU:HD12	1:B:51:VAL:HG11	1.90	0.53
1:B:34:VAL:O	1:B:38:VAL:HG23	2.07	0.53
1:B:185:ILE:O	1:B:185:ILE:HG12	2.08	0.53
1:B:459:TRP:CE2	1:B:466:LYS:NZ	2.77	0.53
1:B:667:SER:OG	1:B:668:PRO:HD2	2.08	0.53
1:A:189:VAL:O	1:A:193:THR:HB	2.09	0.53
1:A:738:LYS:O	1:A:739:GLU:HB2	2.09	0.53
1:A:748:ILE:CG1	1:A:749:LEU:N	2.71	0.53
1:B:124:GLY:HA2	1:B:127:THR:CG2	2.38	0.53
1:B:182:LEU:CD1	1:B:218:VAL:HG11	2.38	0.53
1:B:231:PRO:C	1:B:233:CYS:H	2.11	0.53
1:B:283:VAL:CG2	1:B:284:VAL:N	2.72	0.53
1:B:402:THR:HG21	1:B:432:ARG:HH21	1.71	0.53
1:A:59:VAL:O	1:A:60:ASP:O	2.26	0.53
1:A:120:GLY:O	1:A:123:THR:CG2	2.54	0.53
1:A:500:GLU:OE2	1:A:735:ARG:NH2	2.40	0.53
1:A:711:LEU:HD22	1:A:720:PHE:CZ	2.44	0.53
1:B:184:ARG:HA	1:B:187:GLU:OE2	2.09	0.53
1:B:407:ASN:O	1:B:439:GLY:HA2	2.09	0.53
1:B:549:ILE:O	1:B:553:CYS:HB2	2.09	0.53
1:B:709:CYS:HA	1:B:722:PRO:HA	1.89	0.53
1:A:124:GLY:O	1:A:127:THR:HG23	2.09	0.53
1:B:84:ILE:HD12	1:B:84:ILE:N	2.24	0.53
1:B:213:GLY:HA3	1:B:230:ILE:HG22	1.89	0.53
1:A:35:ARG:HD3	1:A:77:LEU:CD1	2.38	0.53
1:A:57:GLY:HA2	1:A:64:HIS:CD2	2.44	0.53
1:A:436:VAL:CG1	1:A:442:GLY:HA3	2.38	0.53
1:A:572:THR:O	1:A:629:GLU:HB3	2.08	0.53
1:B:407:ASN:HA	1:B:496:ILE:O	2.09	0.53
1:B:738:LYS:O	1:B:739:GLU:HB2	2.08	0.53
1:A:751:ILE:HD13	1:A:752:LEU:H	1.67	0.53
1:B:319:GLU:HG2	1:B:343:ALA:HB1	1.90	0.53
1:B:470:LYS:HG3	1:B:472:THR:HG23	1.90	0.53
1:A:746:ARG:N	1:A:747:PRO:HD2	2.24	0.52
1:B:41:GLY:O	1:B:44:THR:CG2	2.53	0.52
1:B:632:ASN:OD1	1:B:632:ASN:C	2.47	0.52
1:A:265:GLY:O	1:A:267:ILE:HG23	2.08	0.52
1:B:257:LEU:HD23	1:B:257:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:HD12	1:B:641:PHE:HA	1.91	0.52
1:B:358:VAL:HA	1:B:373:LEU:HD13	1.91	0.52
1:B:402:THR:CB	1:B:432:ARG:HH21	2.22	0.52
1:A:239:TRP:CD1	1:A:240:GLU:N	2.78	0.52
1:A:379:MET:O	1:A:383:GLU:HG2	2.09	0.52
1:A:509:MET:O	1:A:512:ARG:HB2	2.09	0.52
1:A:360:LYS:O	1:A:363:ASP:N	2.42	0.52
1:A:604:ASP:O	1:A:607:ALA:N	2.43	0.52
1:A:165:ILE:N	1:A:165:ILE:HD13	2.23	0.52
1:A:371:MET:CE	1:A:382:TRP:CD1	2.93	0.52
1:A:706:ASP:OD1	1:A:706:ASP:N	2.41	0.52
1:B:649:LYS:C	1:B:651:ILE:H	2.13	0.52
1:A:228:VAL:CG1	1:A:229:PHE:N	2.71	0.52
1:A:380:ASN:HD22	1:A:678:LYS:HE2	1.75	0.52
1:A:485:ILE:O	1:A:485:ILE:HG13	2.08	0.52
1:A:185:ILE:O	1:A:189:VAL:HG23	2.10	0.52
1:A:364:GLU:C	1:A:366:ARG:N	2.62	0.52
1:A:437:HIS:O	1:A:438:ASP:HB2	2.10	0.52
1:A:506:LEU:CD2	1:A:723:VAL:HB	2.39	0.52
1:B:126:ASP:O	1:B:129:ARG:HG3	2.09	0.52
1:A:247:LEU:HA	1:A:250:THR:CG2	2.40	0.52
1:A:374:ARG:HG2	1:A:378:PHE:CD2	2.45	0.51
1:A:689:GLY:O	1:A:692:LYS:N	2.43	0.51
1:B:55:TYR:O	1:B:58:LEU:N	2.42	0.51
1:B:145:ILE:C	1:B:147:ALA:H	2.13	0.51
1:B:419:VAL:HG11	1:B:467:LEU:CD1	2.37	0.51
1:B:459:TRP:O	1:B:462:GLN:HG3	2.09	0.51
1:B:664:GLN:O	1:B:666:GLY:N	2.43	0.51
1:B:687:MET:O	1:B:691:ILE:HG12	2.10	0.51
1:B:9:ALA:HB3	1:B:12:LEU:H	1.76	0.51
1:B:214:TYR:CZ	1:B:218:VAL:HG21	2.46	0.51
1:B:713:MET:HG3	1:B:718:LEU:CD1	2.40	0.51
1:A:138:ASP:C	1:A:140:GLN:H	2.14	0.51
1:A:139:LEU:O	1:A:143:GLY:HA3	2.10	0.51
1:B:262:VAL:HG12	1:B:263:ALA:O	2.10	0.51
1:A:39:ARG:HD2	1:A:70:TRP:CZ2	2.44	0.51
1:A:557:LYS:O	1:A:558:GLN:NE2	2.44	0.51
1:A:748:ILE:HG12	1:A:749:LEU:N	2.26	0.51
1:B:153:SER:O	1:B:155:TYR:N	2.43	0.51
1:B:212:CYS:HA	1:B:232:GLU:OE2	2.11	0.51
1:B:731:ASP:OD1	1:B:731:ASP:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB3	1:A:116:ILE:HD13	1.92	0.51
1:B:110:ILE:H	1:B:110:ILE:CD1	2.22	0.51
1:B:624:LEU:HD12	1:B:625:VAL:H	1.73	0.51
1:A:601:THR:O	1:A:601:THR:HG23	2.09	0.51
1:B:11:THR:HA	1:B:14:VAL:HG23	1.92	0.51
1:B:515:PHE:N	1:B:515:PHE:CD1	2.78	0.51
1:B:234:PRO:HG3	1:B:367:PHE:CZ	2.45	0.51
1:B:433:VAL:C	1:B:434:LEU:HD12	2.30	0.51
1:B:615:LYS:HB3	1:B:620:VAL:HG21	1.93	0.51
1:B:415:MET:O	1:B:419:VAL:HG23	2.10	0.51
1:B:551:THR:O	1:B:554:ASP:N	2.42	0.51
2:A:763:ATP:O5'	2:A:763:ATP:H8	1.93	0.51
1:B:311:ILE:HG23	1:B:586:LEU:HD23	1.93	0.51
1:B:595:ILE:N	1:B:595:ILE:CD1	2.74	0.51
1:A:227:TRP:CD1	1:A:228:VAL:N	2.79	0.50
1:A:259:ILE:CG2	1:A:261:ILE:CD1	2.82	0.50
1:A:316:MET:HE3	1:A:337:SER:HA	1.92	0.50
1:B:328:THR:HB	1:B:329:PRO:HD2	1.93	0.50
1:B:435:VAL:HG22	1:B:451:ALA:HB2	1.92	0.50
1:B:665:GLY:O	1:B:666:GLY:O	2.28	0.50
1:A:66:ARG:HH21	1:A:108:ARG:HH22	1.56	0.50
1:A:214:TYR:O	1:A:218:VAL:HG23	2.12	0.50
1:B:165:ILE:HD11	1:B:208:MET:HG2	1.93	0.50
1:A:165:ILE:H	1:A:165:ILE:CD1	2.24	0.50
1:B:435:VAL:CB	1:B:467:LEU:HD21	2.41	0.50
1:B:731:ASP:OD2	1:B:734:HIS:HD2	1.94	0.50
1:A:95:ARG:C	1:A:97:GLY:N	2.65	0.50
1:A:392:ARG:HB2	1:A:393:PRO:HA	1.87	0.50
1:B:248:SER:O	1:B:252:THR:HG22	2.10	0.50
1:B:294:THR:HG22	1:B:295:VAL:N	2.27	0.50
1:B:568:PHE:CD1	1:B:568:PHE:N	2.78	0.50
1:B:729:GLN:O	1:B:738:LYS:HG3	2.12	0.50
1:A:371:MET:SD	1:A:378:PHE:HE2	2.35	0.50
1:A:576:TYR:HD2	1:A:596:PHE:CD1	2.28	0.50
1:A:601:THR:O	1:A:603:ARG:N	2.44	0.50
1:B:63:ASP:C	1:B:65:ILE:H	2.15	0.50
1:B:281:ASP:C	1:B:283:VAL:N	2.63	0.50
1:A:596:PHE:C	1:A:596:PHE:CD2	2.84	0.50
1:A:645:SER:O	1:A:646:GLU:C	2.49	0.50
1:A:189:VAL:HG22	1:A:205:LEU:CD1	2.42	0.50
1:A:596:PHE:O	1:A:598:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:VAL:HG12	1:B:427:LEU:CD1	2.42	0.50
1:B:38:VAL:HG21	1:B:73:VAL:HG11	1.94	0.50
1:B:192:ILE:HG23	1:B:203:PHE:CE2	2.47	0.50
1:B:403:VAL:HG12	1:B:404:ALA:N	2.27	0.50
1:A:23:SER:HB3	1:A:121:SER:HB3	1.94	0.50
1:A:387:LEU:HD23	1:A:428:ILE:CD1	2.42	0.50
1:B:496:ILE:HG12	1:B:525:ILE:HD12	1.94	0.50
1:A:120:GLY:HA2	1:A:123:THR:CG2	2.40	0.49
1:A:481:ILE:O	1:A:485:ILE:HG23	2.12	0.49
1:A:628:ASN:HB3	1:A:631:CYS:HB3	1.94	0.49
1:B:280:LYS:HB2	1:B:293:VAL:HG21	1.93	0.49
1:B:289:TYR:O	1:B:291:THR:N	2.45	0.49
1:B:344:VAL:HG23	1:B:344:VAL:O	2.11	0.49
1:B:531:ASN:HD21	1:B:538:PHE:CA	2.25	0.49
1:B:47:ARG:HD2	1:B:67:GLU:CD	2.32	0.49
1:B:421:SER:O	1:B:425:ILE:N	2.39	0.49
1:A:295:VAL:HG12	1:A:295:VAL:O	2.10	0.49
1:B:741:TRP:CG	1:B:742:TRP:N	2.80	0.49
1:A:393:PRO:HB3	1:A:453:TRP:CE3	2.47	0.49
1:B:159:VAL:CG2	1:B:324:LEU:HD23	2.34	0.49
1:B:234:PRO:HB2	1:B:268:ASP:C	2.33	0.49
1:B:562:GLY:O	1:B:564:LYS:N	2.45	0.49
1:A:50:PHE:CZ	1:A:84:ILE:HD11	2.47	0.49
1:B:9:ALA:C	1:B:11:THR:N	2.65	0.49
1:B:564:LYS:O	1:B:565:ARG:C	2.50	0.49
1:A:388:LEU:CD2	1:A:424:ARG:HB2	2.42	0.49
1:A:418:ALA:HB2	1:A:676:ALA:HB1	1.94	0.49
1:A:482:SER:HA	1:A:485:ILE:HG23	1.94	0.49
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.93	0.49
1:A:65:ILE:HB	1:A:108:ARG:HH12	1.78	0.49
1:A:125:ALA:O	1:A:128:PHE:HB3	2.13	0.49
1:B:41:GLY:C	1:B:44:THR:HG22	2.33	0.49
1:B:618:THR:CG2	1:B:619:THR:H	2.16	0.49
1:B:169:PHE:CZ	1:B:351:CYS:HB3	2.48	0.49
1:A:70:TRP:CZ2	1:A:754:LYS:HB2	2.48	0.49
1:A:130:SER:C	1:A:132:TRP:H	2.17	0.49
1:A:328:THR:C	1:A:330:ASP:H	2.16	0.49
1:B:456:VAL:HA	1:B:459:TRP:CE2	2.48	0.49
1:A:169:PHE:CZ	1:A:351:CYS:HB3	2.48	0.49
1:A:714:ARG:HG3	1:A:719:VAL:HG13	1.95	0.49
1:B:352:VAL:O	1:B:355:THR:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:NH2	1:A:108:ARG:NH2	2.61	0.48
1:A:336:VAL:HA	1:A:344:VAL:O	2.13	0.48
1:A:367:PHE:O	1:A:370:ALA:HB3	2.14	0.48
1:B:283:VAL:CG2	1:B:284:VAL:H	2.26	0.48
1:B:360:LYS:O	1:B:363:ASP:N	2.44	0.48
1:B:193:THR:CG2	1:B:194:THR:N	2.76	0.48
1:B:734:HIS:O	1:B:736:ILE:N	2.46	0.48
1:A:216:ALA:O	1:A:219:THR:HG22	2.14	0.48
1:A:407:ASN:HA	1:A:496:ILE:O	2.12	0.48
1:A:669:THR:HB	1:A:670:PRO:HD2	1.96	0.48
1:A:696:ARG:HH11	1:A:696:ARG:CG	2.21	0.48
1:B:231:PRO:C	1:B:233:CYS:N	2.67	0.48
1:B:400:SER:HB2	1:B:431:ASN:HA	1.94	0.48
1:B:424:ARG:HD2	1:B:453:TRP:CZ2	2.48	0.48
1:B:510:GLU:HA	1:B:510:GLU:OE1	2.13	0.48
1:A:696:ARG:NH1	1:A:696:ARG:CG	2.76	0.48
1:B:69:THR:HG23	1:B:72:SER:CB	2.41	0.48
1:B:567:VAL:HG22	1:B:616:MET:CE	2.42	0.48
1:B:679:MET:O	1:B:680:GLY:C	2.51	0.48
1:B:41:GLY:HA2	1:B:44:THR:HG22	1.94	0.48
1:B:247:LEU:CA	1:B:250:THR:HG22	2.43	0.48
1:B:426:GLY:HA2	1:B:684:MET:HE2	1.94	0.48
1:A:73:VAL:HG12	1:A:76:MET:SD	2.53	0.48
1:A:82:THR:HG21	1:A:86:SER:CB	2.41	0.48
1:A:635:TYR:N	1:A:635:TYR:CD2	2.79	0.48
1:B:435:VAL:HG12	1:B:467:LEU:HD21	1.95	0.48
1:A:65:ILE:HB	1:A:108:ARG:NH1	2.29	0.48
1:A:239:TRP:O	1:A:242:HIS:HB3	2.14	0.48
1:A:304:THR:OG1	1:A:305:PRO:HD2	2.14	0.48
1:A:679:MET:CE	1:A:718:LEU:HD11	2.44	0.48
1:B:21:LEU:HB2	1:B:51:VAL:HB	1.94	0.48
1:B:122:LEU:O	1:B:125:ALA:HB3	2.13	0.48
1:B:747:PRO:O	1:B:751:ILE:HG23	2.14	0.48
1:B:751:ILE:HD11	1:B:752:LEU:HD23	1.95	0.48
1:B:111:THR:O	1:B:156:LEU:HD12	2.13	0.48
1:B:307:ALA:H	1:B:547:ASN:ND2	2.10	0.48
1:B:376:ARG:HH21	1:B:376:ARG:CB	2.26	0.48
1:B:741:TRP:CD2	1:B:742:TRP:N	2.82	0.48
1:B:751:ILE:CD1	1:B:752:LEU:HD23	2.43	0.48
1:A:69:THR:O	1:A:72:SER:OG	2.30	0.48
1:A:282:LEU:HG	1:A:283:VAL:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:HG3	1:A:336:VAL:CG1	2.44	0.48
1:A:580:LEU:O	1:A:581:ALA:C	2.51	0.48
1:B:312:LEU:O	1:B:316:MET:HG2	2.14	0.48
1:B:450:GLU:HG3	1:B:451:ALA:N	2.24	0.48
1:B:547:ASN:O	1:B:550:CYS:N	2.47	0.48
1:B:165:ILE:HB	1:B:181:ALA:HB2	1.96	0.47
1:B:214:TYR:O	1:B:216:ALA:N	2.46	0.47
1:B:470:LYS:HE2	1:B:471:ARG:N	2.26	0.47
1:A:49:PHE:CD1	1:A:110:ILE:CD1	2.97	0.47
1:A:391:ILE:CD1	1:A:392:ARG:N	2.73	0.47
1:B:116:ILE:HG12	1:B:161:LEU:HB3	1.95	0.47
1:B:560:ALA:C	1:B:622:ARG:HH22	2.18	0.47
1:A:42:ILE:O	1:A:45:GLY:N	2.47	0.47
1:A:104:ASN:O	1:A:108:ARG:HG2	2.13	0.47
1:A:391:ILE:O	1:A:392:ARG:O	2.32	0.47
1:B:84:ILE:N	1:B:84:ILE:CD1	2.78	0.47
1:B:205:LEU:CD2	1:B:294:THR:HB	2.42	0.47
1:A:275:THR:HG23	1:A:278:GLY:H	1.80	0.47
1:B:364:GLU:C	1:B:366:ARG:H	2.17	0.47
1:A:212:CYS:SG	1:A:214:TYR:HB2	2.54	0.47
1:A:440:PHE:C	1:A:442:GLY:N	2.65	0.47
1:A:475:LYS:C	1:A:477:SER:H	2.18	0.47
1:A:570:ILE:HA	1:A:657:ASN:O	2.14	0.47
1:A:742:TRP:CZ3	1:A:743:LEU:HG	2.50	0.47
1:B:30:MET:O	1:B:34:VAL:HG23	2.14	0.47
1:B:360:LYS:O	1:B:362:MET:N	2.48	0.47
1:A:440:PHE:C	1:A:442:GLY:H	2.14	0.47
1:B:549:ILE:CD1	1:B:659:LEU:HD13	2.38	0.47
1:A:66:ARG:NH1	1:A:67:GLU:H	2.11	0.47
1:A:239:TRP:CH2	1:A:274:ILE:HD12	2.49	0.47
1:B:234:PRO:HG3	1:B:367:PHE:CE1	2.49	0.47
1:B:247:LEU:CD2	1:B:258:ASN:ND2	2.72	0.47
1:B:370:ALA:O	1:B:374:ARG:N	2.48	0.47
1:B:402:THR:CG2	1:B:491:GLN:HE21	2.28	0.47
1:B:403:VAL:HG21	1:B:684:MET:HE3	1.97	0.47
1:B:477:SER:O	1:B:481:ILE:HG23	2.14	0.47
1:B:512:ARG:NH2	1:B:707:SER:HB2	2.27	0.47
1:A:335:VAL:HG23	1:A:348:LEU:CG	2.39	0.47
1:A:435:VAL:CG1	1:A:467:LEU:CD2	2.93	0.47
1:A:457:GLY:HA2	4:A:767:PO4:O3	2.15	0.47
1:A:565:ARG:NH1	1:A:618:THR:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:GLY:O	1:A:691:ILE:N	2.48	0.47
1:B:153:SER:C	1:B:155:TYR:N	2.68	0.47
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.72	0.47
1:B:578:GLY:H	1:B:597:GLU:CD	2.18	0.47
1:A:120:GLY:C	1:A:123:THR:HG22	2.35	0.47
1:A:475:LYS:C	1:A:477:SER:N	2.69	0.47
1:A:613:VAL:C	1:A:615:LYS:H	2.17	0.47
1:B:11:THR:HG23	1:B:12:LEU:N	2.30	0.47
1:B:100:ARG:O	1:B:104:ASN:ND2	2.47	0.47
1:B:562:GLY:C	1:B:564:LYS:N	2.68	0.47
1:B:756:GLU:O	1:B:756:GLU:HG2	2.14	0.47
1:A:571:GLU:HB3	1:A:658:VAL:HG22	1.97	0.47
1:A:679:MET:O	1:A:680:GLY:C	2.51	0.47
1:B:27:ALA:O	1:B:30:MET:HG3	2.15	0.47
1:B:149:GLU:O	1:B:153:SER:HB3	2.15	0.47
1:B:610:GLU:O	1:B:614:GLN:HG2	2.15	0.47
1:A:193:THR:CG2	1:A:194:THR:N	2.78	0.46
1:A:424:ARG:HD2	1:A:453:TRP:CE2	2.50	0.46
1:B:531:ASN:ND2	1:B:538:PHE:HA	2.28	0.46
1:B:595:ILE:HD11	1:B:598:GLU:HB3	1.97	0.46
1:A:473:LEU:HD22	1:A:474:PRO:HD2	1.97	0.46
1:B:420:ARG:NH1	1:B:460:THR:HG21	2.30	0.46
1:B:605:LEU:O	1:B:609:VAL:HG23	2.15	0.46
1:A:382:TRP:CE2	1:A:386:LYS:HD2	2.50	0.46
1:A:435:VAL:HG13	1:A:467:LEU:HD22	1.97	0.46
1:A:714:ARG:HG3	1:A:719:VAL:CG1	2.46	0.46
1:B:214:TYR:C	1:B:216:ALA:H	2.18	0.46
1:B:279:VAL:O	1:B:281:ASP:N	2.47	0.46
1:B:340:GLY:O	1:B:342:GLN:HG3	2.16	0.46
1:B:358:VAL:HG12	1:B:358:VAL:O	2.15	0.46
1:B:402:THR:HG21	1:B:489:ASN:HD22	1.81	0.46
1:A:35:ARG:CD	1:A:77:LEU:HD13	2.45	0.46
1:A:117:GLY:O	1:A:163:GLY:N	2.46	0.46
1:A:393:PRO:HB3	1:A:453:TRP:CZ3	2.50	0.46
1:B:279:VAL:O	1:B:283:VAL:HG13	2.16	0.46
1:B:308:PHE:CZ	1:B:312:LEU:HD22	2.51	0.46
1:B:560:ALA:O	1:B:622:ARG:NH2	2.47	0.46
1:B:566:ARG:CD	1:B:653:ASP:HB3	2.45	0.46
1:B:605:LEU:HD12	1:B:605:LEU:HA	1.75	0.46
1:B:660:GLY:O	1:B:662:MET:N	2.47	0.46
1:A:235:PRO:O	1:A:236:ASP:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:O	1:B:253:ARG:N	2.48	0.46
1:B:378:PHE:C	1:B:378:PHE:CD2	2.89	0.46
1:B:601:THR:O	1:B:604:ASP:N	2.42	0.46
1:A:517:GLU:C	1:A:519:CYS:H	2.18	0.46
1:A:628:ASN:O	1:A:630:LYS:N	2.49	0.46
1:A:719:VAL:HG22	1:A:721:GLN:HG2	1.98	0.46
1:B:277:GLU:O	1:B:280:LYS:HB3	2.16	0.46
1:B:323:ALA:HA	1:B:345:ARG:NH1	2.31	0.46
1:B:387:LEU:CD2	1:B:428:ILE:HG21	2.45	0.46
1:B:509:MET:CE	1:B:705:PRO:HA	2.45	0.46
1:B:658:VAL:O	1:B:658:VAL:CG1	2.54	0.46
2:B:763:ATP:O5'	2:B:763:ATP:H8	1.98	0.46
1:A:58:LEU:CD1	1:A:105:LEU:HD21	2.40	0.46
1:A:239:TRP:CD1	1:A:239:TRP:C	2.89	0.46
1:B:302:GLY:O	1:B:303:GLY:O	2.33	0.46
1:B:387:LEU:HD23	1:B:428:ILE:HD13	1.98	0.46
1:B:459:TRP:CG	1:B:466:LYS:NZ	2.83	0.46
1:B:512:ARG:HG2	1:B:519:CYS:SG	2.56	0.46
1:B:618:THR:CG2	1:B:619:THR:N	2.64	0.46
1:B:687:MET:HE3	1:B:687:MET:C	2.36	0.46
1:A:243:LEU:CD1	1:A:247:LEU:HD12	2.46	0.46
