WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 03:24 pm GMT

PDB ID	:	2CDE
Title	:	Structure and binding kinetics of three different human CD1d-alpha- Galactosylceramide specific T cell receptors - iNKT-TCR
Authors	:	Gadola, S.D.; Koch, M.; Marles-Wright, J.; Lissin, N.M.; Sheperd, D.; Matulis, G.; Harlos, K.; Villiger, P.M.; Stuart, D.I.; Jakobsen, B.K.; Cerundolo, V.; Jones, E.Y.
Deposited on	:	2006-01-23
Resolution	:	3.50 Å(reported)

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

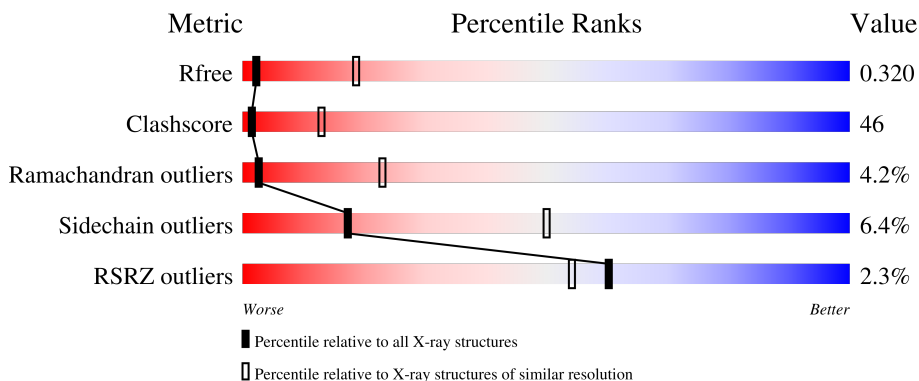|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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.
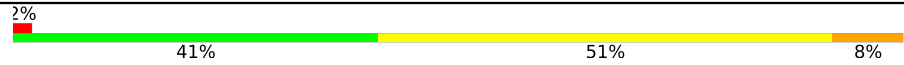
Metric	Percentile Ranks	Value
Rfree		0.320
Clashscore		46
Ramachandran outliers		4.2%
Sidechain outliers		6.4%
RSRZ outliers		2.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	192	4% / 40% / 53% / 6% •
1	C	192	3% / 36% / 57% / 6% •
1	E	192	% / 38% / 56% / 6% •
2	B	244	2% / 42% / 51% / 7%
2	D	244	2% / 42% / 49% / 8% •

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Mol	Chain	Length	Quality of chain
2	F	244	2% 41% 51% 8%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10330 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 INKT-TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1495	923	256	308	8			
1	C	192	Total	C	N	O	S	0	0	0
			1495	923	256	308	8			
1	E	192	Total	C	N	O	S	0	0	0
			1483	915	255	305	8			

- Molecule 2 is a protein called INKT-TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1952	1227	334	384	7			
2	D	244	Total	C	N	O	S	0	0	0
			1952	1227	334	384	7			
2	F	244	Total	C	N	O	S	0	0	0
			1953	1227	334	385	7			

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: INKT-TCR
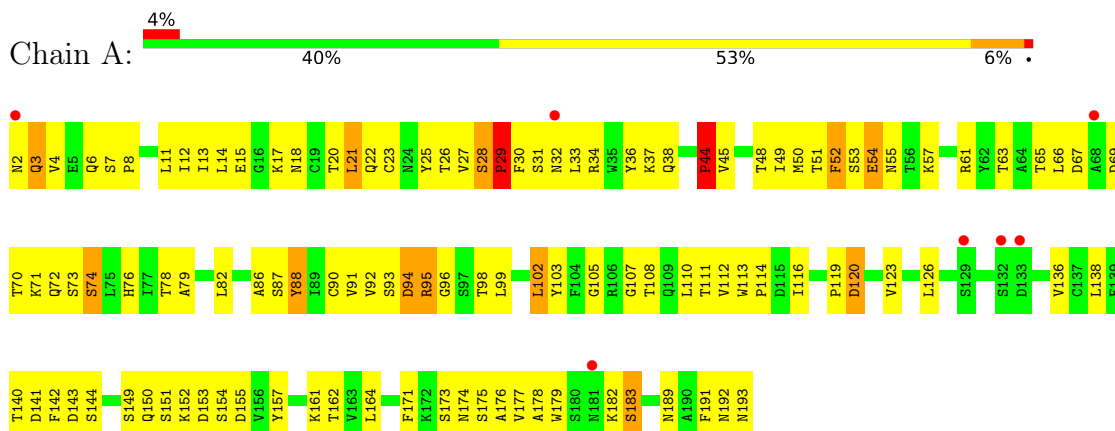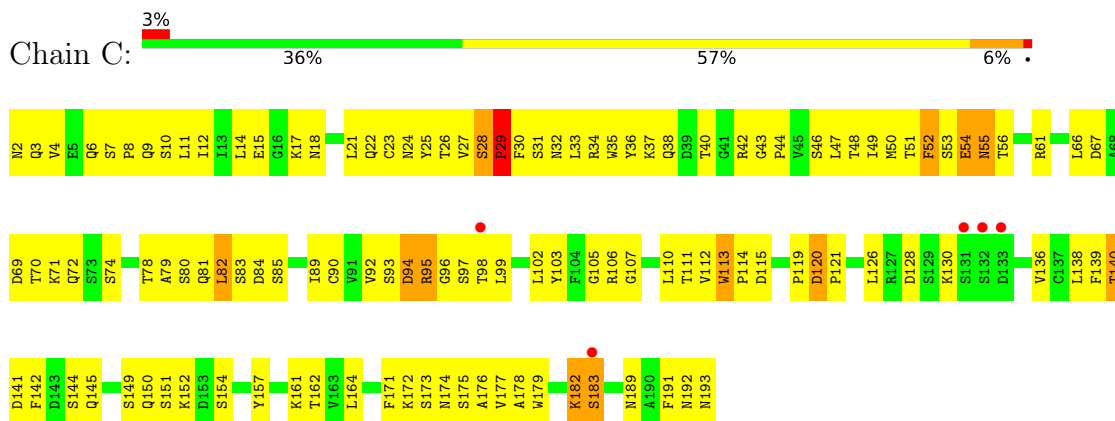
Chain A:

- Molecule 1: INKT-TCR

Chain C:

- Molecule 1: INKT-TCR

Chain E:

• Molecule 2: INKT-TCR
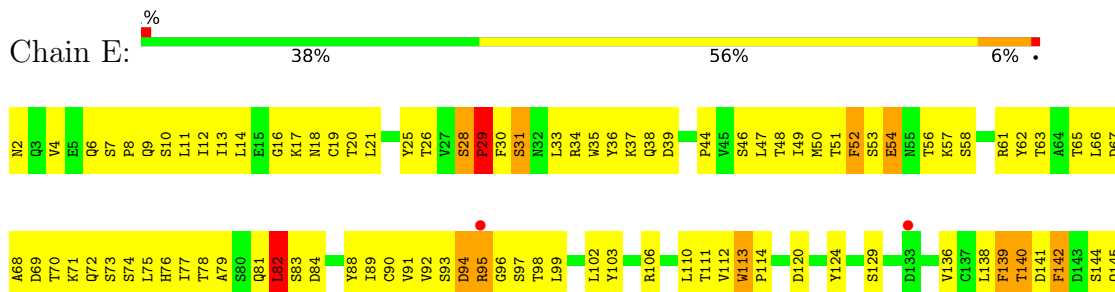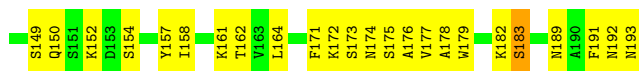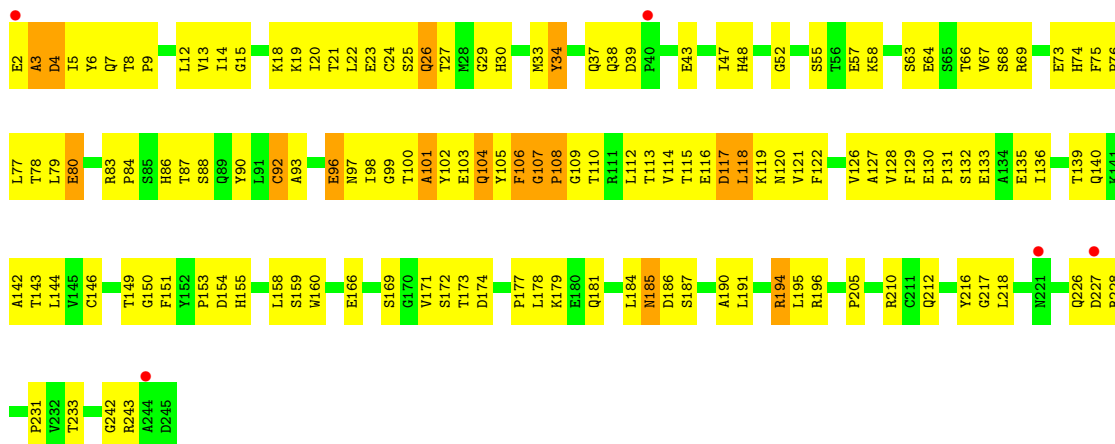
Chain B:

2%
42% 51% 7%

• Molecule 2: INKT-TCR

Chain D:

2%
42% 49% 8%

• Molecule 2: INKT-TCR

Chain F:

2%
41% 51% 8%
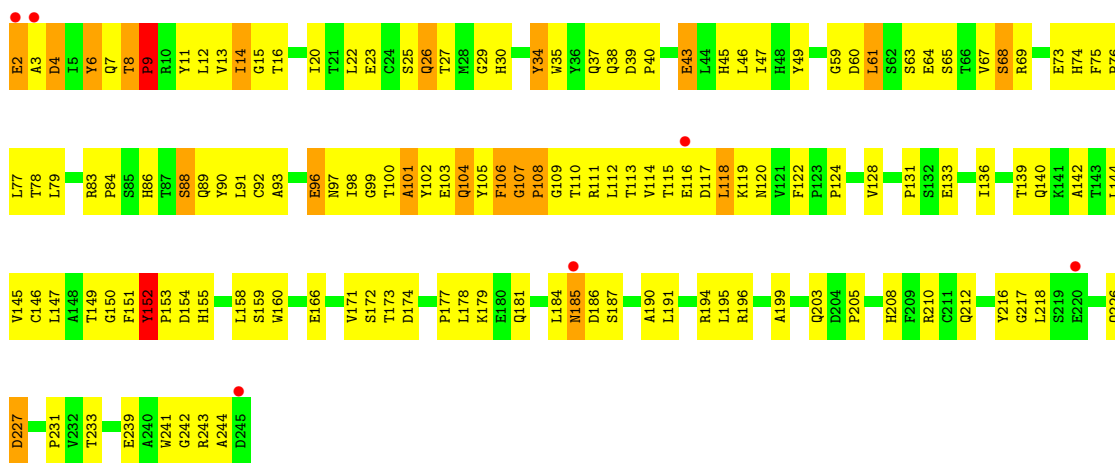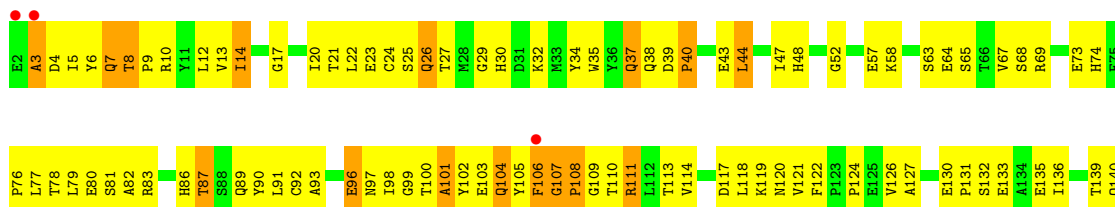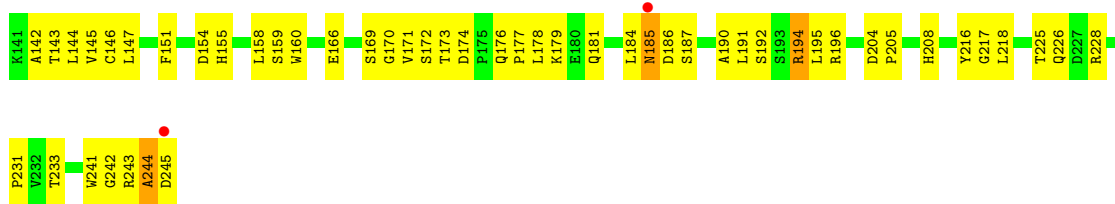
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	289.36Å 84.95Å 78.86Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 19.99 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-3.50) 97.9 (19.99-3.48)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.283 , 0.350 0.268 , 0.320	Depositor DCC
R_{free} test set	1203 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.1	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.035 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.34	0/1522	0.59	0/2064
1	C	0.35	0/1522	0.58	0/2064
1	E	0.39	0/1509	0.62	1/2046 (0.0%)
2	B	0.34	0/2006	0.59	0/2733
2	D	0.35	0/2006	0.61	1/2733 (0.0%)
2	F	0.36	0/2007	0.61	0/2733
All	All	0.36	0/10572	0.60	2/14373 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	114	PRO	N-CA-CB	5.53	109.94	103.30
2	D	152	TYR	C-N-CD	5.03	138.96	128.40

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	1495	0	1434	160	0
1	C	1495	0	1434	160	0
1	E	1483	0	1411	165	0
2	B	1952	0	1840	180	0
2	D	1952	0	1840	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1953	0	1840	169	0
All	All	10330	0	9799	930	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 46.

