



Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 08:06 AM EST

PDB ID : 6X5Z
EMDB ID : EMD-22067
Title : Bovine Cardiac Myosin in Complex with Chicken Skeletal Actin and Human Cardiac Tropomyosin in the Rigor State
Authors : Doran, M.H.; Lehman, W.; Rynkiewicz, M.J.; Bullitt, E.
Deposited on : 2020-05-27
Resolution : 4.24 Å (reported)
Based on initial models : 6KN8, 3I5G

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

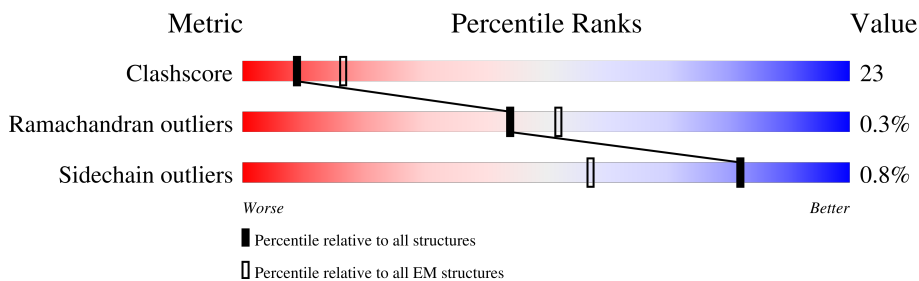
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.24 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	
2	O	284	
2	P	284	
3	D	850	
3	G	850	
3	J	850	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28416 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	369	2880	1823	487	549	21	0	0
1	A	369	2880	1823	487	549	21	0	0
1	C	369	2880	1823	487	549	21	0	0

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	O	166	1326	806	230	287	3	0	0
2	P	166	1326	806	230	287	3	0	0

- Molecule 3 is a protein called Myosin-7.

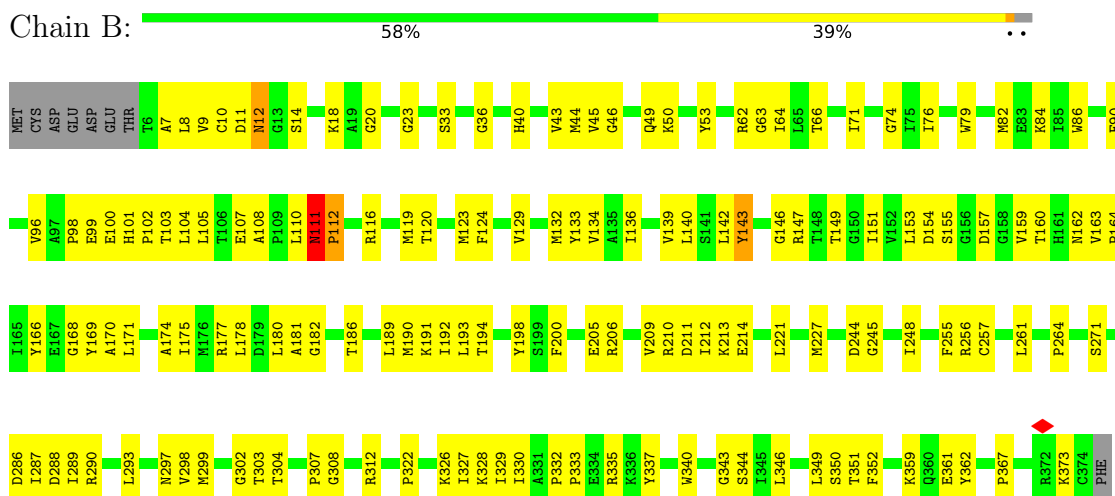
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	705	5680	3636	958	1056	30	0	0
3	D	705	5680	3636	958	1056	30	0	0
3	J	705	5680	3636	958	1056	30	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

3 Residue-property plots i

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Actin, alpha skeletal muscle