1:A:594:TYR:OH	1:A:608:ASN:ND2	2.46	0.46
1:B:192:ILE:HG23	1:B:203:PHE:CZ	2.50	0.46
1:B:336:VAL:HG23	1:B:336:VAL:O	2.16	0.46
1:A:50:PHE:CD2	1:A:84:ILE:HD11	2.51	0.46
1:A:673:ARG:O	1:A:677:THR:HB	2.15	0.46
1:A:742:TRP:C	1:A:744:LYS:N	2.69	0.46
1:B:342:GLN:NE2	1:B:715:LYS:HD2	2.31	0.46
1:A:165:ILE:N	1:A:165:ILE:CD1	2.79	0.46
1:B:214:TYR:C	1:B:216:ALA:N	2.69	0.46
1:B:621:LYS:O	1:B:622:ARG:HD2	2.16	0.46
1:A:662:MET:O	1:A:663:GLN:C	2.54	0.45
1:B:565:ARG:HA	1:B:621:LYS:O	2.16	0.45
1:A:56:GLN:O	1:A:58:LEU:N	2.50	0.45
1:A:328:THR:O	1:A:330:ASP:N	2.49	0.45
1:B:364:GLU:C	1:B:366:ARG:N	2.70	0.45
1:A:371:MET:HE2	1:A:382:TRP:CD1	2.52	0.45
1:B:184:ARG:HD3	1:B:187:GLU:OE2	2.16	0.45
1:B:560:ALA:C	1:B:562:GLY:H	2.20	0.45
1:B:601:THR:O	1:B:602:ILE:C	2.54	0.45
1:B:609:VAL:HG22	1:B:644:TYR:CD2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD23	1:A:325:LEU:HD13	1.98	0.45
1:A:42:ILE:O	1:A:44:THR:N	2.49	0.45
1:A:506:LEU:HD23	1:A:723:VAL:HB	1.98	0.45
1:A:556:ILE:O	1:A:558:GLN:N	2.45	0.45
1:A:748:ILE:HG12	1:A:749:LEU:H	1.82	0.45
1:B:299:VAL:O	1:B:302:GLY:N	2.37	0.45
1:A:392:ARG:HB3	1:A:393:PRO:C	2.36	0.45
1:A:606:GLN:OE1	1:B:606:GLN:OE1	2.35	0.45
1:B:380:ASN:O	1:B:381:ASN:C	2.55	0.45
1:B:404:ALA:HB2	1:B:490:ILE:CD1	2.46	0.45
1:B:484:ASN:C	1:B:486:THR:N	2.69	0.45
1:B:566:ARG:O	1:B:616:MET:HE1	2.17	0.45
1:B:748:ILE:O	1:B:752:LEU:HG	2.16	0.45
1:A:21:LEU:HD23	1:A:22:THR:N	2.32	0.45
1:A:339:SER:OG	1:A:344:VAL:HG11	2.16	0.45
1:A:280:LYS:HB2	1:A:293:VAL:CG2	2.47	0.45
1:A:564:LYS:O	1:A:565:ARG:O	2.35	0.45
1:A:690:LYS:HE3	1:A:706:ASP:HB2	1.98	0.45
1:B:376:ARG:HB3	1:B:376:ARG:NH2	2.31	0.45
1:A:414:GLY:HA3	1:A:540:VAL:CG1	2.46	0.45
1:B:376:ARG:NH2	1:B:376:ARG:HB2	2.32	0.45
1:B:459:TRP:HD1	1:B:459:TRP:N	2.05	0.45
1:B:502:TYR:OH	1:B:730:THR:CG2	2.64	0.45
1:B:552:THR:HG21	1:B:659:LEU:CD2	2.47	0.45
1:A:413:ALA:HB1	1:A:668:PRO:HA	1.98	0.45
1:B:340:GLY:O	1:B:342:GLN:N	2.51	0.45
1:B:403:VAL:HG21	1:B:684:MET:CE	2.46	0.45
1:B:508:LEU:O	1:B:509:MET:C	2.55	0.45
1:B:638:ASP:OD1	1:B:638:ASP:N	2.49	0.45
1:B:734:HIS:O	1:B:735:ARG:C	2.54	0.45
1:A:203:PHE:CD1	1:A:203:PHE:N	2.85	0.44
1:A:391:ILE:CD1	2:A:765:ATP:PG	3.02	0.44
1:A:486:THR:HG22	1:A:487:LYS:N	2.32	0.44
1:A:502:TYR:OH	1:A:730:THR:HG21	2.17	0.44
1:A:652:PHE:HD1	1:A:653:ASP:O	1.99	0.44
1:B:83:VAL:HG12	1:B:84:ILE:HD12	1.99	0.44
1:B:551:THR:HG22	1:B:552:THR:H	1.80	0.44
1:A:319:GLU:HG3	1:A:336:VAL:HB	1.99	0.44
1:A:500:GLU:CD	1:A:735:ARG:HH21	2.19	0.44
1:A:571:GLU:HA	1:A:627:ARG:O	2.17	0.44
1:B:333:ALA:HB3	1:B:348:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:ARG:HB3	1:B:697:ASN:H	1.51	0.44
1:A:407:ASN:HB3	1:A:469:SER:HB3	1.99	0.44
1:A:596:PHE:C	1:A:598:GLU:H	2.21	0.44
1:B:69:THR:O	1:B:70:TRP:C	2.55	0.44
1:B:433:VAL:O	1:B:434:LEU:HD12	2.17	0.44
1:B:659:LEU:HD23	1:B:659:LEU:HA	1.73	0.44
1:A:159:VAL:HG11	1:A:320:ALA:HA	1.99	0.44
1:A:711:LEU:CD1	1:A:718:LEU:HG	2.46	0.44
1:A:745:LEU:C	1:A:747:PRO:HD2	2.37	0.44
1:B:84:ILE:HG22	1:B:84:ILE:O	2.17	0.44
1:B:644:TYR:O	1:B:645:SER:C	2.54	0.44
1:A:13:GLY:O	1:A:46:ALA:HA	2.17	0.44
1:A:354:VAL:C	1:A:356:LYS:N	2.71	0.44
1:A:375:GLY:HA2	1:A:379:MET:HE2	2.00	0.44
1:A:537:ASP:OD1	1:A:714:ARG:NH2	2.37	0.44
1:B:190:ASP:O	1:B:193:THR:HG22	2.17	0.44
1:B:215:LEU:O	1:B:219:THR:HG21	2.16	0.44
1:A:629:GLU:O	1:A:630:LYS:HG3	2.17	0.44
1:A:165:ILE:HD13	1:A:165:ILE:H	1.82	0.44
1:A:377:SER:O	1:A:378:PHE:C	2.55	0.44
1:A:459:TRP:NE1	1:A:466:LYS:NZ	2.65	0.44
1:A:742:TRP:CE3	1:A:743:LEU:HG	2.53	0.44
1:B:185:ILE:C	1:B:185:ILE:HD13	2.37	0.44
1:B:279:VAL:C	1:B:281:ASP:N	2.70	0.44
1:A:252:THR:C	1:A:254:GLY:H	2.20	0.44
1:A:294:THR:CG2	1:A:295:VAL:N	2.81	0.44
1:A:524:VAL:HB	1:A:710:VAL:CG2	2.47	0.44
1:A:582:THR:OG1	1:A:746:ARG:NH1	2.50	0.44
1:A:745:LEU:O	1:A:746:ARG:C	2.55	0.44
1:B:56:GLN:O	1:B:60:ASP:OD2	2.36	0.44
1:A:41:GLY:O	1:A:44:THR:HG22	2.17	0.44
1:A:408:VAL:O	1:A:497:GLY:CA	2.66	0.44
1:A:579:TYR:HD1	1:A:742:TRP:CD1	2.36	0.44
1:B:180:SER:O	1:B:181:ALA:C	2.56	0.44
1:B:245:ARG:HH11	1:B:245:ARG:HG2	1.83	0.44
1:B:416:ASN:O	1:B:417:ALA:C	2.55	0.44
1:B:696:ARG:O	1:B:698:GLY:N	2.50	0.44
1:B:730:THR:O	1:B:738:LYS:HD2	2.17	0.44
1:B:754:LYS:O	1:B:755:TYR:O	2.36	0.44
1:A:371:MET:O	1:A:379:MET:HE2	2.18	0.43
1:A:140:GLN:NE2	1:A:144:LYS:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:OE2	1:A:374:ARG:NE	2.51	0.43
1:A:360:LYS:C	1:A:362:MET:N	2.71	0.43
1:A:435:VAL:CG1	1:A:467:LEU:HD22	2.48	0.43
1:B:78:GLN:H	1:B:78:GLN:CD	2.20	0.43
1:B:404:ALA:CB	1:B:490:ILE:HD12	2.47	0.43
1:B:555:ARG:HG2	1:B:556:ILE:N	2.34	0.43
1:A:598:GLU:HA	1:A:599:PRO:HD2	1.83	0.43
1:A:613:VAL:C	1:A:615:LYS:N	2.71	0.43
1:B:205:LEU:HB2	1:B:261:ILE:HD13	2.00	0.43
1:B:352:VAL:HA	1:B:355:THR:HB	1.99	0.43
1:B:393:PRO:HD3	1:B:453:TRP:CD2	2.53	0.43
1:A:239:TRP:CG	1:A:240:GLU:N	2.86	0.43
1:A:387:LEU:CD2	1:A:428:ILE:HD13	2.45	0.43
1:A:413:ALA:HB1	1:A:668:PRO:CA	2.49	0.43
1:B:193:THR:HA	1:B:257:LEU:HD11	2.00	0.43
1:A:21:LEU:HD23	1:A:21:LEU:C	2.38	0.43
1:A:257:LEU:HD23	1:A:257:LEU:N	2.20	0.43
1:A:358:VAL:HG22	1:A:373:LEU:HB3	2.00	0.43
1:A:509:MET:O	1:A:512:ARG:N	2.50	0.43
1:B:240:GLU:CG	1:B:282:LEU:HD22	2.49	0.43
1:B:307:ALA:O	1:B:311:ILE:HG12	2.18	0.43
1:B:481:ILE:HD12	1:B:485:ILE:HG23	2.00	0.43
1:B:528:THR:HG23	1:B:528:THR:O	2.19	0.43
1:B:576:TYR:CE1	1:B:630:LYS:HD2	2.53	0.43
1:A:186:THR:HG22	1:A:190:ASP:OD2	2.18	0.43
1:A:686:TRP:HZ3	1:A:687:MET:HG2	1.82	0.43
1:B:109:GLY:O	1:B:110:ILE:C	2.57	0.43
1:B:243:LEU:HD12	1:B:243:LEU:O	2.17	0.43
1:B:424:ARG:HD2	1:B:453:TRP:CH2	2.54	0.43
1:B:485:ILE:CG1	1:B:517:GLU:HB3	2.48	0.43
1:B:609:VAL:HG22	1:B:644:TYR:CZ	2.50	0.43
1:B:742:TRP:C	1:B:744:LYS:H	2.21	0.43
1:A:679:MET:HG2	1:A:718:LEU:HD21	2.01	0.43
1:A:38:VAL:O	1:A:42:ILE:HG12	2.19	0.43
1:A:185:ILE:CD1	1:A:215:LEU:HD23	2.49	0.43
1:B:193:THR:O	1:B:195:THR:N	2.52	0.43
1:B:355:THR:HG22	1:B:356:LYS:N	2.34	0.43
1:B:547:ASN:O	1:B:548:THR:C	2.57	0.43
1:B:566:ARG:HD2	1:B:653:ASP:OD2	2.18	0.43
1:B:615:LYS:HB3	1:B:620:VAL:CG2	2.48	0.43
1:A:13:GLY:CA	1:A:44:THR:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASN:O	1:A:259:ILE:HD12	2.18	0.43
1:A:558:GLN:O	1:A:559:SER:O	2.37	0.43
1:B:295:VAL:O	1:B:296:LEU:C	2.54	0.43
1:B:414:GLY:HA3	1:B:540:VAL:CG1	2.49	0.43
1:B:510:GLU:C	1:B:512:ARG:N	2.72	0.43
1:A:544:THR:OG1	1:A:669:THR:HG23	2.19	0.43
1:A:684:MET:O	1:A:684:MET:HG3	2.19	0.43
1:B:78:GLN:OE1	1:B:78:GLN:N	2.37	0.43
1:B:113:LEU:O	1:B:158:ILE:HA	2.19	0.43
1:A:275:THR:HG23	1:A:278:GLY:N	2.34	0.42
1:A:503:THR:CG2	1:A:504:GLY:N	2.79	0.42
1:B:200:GLN:HA	1:B:256:ARG:O	2.19	0.42
1:B:402:THR:CG2	1:B:432:ARG:HH21	2.30	0.42
1:B:510:GLU:C	1:B:512:ARG:H	2.22	0.42
1:B:520:ILE:HA	1:B:521:PRO:HD3	1.84	0.42
1:A:234:PRO:HG3	1:A:367:PHE:CZ	2.53	0.42
1:A:564:LYS:HE2	1:A:564:LYS:CA	2.50	0.42
1:A:679:MET:C	1:A:681:ALA:N	2.72	0.42
1:A:742:TRP:C	1:A:744:LYS:H	2.21	0.42
1:B:89:CYS:O	1:B:89:CYS:SG	2.77	0.42
1:B:242:HIS:O	1:B:246:ARG:HG2	2.19	0.42
1:A:112:ASN:HB3	1:A:324:LEU:HD13	2.01	0.42
1:A:307:ALA:O	1:A:311:ILE:HG13	2.19	0.42
1:A:634:ASN:HB2	1:B:646:GLU:CG	2.48	0.42
1:A:669:THR:CB	1:A:670:PRO:HD2	2.49	0.42
1:B:218:VAL:HG12	1:B:219:THR:N	2.35	0.42
1:B:328:THR:CB	1:B:329:PRO:CD	2.93	0.42
1:A:120:GLY:O	1:A:121:SER:C	2.58	0.42
1:A:158:ILE:HD13	1:A:158:ILE:H	1.84	0.42
1:A:319:GLU:CG	1:A:336:VAL:HB	2.50	0.42
1:A:429:GLN:HE22	1:A:685:ASN:HA	1.85	0.42
1:A:564:LYS:HB3	1:A:565:ARG:H	1.72	0.42
1:A:604:ASP:O	1:A:606:GLN:N	2.52	0.42
1:B:319:GLU:HG3	1:B:336:VAL:HB	2.01	0.42
1:B:359:THR:O	1:B:362:MET:HB2	2.19	0.42
1:B:549:ILE:HD12	1:B:659:LEU:CD1	2.37	0.42
1:A:227:TRP:HB3	1:A:260:ILE:HG23	2.00	0.42
1:B:29:GLY:HA3	1:B:176:ILE:CG2	2.49	0.42
1:B:185:ILE:CD1	1:B:219:THR:HB	2.49	0.42
1:B:554:ASP:O	1:B:557:LYS:HB3	2.19	0.42
1:A:65:ILE:HG22	1:A:65:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:O	1:A:77:LEU:C	2.58	0.42
1:A:388:LEU:HD23	1:A:424:ARG:CB	2.49	0.42
1:A:491:GLN:CB	1:A:700:ILE:HD11	2.39	0.42
1:B:284:VAL:HA	1:B:288:GLY:HA2	2.02	0.42
1:A:193:THR:CG2	1:A:194:THR:HG23	2.50	0.42
1:A:352:VAL:O	1:A:355:THR:HG22	2.20	0.42
1:A:751:ILE:HD11	1:A:752:LEU:HD23	2.02	0.42
1:B:132:TRP:CE3	1:B:156:LEU:HD22	2.55	0.42
1:B:192:ILE:HD13	1:B:192:ILE:N	2.34	0.42
1:B:240:GLU:HG2	1:B:282:LEU:HD22	2.02	0.42
1:B:481:ILE:HD12	1:B:485:ILE:CG2	2.50	0.42
1:B:509:MET:HE3	1:B:705:PRO:HA	2.02	0.42
1:A:13:GLY:N	1:A:44:THR:O	2.53	0.42
1:A:18:ILE:CG2	1:A:112:ASN:HB2	2.41	0.42
1:A:360:LYS:O	1:A:362:MET:N	2.52	0.42
1:A:575:GLY:HA2	1:A:630:LYS:HE2	2.02	0.42
1:B:204:VAL:HB	1:B:293:VAL:HG22	2.01	0.42
1:B:502:TYR:O	1:B:505:GLY:N	2.42	0.42
1:A:261:ILE:HD12	1:A:261:ILE:N	2.35	0.42
1:A:328:THR:C	1:A:330:ASP:N	2.73	0.42
1:B:110:ILE:HD12	1:B:110:ILE:N	2.33	0.42
1:B:342:GLN:HE21	1:B:715:LYS:HD2	1.84	0.42
1:B:628:ASN:HB3	1:B:631:CYS:HB3	2.01	0.42
1:A:193:THR:HG23	1:A:194:THR:HG23	2.01	0.42
1:A:248:SER:O	1:A:249:GLU:C	2.59	0.42
1:A:344:VAL:HG23	1:A:346:LEU:HG	2.01	0.42
1:A:375:GLY:HA2	1:A:379:MET:HE3	2.02	0.42
1:A:565:ARG:HH21	1:A:565:ARG:CG	2.32	0.42
1:B:84:ILE:O	1:B:84:ILE:CG2	2.68	0.42
1:B:184:ARG:HA	1:B:184:ARG:HD3	1.76	0.42
1:B:228:VAL:HG23	1:B:385:TYR:CE2	2.55	0.42
1:B:280:LYS:C	1:B:283:VAL:HG22	2.40	0.42
1:A:323:ALA:HA	1:A:345:ARG:NH1	2.35	0.41
1:A:509:MET:O	1:A:510:GLU:C	2.59	0.41
1:A:604:ASP:O	1:A:605:LEU:C	2.57	0.41
1:A:634:ASN:HB2	1:B:646:GLU:HG2	2.02	0.41
1:A:158:ILE:HD13	1:A:158:ILE:O	2.20	0.41
1:A:264:GLU:C	1:A:266:ALA:H	2.23	0.41
1:A:377:SER:O	1:A:380:ASN:N	2.53	0.41
1:A:524:VAL:HB	1:A:710:VAL:HG22	2.02	0.41
1:B:280:LYS:HB2	1:B:293:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LYS:C	1:B:477:SER:H	2.23	0.41
1:B:585:GLY:CA	1:B:626:LEU:HD12	2.47	0.41
1:A:39:ARG:CD	1:A:70:TRP:CE2	3.02	0.41
1:B:41:GLY:CA	1:B:44:THR:HG22	2.49	0.41
1:B:69:THR:O	1:B:72:SER:N	2.41	0.41
1:B:742:TRP:C	1:B:744:LYS:N	2.74	0.41
1:A:22:THR:HG23	1:A:85:GLY:O	2.21	0.41
1:B:59:VAL:HA	1:B:101:ALA:HB2	2.03	0.41
1:B:132:TRP:CD2	1:B:156:LEU:HD22	2.56	0.41
1:A:505:GLY:O	1:A:508:LEU:N	2.42	0.41
1:A:618:THR:HG22	1:A:619:THR:N	2.35	0.41
1:B:251:ARG:C	1:B:253:ARG:H	2.23	0.41
1:B:426:GLY:CA	1:B:684:MET:HE2	2.50	0.41
1:B:578:GLY:HA3	1:B:595:ILE:HB	2.02	0.41
1:B:627:ARG:HG2	1:B:627:ARG:HH11	1.85	0.41
1:A:50:PHE:O	1:A:51:VAL:CG2	2.67	0.41
1:A:169:PHE:CE2	1:A:351:CYS:HB3	2.56	0.41
1:A:435:VAL:CG1	1:A:467:LEU:HD21	2.51	0.41
1:A:454:SER:O	1:A:455:TYR:C	2.59	0.41
1:A:544:THR:O	1:A:545:ALA:C	2.56	0.41
1:A:581:ALA:O	1:A:585:GLY:N	2.50	0.41
1:A:597:GLU:H	1:A:597:GLU:CD	2.21	0.41
1:A:609:VAL:HG22	1:A:644:TYR:CZ	2.55	0.41
1:B:63:ASP:O	1:B:65:ILE:N	2.53	0.41
1:B:101:ALA:O	1:B:104:ASN:HB2	2.21	0.41
1:B:181:ALA:O	1:B:185:ILE:HG22	2.21	0.41
1:B:244:CYS:C	1:B:246:ARG:N	2.74	0.41
1:B:520:ILE:CG2	1:B:700:ILE:HD11	2.40	0.41
1:A:515:PHE:CD1	1:A:515:PHE:N	2.89	0.41
1:B:124:GLY:C	1:B:127:THR:HG22	2.41	0.41
1:B:193:THR:HA	1:B:257:LEU:CD1	2.50	0.41
1:B:402:THR:HB	1:B:432:ARG:HE	1.85	0.41
1:B:551:THR:CG2	1:B:552:THR:N	2.78	0.41
1:A:162:VAL:CG1	1:A:175:THR:HG22	2.50	0.41
1:A:215:LEU:O	1:A:219:THR:HB	2.21	0.41
1:A:473:LEU:HA	1:A:473:LEU:HD23	1.63	0.41
1:A:517:GLU:C	1:A:519:CYS:N	2.74	0.41
1:B:419:VAL:CG1	1:B:467:LEU:HD11	2.43	0.41
1:B:524:VAL:HB	1:B:710:VAL:HG22	2.02	0.41
1:B:632:ASN:OD1	1:B:634:ASN:N	2.54	0.41
1:A:181:ALA:O	1:A:185:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD11	1:A:260:ILE:HD11	2.03	0.41
1:A:491:GLN:HE21	1:A:700:ILE:HD13	1.86	0.41
1:A:596:PHE:C	1:A:598:GLU:N	2.74	0.41
1:B:22:THR:HG21	1:B:82:THR:OG1	2.20	0.41
1:B:39:ARG:HG3	1:B:39:ARG:NH1	2.33	0.41
1:B:251:ARG:C	1:B:253:ARG:N	2.75	0.41
1:B:299:VAL:CG2	1:B:300:GLN:N	2.84	0.41
1:B:423:VAL:HG12	1:B:427:LEU:HD11	2.02	0.41
1:A:388:LEU:HD23	1:A:424:ARG:HB2	2.02	0.41
1:B:230:ILE:HA	1:B:231:PRO:HD3	1.87	0.41
1:B:440:PHE:C	1:B:443:PRO:HD2	2.40	0.41
1:B:471:ARG:NH2	4:B:768:PO4:O1	2.53	0.41
1:A:153:SER:C	1:A:155:TYR:N	2.70	0.40
1:A:403:VAL:CG1	1:A:404:ALA:N	2.84	0.40
1:A:414:GLY:HA3	1:A:540:VAL:HG11	2.03	0.40
1:A:493:LEU:O	1:A:522:PHE:HA	2.21	0.40
1:B:229:PHE:HZ	1:B:239:TRP:CZ3	2.39	0.40
1:B:679:MET:HE3	1:B:718:LEU:HD11	2.01	0.40
1:A:101:ALA:O	1:A:104:ASN:HB2	2.22	0.40
1:A:184:ARG:HD2	1:A:302:GLY:O	2.21	0.40
1:A:208:MET:CG	1:A:209:GLY:H	2.33	0.40
1:A:473:LEU:HB3	1:A:474:PRO:HD2	2.03	0.40
1:A:602:ILE:O	1:A:602:ILE:HG13	2.21	0.40
1:B:723:VAL:HG23	1:B:724:THR:H	1.86	0.40
1:A:473:LEU:HD22	1:A:504:GLY:HA2	2.02	0.40
1:B:377:SER:O	1:B:380:ASN:N	2.52	0.40
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.94	0.40
1:B:649:LYS:HD2	1:B:649:LYS:HA	1.88	0.40
1:A:109:GLY:C	1:A:110:ILE:HG12	2.41	0.40
1:A:186:THR:O	1:A:190:ASP:HB2	2.21	0.40
1:B:235:PRO:HB2	1:B:239:TRP:CB	2.52	0.40
1:A:173:ASP:HB3	3:A:764:ADP:H4'	2.02	0.40
1:B:193:THR:C	1:B:195:THR:N	2.75	0.40
1:B:403:VAL:HG12	1:B:404:ALA:H	1.85	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	746/762 (98%)	564 (76%)	123 (16%)	59 (8%)	1	6
1	B	746/762 (98%)	565 (76%)	119 (16%)	62 (8%)	1	5
All	All	1492/1524 (98%)	1129 (76%)	242 (16%)	121 (8%)	1	5