All (930) 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)
2:D:8:THR:HB	2:D:9:PRO:HD2	1.16	1.12
1:C:136:VAL:HG12	1:C:179:TRP:HB3	1.35	1.07
1:E:82:LEU:H	1:E:82:LEU:HD23	1.21	1.06
2:F:34:TYR:HB2	2:F:93:ALA:HB3	1.37	1.03
1:E:13:ILE:HG12	1:E:17:LYS:HD2	1.40	1.03
1:C:152:LYS:HA	1:E:152:LYS:HA	1.36	1.02
2:F:111:ARG:HH12	2:F:154:ASP:HB3	1.22	1.00
1:E:14:LEU:HB2	1:E:17:LYS:HE3	1.44	0.99
1:C:38:GLN:HE21	1:C:44:PRO:HD3	1.28	0.98
1:E:6:GLN:NE2	1:E:90:CYS:H	1.63	0.97
2:F:44:LEU:HD23	2:F:44:LEU:H	1.31	0.96
1:C:66:LEU:HD11	1:C:70:THR:HG23	1.45	0.95
1:A:50:MET:HG2	1:A:57:LYS:HD2	1.49	0.94
1:E:51:THR:HG22	1:E:52:PHE:H	1.32	0.92
1:C:51:THR:HG22	1:C:52:PHE:H	1.31	0.92
2:F:37:GLN:HB3	2:F:47:ILE:HD11	1.51	0.92
2:D:67:VAL:HG12	2:D:68:SER:H	1.32	0.92
1:C:140:THR:HG23	1:C:175:SER:HB3	1.51	0.91
1:A:55:ASN:HA	1:A:66:LEU:H	1.34	0.91
1:A:162:THR:HG22	2:B:172:SER:HB2	1.50	0.91
1:A:51:THR:HG22	1:A:52:PHE:H	1.33	0.91
1:E:66:LEU:HD11	1:E:70:THR:HG23	1.51	0.90
1:A:136:VAL:HG12	1:A:179:TRP:HB3	1.51	0.90
1:E:38:GLN:HB2	1:E:44:PRO:HB3	1.52	0.90
2:D:117:ASP:HB3	2:D:120:ASN:CG	1.92	0.90
2:B:217:GLY:H	2:B:233:THR:HA	1.37	0.90
1:E:136:VAL:HG12	1:E:179:TRP:HB3	1.54	0.89
1:A:140:THR:HG23	1:A:175:SER:HB3	1.51	0.89
1:E:162:THR:HG22	2:F:172:SER:HB2	1.53	0.89
2:B:216:TYR:HA	2:B:233:THR:HG23	1.55	0.88
1:E:140:THR:HG23	1:E:175:SER:HB3	1.55	0.87
2:D:118:LEU:HD23	2:D:118:LEU:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:H	1:C:17:LYS:HD2	1.40	0.87
1:E:106:ARG:HA	2:F:43:GLU:HG2	1.54	0.87
1:E:138:LEU:HD11	1:E:175:SER:HB2	1.56	0.87
2:F:111:ARG:NH1	2:F:154:ASP:HB3	1.89	0.86
1:E:18:ASN:HB3	1:E:76:HIS:HE1	1.41	0.86
1:C:44:PRO:HG3	2:D:105:TYR:OH	1.78	0.84
2:B:7:GLN:HE21	2:B:107:GLY:HA3	1.41	0.84
1:E:37:LYS:HB2	1:E:47:LEU:HD11	1.60	0.84
2:B:118:LEU:H	2:B:118:LEU:HD23	1.41	0.84
1:C:18:ASN:ND2	1:C:78:THR:HA	1.93	0.84
2:F:83:ARG:H	2:F:86:HIS:HD2	1.19	0.83
1:A:44:PRO:HG2	2:B:105:TYR:OH	1.79	0.83
1:C:7:SER:HB2	1:E:13:ILE:HD11	1.61	0.83
2:D:115:THR:HG22	2:D:117:ASP:H	1.43	0.83
1:C:33:LEU:HD13	1:C:92:VAL:HG22	1.58	0.82
1:C:38:GLN:NE2	1:C:44:PRO:HD3	1.93	0.82
1:E:71:LYS:HG3	1:E:72:GLN:HG2	1.60	0.82
2:D:25:SER:HB3	2:D:74:HIS:ND1	1.94	0.82
2:B:37:GLN:CB	2:B:47:ILE:HD11	2.10	0.81
1:C:9:GLN:NE2	1:E:14:LEU:HG	1.95	0.81
2:F:23:GLU:HG2	2:F:76:PRO:HB3	1.61	0.81
2:F:37:GLN:CB	2:F:47:ILE:HD11	2.10	0.80
1:A:6:GLN:NE2	1:A:90:CYS:H	1.80	0.80
2:F:8:THR:HB	2:F:9:PRO:HD3	1.62	0.80
2:D:77:LEU:HD13	2:D:78:THR:N	1.97	0.80
1:C:6:GLN:HE21	1:C:105:GLY:HA3	1.47	0.80
2:D:8:THR:CB	2:D:9:PRO:HD2	2.03	0.80
2:B:14:ILE:HG23	2:B:18:LYS:HD2	1.61	0.80
2:D:131:PRO:HD3	2:D:144:LEU:CD2	2.11	0.80
2:B:37:GLN:HB3	2:B:47:ILE:HD11	1.62	0.79
1:A:116:ILE:HD13	1:A:143:ASP:HB2	1.63	0.79
2:F:87:THR:HG23	2:F:113:THR:HA	1.63	0.79
1:C:162:THR:HG22	2:D:172:SER:HB2	1.64	0.78
2:B:22:LEU:HD22	2:B:110:THR:HG21	1.66	0.78
1:A:50:MET:HA	1:A:57:LYS:NZ	1.98	0.78
2:B:210:ARG:HH12	2:B:212:GLN:HB2	1.48	0.78
2:F:216:TYR:HA	2:F:233:THR:HG23	1.65	0.77
2:B:93:ALA:CB	2:B:105:TYR:HB3	2.14	0.77
1:C:110:LEU:HD12	1:C:111:THR:H	1.48	0.77
1:A:25:TYR:OH	1:A:70:THR:HG22	1.83	0.77
1:E:82:LEU:HD23	1:E:82:LEU:N	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:THR:HG22	1:E:141:ASP:H	1.49	0.77
1:C:31:SER:HB3	1:C:95:ARG:HB2	1.67	0.77
2:F:14:ILE:HD11	2:F:114:VAL:HG22	1.67	0.77
2:D:184:LEU:HB3	2:D:186:ASP:OD2	1.84	0.77
2:D:8:THR:HB	2:D:9:PRO:CD	2.08	0.77
1:A:31:SER:HB3	1:A:95:ARG:HB2	1.67	0.77
2:B:3:ALA:HB3	2:B:27:THR:OG1	1.85	0.76
1:A:34:ARG:HG2	1:A:49:ILE:HG12	1.66	0.76
2:B:171:VAL:HG22	2:B:195:LEU:HD13	1.67	0.76
1:C:33:LEU:HD11	1:C:90:CYS:SG	2.26	0.76
1:E:31:SER:HB3	1:E:95:ARG:HB2	1.66	0.76
2:B:158:LEU:HD23	2:B:159:SER:N	2.00	0.75
2:F:217:GLY:H	2:F:233:THR:HA	1.50	0.75
2:D:131:PRO:HD3	2:D:144:LEU:HD23	1.68	0.75
1:C:152:LYS:HA	1:E:152:LYS:CA	2.16	0.74
1:A:44:PRO:HD2	2:B:105:TYR:CE1	2.23	0.74
2:D:22:LEU:HB2	2:D:77:LEU:HB3	1.68	0.74
2:D:216:TYR:HA	2:D:233:THR:HG23	1.69	0.74
1:C:82:LEU:HA	1:C:112:VAL:HB	1.70	0.74
2:B:90:TYR:HE2	2:B:112:LEU:HD23	1.53	0.74
2:B:131:PRO:HG3	2:B:142:ALA:HB1	1.70	0.74
1:A:13:ILE:HG22	1:A:14:LEU:N	2.04	0.73
1:A:55:ASN:O	1:A:65:THR:HA	1.87	0.73
2:B:131:PRO:HD3	2:B:144:LEU:HD23	1.70	0.73
1:C:38:GLN:HB2	1:C:44:PRO:HB3	1.70	0.73
1:A:20:THR:HG22	1:A:76:HIS:HA	1.69	0.73
1:C:152:LYS:CA	1:E:152:LYS:HA	2.18	0.73
2:D:11:TYR:CE1	2:D:111:ARG:HD2	2.23	0.73
1:A:140:THR:HG22	1:A:141:ASP:H	1.54	0.73
1:E:56:THR:HG22	1:E:58:SER:H	1.52	0.72
2:D:210:ARG:HH12	2:D:212:GLN:HB2	1.53	0.72
1:A:13:ILE:CG2	1:A:17:LYS:HD2	2.20	0.72
1:E:142:PHE:CE1	1:E:174:ASN:HB2	2.25	0.72
2:B:14:ILE:HD13	2:B:20:ILE:HG12	1.72	0.72
1:C:82:LEU:HD23	1:C:82:LEU:N	2.05	0.72
2:F:184:LEU:HB3	2:F:186:ASP:OD2	1.90	0.72
2:B:23:GLU:HG2	2:B:76:PRO:HB3	1.71	0.72
1:A:50:MET:HA	1:A:57:LYS:HZ2	1.51	0.72
2:D:146:CYS:HB2	2:D:160:TRP:CZ2	2.25	0.71
1:C:11:LEU:HD12	1:C:12:ILE:H	1.55	0.71
1:A:66:LEU:HD11	1:A:70:THR:HG23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD11	1:A:175:SER:HB2	1.73	0.71
1:A:67:ASP:HB2	1:A:72:GLN:O	1.91	0.71
2:D:185:ASN:N	2:D:185:ASN:HD22	1.87	0.71
1:C:25:TYR:OH	1:C:70:THR:HG22	1.91	0.70
1:E:79:ALA:O	1:E:81:GLN:HG3	1.91	0.70
2:F:7:GLN:CB	2:F:10:ARG:HH12	2.04	0.70
2:F:83:ARG:N	2:F:86:HIS:HD2	1.88	0.70
2:B:77:LEU:HD12	2:B:78:THR:H	1.56	0.70
1:C:140:THR:HG22	1:C:141:ASP:H	1.55	0.70
1:A:18:ASN:ND2	1:A:78:THR:HG23	2.05	0.70
2:F:7:GLN:HB2	2:F:10:ARG:HH12	1.57	0.70
1:C:9:GLN:HE21	1:E:17:LYS:NZ	1.89	0.70
2:D:217:GLY:H	2:D:233:THR:HA	1.55	0.70
2:B:185:ASN:N	2:B:185:ASN:HD22	1.87	0.70
1:C:85:SER:HB3	1:C:112:VAL:HG23	1.74	0.70
1:E:82:LEU:H	1:E:82:LEU:CD2	1.93	0.70
1:A:182:LYS:HG2	1:A:183:SER:H	1.57	0.69
2:F:38:GLN:HB3	2:F:44:LEU:HA	1.72	0.69
1:A:2:ASN:N	1:A:27:VAL:HG12	2.06	0.69
2:F:9:PRO:O	2:F:110:THR:HG23	1.92	0.69
2:B:118:LEU:HD23	2:B:118:LEU:N	2.07	0.69
2:D:139:THR:HG21	2:D:196:ARG:HH21	1.57	0.69
2:B:34:TYR:HB2	2:B:93:ALA:HB3	1.73	0.69
2:B:26:GLN:OE1	2:B:30:HIS:HB2	1.93	0.69
2:B:174:ASP:HB2	2:B:191:LEU:CD1	2.23	0.69
2:F:3:ALA:HB1	2:F:6:TYR:OH	1.92	0.69
2:F:98:ILE:HG22	2:F:99:GLY:N	2.08	0.69
2:D:26:GLN:OE1	2:D:30:HIS:HB2	1.94	0.68
2:B:9:PRO:O	2:B:110:THR:HG23	1.92	0.68
2:B:205:PRO:HA	2:B:242:GLY:O	1.93	0.68
2:D:14:ILE:HD13	2:D:14:ILE:H	1.57	0.68
2:F:131:PRO:HG2	2:F:142:ALA:HB1	1.75	0.68
1:A:21:LEU:HD23	1:A:21:LEU:N	2.09	0.68
2:D:98:ILE:HG22	2:D:99:GLY:N	2.08	0.68
2:F:8:THR:HB	2:F:9:PRO:CD	2.24	0.68
2:D:115:THR:CG2	2:D:117:ASP:HB2	2.24	0.68
2:D:218:LEU:HD13	2:D:231:PRO:O	1.94	0.68
2:F:119:LYS:HE2	2:F:226:GLN:NE2	2.09	0.68
2:B:19:LYS:HA	2:B:80:GLU:O	1.94	0.68
1:E:14:LEU:HD23	1:E:113:TRP:HB2	1.76	0.68
2:F:26:GLN:OE1	2:F:30:HIS:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ILE:HG22	2:B:99:GLY:N	2.09	0.67
2:F:96:GLU:HB2	2:F:102:TYR:HB3	1.75	0.67
1:C:138:LEU:HD12	1:C:176:ALA:O	1.93	0.67
1:C:176:ALA:HB3	1:C:191:PHE:HE2	1.59	0.67
2:D:96:GLU:HB2	2:D:102:TYR:HB3	1.77	0.67
2:D:158:LEU:HD23	2:D:159:SER:N	2.10	0.67
2:F:185:ASN:N	2:F:185:ASN:HD22	1.90	0.67
1:A:86:ALA:O	1:A:110:LEU:HB3	1.94	0.67
1:A:7:SER:HA	1:A:8:PRO:O	1.95	0.67
2:B:83:ARG:HB2	2:B:86:HIS:CD2	2.30	0.67
2:D:83:ARG:H	2:D:86:HIS:HD2	1.43	0.67
2:D:131:PRO:HG3	2:D:142:ALA:HB1	1.77	0.67
1:C:38:GLN:HA	1:C:44:PRO:HA	1.77	0.66
1:E:35:TRP:HA	1:E:89:ILE:O	1.95	0.66
2:D:118:LEU:O	2:D:119:LYS:HB2	1.95	0.66
2:F:133:GLU:HA	2:F:136:ILE:HD12	1.78	0.66
2:D:3:ALA:HB3	2:D:27:THR:OG1	1.94	0.66
1:A:94:ASP:OD1	1:A:103:TYR:HE1	1.78	0.66
2:B:22:LEU:CD2	2:B:110:THR:HG21	2.24	0.66
2:B:139:THR:HG21	2:B:196:ARG:HH21	1.60	0.66
2:F:77:LEU:HD13	2:F:78:THR:N	2.11	0.66
1:C:8:PRO:HD2	1:C:21:LEU:HD23	1.76	0.66
1:E:182:LYS:HG2	1:E:183:SER:H	1.61	0.66
1:A:116:ILE:HG21	1:A:143:ASP:HB3	1.78	0.66
1:A:171:PHE:CZ	1:A:173:SER:HB3	2.31	0.66
2:B:133:GLU:HA	2:B:136:ILE:HD12	1.78	0.66
1:C:164:LEU:HD12	1:C:164:LEU:O	1.96	0.66
1:E:65:THR:HB	1:E:74:SER:OG	1.95	0.66
2:B:67:VAL:HG22	2:B:77:LEU:HD13	1.77	0.66
2:B:113:THR:HG21	2:B:153:PRO:HB3	1.76	0.65
2:B:131:PRO:HD3	2:B:144:LEU:CD2	2.26	0.65
1:C:36:TYR:HB3	1:C:44:PRO:HB2	1.78	0.65
2:B:96:GLU:HB2	2:B:102:TYR:HB3	1.76	0.65
1:C:15:GLU:OE2	1:C:114:PRO:HA	1.96	0.65
1:C:138:LEU:HD11	1:C:175:SER:HB2	1.79	0.65
2:B:79:LEU:HD21	2:B:86:HIS:CD2	2.32	0.65
2:D:174:ASP:HB2	2:D:191:LEU:CD1	2.26	0.65
1:C:11:LEU:HD11	1:E:8:PRO:HB3	1.78	0.65
1:E:63:THR:HB	1:E:76:HIS:HB3	1.79	0.65
2:F:48:HIS:CE1	2:F:58:LYS:HG2	2.32	0.65
2:F:106:PHE:O	2:F:107:GLY:C	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:GLY:H	2:B:18:LYS:HZ2	1.45	0.64
1:E:31:SER:HB3	1:E:95:ARG:CB	2.27	0.64
1:A:8:PRO:HG2	1:A:108:THR:HG21	1.79	0.64
2:D:9:PRO:O	2:D:110:THR:HG23	1.98	0.64
2:F:205:PRO:HA	2:F:242:GLY:O	1.97	0.64
1:A:28:SER:OG	1:A:29:PRO:HD3	1.98	0.64
2:D:118:LEU:HD23	2:D:118:LEU:N	2.12	0.64
2:F:38:GLN:HB3	2:F:44:LEU:CA	2.27	0.64
1:C:138:LEU:HD13	1:C:177:VAL:HG22	1.78	0.64
1:C:67:ASP:HB2	1:C:72:GLN:O	1.98	0.64
2:D:106:PHE:O	2:D:107:GLY:C	2.36	0.64
1:E:28:SER:OG	1:E:29:PRO:HD3	1.98	0.64
1:E:62:TYR:HD2	1:E:77:ILE:HG12	1.61	0.64
2:F:139:THR:HG21	2:F:196:ARG:HH21	1.63	0.64
1:A:13:ILE:HG22	1:A:14:LEU:H	1.62	0.64
1:C:102:LEU:HD12	1:C:102:LEU:N	2.13	0.64
1:E:69:ASP:OD1	1:E:71:LYS:HG2	1.98	0.64
2:F:171:VAL:HG22	2:F:195:LEU:HD13	1.79	0.64
1:C:6:GLN:NE2	1:C:105:GLY:HA3	2.12	0.64
1:C:8:PRO:CB	1:E:11:LEU:HD11	2.28	0.64
2:B:15:GLY:H	2:B:18:LYS:NZ	1.95	0.64
2:D:185:ASN:ND2	2:D:185:ASN:H	1.96	0.64
2:F:48:HIS:HA	2:F:57:GLU:O	1.98	0.64
2:F:7:GLN:HG3	2:F:24:CYS:HB3	1.80	0.64
1:C:51:THR:HG22	1:C:52:PHE:N	2.09	0.63
2:B:38:GLN:HG3	2:B:38:GLN:O	1.98	0.63
1:A:102:LEU:HD23	1:A:102:LEU:N	2.13	0.63
2:F:158:LEU:HD23	2:F:159:SER:N	2.13	0.63
1:C:10:SER:OG	1:E:12:ILE:HB	1.97	0.63
2:D:115:THR:HG22	2:D:117:ASP:HB2	1.79	0.63
1:A:31:SER:HB3	1:A:95:ARG:CB	2.29	0.63
2:B:184:LEU:HB3	2:B:186:ASP:OD2	1.99	0.63
2:D:39:ASP:HB3	2:D:40:PRO:HD2	1.81	0.63
2:D:152:TYR:O	2:D:153:PRO:C	2.31	0.63
1:E:33:LEU:HD12	1:E:92:VAL:HG22	1.81	0.62