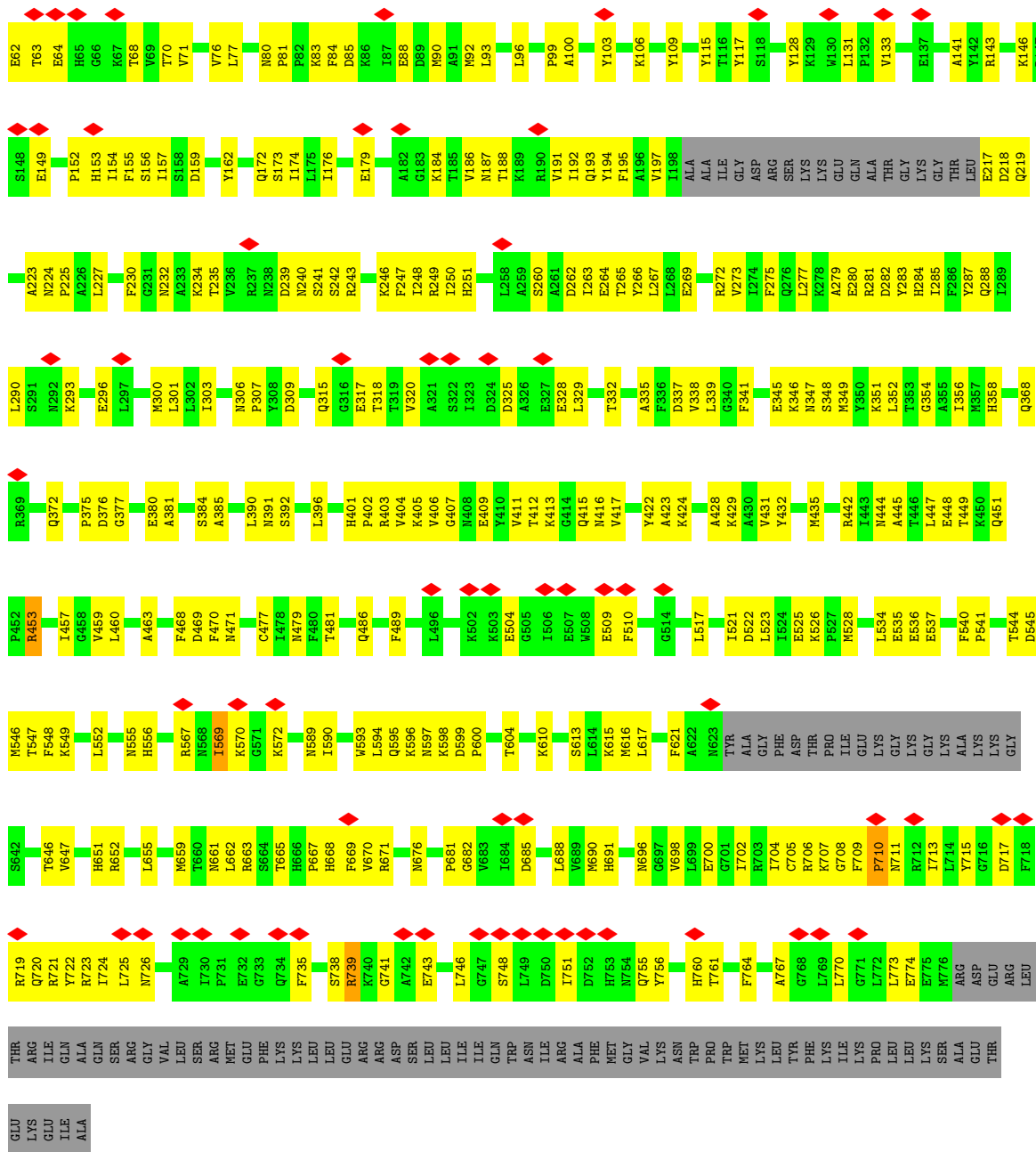


- Molecule 1: Actin, alpha skeletal muscle

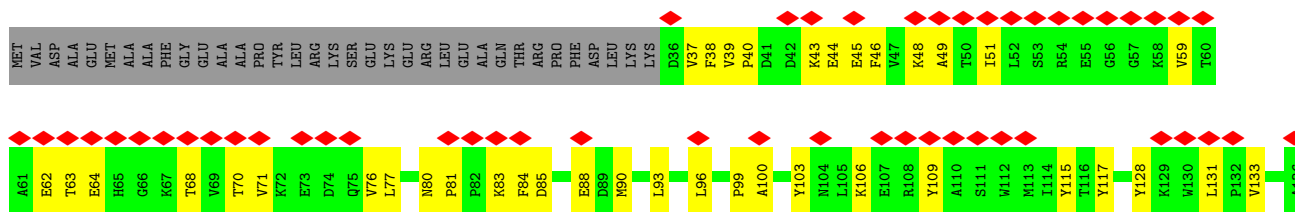