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	51	VAL
1	A	54	GLY
1	A	60	ASP
1	A	153	SER
1	A	198	SER
1	A	214	TYR
1	A	238	ASN
1	A	297	GLY
1	A	298	HIS
1	A	365	LYS
1	A	375	GLY
1	A	392	ARG
1	A	559	SER
1	A	565	ARG
1	B	60	ASP
1	B	62	GLY
1	B	232	GLU
1	B	291	THR
1	B	303	GLY
1	B	390	HIS
1	B	445	LYS
1	B	466	LYS
1	B	602	ILE
1	B	645	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	664	GLN
1	B	735	ARG
1	B	753	ALA
1	A	56	GLN
1	A	57	GLY
1	A	142	ALA
1	A	143	GLY
1	A	152	ARG
1	A	154	SER
1	A	196	ALA
1	A	236	ASP
1	A	476	LYS
1	A	564	LYS
1	A	629	GLU
1	A	647	GLU
1	A	663	GLN
1	A	666	GLY
1	A	680	GLY
1	A	690	LYS
1	B	12	LEU
1	B	64	HIS
1	B	107	LYS
1	B	110	ILE
1	B	154	SER
1	B	194	THR
1	B	201	ARG
1	B	208	MET
1	B	237	ASP
1	B	247	LEU
1	B	280	LYS
1	B	282	LEU
1	B	290	ASP
1	B	332	PRO
1	B	341	ASN
1	B	361	ALA
1	B	365	LYS
1	B	397	LYS
1	B	465	SER
1	B	476	LYS
1	B	511	GLY
1	B	551	THR
1	B	563	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	565	ARG
1	B	589	GLY
1	B	597	GLU
1	B	618	THR
1	B	661	HIS
1	B	666	GLY
1	B	755	TYR
1	A	126	ASP
1	A	208	MET
1	A	235	PRO
1	A	272	LYS
1	A	273	PRO
1	A	296	LEU
1	A	390	HIS
1	A	560	ALA
1	A	597	GLU
1	A	602	ILE
1	A	605	LEU
1	A	645	SER
1	B	16	LYS
1	B	75	MET
1	B	141	LYS
1	B	146	THR
1	B	555	ARG
1	B	559	SER
1	B	564	LYS
1	B	662	MET
1	A	28	GLN
1	A	109	GLY
1	A	131	GLU
1	A	619	THR
1	A	646	GLU
1	B	198	SER
1	B	215	LEU
1	B	382	TRP
1	B	510	GLU
1	B	697	ASN
1	A	200	GLN
1	A	371	MET
1	A	580	LEU
1	A	618	THR
1	A	641	PHE