2:B:14:ILE:CG2	2:B:18:LYS:HD2	2.28	0.62
2:D:11:TYR:HE1	2:D:111:ARG:HD2	1.61	0.62
2:B:106:PHE:O	2:B:107:GLY:C	2.37	0.62
1:C:113:TRP:HA	1:C:113:TRP:CE3	2.35	0.62
2:B:146:CYS:HB2	2:B:160:TRP:CZ2	2.34	0.62
1:A:7:SER:HA	1:A:8:PRO:C	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:HG2	1:C:49:ILE:HG12	1.79	0.62
2:F:39:ASP:HB3	2:F:40:PRO:HD2	1.82	0.62
1:A:55:ASN:HA	1:A:66:LEU:N	2.12	0.62
2:B:37:GLN:HB2	2:B:47:ILE:HD11	1.81	0.62
1:C:113:TRP:HA	1:C:113:TRP:HE3	1.65	0.62
1:C:177:VAL:HG12	1:C:178:ALA:N	2.13	0.62
1:E:25:TYR:OH	1:E:70:THR:HG22	2.00	0.62
1:E:176:ALA:HB3	1:E:191:PHE:HE2	1.65	0.62
2:B:7:GLN:NE2	2:B:92:CYS:H	1.98	0.62
1:C:31:SER:HB3	1:C:95:ARG:CB	2.29	0.62
2:F:96:GLU:HB3	2:F:102:TYR:H	1.65	0.62
1:A:51:THR:C	1:A:53:SER:H	2.03	0.61
1:A:92:VAL:O	1:A:102:LEU:HA	1.99	0.61
2:B:13:VAL:HG22	2:B:153:PRO:HG3	1.82	0.61
1:C:82:LEU:CD2	1:C:82:LEU:H	2.14	0.61
1:E:13:ILE:CG1	1:E:17:LYS:HD2	2.24	0.61
2:F:92:CYS:O	2:F:105:TYR:HB2	2.00	0.61
2:B:93:ALA:HA	2:B:105:TYR:CB	2.31	0.61
1:C:28:SER:OG	1:C:29:PRO:HD3	2.01	0.61
2:D:205:PRO:HA	2:D:242:GLY:O	2.01	0.61
1:A:55:ASN:HB3	1:A:66:LEU:O	2.01	0.61
1:C:61:ARG:HH22	1:C:84:ASP:CG	2.04	0.61
2:D:38:GLN:O	2:D:38:GLN:HG3	2.01	0.61
2:D:139:THR:HG21	2:D:196:ARG:NH2	2.16	0.61
1:E:51:THR:HG22	1:E:52:PHE:N	2.10	0.61
1:C:38:GLN:HE21	1:C:44:PRO:CD	2.10	0.60
2:D:14:ILE:HD11	2:D:114:VAL:HG22	1.83	0.60
2:D:13:VAL:HA	2:D:113:THR:O	2.01	0.60
1:A:55:ASN:HB2	1:A:65:THR:HG23	1.84	0.60
2:D:16:THR:HG22	2:D:84:PRO:HD3	1.83	0.60
2:D:146:CYS:HB2	2:D:160:TRP:CH2	2.36	0.60
2:F:118:LEU:C	2:F:120:ASN:H	2.05	0.60
1:E:164:LEU:HB3	2:F:172:SER:HB3	1.84	0.60
1:A:14:LEU:HB2	1:A:17:LYS:HE3	1.83	0.60
2:B:96:GLU:HB3	2:B:102:TYR:H	1.66	0.60
1:A:28:SER:CB	1:A:29:PRO:HD3	2.32	0.60
1:E:28:SER:CB	1:E:29:PRO:HD3	2.32	0.60
2:F:4:ASP:OD1	2:F:5:ILE:HG22	2.01	0.60
2:B:217:GLY:H	2:B:233:THR:CA	2.12	0.60
1:A:6:GLN:HE21	1:A:105:GLY:HA3	1.67	0.60
1:A:51:THR:HG22	1:A:52:PHE:N	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:185:ASN:H	2:F:185:ASN:ND2	1.99	0.59
2:D:16:THR:HG21	2:D:116:GLU:HG2	1.84	0.59
2:B:93:ALA:CA	2:B:105:TYR:HB3	2.32	0.59
1:C:28:SER:CB	1:C:29:PRO:HD3	2.33	0.59
2:B:9:PRO:HG2	2:B:12:LEU:HD22	1.84	0.59
1:C:97:SER:HB3	2:D:99:GLY:O	2.03	0.59
1:E:25:TYR:HH	1:E:70:THR:HG22	1.66	0.59
1:E:150:GLN:O	1:E:152:LYS:HG3	2.02	0.59
2:F:37:GLN:HG3	2:F:90:TYR:CE1	2.37	0.59
1:C:6:GLN:NE2	1:C:90:CYS:H	1.99	0.59
2:D:136:ILE:O	2:D:140:GLN:N	2.34	0.59
2:D:185:ASN:HD22	2:D:185:ASN:H	1.49	0.59
2:F:146:CYS:HB2	2:F:160:TRP:CZ2	2.36	0.59
2:B:7:GLN:HG2	2:B:24:CYS:HB3	1.85	0.59
1:C:11:LEU:HD11	1:E:8:PRO:CB	2.33	0.59
1:A:116:ILE:HG21	1:A:143:ASP:HA	1.85	0.59
2:B:39:ASP:HA	2:B:88:SER:HB2	1.83	0.59
1:C:51:THR:C	1:C:53:SER:H	2.06	0.59
1:A:162:THR:CG2	2:B:172:SER:HB2	2.29	0.59
2:B:146:CYS:HB2	2:B:160:TRP:CH2	2.38	0.59
2:B:185:ASN:ND2	2:B:185:ASN:H	2.01	0.59
1:C:136:VAL:HG12	1:C:179:TRP:CB	2.23	0.59
1:E:98:THR:O	2:F:32:LYS:HE3	2.01	0.59
1:E:157:TYR:O	1:E:178:ALA:HA	2.03	0.59
1:E:162:THR:CG2	2:F:172:SER:HB2	2.30	0.59
1:A:67:ASP:HB3	1:A:71:LYS:H	1.68	0.58
2:F:174:ASP:HB2	2:F:191:LEU:CD1	2.32	0.58
2:B:151:PHE:HE1	2:B:190:ALA:HA	1.68	0.58
2:B:218:LEU:HD13	2:B:231:PRO:O	2.04	0.58
1:A:116:ILE:CD1	1:A:144:SER:H	2.16	0.58
2:D:185:ASN:N	2:D:185:ASN:ND2	2.50	0.58
1:E:138:LEU:HD12	1:E:176:ALA:O	2.03	0.58
1:A:6:GLN:OE1	1:A:107:GLY:HA2	2.02	0.58
2:B:185:ASN:N	2:B:185:ASN:ND2	2.49	0.58
2:D:96:GLU:HB3	2:D:102:TYR:H	1.66	0.58
1:A:18:ASN:HD21	1:A:78:THR:HG23	1.65	0.58
1:A:6:GLN:HE22	1:A:90:CYS:H	1.48	0.58
1:A:22:GLN:HG2	1:A:74:SER:HB2	1.86	0.58
1:C:82:LEU:N	1:C:82:LEU:CD2	2.67	0.58
1:E:97:SER:HA	2:F:101:ALA:HB2	1.84	0.58
1:A:13:ILE:HG23	1:A:17:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ALA:HA	2:B:105:TYR:HB3	1.86	0.58
1:E:11:LEU:HD12	1:E:12:ILE:H	1.68	0.58
1:A:177:VAL:HG12	1:A:178:ALA:N	2.19	0.58
1:E:177:VAL:HG12	1:E:178:ALA:N	2.19	0.58
1:A:54:GLU:O	1:A:66:LEU:HB3	2.04	0.58
2:B:63:SER:O	2:B:64:GLU:HB2	2.04	0.58
2:F:12:LEU:HD12	2:F:13:VAL:H	1.69	0.58
2:F:39:ASP:HB3	2:F:40:PRO:CD	2.34	0.58
2:F:111:ARG:HD2	2:F:155:HIS:CD2	2.39	0.58
2:D:14:ILE:HD13	2:D:14:ILE:N	2.18	0.57
1:C:82:LEU:HD23	1:C:82:LEU:H	1.68	0.57
1:C:119:PRO:O	1:C:120:ASP:HB2	2.04	0.57
2:B:136:ILE:O	2:B:140:GLN:N	2.37	0.57
2:D:93:ALA:HA	2:D:105:TYR:CB	2.34	0.57
2:F:34:TYR:CB	2:F:93:ALA:HB3	2.26	0.57
2:B:26:GLN:HE22	2:B:29:GLY:CA	2.17	0.57
2:F:185:ASN:N	2:F:185:ASN:ND2	2.51	0.57
2:F:93:ALA:HA	2:F:105:TYR:CB	2.35	0.57
1:A:138:LEU:HD12	1:A:176:ALA:O	2.04	0.57
2:D:26:GLN:HE22	2:D:29:GLY:CA	2.17	0.57
2:B:33:MET:SD	2:B:75:PHE:HB2	2.45	0.57
2:D:67:VAL:HG12	2:D:68:SER:N	2.11	0.57
1:A:31:SER:OG	1:A:95:ARG:HA	2.05	0.57
1:C:171:PHE:CZ	1:C:173:SER:HB3	2.39	0.57
1:E:31:SER:OG	1:E:95:ARG:HA	2.04	0.57
1:E:92:VAL:HG12	1:E:93:SER:H	1.69	0.57
2:F:26:GLN:HE22	2:F:29:GLY:CA	2.17	0.57
2:F:151:PHE:HE1	2:F:190:ALA:HA	1.69	0.57
2:B:12:LEU:HD23	2:B:12:LEU:N	2.19	0.57
2:D:171:VAL:HG22	2:D:195:LEU:HD13	1.87	0.57
1:E:18:ASN:HB3	1:E:76:HIS:CE1	2.31	0.57
1:A:36:TYR:HA	1:A:45:VAL:O	2.04	0.56
2:D:139:THR:O	2:D:140:GLN:HB2	2.05	0.56
1:E:189:ASN:O	1:E:192:ASN:HB2	2.04	0.56
1:C:14:LEU:O	1:C:17:LYS:HB2	2.05	0.56
2:D:63:SER:O	2:D:64:GLU:HB2	2.05	0.56
2:D:181:GLN:O	2:D:187:SER:HB2	2.05	0.56
1:A:92:VAL:HG12	1:A:93:SER:H	1.70	0.56
2:B:112:LEU:HD12	2:B:113:THR:N	2.20	0.56
2:B:139:THR:HG21	2:B:196:ARG:NH2	2.20	0.56
1:C:92:VAL:HG12	1:C:93:SER:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:LEU:HD13	2:D:77:LEU:C	2.23	0.56
1:E:34:ARG:NH2	2:F:101:ALA:O	2.38	0.56
1:E:51:THR:HG22	1:E:52:PHE:HD1	1.70	0.56
1:E:51:THR:C	1:E:53:SER:H	2.07	0.56
1:E:69:ASP:OD2	1:E:71:LYS:HB3	2.05	0.56
2:F:131:PRO:CG	2:F:142:ALA:HB1	2.34	0.56
1:C:121:PRO:HA	1:C:140:THR:O	2.06	0.56
2:F:98:ILE:CG2	2:F:99:GLY:N	2.69	0.56
1:A:32:ASN:OD1	2:B:100:THR:HG23	2.05	0.56
2:B:83:ARG:H	2:B:86:HIS:HD2	1.53	0.56
2:D:115:THR:HG22	2:D:117:ASP:N	2.18	0.56
1:E:139:PHE:CE1	1:E:142:PHE:HD2	2.23	0.56
1:C:17:LYS:NZ	1:E:9:GLN:HE21	2.03	0.56
1:E:136:VAL:HG11	2:F:147:LEU:HD11	1.88	0.56
2:F:12:LEU:HD12	2:F:13:VAL:N	2.21	0.56
1:A:82:LEU:HA	1:A:112:VAL:HB	1.85	0.56
1:A:140:THR:HG22	1:A:141:ASP:N	2.19	0.56
2:B:3:ALA:HB1	2:B:6:TYR:OH	2.05	0.56
2:B:210:ARG:NH1	2:B:212:GLN:HB2	2.21	0.55
1:C:9:GLN:HE21	1:E:14:LEU:HG	1.68	0.55
2:D:115:THR:HG22	2:D:117:ASP:CB	2.36	0.55
1:E:6:GLN:HE22	1:E:89:ILE:HA	1.70	0.55
1:E:62:TYR:CD2	1:E:77:ILE:HG12	2.41	0.55
2:F:93:ALA:CB	2:F:105:TYR:HB3	2.36	0.55
2:B:23:GLU:HG2	2:B:76:PRO:CB	2.34	0.55
2:D:117:ASP:HB3	2:D:120:ASN:CB	2.37	0.55
1:A:150:GLN:O	1:A:152:LYS:HG3	2.06	0.55
2:D:46:LEU:HD11	2:D:49:TYR:HB3	1.89	0.55
1:E:67:ASP:OD1	1:E:69:ASP:OD1	2.24	0.55
1:E:113:TRP:HA	1:E:113:TRP:CE3	2.41	0.55
1:E:113:TRP:HA	1:E:113:TRP:HE3	1.72	0.55
1:E:171:PHE:CZ	1:E:173:SER:HB3	2.41	0.55
2:B:178:LEU:HD23	2:B:179:LYS:N	2.22	0.55
1:C:51:THR:HG22	1:C:52:PHE:HD1	1.71	0.55
1:E:13:ILE:O	1:E:112:VAL:HA	2.07	0.55
1:E:164:LEU:HD12	1:E:164:LEU:O	2.07	0.55
1:C:31:SER:OG	1:C:95:ARG:HA	2.07	0.55
1:A:67:ASP:OD1	1:A:69:ASP:OD1	2.24	0.55
1:E:120:ASP:O	1:E:141:ASP:HB2	2.06	0.55
2:B:130:GLU:OE1	2:B:243:ARG:HD3	2.06	0.55
1:C:67:ASP:OD1	1:C:69:ASP:OD1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:SER:HB3	1:E:17:LYS:HD3	1.89	0.55
1:C:9:GLN:HE21	1:E:17:LYS:HZ1	1.54	0.55
2:D:65:SER:HB2	2:D:77:LEU:HD21	1.88	0.55
1:A:189:ASN:O	1:A:192:ASN:HB2	2.08	0.54
2:D:98:ILE:CG2	2:D:99:GLY:N	2.69	0.54
1:C:18:ASN:HD21	1:C:78:THR:HG23	1.72	0.54
2:F:139:THR:HG21	2:F:196:ARG:NH2	2.22	0.54
1:A:14:LEU:HD23	1:A:113:TRP:HB2	1.89	0.54
1:C:140:THR:HG22	1:C:141:ASP:N	2.22	0.54
1:A:88:TYR:N	1:A:88:TYR:CD2	2.76	0.54
1:C:38:GLN:HG3	1:C:43:GLY:C	2.28	0.54
2:D:118:LEU:O	2:D:119:LYS:CB	2.56	0.54
2:F:5:ILE:HD11	2:F:92:CYS:SG	2.48	0.54
2:F:14:ILE:HG13	2:F:20:ILE:HD11	1.90	0.54
1:C:11:LEU:HD12	1:C:12:ILE:N	2.21	0.54
1:C:102:LEU:N	1:C:102:LEU:CD1	2.71	0.54
2:D:34:TYR:CD1	2:D:34:TYR:N	2.75	0.54
1:A:34:ARG:CG	1:A:49:ILE:HG12	2.36	0.54
2:D:173:THR:HG22	2:D:174:ASP:N	2.23	0.54
1:E:6:GLN:HE22	1:E:90:CYS:H	1.49	0.54
2:F:96:GLU:HB2	2:F:102:TYR:CB	2.37	0.54
1:A:51:THR:HG22	1:A:52:PHE:HD1	1.71	0.54
2:B:98:ILE:CG2	2:B:99:GLY:N	2.70	0.54
2:B:154:ASP:OD2	2:B:177:PRO:HG3	2.07	0.54
1:C:189:ASN:O	1:C:192:ASN:HB2	2.08	0.54
1:E:44:PRO:HG2	2:F:105:TYR:CE1	2.44	0.53
1:A:3:GLN:O	1:A:25:TYR:HA	2.07	0.53
2:D:122:PHE:O	2:D:151:PHE:HA	2.06	0.53
2:F:48:HIS:HE1	2:F:58:LYS:HE2	1.74	0.53
1:A:34:ARG:HH12	2:B:103:GLU:HB2	1.72	0.53
1:A:164:LEU:O	1:A:164:LEU:HD12	2.08	0.53
2:B:90:TYR:CE2	2:B:112:LEU:HD23	2.40	0.53
2:D:7:GLN:HE22	2:D:109:GLY:HA2	1.74	0.53
1:A:116:ILE:HD13	1:A:143:ASP:CB	2.35	0.53
2:D:133:GLU:HA	2:D:136:ILE:HD12	1.90	0.53
2:D:174:ASP:OD2	2:D:191:LEU:HD12	2.08	0.53
1:A:142:PHE:CE1	1:A:174:ASN:HB2	2.43	0.53
1:C:110:LEU:HD12	1:C:111:THR:N	2.22	0.53
1:A:88:TYR:N	1:A:88:TYR:HD2	2.06	0.53
2:F:47:ILE:O	2:F:58:LYS:HA	2.07	0.53
1:A:138:LEU:HD13	1:A:177:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ARG:HD3	1:E:145:GLN:NE2	2.24	0.53
1:A:116:ILE:HG21	1:A:143:ASP:CB	2.39	0.53
2:B:67:VAL:HG11	2:B:75:PHE:CE1	2.43	0.53
2:B:96:GLU:HB2	2:B:102:TYR:CB	2.38	0.53
1:C:142:PHE:CE1	1:C:174:ASN:HB2	2.44	0.53
2:F:131:PRO:HD3	2:F:144:LEU:CD2	2.38	0.53
1:A:55:ASN:CA	1:A:66:LEU:H	2.16	0.53
1:A:71:LYS:HG3	1:A:72:GLN:HG2	1.91	0.53
2:F:122:PHE:O	2:F:151:PHE:HA	2.08	0.52
1:A:51:THR:C	1:A:53:SER:N	2.62	0.52
1:C:6:GLN:OE1	1:C:107:GLY:HA2	2.09	0.52
1:C:32:ASN:OD1	2:D:100:THR:HG23	2.09	0.52
2:D:96:GLU:HB2	2:D:102:TYR:CB	2.38	0.52
1:E:34:ARG:HG2	1:E:49:ILE:HG23	1.91	0.52
1:E:140:THR:HG22	1:E:141:ASP:N	2.21	0.52
1:A:34:ARG:HD3	1:A:49:ILE:HG12	1.92	0.52
2:D:151:PHE:HE1	2:D:190:ALA:HA	1.73	0.52
1:A:44:PRO:HD2	2:B:105:TYR:HE1	1.71	0.52
2:B:119:LYS:HE2	2:B:226:GLN:NE2	2.24	0.52
2:D:37:GLN:NE2	2:D:90:TYR:OH	2.43	0.52
2:F:218:LEU:HD13	2:F:231:PRO:O	2.10	0.52
1:A:177:VAL:HG12	1:A:178:ALA:H	1.74	0.52
2:D:6:TYR:N	2:D:6:TYR:CD1	2.78	0.52