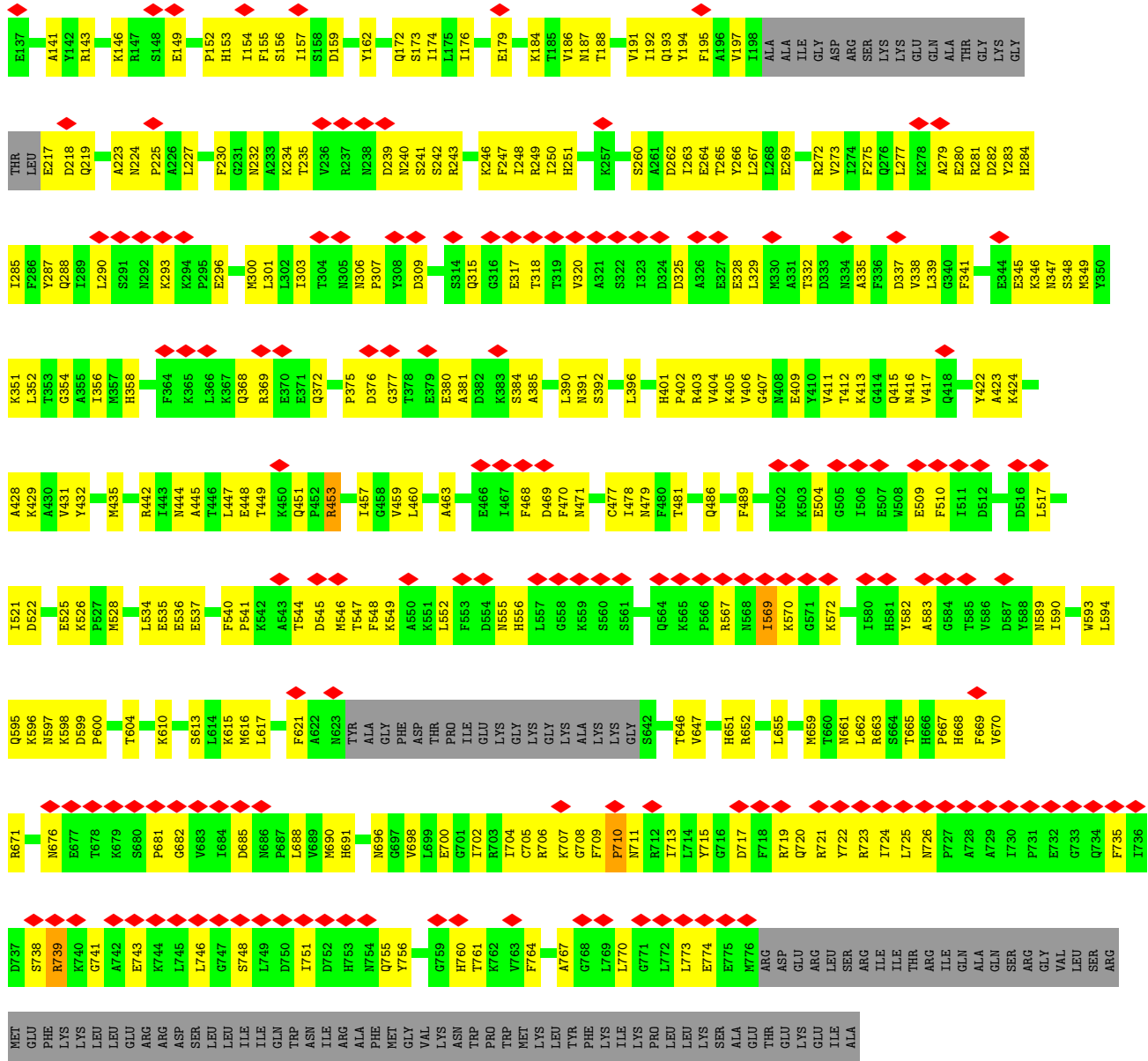
- Molecule 1: Actin, alpha skeletal muscle