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Mol	Chain	Res	Type
1	A	662	MET
1	A	693	GLU
1	B	199	HIS
1	B	396	PRO
1	B	561	ALA
1	B	579	TYR
1	A	201	ARG
1	B	446	GLY
1	A	42	ILE
1	B	698	GLY
1	A	62	GLY
1	A	329	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	605/618 (98%)	530 (88%)	75 (12%)	<b>4</b> <b>21</b>
1	B	605/618 (98%)	537 (89%)	68 (11%)	<b>6</b> <b>25</b>
All	All	1210/1236 (98%)	1067 (88%)	143 (12%)	<b>5</b> <b>23</b>

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	22	THR
1	A	28	GLN
1	A	64	HIS
1	A	73	VAL
1	A	77	LEU
1	A	78	GLN
1	A	84	ILE
1	A	119	ASP
1	A	126	ASP
1	A	127	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	138	ASP
1	A	140	GLN
1	A	155	TYR
1	A	158	ILE
1	A	164	SER
1	A	165	ILE
1	A	178	THR
1	A	180	SER
1	A	190	ASP
1	A	193	THR
1	A	200	GLN
1	A	226	ASP
1	A	239	TRP
1	A	242	HIS
1	A	243	LEU
1	A	257	LEU
1	A	275	THR
1	A	276	SER
1	A	277	GLU
1	A	304	THR
1	A	314	SER
1	A	348	LEU
1	A	352	VAL
1	A	391	ILE
1	A	402	THR
1	A	405	VAL
1	A	428	ILE
1	A	460	THR
1	A	481	ILE
1	A	485	ILE
1	A	486	THR
1	A	493	LEU
1	A	495	ILE
1	A	503	THR
1	A	507	GLU
1	A	516	ASP
1	A	523	VAL
1	A	531	ASN
1	A	547	ASN
1	A	551	THR
1	A	552	THR
1	A	553	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	564	LYS
1	A	565	ARG
1	A	566	ARG
1	A	614	GLN
1	A	621	LYS
1	A	649	LYS
1	A	657	ASN
1	A	669	THR
1	A	677	THR
1	A	685	ASN
1	A	687	MET
1	A	693	GLU
1	A	699	ARG
1	A	700	ILE
1	A	706	ASP
1	A	710	VAL
1	A	714	ARG
1	A	719	VAL
1	A	730	THR
1	A	731	ASP
1	A	740	GLN
1	A	751	ILE
1	B	18	ILE
1	B	21	LEU
1	B	22	THR
1	B	26	ASP
1	B	69	THR
1	B	78	GLN
1	B	89	CYS
1	B	129	ARG
1	B	138	ASP
1	B	158	ILE
1	B	165	ILE
1	B	173	ASP
1	B	178	THR
1	B	185	ILE
1	B	189	VAL
1	B	200	GLN
1	B	208	MET
1	B	210	ARG
1	B	219	THR
1	B	238	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	253	ARG
1	B	274	ILE
1	B	275	THR
1	B	348	LEU
1	B	368	ASP
1	B	373	LEU
1	B	374	ARG
1	B	402	THR
1	B	411	PRO
1	B	420	ARG
1	B	435	VAL
1	B	450	GLU
1	B	454	SER
1	B	460	THR
1	B	462	GLN
1	B	466	LYS
1	B	467	LEU
1	B	470	LYS
1	B	481	ILE
1	B	485	ILE
1	B	500	GLU
1	B	503	THR
1	B	509	MET
1	B	512	ARG
1	B	514	GLN
1	B	517	GLU
1	B	530	SER
1	B	550	CYS
1	B	553	CYS
1	B	566	ARG
1	B	573	MET
1	B	595	ILE
1	B	621	LYS
1	B	622	ARG
1	B	638	ASP
1	B	642	ASN
1	B	703	ASN
1	B	707	SER
1	B	713	MET
1	B	714	ARG
1	B	719	VAL
1	B	723	VAL