2:D:93:ALA:HA	2:D:105:TYR:HB3	1.91	0.52
1:A:55:ASN:HB2	1:A:65:THR:CG2	2.40	0.52
2:D:8:THR:OG1	2:D:23:GLU:HB2	2.09	0.52
2:D:46:LEU:O	2:D:59:GLY:HA3	2.10	0.52
2:B:122:PHE:O	2:B:151:PHE:HA	2.10	0.52
1:C:10:SER:O	1:E:11:LEU:HD12	2.10	0.52
2:F:14:ILE:HD13	2:F:14:ILE:H	1.74	0.52
2:F:63:SER:O	2:F:64:GLU:HG2	2.10	0.52
1:E:44:PRO:HG2	2:F:105:TYR:CZ	2.46	0.51
2:B:178:LEU:HD23	2:B:178:LEU:C	2.31	0.51
2:D:88:SER:OG	2:D:89:GLN:N	2.41	0.51
1:A:13:ILE:CG2	1:A:14:LEU:H	2.23	0.51
1:A:13:ILE:CG2	1:A:14:LEU:N	2.71	0.51
1:C:48:THR:HG22	1:C:49:ILE:N	2.25	0.51
1:C:80:SER:O	1:C:81:GLN:HG3	2.09	0.51
2:D:15:GLY:HA2	2:D:115:THR:O	2.10	0.51
2:B:5:ILE:HG22	2:B:6:TYR:N	2.25	0.51
2:B:48:HIS:CE1	2:B:58:LYS:HG2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ARG:HD3	1:E:145:GLN:HE22	1.75	0.51
1:C:128:ASP:OD1	1:C:130:LYS:N	2.42	0.51
1:C:151:SER:O	1:C:152:LYS:HB2	2.10	0.51
2:D:90:TYR:O	2:D:109:GLY:HA2	2.10	0.51
2:F:44:LEU:H	2:F:44:LEU:CD2	2.11	0.51
1:A:157:TYR:O	1:A:178:ALA:HA	2.10	0.51
1:C:37:LYS:HB2	1:C:47:LEU:HD11	1.92	0.51
2:D:152:TYR:CD1	2:D:153:PRO:N	2.79	0.51
1:E:158:ILE:HG12	1:E:178:ALA:HB2	1.92	0.51
2:D:178:LEU:HD23	2:D:179:LYS:N	2.26	0.51
1:A:34:ARG:HD3	1:A:49:ILE:CD1	2.40	0.51
1:C:8:PRO:HB2	1:E:11:LEU:HD11	1.91	0.51
2:D:35:TRP:O	2:D:47:ILE:HG12	2.11	0.51
2:F:80:GLU:OE1	2:F:80:GLU:HA	2.10	0.51
1:A:63:THR:HB	1:A:76:HIS:HB3	1.92	0.51
1:A:177:VAL:CG2	2:B:194:ARG:HD3	2.40	0.51
2:B:173:THR:HG22	2:B:174:ASP:N	2.26	0.51
1:C:34:ARG:HG2	1:C:49:ILE:HG23	1.93	0.51
2:D:69:ARG:HD3	2:D:75:PHE:CD1	2.46	0.51
2:D:93:ALA:CB	2:D:105:TYR:HB3	2.41	0.51
1:E:93:SER:HB3	1:E:102:LEU:HD13	1.92	0.51
1:A:116:ILE:HD11	1:A:144:SER:H	1.75	0.51
2:B:7:GLN:HE21	2:B:107:GLY:CA	2.19	0.51
1:C:164:LEU:HB3	2:D:172:SER:HB3	1.93	0.51
2:D:91:LEU:HD23	2:D:109:GLY:HA3	1.93	0.51
2:D:217:GLY:H	2:D:233:THR:CA	2.23	0.51
1:E:67:ASP:HB2	1:E:72:GLN:O	2.11	0.51
2:D:178:LEU:HD23	2:D:178:LEU:C	2.32	0.50
1:A:144:SER:O	1:A:161:LYS:NZ	2.44	0.50
2:B:48:HIS:HA	2:B:57:GLU:O	2.11	0.50
1:C:106:ARG:NH1	1:E:145:GLN:NE2	2.59	0.50
2:F:83:ARG:HB2	2:F:86:HIS:CD2	2.46	0.50
1:A:94:ASP:OD1	1:A:103:TYR:CE1	2.63	0.50
1:A:48:THR:HG22	1:A:49:ILE:N	2.27	0.50
2:F:158:LEU:HD23	2:F:158:LEU:C	2.32	0.50
1:C:51:THR:C	1:C:53:SER:N	2.65	0.50
1:E:48:THR:HG22	1:E:49:ILE:N	2.26	0.50
1:E:51:THR:C	1:E:53:SER:N	2.65	0.50
1:E:158:ILE:HG12	1:E:178:ALA:CB	2.41	0.50
2:B:12:LEU:HD12	2:B:14:ILE:HD11	1.94	0.50
2:B:21:THR:HG23	2:B:78:THR:OG1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:THR:HG21	2:B:153:PRO:CB	2.42	0.50
1:C:44:PRO:CG	2:D:105:TYR:OH	2.57	0.50
2:D:16:THR:CG2	2:D:84:PRO:HD3	2.41	0.50
1:E:34:ARG:HH12	2:F:103:GLU:HB2	1.76	0.50
2:F:6:TYR:O	2:F:24:CYS:HA	2.11	0.50
2:D:131:PRO:HD3	2:D:144:LEU:HD21	1.93	0.50
2:B:139:THR:O	2:B:140:GLN:HB2	2.12	0.50
1:C:21:LEU:O	1:C:74:SER:HA	2.12	0.50
1:C:136:VAL:HG11	2:D:147:LEU:HD11	1.93	0.50
2:D:218:LEU:N	2:D:218:LEU:HD12	2.26	0.50
1:E:19:CYS:O	1:E:77:ILE:N	2.44	0.50
1:E:92:VAL:HG12	1:E:93:SER:N	2.26	0.50
1:A:34:ARG:NH1	2:B:103:GLU:HB2	2.26	0.49
2:B:121:VAL:O	2:B:228:ARG:NH2	2.40	0.49
2:B:169:SER:O	2:B:171:VAL:HG23	2.12	0.49
1:C:150:GLN:O	1:C:152:LYS:HG3	2.12	0.49
2:F:217:GLY:H	2:F:233:THR:CA	2.20	0.49
2:B:67:VAL:HG12	2:B:68:SER:N	2.27	0.49
2:D:115:THR:HG21	2:D:117:ASP:HB2	1.94	0.49
2:F:25:SER:HB3	2:F:74:HIS:ND1	2.27	0.49
2:F:35:TRP:CE2	2:F:77:LEU:HB2	2.47	0.49
1:A:92:VAL:HG12	1:A:93:SER:N	2.27	0.49
1:C:162:THR:CG2	2:D:172:SER:HB2	2.39	0.49
2:F:136:ILE:O	2:F:140:GLN:N	2.40	0.49
2:F:146:CYS:HB2	2:F:160:TRP:CH2	2.47	0.49
2:D:210:ARG:NH1	2:D:212:GLN:HB2	2.25	0.49
1:E:6:GLN:NE2	1:E:90:CYS:N	2.47	0.49
2:D:14:ILE:N	2:D:14:ILE:CD1	2.76	0.49
1:E:20:THR:HA	1:E:75:LEU:O	2.12	0.49
2:F:185:ASN:HD22	2:F:186:ASP:N	2.10	0.49
1:C:145:GLN:HE22	1:E:106:ARG:NE	2.09	0.49
2:F:20:ILE:O	2:F:78:THR:HG23	2.13	0.49
2:F:178:LEU:HD23	2:F:178:LEU:C	2.33	0.49
1:A:8:PRO:HG2	1:A:108:THR:CG2	2.43	0.49
1:A:15:GLU:OE2	1:A:114:PRO:HA	2.13	0.49
2:D:2:GLU:CD	2:D:3:ALA:H	2.16	0.49
1:E:81:GLN:O	1:E:84:ASP:N	2.45	0.49
1:A:13:ILE:HG22	1:A:17:LYS:HD2	1.95	0.49
2:B:93:ALA:CB	2:B:105:TYR:CB	2.88	0.49
2:B:83:ARG:C	2:B:114:VAL:HG11	2.33	0.48
2:B:112:LEU:HD12	2:B:113:THR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:THR:HG21	2:D:116:GLU:CG	2.43	0.48
1:E:124:TYR:HB3	2:F:132:SER:CB	2.43	0.48
2:D:7:GLN:NE2	2:D:109:GLY:HA2	2.27	0.48
2:D:20:ILE:O	2:D:78:THR:HA	2.13	0.48
2:F:20:ILE:HG22	2:F:21:THR:N	2.27	0.48
2:F:131:PRO:HD3	2:F:144:LEU:HD21	1.94	0.48
1:A:87:SER:C	1:A:88:TYR:HD2	2.15	0.48
1:C:18:ASN:CG	1:C:78:THR:HA	2.33	0.48
1:E:124:TYR:CE2	2:F:135:GLU:HG3	2.48	0.48
2:D:158:LEU:HD23	2:D:158:LEU:C	2.33	0.48
2:F:68:SER:O	2:F:76:PRO:HD2	2.14	0.48
2:F:139:THR:O	2:F:140:GLN:HB2	2.13	0.48
1:C:9:GLN:HE22	1:E:14:LEU:HG	1.76	0.48
1:E:106:ARG:HG2	1:E:106:ARG:HH11	1.79	0.48
1:A:116:ILE:HG21	1:A:143:ASP:CA	2.43	0.48
2:F:191:LEU:HD12	2:F:192:SER:H	1.79	0.48
1:C:67:ASP:HB3	1:C:70:THR:HA	1.96	0.48
1:E:124:TYR:CZ	2:F:135:GLU:HA	2.48	0.48
2:F:83:ARG:N	2:F:86:HIS:CD2	2.76	0.48
1:A:176:ALA:HB3	1:A:191:PHE:HE2	1.78	0.48
2:B:7:GLN:O	2:B:8:THR:HG23	2.13	0.48
1:E:38:GLN:CB	1:E:44:PRO:HB3	2.36	0.48
2:B:14:ILE:HG23	2:B:18:LYS:CD	2.41	0.48
1:C:92:VAL:HG12	1:C:93:SER:N	2.28	0.48
2:D:14:ILE:HG13	2:D:20:ILE:HD11	1.96	0.48
1:C:54:GLU:O	1:C:56:THR:HG22	2.14	0.47
1:E:18:ASN:OD1	1:E:78:THR:HA	2.13	0.47
1:E:91:VAL:HG13	1:E:103:TYR:O	2.14	0.47
2:F:7:GLN:HG3	2:F:24:CYS:CB	2.44	0.47
2:F:37:GLN:HB2	2:F:47:ILE:HD11	1.96	0.47
2:F:118:LEU:C	2:F:120:ASN:N	2.67	0.47
1:A:23:CYS:O	1:A:72:GLN:HA	2.14	0.47
2:B:103:GLU:CD	2:B:104:GLN:N	2.68	0.47
2:D:103:GLU:CD	2:D:104:GLN:N	2.68	0.47
2:F:17:GLY:HA2	2:F:81:SER:HB2	1.97	0.47
1:A:51:THR:O	1:A:53:SER:N	2.47	0.47
2:B:66:THR:O	2:B:77:LEU:HD12	2.14	0.47
2:B:121:VAL:HG12	2:B:231:PRO:HB2	1.97	0.47
2:B:93:ALA:HB1	2:B:105:TYR:HB3	1.95	0.47
2:D:92:CYS:O	2:D:105:TYR:HB2	2.15	0.47
1:E:2:ASN:HB2	1:E:26:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:PHE:N	2:B:76:PRO:CD	2.78	0.47
2:B:194:ARG:N	2:B:194:ARG:HE	2.12	0.47
1:C:144:SER:O	1:C:161:LYS:NZ	2.48	0.47
2:D:13:VAL:HG13	2:D:13:VAL:O	2.15	0.47
1:E:21:LEU:O	1:E:74:SER:HA	2.15	0.47
1:E:51:THR:CG2	1:E:52:PHE:H	2.15	0.47
2:B:7:GLN:NE2	2:B:92:CYS:HB3	2.29	0.47
2:B:13:VAL:C	2:B:14:ILE:HG13	2.34	0.47
1:E:7:SER:HA	1:E:8:PRO:O	2.15	0.47
2:F:126:VAL:HG12	2:F:127:ALA:N	2.28	0.47
1:A:126:LEU:HD23	2:B:132:SER:HB2	1.97	0.47
2:B:83:ARG:O	2:B:114:VAL:HG21	2.14	0.47
2:B:143:THR:HA	2:B:195:LEU:O	2.15	0.47
2:B:181:GLN:O	2:B:187:SER:HB2	2.14	0.47
2:D:115:THR:C	2:D:117:ASP:H	2.16	0.47
1:E:138:LEU:HD13	1:E:177:VAL:HG22	1.97	0.47
2:F:154:ASP:CG	2:F:177:PRO:HG3	2.35	0.47
1:C:51:THR:O	1:C:53:SER:N	2.48	0.47
1:C:177:VAL:HG12	1:C:178:ALA:H	1.79	0.47
1:E:81:GLN:N	1:E:84:ASP:OD2	2.47	0.47
2:F:135:GLU:O	2:F:139:THR:HB	2.14	0.47
2:F:181:GLN:O	2:F:187:SER:HB2	2.14	0.47
1:A:37:LYS:O	1:A:37:LYS:HG2	2.15	0.46
1:A:119:PRO:O	1:A:120:ASP:HB2	2.14	0.46
2:B:13:VAL:CG2	2:B:153:PRO:HG3	2.45	0.46
1:E:16:GLY:O	1:E:79:ALA:HA	2.15	0.46
2:F:93:ALA:HA	2:F:105:TYR:HB3	1.96	0.46
1:A:67:ASP:OD2	1:A:71:LYS:NZ	2.47	0.46
2:B:3:ALA:HB3	2:B:27:THR:HG1	1.76	0.46
1:C:44:PRO:HD2	2:D:105:TYR:CE1	2.50	0.46
2:D:20:ILE:HB	2:D:79:LEU:HB2	1.96	0.46
1:E:50:MET:HG2	1:E:57:LYS:HD2	1.97	0.46
2:F:98:ILE:HG22	2:F:99:GLY:H	1.80	0.46
2:F:106:PHE:O	2:F:108:PRO:N	2.48	0.46
1:C:82:LEU:HD22	1:C:172:LYS:HZ3	1.80	0.46
2:B:174:ASP:HB2	2:B:191:LEU:HD11	1.98	0.46
2:F:98:ILE:CG2	2:F:99:GLY:H	2.28	0.46
2:F:178:LEU:HD23	2:F:179:LYS:N	2.29	0.46
2:B:66:THR:HG22	2:B:67:VAL:N	2.31	0.46
1:E:61:ARG:HB3	1:E:78:THR:O	2.15	0.46
2:B:115:THR:HG22	2:B:117:ASP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:HD23	2:B:158:LEU:C	2.35	0.46
2:F:143:THR:HA	2:F:195:LEU:O	2.15	0.46
1:A:6:GLN:NE2	1:A:105:GLY:HA3	2.30	0.46
2:D:30:HIS:HA	2:D:97:ASN:HD21	1.81	0.46
2:D:210:ARG:HG3	2:D:239:GLU:HB3	1.97	0.46
2:F:13:VAL:HA	2:F:113:THR:O	2.16	0.46
1:A:67:ASP:CG	1:A:71:LYS:HG2	2.37	0.46
2:B:67:VAL:HG12	2:B:68:SER:H	1.81	0.46
1:C:69:ASP:OD1	1:C:71:LYS:HE2	2.16	0.46
2:F:22:LEU:HD13	2:F:110:THR:HG21	1.97	0.46
2:B:7:GLN:HG2	2:B:24:CYS:CB	2.46	0.46
1:C:9:GLN:HE22	1:E:14:LEU:CG	2.29	0.46
2:D:119:LYS:HD3	2:D:226:GLN:CD	2.36	0.46
1:E:56:THR:HG23	1:E:63:THR:HG23	1.98	0.46
1:E:177:VAL:CG2	2:F:194:ARG:HD3	2.46	0.46
2:F:169:SER:O	2:F:171:VAL:HG23	2.16	0.46
2:F:244:ALA:O	2:F:245:ASP:HB2	2.16	0.46
1:A:149:SER:CB	1:A:193:ASN:O	2.63	0.46
2:B:83:ARG:HB2	2:B:86:HIS:NE2	2.30	0.46
1:A:50:MET:HA	1:A:57:LYS:HZ3	1.78	0.45
2:D:144:LEU:N	2:D:195:LEU:O	2.45	0.45
2:F:103:GLU:CD	2:F:104:GLN:N	2.69	0.45
1:A:96:GLY:C	1:A:98:THR:H	2.20	0.45
1:C:89:ILE:HG12	1:C:107:GLY:HA3	1.97	0.45
2:D:90:TYR:HE2	2:D:112:LEU:HD23	1.80	0.45
1:E:51:THR:O	1:E:53:SER:N	2.49	0.45
2:F:77:LEU:HD13	2:F:77:LEU:C	2.36	0.45
1:A:7:SER:CA	1:A:8:PRO:O	2.63	0.45
1:A:78:THR:HG22	1:A:79:ALA:N	2.31	0.45
2:B:93:ALA:CA	2:B:105:TYR:CB	2.94	0.45
2:F:10:ARG:NH1	2:F:108:PRO:HG2	2.31	0.45
1:A:164:LEU:HB3	2:B:172:SER:HB3	1.98	0.45
2:B:118:LEU:N	2:B:118:LEU:CD2	2.78	0.45
2:B:174:ASP:OD2	2:B:191:LEU:HD12	2.16	0.45
2:D:63:SER:O	2:D:64:GLU:CB	2.64	0.45
2:D:195:LEU:HD12	2:D:196:ARG:N	2.31	0.45
2:F:145:VAL:HG22	2:F:194:ARG:HG3	1.98	0.45
1:A:136:VAL:HG12	1:A:179:TRP:CB	2.35	0.45
2:B:98:ILE:HG22	2:B:99:GLY:H	1.81	0.45
1:C:17:LYS:HZ3	1:E:9:GLN:HE21	1.63	0.45
1:C:36:TYR:CD1	1:C:46:SER:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:CG2	1:A:143:ASP:HA	2.45	0.45
2:D:128:VAL:HA	2:D:145:VAL:O	2.17	0.45
1:E:96:GLY:C	1:E:98:THR:N	2.70	0.45
1:E:56:THR:HG22	1:E:57:LYS:N	2.31	0.45
1:A:82:LEU:N	1:A:82:LEU:HD23	2.32	0.45
2:B:7:GLN:HE22	2:B:92:CYS:H	1.65	0.45
1:C:4:VAL:HG21	1:C:103:TYR:O	2.17	0.45
1:C:96:GLY:C	1:C:98:THR:N	2.70	0.45
2:D:35:TRP:CD1	2:D:75:PHE:CD2	3.05	0.45
2:D:115:THR:C	2:D:117:ASP:N	2.70	0.45
1:A:65:THR:O	1:A:73:SER:HA	2.17	0.45
1:A:96:GLY:C	1:A:98:THR:N	2.71	0.45
2:B:30:HIS:HA	2:B:97:ASN:HD21	1.82	0.45