• Molecule 3: Myosin-7





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.4°, rise=27.5 Å, axial sym=C1	Depositor
Number of segments used	32158	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

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: ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/2942	0.54	0/3986
1	B	0.45	0/2942	0.54	0/3986
1	C	0.45	0/2942	0.54	0/3986
2	O	0.64	0/1328	0.97	10/1770 (0.6%)
2	P	0.64	0/1328	0.97	10/1770 (0.6%)
3	D	0.33	0/5803	0.53	0/7825
3	G	0.33	0/5803	0.53	0/7825
3	J	0.33	0/5803	0.53	0/7825
All	All	0.41	0/28891	0.59	20/38973 (0.1%)

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	2
1	B	0	2
1	C	0	2
3	D	0	2
3	G	0	2
3	J	0	2
All	All	0	12

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	178	ARG	NE-CZ-NH1	7.41	124.00	120.30
2	P	182	ARG	NE-CZ-NH1	6.99	123.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	101	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	P	90	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	O	182	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	P	167	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	O	91	ARG	NE-CZ-NH2	6.55	123.57	120.30
2	O	167	ARG	NE-CZ-NH2	6.53	123.56	120.30
2	O	160	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	P	160	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	O	178	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	P	105	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	P	91	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	P	101	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	O	90	ARG	NE-CZ-NH2	5.85	123.22	120.30
2	O	125	ARG	NE-CZ-NH1	5.69	123.14	120.30
2	O	105	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	P	133	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	O	133	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	P	125	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	LEU	Peptide
1	A	111	ASN	Peptide
1	B	110	LEU	Peptide
1	B	111	ASN	Peptide
1	C	110	LEU	Peptide
1	C	111	ASN	Peptide
3	D	569	ILE	Peptide
3	D	726	ASN	Peptide
3	G	569	ILE	Peptide
3	G	726	ASN	Peptide
3	J	569	ILE	Peptide
3	J	726	ASN	Peptide

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	2880	0	2852	205	0
1	B	2880	0	2852	245	0
1	C	2880	0	2853	179	0
2	O	1326	0	1330	45	0
2	P	1326	0	1332	63	0
3	D	5680	0	5633	272	0
3	G	5680	0	5633	259	0
3	J	5680	0	5635	269	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	28416	0	28156	1311	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 23.