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Mol	Chain	Res	Type
1	B	724	THR
1	B	730	THR
1	B	731	ASP
1	B	743	LEU
1	B	749	LEU
1	B	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	64	HIS
1	A	104	ASN
1	A	380	ASN
1	A	429	GLN
1	A	431	ASN
1	A	437	HIS
1	A	447	GLN
1	A	462	GLN
1	A	489	ASN
1	A	491	GLN
1	A	514	GLN
1	A	531	ASN
1	A	608	ASN
1	A	634	ASN
1	A	642	ASN
1	A	661	HIS
1	A	674	ASN
1	A	703	ASN
1	A	734	HIS
1	A	740	GLN
1	B	104	ASN
1	B	183	HIS
1	B	242	HIS
1	B	258	ASN
1	B	342	GLN
1	B	431	ASN
1	B	437	HIS
1	B	489	ASN
1	B	491	GLN
1	B	514	GLN
1	B	531	ASN

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Mol	Chain	Res	Type
1	B	547	ASN
1	B	634	ASN
1	B	642	ASN
1	B	674	ASN
1	B	703	ASN
1	B	727	GLN
1	B	734	HIS

### 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](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 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
2	ATP	B	763	-	26,33,33	0.95	1 (3%)	31,52,52	1.47	4 (12%)
4	PO4	B	766	-	4,4,4	1.99	3 (75%)	6,6,6	1.26	2 (33%)
4	PO4	B	768	-	4,4,4	1.96	3 (75%)	6,6,6	1.20	1 (16%)
4	PO4	A	767	-	4,4,4	1.94	3 (75%)	6,6,6	1.41	2 (33%)
4	PO4	A	768	-	4,4,4	1.94	3 (75%)	6,6,6	1.36	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	B	764	-	24,29,29	0.94	1 (4%)	29,45,45	1.40	3 (10%)
2	ATP	A	763	-	26,33,33	0.98	1 (3%)	31,52,52	1.48	4 (12%)
4	PO4	A	766	-	4,4,4	1.96	3 (75%)	6,6,6	1.33	1 (16%)
4	PO4	B	767	-	4,4,4	1.96	3 (75%)	6,6,6	1.21	1 (16%)
2	ATP	B	765	-	26,33,33	0.93	0	31,52,52	1.94	8 (25%)
2	ATP	A	765	-	26,33,33	0.95	1 (3%)	31,52,52	2.22	12 (38%)
3	ADP	A	764	-	24,29,29	0.95	1 (4%)	29,45,45	1.87	8 (27%)

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	ATP	B	763	-	-	2/18/38/38	0/3/3/3
3	ADP	B	764	-	-	2/12/32/32	0/3/3/3
2	ATP	A	763	-	-	4/18/38/38	0/3/3/3
2	ATP	B	765	-	-	2/18/38/38	0/3/3/3
2	ATP	A	765	-	-	5/18/38/38	0/3/3/3
3	ADP	A	764	-	-	2/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	763	ATP	O4'-C1'	2.44	1.44	1.41
2	B	763	ATP	O4'-C1'	2.36	1.44	1.41
3	A	764	ADP	O4'-C1'	2.31	1.44	1.41
4	B	766	PO4	P-O2	2.30	1.61	1.54
4	B	766	PO4	P-O3	2.30	1.61	1.54
4	A	766	PO4	P-O3	2.29	1.61	1.54
4	A	768	PO4	P-O3	2.28	1.61	1.54
3	B	764	ADP	O4'-C1'	2.26	1.44	1.41
4	A	766	PO4	P-O2	2.26	1.61	1.54
4	B	767	PO4	P-O2	2.25	1.61	1.54
4	B	767	PO4	P-O3	2.23	1.61	1.54
2	A	765	ATP	O4'-C1'	2.23	1.44	1.41
4	B	768	PO4	P-O2	2.23	1.61	1.54
4	A	767	PO4	P-O3	2.23	1.61	1.54
4	A	767	PO4	P-O2	2.22	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	768	PO4	P-O3	2.20	1.61	1.54
4	A	768	PO4	P-O2	2.18	1.61	1.54
4	B	768	PO4	P-O4	-2.10	1.48	1.54
4	B	767	PO4	P-O4	-2.09	1.48	1.54
4	B	766	PO4	P-O4	-2.07	1.48	1.54
4	A	766	PO4	P-O4	-2.04	1.48	1.54
4	A	768	PO4	P-O4	-2.03	1.48	1.54
4	A	767	PO4	P-O4	-2.03	1.48	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	763	ATP	N3-C2-N1	-4.52	121.61	128.68
2	B	765	ATP	N3-C2-N1	-4.48	121.68	128.68
3	A	764	ADP	N3-C2-N1	-4.44	121.73	128.68
2	B	763	ATP	N3-C2-N1	-4.41	121.79	128.68
3	B	764	ADP	N3-C2-N1	-4.38	121.83	128.68
2	A	765	ATP	N3-C2-N1	-4.30	121.95	128.68
2	B	763	ATP	PB-O3B-PG	-4.25	118.24	132.83
2	B	765	ATP	PA-O3A-PB	-4.19	118.44	132.83
2	A	763	ATP	PB-O3B-PG	-4.11	118.72	132.83
2	A	765	ATP	PA-O3A-PB	-4.03	119.00	132.83
2	A	765	ATP	O2A-PA-O5'	-4.00	89.19	107.75
2	B	765	ATP	PB-O3B-PG	-3.95	119.27	132.83
2	B	765	ATP	O4'-C1'-C2'	-3.82	101.35	106.93
2	A	765	ATP	O2G-PG-O3B	-3.59	92.59	104.64
3	B	764	ADP	PA-O3A-PB	-3.58	120.53	132.83
2	A	765	ATP	PB-O3B-PG	-3.57	120.59	132.83
2	B	765	ATP	O2A-PA-O5'	-3.56	91.22	107.75
2	A	765	ATP	O3G-PG-O3B	-3.38	93.29	104.64
3	A	764	ADP	PA-O3A-PB	-3.37	121.27	132.83
3	A	764	ADP	O2B-PB-O3A	-3.35	93.39	104.64
3	A	764	ADP	O3B-PB-O3A	-3.34	93.43	104.64
2	B	763	ATP	PA-O3A-PB	-3.32	121.43	132.83
2	B	765	ATP	O5'-PA-O1A	-3.24	96.42	109.07
2	A	765	ATP	O2G-PG-O1G	3.13	122.93	110.68
2	A	765	ATP	C5'-C4'-C3'	-3.08	103.63	115.18
2	A	765	ATP	O5'-PA-O1A	-3.02	97.25	109.07
2	A	763	ATP	PA-O3A-PB	-3.01	122.50	132.83
3	A	764	ADP	O3B-PB-O1B	2.93	122.16	110.68
2	B	765	ATP	C3'-C2'-C1'	-2.86	96.67	100.98
3	A	764	ADP	O2B-PB-O1B	2.85	121.84	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	765	ATP	O3G-PG-O1G	2.74	121.40	110.68
4	A	768	PO4	O4-P-O1	2.63	120.52	110.89
4	A	767	PO4	O3-P-O2	-2.59	99.65	107.97
3	B	764	ADP	O4'-C1'-C2'	-2.49	103.28	106.93
4	A	766	PO4	O4-P-O1	2.49	120.00	110.89
2	A	763	ATP	C2'-C3'-C4'	-2.30	98.17	102.64
4	B	767	PO4	O4-P-O1	2.29	119.26	110.89
3	A	764	ADP	C3'-C2'-C1'	-2.17	97.71	100.98
3	A	764	ADP	O3A-PB-O1B	-2.16	99.19	111.19
4	A	767	PO4	O4-P-O1	2.16	118.78	110.89
2	A	765	ATP	O3B-PG-O1G	-2.15	99.28	111.19
4	B	766	PO4	O3-P-O2	-2.13	101.13	107.97
4	B	766	PO4	O4-P-O1	2.10	118.58	110.89
4	B	768	PO4	O4-P-O1	2.09	118.53	110.89
2	B	763	ATP	C2'-C3'-C4'	-2.08	98.60	102.64
2	A	765	ATP	O2A-PA-O1A	2.05	122.37	112.24
2	B	765	ATP	O2A-PA-O1A	2.02	122.24	112.24