2:B:100:THR:O	2:B:101:ALA:C	2.55	0.45
1:C:139:PHE:CE1	1:C:142:PHE:HD2	2.35	0.45
2:D:25:SER:HA	2:D:73:GLU:O	2.16	0.45
2:D:98:ILE:CG2	2:D:99:GLY:H	2.29	0.45
1:E:177:VAL:HG12	1:E:178:ALA:H	1.83	0.45
2:F:100:THR:O	2:F:101:ALA:C	2.55	0.45
1:A:34:ARG:CD	1:A:49:ILE:HG12	2.46	0.44
1:C:15:GLU:OE1	1:C:172:LYS:NZ	2.44	0.44
1:C:96:GLY:C	1:C:98:THR:H	2.19	0.44
1:E:14:LEU:H	1:E:17:LYS:HZ2	1.64	0.44
1:E:110:LEU:HD12	1:E:111:THR:H	1.82	0.44
2:F:8:THR:CB	2:F:9:PRO:CD	2.94	0.44
1:A:21:LEU:N	1:A:21:LEU:CD2	2.78	0.44
1:A:151:SER:C	1:A:153:ASP:H	2.20	0.44
2:F:124:PRO:HA	2:F:151:PHE:HB3	1.99	0.44
1:A:33:LEU:HD21	1:A:73:SER:CB	2.47	0.44
2:B:106:PHE:O	2:B:108:PRO:N	2.50	0.44
2:B:218:LEU:N	2:B:218:LEU:HD12	2.32	0.44
1:C:157:TYR:O	1:C:178:ALA:HA	2.17	0.44
1:C:164:LEU:HD12	1:C:164:LEU:C	2.37	0.44
1:C:177:VAL:CG1	1:C:178:ALA:N	2.80	0.44
2:D:37:GLN:HB2	2:D:90:TYR:CD1	2.52	0.44
1:E:14:LEU:CD2	1:E:113:TRP:HB2	2.45	0.44
1:E:96:GLY:C	1:E:98:THR:H	2.20	0.44
1:A:55:ASN:O	1:A:65:THR:HG23	2.17	0.44
1:A:94:ASP:O	1:A:95:ARG:C	2.55	0.44
2:B:4:ASP:HB3	2:B:5:ILE:H	1.61	0.44
2:B:25:SER:HB3	2:B:74:HIS:ND1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ARG:N	2:B:86:HIS:HD2	2.16	0.44
2:B:107:GLY:O	2:B:109:GLY:N	2.50	0.44
2:D:106:PHE:O	2:D:108:PRO:N	2.50	0.44
2:F:3:ALA:HB3	2:F:27:THR:OG1	2.18	0.44
2:F:191:LEU:HD12	2:F:192:SER:N	2.32	0.44
1:C:67:ASP:CB	1:C:72:GLN:O	2.65	0.44
2:D:100:THR:O	2:D:101:ALA:C	2.56	0.44
2:D:174:ASP:HB2	2:D:191:LEU:HD11	2.00	0.44
1:E:144:SER:O	1:E:161:LYS:NZ	2.51	0.44
2:F:44:LEU:HD23	2:F:44:LEU:N	2.14	0.44
2:F:111:ARG:NH2	2:F:154:ASP:OD1	2.47	0.44
2:D:45:HIS:O	2:D:47:ILE:HG23	2.18	0.44
2:D:184:LEU:HB2	2:D:187:SER:HB2	1.99	0.44
2:B:98:ILE:CG2	2:B:99:GLY:H	2.30	0.44
1:E:47:LEU:HD23	1:E:47:LEU:N	2.33	0.44
1:E:94:ASP:O	1:E:95:ARG:C	2.55	0.44
1:C:106:ARG:NH1	1:E:145:GLN:HE21	2.16	0.44
1:E:4:VAL:HG12	1:E:25:TYR:HB3	2.00	0.44
1:E:61:ARG:HD2	1:E:78:THR:O	2.17	0.44
1:E:81:GLN:O	1:E:83:SER:N	2.50	0.44
1:A:33:LEU:O	1:A:49:ILE:HA	2.17	0.44
1:A:50:MET:CE	1:A:57:LYS:HG3	2.47	0.44
2:B:128:VAL:HG12	2:B:129:PHE:N	2.33	0.44
1:C:81:GLN:C	1:C:83:SER:N	2.72	0.44
1:C:85:SER:HB3	1:C:112:VAL:N	2.33	0.44
1:C:126:LEU:HD22	2:D:131:PRO:HA	1.99	0.44
1:A:20:THR:HG22	1:A:76:HIS:CA	2.46	0.43
2:B:93:ALA:HB2	2:B:105:TYR:CB	2.48	0.43
2:B:154:ASP:CG	2:B:177:PRO:HG3	2.38	0.43
1:E:164:LEU:HD12	1:E:164:LEU:C	2.38	0.43
2:F:77:LEU:HD22	2:F:78:THR:H	1.83	0.43
2:F:89:GLN:HE21	2:F:91:LEU:HD21	1.83	0.43
1:A:116:ILE:CD1	1:A:144:SER:N	2.81	0.43
2:B:160:TRP:O	2:B:166:GLU:HA	2.19	0.43
1:C:149:SER:CB	1:C:193:ASN:O	2.66	0.43
2:D:26:GLN:HE22	2:D:29:GLY:N	2.16	0.43
2:D:124:PRO:CA	2:D:151:PHE:HB3	2.48	0.43
1:A:38:GLN:HG3	1:A:44:PRO:CD	2.48	0.43
1:A:103:TYR:N	1:A:103:TYR:CD1	2.86	0.43
1:C:53:SER:O	1:C:54:GLU:O	2.36	0.43
1:C:97:SER:HA	2:D:101:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:126:VAL:HG13	2:F:146:CYS:SG	2.58	0.43
2:F:174:ASP:OD2	2:F:191:LEU:HD12	2.18	0.43
2:B:7:GLN:NE2	2:B:107:GLY:HA3	2.21	0.43
2:B:84:PRO:HA	2:B:114:VAL:HB	2.01	0.43
1:C:50:MET:CE	1:C:55:ASN:HA	2.48	0.43
2:D:149:THR:HG22	2:D:150:GLY:N	2.34	0.43
2:D:154:ASP:OD2	2:D:177:PRO:HG3	2.17	0.43
1:C:120:ASP:O	1:C:141:ASP:HB2	2.19	0.43
2:D:93:ALA:CA	2:D:105:TYR:HB3	2.48	0.43
2:B:26:GLN:HE22	2:B:29:GLY:N	2.16	0.43
1:C:9:GLN:NE2	1:E:14:LEU:CG	2.74	0.43
1:C:9:GLN:HE21	1:E:17:LYS:HZ2	1.62	0.43
1:E:14:LEU:HG	1:E:17:LYS:HZ2	1.83	0.43
2:F:30:HIS:HA	2:F:97:ASN:HD21	1.83	0.43
2:F:130:GLU:OE1	2:F:243:ARG:HD3	2.18	0.43
2:F:7:GLN:HA	2:F:24:CYS:HB3	2.00	0.43
1:C:2:ASN:N	1:C:27:VAL:HG12	2.34	0.43
2:D:103:GLU:CD	2:D:103:GLU:C	2.77	0.43
1:E:129:SER:HA	2:F:130:GLU:OE2	2.18	0.43
1:E:182:LYS:O	1:E:183:SER:HB2	2.19	0.43
2:F:107:GLY:O	2:F:109:GLY:N	2.52	0.43
2:B:63:SER:O	2:B:64:GLU:CB	2.66	0.43
2:B:126:VAL:HG13	2:B:146:CYS:SG	2.59	0.43
1:C:17:LYS:NZ	1:E:9:GLN:NE2	2.66	0.43
1:C:44:PRO:CG	2:D:105:TYR:CZ	3.01	0.43
1:C:94:ASP:O	1:C:95:ARG:C	2.57	0.43
2:D:61:LEU:N	2:D:61:LEU:HD23	2.33	0.43
1:E:28:SER:OG	1:E:29:PRO:CD	2.66	0.43
2:B:116:GLU:O	2:B:117:ASP:HB2	2.19	0.43
2:B:178:LEU:HD23	2:B:179:LYS:C	2.39	0.43
1:C:22:GLN:HG2	1:C:74:SER:HB3	2.01	0.43
1:C:182:LYS:O	1:C:183:SER:HB2	2.18	0.43
2:D:107:GLY:O	2:D:109:GLY:N	2.52	0.43
1:E:36:TYR:O	1:E:88:TYR:HA	2.18	0.43
2:F:34:TYR:N	2:F:34:TYR:CD2	2.86	0.43
1:A:11:LEU:HD12	1:A:12:ILE:H	1.84	0.42
1:A:151:SER:O	1:A:152:LYS:HB2	2.19	0.42
2:B:48:HIS:HE1	2:B:58:LYS:HE2	1.84	0.42
1:E:68:ALA:C	1:E:70:THR:H	2.21	0.42
1:A:153:ASP:O	1:A:155:ASP:N	2.52	0.42
2:D:154:ASP:CG	2:D:177:PRO:HG3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:LEU:N	2:D:218:LEU:CD1	2.82	0.42
1:E:18:ASN:C	1:E:19:CYS:SG	2.98	0.42
2:F:160:TRP:O	2:F:166:GLU:HA	2.19	0.42
1:A:28:SER:OG	1:A:29:PRO:CD	2.66	0.42
1:A:55:ASN:CB	1:A:66:LEU:O	2.67	0.42
2:B:7:GLN:CD	2:B:92:CYS:HB3	2.40	0.42
2:B:47:ILE:O	2:B:58:LYS:HA	2.20	0.42
1:C:7:SER:HA	1:C:8:PRO:C	2.39	0.42
1:E:28:SER:CB	1:E:29:PRO:CD	2.97	0.42
2:F:26:GLN:HE22	2:F:29:GLY:N	2.17	0.42
1:A:28:SER:CB	1:A:29:PRO:CD	2.98	0.42
2:B:103:GLU:CD	2:B:103:GLU:C	2.78	0.42
2:B:159:SER:O	2:B:212:GLN:N	2.46	0.42
1:C:81:GLN:N	1:C:84:ASP:OD2	2.53	0.42
2:D:160:TRP:O	2:D:166:GLU:HA	2.19	0.42
1:E:26:THR:O	1:E:26:THR:HG22	2.18	0.42
2:F:14:ILE:HD13	2:F:14:ILE:N	2.33	0.42
2:F:83:ARG:H	2:F:86:HIS:CD2	2.11	0.42
2:F:173:THR:HG22	2:F:174:ASP:N	2.34	0.42
2:B:25:SER:HA	2:B:73:GLU:O	2.20	0.42
1:C:17:LYS:NZ	1:E:9:GLN:HG2	2.35	0.42
1:E:82:LEU:HD21	1:E:172:LYS:NZ	2.35	0.42
1:E:149:SER:CB	1:E:193:ASN:O	2.68	0.42
1:C:12:ILE:HD12	1:E:10:SER:OG	2.20	0.42
1:C:23:CYS:HB2	1:C:35:TRP:CH2	2.55	0.42
2:D:67:VAL:CG1	2:D:68:SER:H	2.10	0.42
2:D:83:ARG:C	2:D:114:VAL:HG11	2.40	0.42
2:F:218:LEU:N	2:F:218:LEU:HD12	2.34	0.42
2:F:225:THR:OG1	2:F:226:GLN:NE2	2.53	0.42
2:B:84:PRO:N	2:B:114:VAL:HG11	2.34	0.42
2:D:83:ARG:HA	2:D:84:PRO:HD3	1.93	0.42
2:D:153:PRO:O	2:D:155:HIS:N	2.46	0.42
1:E:37:LYS:NZ	1:E:84:ASP:HA	2.34	0.42
1:E:53:SER:O	1:E:54:GLU:O	2.38	0.42
2:F:117:ASP:CB	2:F:120:ASN:OD1	2.68	0.42
2:F:170:GLY:O	2:F:195:LEU:HD12	2.20	0.42
2:F:208:HIS:HB2	2:F:241:TRP:CZ3	2.54	0.42
1:A:21:LEU:O	1:A:74:SER:HA	2.20	0.42
1:A:69:ASP:O	1:A:70:THR:HB	2.20	0.42
1:A:151:SER:C	1:A:153:ASP:N	2.73	0.42
2:B:107:GLY:HA2	2:B:108:PRO:HD2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:SER:HA	2:F:73:GLU:O	2.20	0.42
2:F:86:HIS:O	2:F:87:THR:C	2.58	0.42
2:F:103:GLU:CD	2:F:103:GLU:C	2.79	0.42
1:A:123:VAL:HA	1:A:138:LEU:O	2.19	0.41
2:D:107:GLY:C	2:D:109:GLY:H	2.23	0.41
1:E:31:SER:CB	1:E:95:ARG:HB2	2.42	0.41
1:E:102:LEU:HD22	1:E:102:LEU:N	2.35	0.41
2:B:107:GLY:C	2:B:109:GLY:H	2.23	0.41
2:B:107:GLY:C	2:B:109:GLY:N	2.73	0.41
2:B:149:THR:HG22	2:B:150:GLY:N	2.35	0.41
2:B:151:PHE:CE1	2:B:190:ALA:HA	2.53	0.41
1:C:106:ARG:HG2	2:D:43:GLU:OE1	2.20	0.41
2:F:65:SER:HB3	2:F:79:LEU:CD2	2.51	0.41
1:A:13:ILE:O	1:A:112:VAL:HA	2.20	0.41
1:A:38:GLN:HB2	1:A:44:PRO:HG3	2.01	0.41
1:A:44:PRO:CG	2:B:105:TYR:OH	2.61	0.41
1:C:26:THR:HG22	1:C:26:THR:O	2.19	0.41
2:F:124:PRO:CA	2:F:151:PHE:HB3	2.50	0.41
2:B:126:VAL:HG12	2:B:127:ALA:N	2.36	0.41
1:C:174:ASN:O	1:C:175:SER:HB3	2.21	0.41
1:E:54:GLU:OE1	1:E:68:ALA:HA	2.21	0.41
1:A:78:THR:O	1:A:79:ALA:C	2.58	0.41
2:B:77:LEU:HD12	2:B:78:THR:N	2.31	0.41
2:D:67:VAL:O	2:D:68:SER:HB3	2.20	0.41
2:D:69:ARG:HG2	2:D:69:ARG:HH11	1.86	0.41
1:C:17:LYS:HZ1	1:E:9:GLN:HG2	1.86	0.41
2:D:199:ALA:O	2:D:203:GLN:HG3	2.20	0.41
2:F:105:TYR:C	2:F:107:GLY:N	2.74	0.41
2:F:107:GLY:C	2:F:109:GLY:H	2.23	0.41
2:F:151:PHE:HE1	2:F:190:ALA:CA	2.33	0.41
1:A:164:LEU:HD12	1:A:164:LEU:C	2.40	0.41
2:B:39:ASP:HA	2:B:88:SER:CB	2.51	0.41
2:B:52:GLY:H	2:B:55:SER:HG	1.68	0.41
2:B:135:GLU:O	2:B:139:THR:HB	2.19	0.41
1:C:110:LEU:CD1	1:C:111:THR:H	2.27	0.41
2:D:2:GLU:CD	2:D:3:ALA:N	2.74	0.41
2:D:12:LEU:O	2:D:113:THR:N	2.47	0.41
2:D:67:VAL:HG13	2:D:76:PRO:O	2.20	0.41
1:E:67:ASP:CG	1:E:71:LYS:HG2	2.40	0.41
2:F:52:GLY:O	2:F:69:ARG:HG2	2.21	0.41
1:A:26:THR:O	1:A:26:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:TYR:CD1	2:B:34:TYR:N	2.88	0.41
1:C:2:ASN:ND2	1:C:26:THR:O	2.54	0.41
1:C:24:ASN:ND2	1:C:72:GLN:HB3	2.35	0.41
1:C:25:TYR:OH	1:C:70:THR:CG2	2.66	0.41
1:C:28:SER:OG	1:C:29:PRO:CD	2.68	0.41
2:F:93:ALA:CA	2:F:105:TYR:HB3	2.50	0.41
1:A:12:ILE:HG23	1:A:111:THR:HB	2.03	0.41
1:A:51:THR:CG2	1:A:52:PHE:H	2.16	0.41
1:A:116:ILE:HD11	1:A:144:SER:N	2.35	0.41
2:B:69:ARG:HG2	2:B:69:ARG:HH11	1.86	0.41
2:B:116:GLU:C	2:B:117:ASP:O	2.58	0.41
2:B:118:LEU:C	2:B:120:ASN:H	2.24	0.41
1:C:110:LEU:CG	1:C:111:THR:N	2.83	0.41
2:D:91:LEU:HD23	2:D:109:GLY:CA	2.50	0.41
2:F:96:GLU:CD	2:F:102:TYR:HB2	2.42	0.41
2:F:107:GLY:C	2:F:109:GLY:N	2.73	0.41
2:F:67:VAL:HG12	2:F:77:LEU:HA	2.03	0.41
2:B:105:TYR:C	2:B:107:GLY:N	2.72	0.40
1:C:28:SER:CB	1:C:29:PRO:CD	2.98	0.40
1:C:40:THR:C	1:C:42:ARG:H	2.24	0.40
2:F:121:VAL:O	2:F:228:ARG:NH2	2.50	0.40
1:A:61:ARG:NH1	1:A:79:ALA:O	2.54	0.40
2:B:154:ASP:O	2:B:155:HIS:HD2	2.04	0.40
2:D:116:GLU:O	2:D:118:LEU:HD23	2.21	0.40
2:D:173:THR:CG2	2:D:174:ASP:N	2.85	0.40
2:F:204:ASP:HA	2:F:205:PRO:HD2	1.86	0.40
1:A:31:SER:CB	1:A:95:ARG:HB2	2.44	0.40
1:A:177:VAL:HG23	2:B:194:ARG:HD3	2.04	0.40
2:D:208:HIS:HB2	2:D:241:TRP:CZ3	2.56	0.40
2:D:227:ASP:O	2:D:227:ASP:OD2	2.39	0.40
1:E:68:ALA:C	1:E:70:THR:N	2.73	0.40
2:D:107:GLY:C	2:D:109:GLY:N	2.75	0.40
1:A:38:GLN:HG3	1:A:44:PRO:HD3	2.02	0.40
1:A:91:VAL:CG1	1:A:102:LEU:HB2	2.51	0.40
2:B:96:GLU:CD	2:B:102:TYR:HB2	2.42	0.40
1:E:136:VAL:HG12	1:E:179:TRP:CB	2.38	0.40
2:F:20:ILE:HD11	2:F:82:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	190/192 (99%)	157 (83%)	25 (13%)	8 (4%)	3	23
1	C	190/192 (99%)	153 (80%)	28 (15%)	9 (5%)	2	20
1	E	190/192 (99%)	155 (82%)	27 (14%)	8 (4%)	3	23
2	B	242/244 (99%)	206 (85%)	27 (11%)	9 (4%)	3	26
2	D	242/244 (99%)	200 (83%)	30 (12%)	12 (5%)	2	19
2	F	242/244 (99%)	203 (84%)	30 (12%)	9 (4%)	3	26
All	All	1296/1308 (99%)	1074 (83%)	167 (13%)	55 (4%)	3	23