All (1311) 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:B:168:GLY:HA2	1:C:44:MET:CE	1.30	1.59
1:B:170:ALA:HB3	1:C:43:VAL:CG1	1.29	1.56
1:B:170:ALA:CB	1:C:43:VAL:HG11	1.28	1.55
1:B:205:GLU:CD	1:A:287:ILE:HD13	1.17	1.55
1:B:205:GLU:CD	1:A:287:ILE:CD1	1.81	1.46
1:B:307:PRO:HB2	2:O:125:ARG:NH1	1.20	1.41
1:B:308:GLY:CA	2:O:125:ARG:NH2	1.81	1.41
1:B:287:ILE:HD13	1:C:205:GLU:CD	1.44	1.37
1:B:64:ILE:CD1	1:A:169:TYR:CD1	2.07	1.35
1:B:307:PRO:CB	2:O:125:ARG:HH12	1.49	1.25
1:B:62:ARG:HG3	1:A:288:ASP:OD2	1.31	1.25
1:B:308:GLY:N	2:O:125:ARG:HH22	1.36	1.23
1:B:169:TYR:CD1	1:C:64:ILE:HD13	1.75	1.22
1:B:308:GLY:HA3	2:O:125:ARG:NH2	1.39	1.21
2:P:91:ARG:NH1	1:A:311:ASP:HB2	1.55	1.20
1:B:169:TYR:CD1	1:C:64:ILE:CD1	2.25	1.20
2:P:171:ILE:HD13	1:C:311:ASP:OD1	1.42	1.18
1:B:168:GLY:CA	1:C:44:MET:CE	2.23	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:90:ARG:CD	1:A:221:LEU:HD23	1.75	1.16
1:B:63:GLY:HA3	1:A:289:ILE:CD1	1.76	1.15
1:B:308:GLY:CA	2:O:125:ARG:HH22	1.45	1.14
1:B:168:GLY:HA2	1:C:44:MET:HE3	1.19	1.14
1:B:44:MET:CE	1:A:168:GLY:HA2	1.77	1.14
1:B:287:ILE:CD1	1:C:205:GLU:CD	2.16	1.13
1:B:40:HIS:CE1	1:A:171:LEU:HD11	1.85	1.12
1:B:205:GLU:OE1	1:A:287:ILE:CD1	1.97	1.11
1:B:170:ALA:N	1:C:43:VAL:HG21	1.66	1.11
1:B:64:ILE:HD13	1:A:169:TYR:CD1	1.77	1.10
2:P:171:ILE:HD13	1:C:311:ASP:CG	1.72	1.10
1:B:205:GLU:CG	1:A:287:ILE:HD13	1.80	1.10
1:B:63:GLY:CA	1:A:289:ILE:HD11	1.81	1.09
1:B:289:ILE:HD11	1:C:63:GLY:HA3	1.31	1.09
1:B:168:GLY:HA2	1:C:44:MET:HE2	1.17	1.07
2:P:91:ARG:CZ	1:A:311:ASP:HB2	1.84	1.07
1:B:168:GLY:CA	1:C:44:MET:HE3	1.83	1.06
1:B:307:PRO:CB	2:O:125:ARG:NH1	2.13	1.04
2:P:90:ARG:HD2	1:A:221:LEU:HD23	1.33	1.04
2:P:90:ARG:HD2	1:A:221:LEU:CD2	1.88	1.04
2:O:173:GLU:HG2	2:P:172:ILE:HD13	1.41	1.02
1:B:205:GLU:OE2	1:A:287:ILE:HD13	1.58	1.02
2:P:91:ARG:NH2	1:A:311:ASP:OD1	1.94	1.01
2:P:171:ILE:CD1	1:C:311:ASP:CG	2.28	1.01
1:B:170:ALA:HB2	1:C:43:VAL:CB	1.92	0.99
1:B:170:ALA:N	1:C:43:VAL:CG2	2.25	0.99
1:B:308:GLY:N	2:O:125:ARG:NH2	2.01	0.99
1:B:44:MET:HE2	1:A:168:GLY:HA2	1.41	0.98
2:O:133:ARG:HB3	3:G:369:ARG:HH22	1.26	0.98
1:B:288:ASP:OD2	1:C:62:ARG:HG3	1.64	0.97
1:B:307:PRO:C	2:O:125:ARG:HH22	1.68	0.97
2:P:91:ARG:CZ	1:A:311:ASP:OD1	2.13	0.96
2:O:169:LEU:CD2	2:O:173:GLU:OE2	2.14	0.95