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	763	ATP	PB-O3B-PG-O3G
2	A	765	ATP	C5'-O5'-PA-O1A
2	A	765	ATP	C5'-O5'-PA-O2A
2	A	765	ATP	C5'-O5'-PA-O3A
2	A	763	ATP	PA-O3A-PB-O1B
3	A	764	ADP	PB-O3A-PA-O1A
2	B	763	ATP	PB-O3A-PA-O1A
2	B	765	ATP	PA-O3A-PB-O1B
2	A	763	ATP	PB-O3A-PA-O2A
3	B	764	ADP	PB-O3A-PA-O1A
2	A	763	ATP	PA-O3A-PB-O2B
3	A	764	ADP	PB-O3A-PA-O2A
2	A	765	ATP	PB-O3A-PA-O2A
2	B	763	ATP	PA-O3A-PB-O2B
2	B	765	ATP	PB-O3A-PA-O1A
3	B	764	ADP	PB-O3A-PA-O2A
2	A	765	ATP	C3'-C4'-C5'-O5'

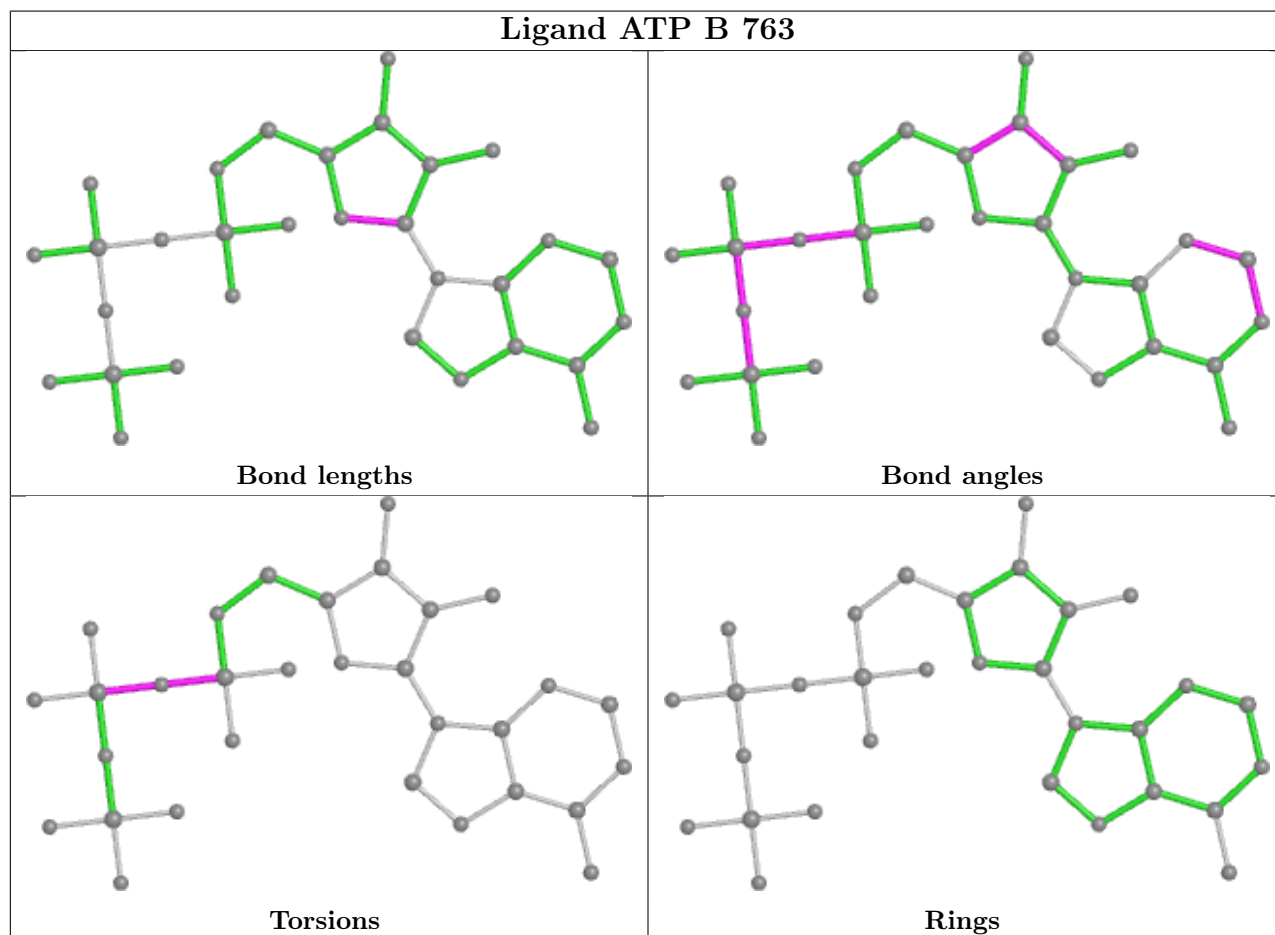
There are no ring outliers.

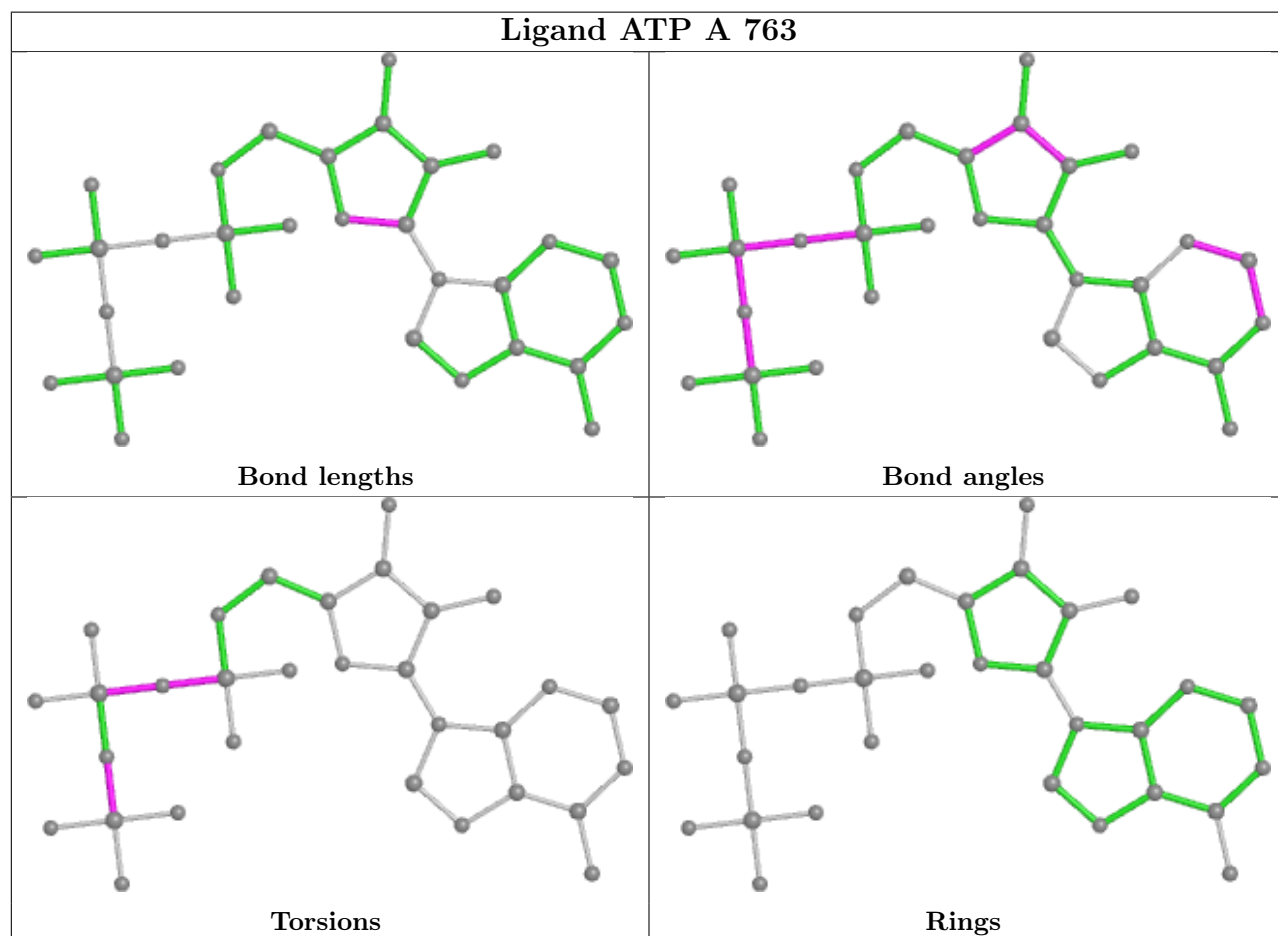
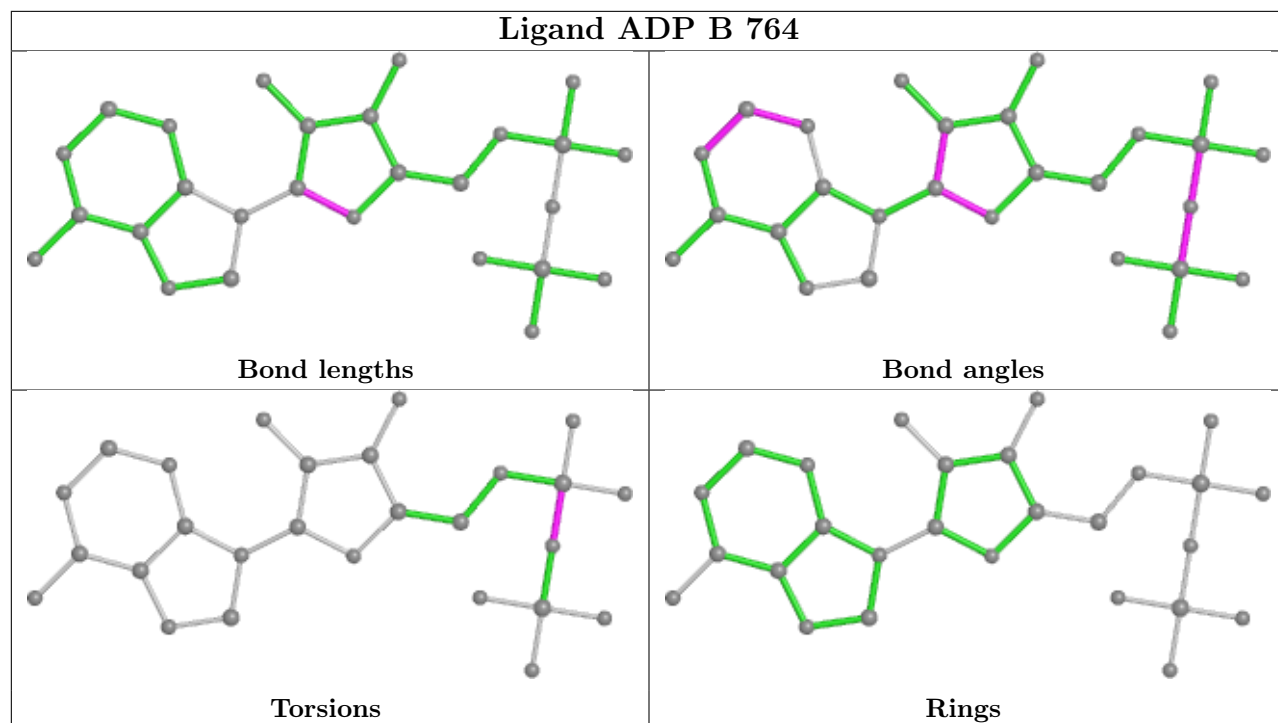
6 monomers are involved in 9 short contacts:

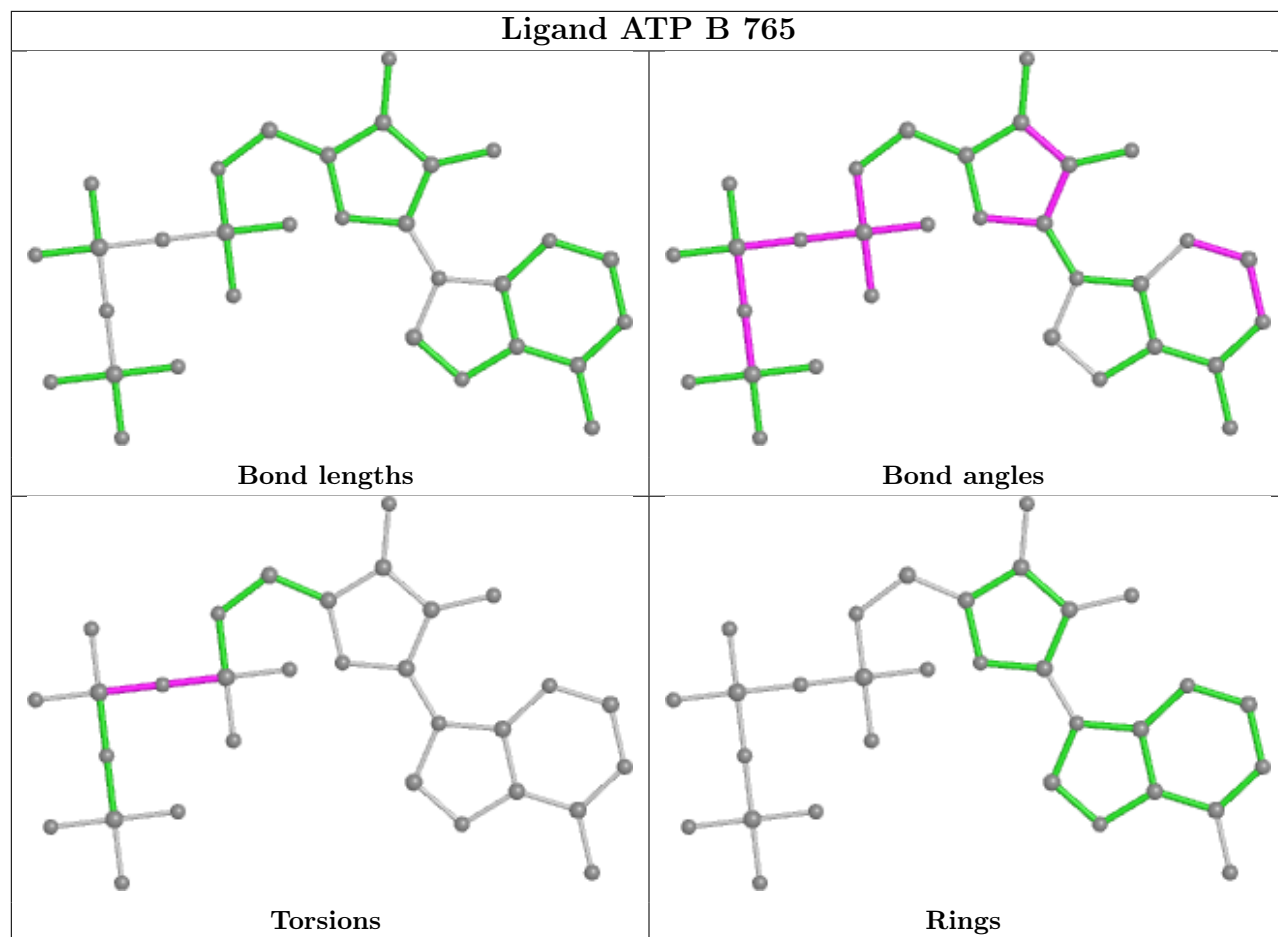


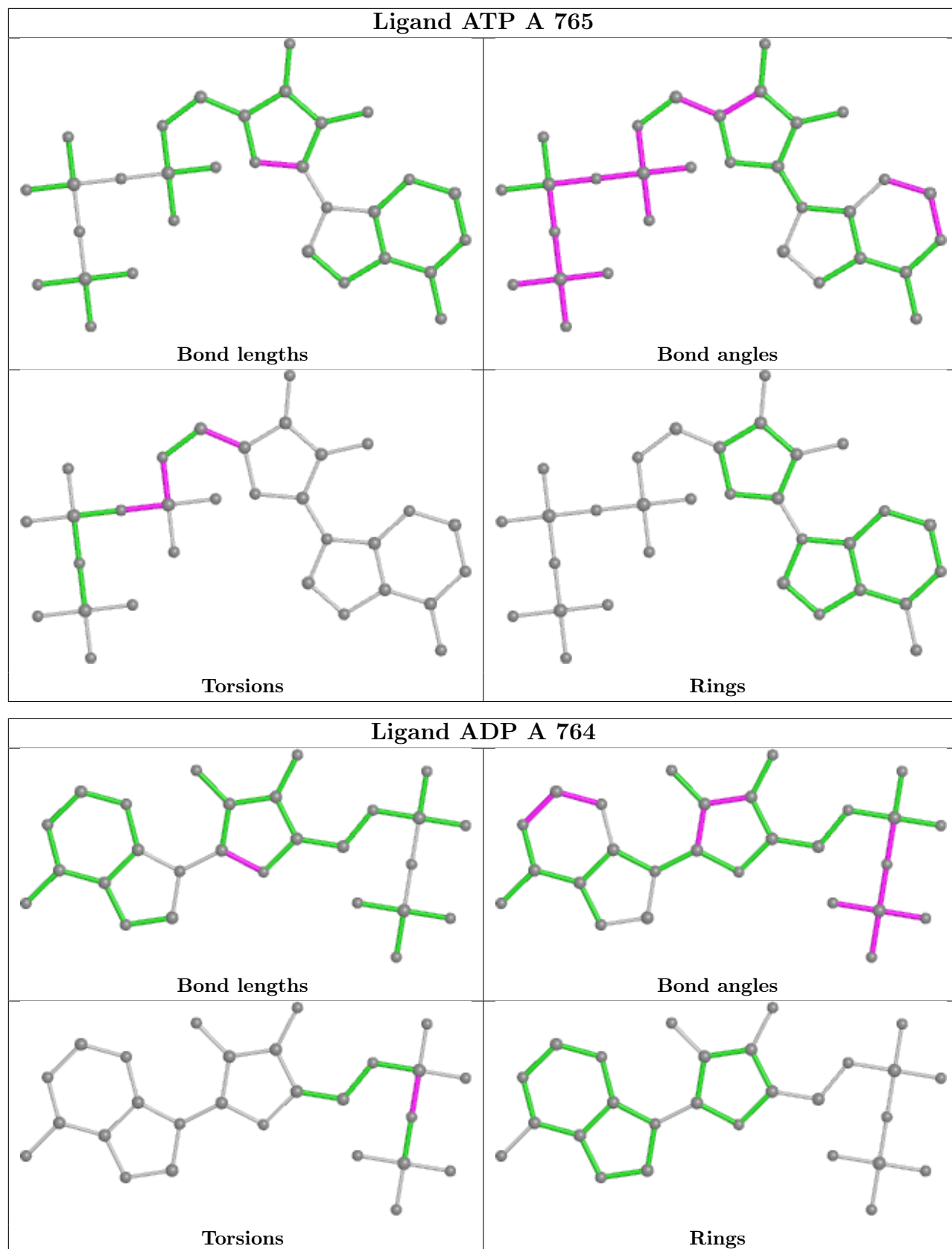
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	763	ATP	1	0
4	B	768	PO4	1	0
4	A	767	PO4	1	0
2	A	763	ATP	2	0
2	A	765	ATP	3	0
3	A	764	ADP	1	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	739/762 (96%)	-0.44	1 (0%) 95 95	14, 57, 138, 202	76 (10%)
1	B	745/762 (97%)	-0.25	12 (1%) 72 59	7, 59, 148, 202	86 (11%)
All	All	1484/1524 (97%)	-0.35	13 (0%) 84 75	7, 58, 144, 202	162 (10%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	SER	6.5
1	B	142	ALA	6.2
1	B	92	PHE	3.9
1	B	59	VAL	3.8
1	B	154	SER	3.4
1	B	291	THR	2.9
1	B	556	ILE	2.9
1	B	143	GLY	2.7
1	B	58	LEU	2.4
1	B	101	ALA	2.3
1	B	153	SER	2.2
1	B	110	ILE	2.2
1	A	361	ALA	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](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

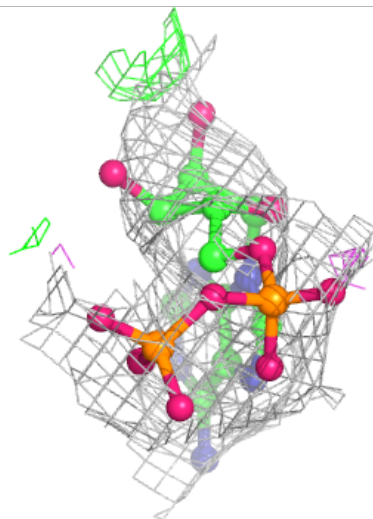
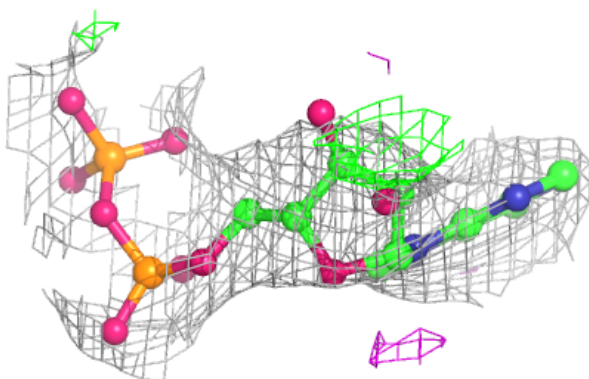
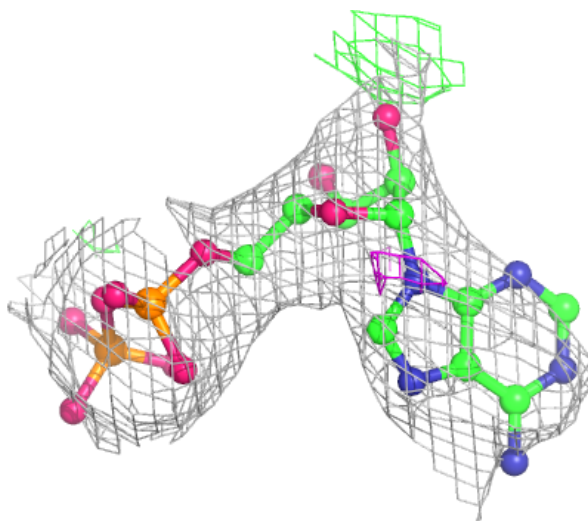
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	B	764	27/27	0.82	0.26	145,148,154,154	0
2	ATP	A	763	31/31	0.85	0.22	82,87,97,98	0
3	ADP	A	764	27/27	0.86	0.29	135,138,144,144	0
2	ATP	B	763	31/31	0.87	0.19	98,100,101,101	0
4	PO4	A	766	5/5	0.88	0.32	99,99,100,101	0
4	PO4	B	767	5/5	0.89	0.32	66,66,69,71	0
4	PO4	B	766	5/5	0.90	0.32	91,92,93,94	0
2	ATP	A	765	31/31	0.93	0.20	58,63,77,78	0
4	PO4	A	767	5/5	0.94	0.28	60,60,61,63	0
2	ATP	B	765	31/31	0.96	0.12	72,77,90,91	0
4	PO4	A	768	5/5	0.97	0.17	55,56,57,58	0
4	PO4	B	768	5/5	0.99	0.15	52,53,55,55	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 ADP B 764:**