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	95	ARG
1	A	154	SER
1	C	54	GLU
1	C	55	ASN
1	C	95	ARG
1	C	120	ASP
1	C	154	SER
2	D	9	PRO
2	D	152	TYR
1	E	54	GLU
1	E	95	ARG
2	F	244	ALA
1	A	44	PRO
2	B	3	ALA
2	B	80	GLU
2	B	107	GLY
2	D	107	GLY
1	E	154	SER
2	F	107	GLY

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Mol	Chain	Res	Type
1	A	29	PRO
1	A	183	SER
2	B	101	ALA
1	C	29	PRO
2	D	68	SER
2	D	96	GLU
2	D	101	ALA
2	D	244	ALA
1	E	29	PRO
1	E	82	LEU
2	F	3	ALA
2	F	87	THR
2	F	101	ALA
1	A	52	PHE
2	B	87	THR
1	C	52	PHE
1	C	79	ALA
1	C	183	SER
2	D	4	ASP
2	D	227	ASP
1	E	52	PHE
2	F	8	THR
2	F	40	PRO
2	F	96	GLU
2	B	96	GLU
2	B	117	ASP
2	B	227	ASP
1	E	31	SER
1	E	183	SER
2	D	88	SER
2	B	108	PRO
2	D	8	THR
2	D	108	PRO
1	A	120	ASP
2	F	108	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	174/174 (100%)	162 (93%)	12 (7%)	15	47
1	C	174/174 (100%)	163 (94%)	11 (6%)	18	51
1	E	170/174 (98%)	157 (92%)	13 (8%)	13	43
2	B	215/215 (100%)	204 (95%)	11 (5%)	24	57
2	D	215/215 (100%)	199 (93%)	16 (7%)	13	44
2	F	215/215 (100%)	204 (95%)	11 (5%)	24	57
All	All	1163/1167 (100%)	1089 (94%)	74 (6%)	17	50