1:B:169:TYR:CE1	1:C:64:ILE:CD1	2.50	0.95
2:O:173:GLU:HG2	2:P:172:ILE:CD1	1.95	0.95
1:B:170:ALA:CB	1:C:43:VAL:HG21	1.95	0.94
1:B:170:ALA:CB	1:C:43:VAL:CB	2.45	0.94
1:B:308:GLY:CA	2:O:125:ARG:HH21	1.75	0.94
1:B:205:GLU:OE2	1:A:287:ILE:CD1	2.13	0.94
1:B:205:GLU:CD	1:A:287:ILE:HD11	1.87	0.94
1:B:170:ALA:CA	1:C:43:VAL:HG21	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ALA:HB2	1:C:43:VAL:HG21	1.50	0.92
2:O:93:GLN:CA	3:D:368:GLN:HE22	1.80	0.92
1:C:142:LEU:HD12	1:C:165:ILE:HD12	1.50	0.92
1:B:287:ILE:HD13	1:C:205:GLU:OE2	1.69	0.91
1:B:64:ILE:CD1	1:A:169:TYR:CE1	2.53	0.91
1:B:244:ASP:OD1	1:A:287:ILE:O	1.88	0.91
2:P:91:ARG:CZ	1:A:311:ASP:CB	2.47	0.91
1:B:169:TYR:CE1	1:C:64:ILE:HD11	2.05	0.91
2:O:93:GLN:HA	3:D:368:GLN:HE22	1.34	0.90
1:B:170:ALA:HB2	1:C:43:VAL:CG2	2.00	0.90
1:B:205:GLU:OE1	1:A:287:ILE:HD11	1.69	0.90
1:B:308:GLY:HA3	2:O:125:ARG:HH21	1.27	0.90
2:P:91:ARG:NH1	1:A:311:ASP:CB	2.34	0.90
3:D:290:LEU:HD21	3:D:307:PRO:HB3	1.53	0.89
1:B:46:GLY:HA3	3:D:540:PHE:CE1	2.07	0.89
1:B:64:ILE:HD11	1:A:169:TYR:CD1	2.08	0.88
1:B:44:MET:HE3	1:A:168:GLY:HA2	1.55	0.88
3:G:290:LEU:HD21	3:G:307:PRO:HB3	1.52	0.88
1:B:64:ILE:HD12	1:A:169:TYR:CD1	2.08	0.88
3:J:290:LEU:HD21	3:J:307:PRO:HB3	1.52	0.88
3:J:569:ILE:HD12	3:J:572:LYS:HG3	1.56	0.87
3:G:368:GLN:HE22	2:P:135:GLN:HB3	1.39	0.87
3:G:569:ILE:HD12	3:G:572:LYS:HG3	1.56	0.87
3:J:174:ILE:HG13	3:J:668:HIS:HE1	1.39	0.87
3:D:569:ILE:HD12	3:D:572:LYS:HG3	1.56	0.87
3:G:174:ILE:HG13	3:G:668:HIS:HE1	1.39	0.86
3:G:723:ARG:HE	3:G:735:PHE:HB2	1.41	0.86
3:D:723:ARG:HE	3:D:735:PHE:HB2	1.41	0.86
2:P:90:ARG:HD2	1:A:221:LEU:CG	2.04	0.86
1:B:287:ILE:CD1	1:C:205:GLU:OE1	2.24	0.86
3:J:723:ARG:HE	3:J:735:PHE:HB2	1.41	0.86
3:D:174:ILE:HG13	3:D:668:HIS:HE1	1.39	0.85
1:B:170:ALA:CB	1:C:43:VAL:CG1	2.09	0.84
1:B:307:PRO:HB2	2:O:125:ARG:HH11	1.40	0.84
1:B:64:ILE:HD11	1:A:169:TYR:CE1	2.14	0.83
1:B:170:ALA:CB	1:C:43:VAL:CG2	2.56	0.83
1:B:245:GLY:HA3	1:A:322:PRO:CG	2.09	0.82
1:B:170:ALA:H	1:C:43:VAL:CG2	1.88	0.82
3:G:288:GLN:NE2	3:G:332:THR:OG1	2.13	0.82
2:P:172:ILE:HA	3:J:369:ARG:HH22	1.41	0.82
3:J:288:GLN:NE2	3:J:332:THR:OG1	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:CG2	1:A:170:ALA:N	2.42	0.82
3:D:288:GLN:NE2	3:D:332:THR:OG1	2.12	0.81