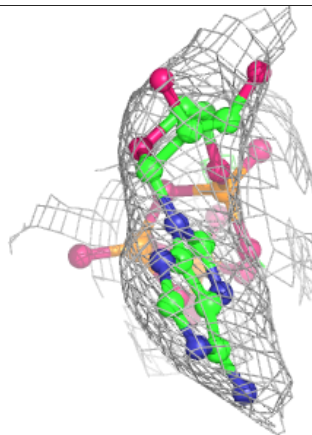
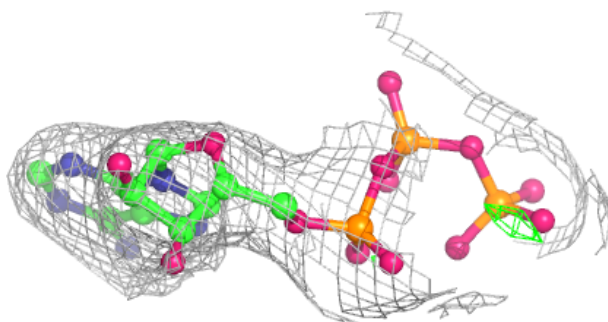
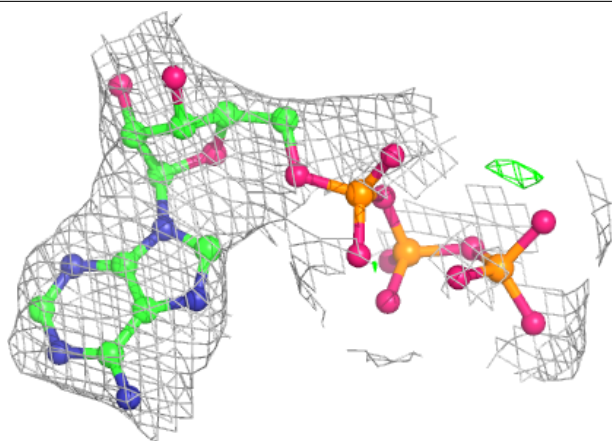
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





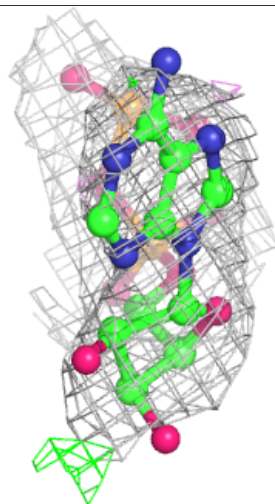
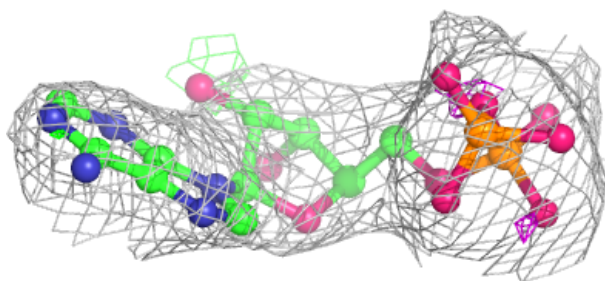
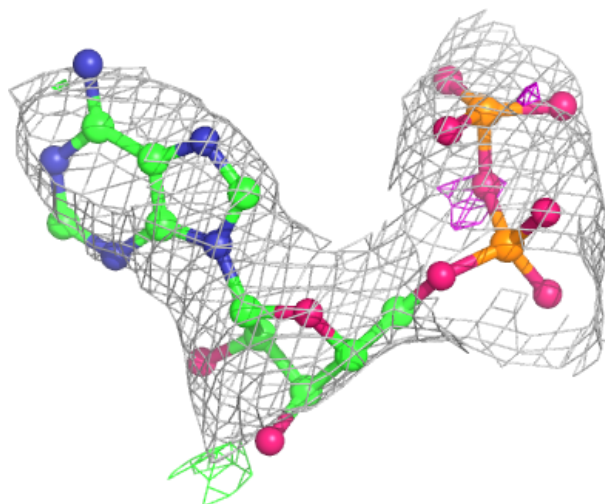
**Electron density around ATP A 763:**

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



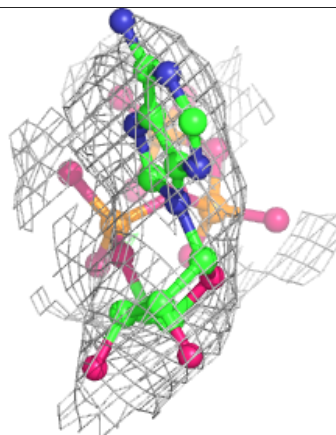
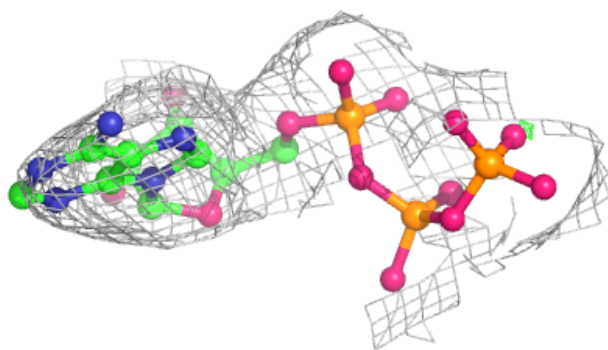
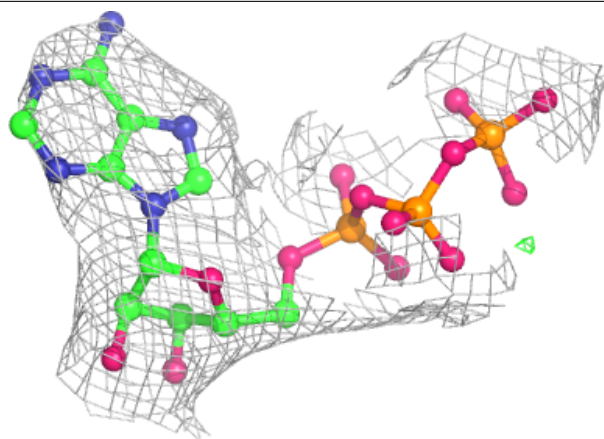
**Electron density around ADP A 764:**

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



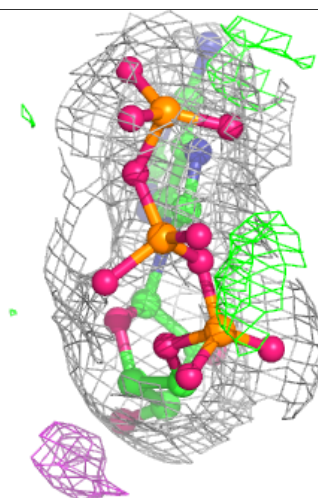
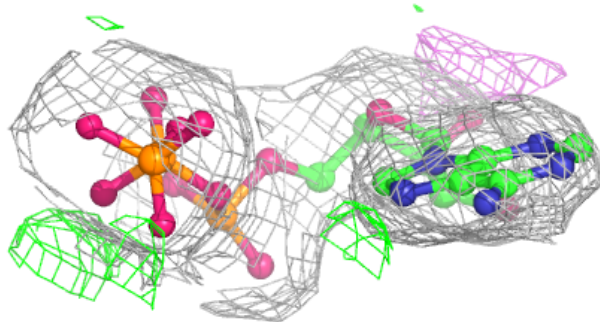
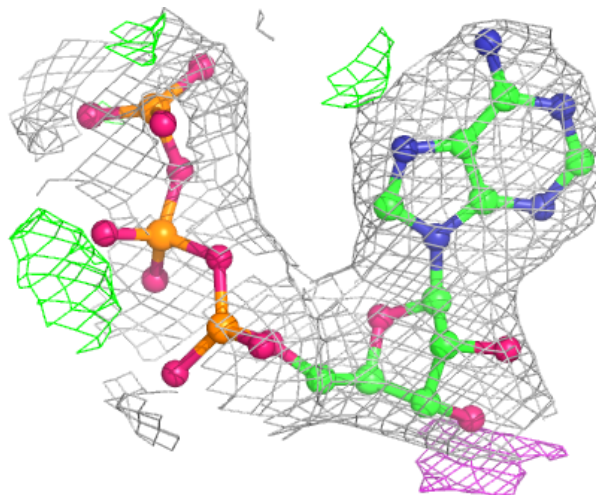
**Electron density around ATP B 763:**

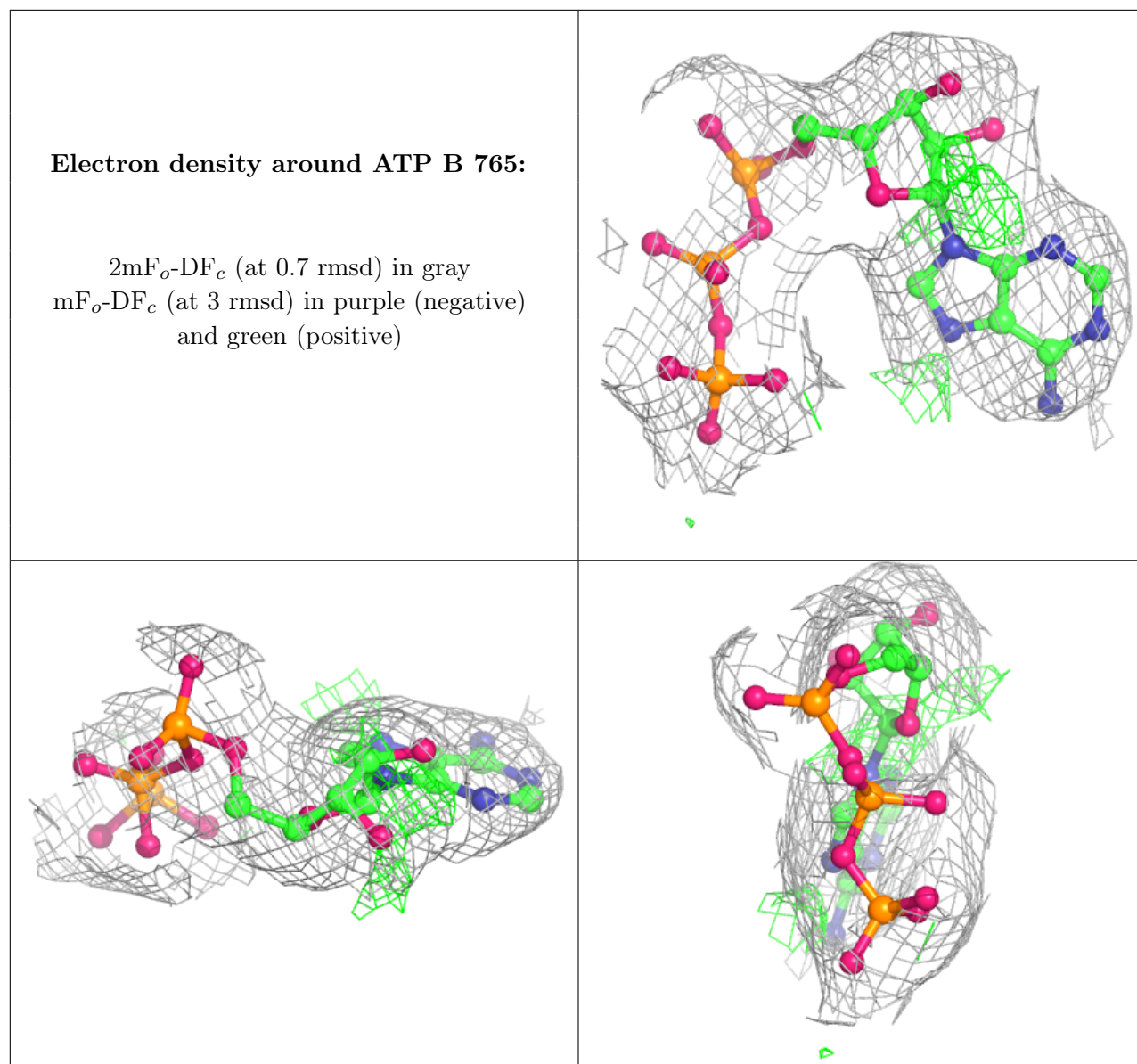
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP A 765:**

$2mF_o-DF_c$  (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.