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	VAL
1	A	21	LEU
1	A	28	SER
1	A	29	PRO
1	A	30	PHE
1	A	44	PRO
1	A	74	SER
1	A	88	TYR
1	A	94	ASP
1	A	99	LEU
1	A	102	LEU
2	B	2	GLU
2	B	4	ASP
2	B	26	GLN
2	B	34	TYR
2	B	43	GLU
2	B	92	CYS
2	B	104	GLN
2	B	106	PHE
2	B	118	LEU
2	B	185	ASN
2	B	194	ARG
1	C	3	GLN
1	C	28	SER
1	C	29	PRO
1	C	30	PHE
1	C	82	LEU

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Mol	Chain	Res	Type
1	C	94	ASP
1	C	99	LEU
1	C	113	TRP
1	C	115	ASP
1	C	140	THR
1	C	182	LYS
2	D	2	GLU
2	D	4	ASP
2	D	6	TYR
2	D	9	PRO
2	D	14	ILE
2	D	26	GLN
2	D	34	TYR
2	D	43	GLU
2	D	60	ASP
2	D	61	LEU
2	D	104	GLN
2	D	106	PHE
2	D	118	LEU
2	D	185	ASN
2	D	194	ARG
2	D	243	ARG
1	E	28	SER
1	E	29	PRO
1	E	30	PHE
1	E	39	ASP
1	E	46	SER
1	E	73	SER
1	E	82	LEU
1	E	94	ASP
1	E	99	LEU
1	E	113	TRP
1	E	139	PHE
1	E	140	THR
1	E	142	PHE
2	F	7	GLN
2	F	14	ILE
2	F	26	GLN
2	F	37	GLN
2	F	44	LEU
2	F	104	GLN
2	F	106	PHE