1:A:143:TYR:OH	3:D:540:PHE:CE1	2.34	0.81
1:A:107:GLU:HG2	1:A:116:ARG:HE	1.46	0.80
1:C:107:GLU:HG2	1:C:116:ARG:HE	1.46	0.80
2:P:79:THR:HG22	1:A:238:LYS:HZ1	1.47	0.79
1:B:107:GLU:HG2	1:B:116:ARG:HE	1.46	0.79
1:B:245:GLY:HA3	1:A:322:PRO:HG3	1.65	0.79
1:B:46:GLY:C	3:D:540:PHE:CZ	2.56	0.79
1:B:40:HIS:CE1	1:A:171:LEU:CD1	2.64	0.79
1:B:123:MET:HE1	1:B:132:MET:HG3	1.66	0.78
3:D:719:ARG:HG3	3:D:738:SER:HA	1.65	0.78
1:B:43:VAL:HG21	1:A:170:ALA:N	1.99	0.77
3:G:719:ARG:HG3	3:G:738:SER:HA	1.65	0.77
2:O:173:GLU:HB3	3:J:368:GLN:HE22	1.49	0.76
3:J:719:ARG:HG3	3:J:738:SER:HA	1.65	0.76
2:P:79:THR:HG22	1:A:238:LYS:NZ	2.00	0.76
2:O:173:GLU:CG	2:P:172:ILE:HD13	2.16	0.76
1:B:40:HIS:CG	1:A:171:LEU:HD12	2.21	0.75
1:B:170:ALA:H	1:C:43:VAL:HG22	1.50	0.75
1:B:43:VAL:HG21	1:A:170:ALA:CA	2.16	0.75
2:P:175:ASP:HB2	3:J:369:ARG:NH2	2.01	0.75
2:O:93:GLN:CB	3:D:368:GLN:HE22	2.00	0.74
1:B:63:GLY:HA3	1:A:289:ILE:HD11	0.85	0.74
1:B:64:ILE:HD13	1:A:169:TYR:HD1	1.44	0.74
3:D:234:LYS:HG3	3:D:239:ASP:HB2	1.69	0.74
3:J:449:THR:OG1	3:J:451:GLN:OE1	2.06	0.73
1:B:287:ILE:HD13	1:C:205:GLU:CG	2.18	0.73
1:B:308:GLY:HA2	2:O:125:ARG:NH2	1.96	0.73
1:B:205:GLU:HG2	1:A:287:ILE:HD13	1.71	0.73
1:C:149:THR:HG23	1:C:166:TYR:HA	1.70	0.73
1:C:123:MET:HE1	1:C:132:MET:HG3	1.68	0.73
1:B:149:THR:HG23	1:B:166:TYR:HA	1.70	0.72
3:D:449:THR:OG1	3:D:451:GLN:OE1	2.06	0.72
1:B:169:TYR:CG	1:C:64:ILE:HD13	2.24	0.72
3:G:234:LYS:HG3	3:G:239:ASP:HB2	1.69	0.72
1:B:45:VAL:O	3:D:540:PHE:CE1	2.43	0.72
1:A:123:MET:HE1	1:A:132:MET:HG3	1.69	0.72
1:A:149:THR:HG23	1:A:166:TYR:HA	1.70	0.72
2:O:93:GLN:HA	3:D:368:GLN:NE2	2.04	0.72
3:G:449:THR:OG1	3:G:451:GLN:OE1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:128:TYR:HD2	3:G:681:PRO:HG3	1.55	0.72
2:P:172:ILE:HG13	3:J:369:ARG:NH2	2.04	0.72
3:J:128:TYR:HD2	3:J:681:PRO:HG3	1.55	0.72
1:A:8:LEU:HD22	1:A:103:THR:HG23	1.72	0.72
1:B:8:LEU:HD22	1:B:103:THR:HG23	1.72	0.72
3:J:234:LYS:HG3	3:J:239:ASP:HB2	1.69	0.72
3:G:535:GLU:OE1	3:G:646:THR:OG1	2.08	0.71
3:D:128:TYR:HD2	3:D:681:PRO:HG3	1.55	0.71
1:C:8:LEU:HD22	1:C:103:THR:HG23	1.72	0.71
3:D:720:GLN:O	3:D:723:ARG:NH2	2.24	0.71
1:B:143:TYR:OH	1:C:45:VAL:O	2.08	0.71
1:B:169:TYR:CD1	1:C:64:ILE:HD11	2.22	0.71
3:G:720:GLN:O	3:G:723:ARG:NH2	2.24	0.71