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Mol	Chain	Res	Type
2	F	111	ARG
2	F	176	GLN
2	F	185	ASN
2	F	194	ARG

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	6	GLN
1	A	38	GLN
1	A	81	GLN
2	B	7	GLN
2	B	86	HIS
2	B	104	GLN
2	B	155	HIS
2	B	176	GLN
2	B	185	ASN
2	B	207	ASN
2	B	226	GLN
1	C	2	ASN
1	C	6	GLN
1	C	9	GLN
1	C	38	GLN
1	C	55	ASN
1	C	145	GLN
2	D	37	GLN
2	D	86	HIS
2	D	104	GLN
2	D	176	GLN
2	D	185	ASN
2	D	207	ASN
2	D	226	GLN
1	E	6	GLN
1	E	9	GLN
1	E	32	ASN
1	E	38	GLN
1	E	76	HIS
1	E	145	GLN
2	F	38	GLN
2	F	86	HIS
2	F	89	GLN
2	F	104	GLN

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Mol	Chain	Res	Type
2	F	155	HIS
2	F	176	GLN
2	F	185	ASN
2	F	207	ASN
2	F	226	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	192/192 (100%)	0.07	7 (3%)	42	38	19, 64, 91, 98	0
1	C	192/192 (100%)	0.01	5 (2%)	56	49	9, 51, 85, 104	0
1	E	192/192 (100%)	-0.23	2 (1%)	82	77	7, 38, 82, 102	0
2	B	244/244 (100%)	-0.05	5 (2%)	65	60	16, 57, 85, 93	0
2	D	244/244 (100%)	-0.16	6 (2%)	57	51	9, 52, 82, 95	0
2	F	244/244 (100%)	-0.28	5 (2%)	65	60	7, 37, 74, 106	0
All	All	1308/1308 (100%)	-0.11	30 (2%)	60	54	7, 51, 85, 106	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	133	ASP	5.2
1	A	133	ASP	4.3
1	C	133	ASP	4.0
2	F	2	GLU	3.9
2	D	185	ASN	3.5
2	D	245	ASP	3.4
2	D	2	GLU	3.4
1	A	181	ASN	3.2
1	C	183	SER	3.2
1	C	131	SER	3.0
1	C	132	SER	2.8
2	F	245	ASP	2.7
2	D	116	GLU	2.7
2	F	3	ALA	2.6
2	B	227	ASP	2.6
1	A	2	ASN	2.5
2	F	106	PHE	2.5
2	D	3	ALA	2.4
2	D	220	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	2	GLU	2.3
1	A	68	ALA	2.3
1	E	95	ARG	2.2
2	B	221	ASN	2.2
2	B	40	PRO	2.2
1	A	32	ASN	2.2
1	A	132	SER	2.2
2	B	244	ALA	2.2
1	C	98	THR	2.1
2	F	185	ASN	2.1
1	A	129	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.