1:B:163:VAL:HG12	1:B:175:ILE:HG12	1.72	0.71
1:A:163:VAL:HG12	1:A:175:ILE:HG12	1.72	0.71
3:D:192:ILE:HD11	3:D:250:ILE:HG21	1.72	0.70
1:C:111:ASN:OD1	1:C:177:ARG:NH1	2.21	0.70
1:C:163:VAL:HG12	1:C:175:ILE:HG12	1.72	0.70
3:J:100:ALA:HA	3:J:103:TYR:CE1	2.26	0.70
2:P:90:ARG:NH1	1:A:221:LEU:HD23	2.06	0.70
3:D:235:THR:HG21	3:D:243:ARG:HH11	1.56	0.70
3:J:235:THR:HG21	3:J:243:ARG:HH11	1.56	0.70
2:P:172:ILE:HA	3:J:369:ARG:NH2	2.07	0.70
3:D:37:VAL:HG21	3:D:51:ILE:HG23	1.73	0.70
3:J:720:GLN:O	3:J:723:ARG:NH2	2.24	0.70
3:J:535:GLU:OE1	3:J:646:THR:OG1	2.08	0.70
3:G:100:ALA:HA	3:G:103:TYR:CE1	2.26	0.70
3:G:192:ILE:HD11	3:G:250:ILE:HG21	1.72	0.70
3:D:535:GLU:OE1	3:D:646:THR:OG1	2.08	0.70
3:G:235:THR:HG21	3:G:243:ARG:HH11	1.56	0.70
3:D:725:LEU:HD11	3:D:773:LEU:HD13	1.74	0.70
2:P:90:ARG:NE	1:A:221:LEU:HD23	2.06	0.69
3:G:37:VAL:HG21	3:G:51:ILE:HG23	1.73	0.69
2:P:79:THR:CG2	1:A:238:LYS:NZ	2.55	0.69
3:J:192:ILE:HD11	3:J:250:ILE:HG21	1.72	0.69
1:B:180:LEU:HD21	1:B:261:LEU:HA	1.74	0.69
2:P:90:ARG:CZ	1:A:221:LEU:HD23	2.21	0.69
1:A:180:LEU:HD21	1:A:261:LEU:HA	1.74	0.69
3:D:100:ALA:HA	3:D:103:TYR:CE1	2.26	0.69
1:C:180:LEU:HD21	1:C:261:LEU:HA	1.74	0.69
3:G:725:LEU:HD11	3:G:773:LEU:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:37:VAL:HG21	3:J:51:ILE:HG23	1.73	0.69
1:B:45:VAL:O	3:D:540:PHE:HE1	1.75	0.69
1:B:170:ALA:HB2	1:C:43:VAL:HB	1.71	0.69
2:P:79:THR:CG2	1:A:238:LYS:HZ1	2.05	0.69
2:P:132:SER:O	2:P:135:GLN:HG2	1.93	0.69
2:O:103:GLN:OE1	1:A:326:LYS:NZ	2.19	0.69
3:G:155:PHE:HB3	3:G:194:TYR:CZ	2.29	0.68
3:D:155:PHE:HB3	3:D:194:TYR:CZ	2.29	0.68
3:J:725:LEU:HD11	3:J:773:LEU:HD13	1.74	0.68
3:J:155:PHE:HB3	3:J:194:TYR:CZ	2.29	0.68
1:B:111:ASN:OD1	1:B:177:ARG:NH1	2.21	0.68
1:B:40:HIS:ND1	1:A:171:LEU:CD1	2.57	0.68
1:B:168:GLY:CA	1:C:44:MET:HE2	2.08	0.68
2:O:133:ARG:HB3	3:G:369:ARG:NH2	2.05	0.68
1:A:142:LEU:HD12	1:A:165:ILE:HD12	1.76	0.68
1:C:11:ASP:OD1	1:C:12:ASN:N	2.27	0.68
2:P:90:ARG:HD2	1:A:221:LEU:HG	1.73	0.67
1:A:11:ASP:OD1	1:A:12:ASN:N	2.27	0.67
1:B:11:ASP:OD1	1:B:12:ASN:N	2.27	0.67
1:B:43:VAL:HG22	1:A:170:ALA:N	2.09	0.67
2:O:93:GLN:CB	3:D:368:GLN:NE2	2.57	0.67
1:C:11:ASP:OD2	1:C:18:LYS:NZ	2.27	0.67
1:A:11:ASP:OD2	1:A:18:LYS:NZ	2.27	0.67
1:B:11:ASP:OD2	1:B:18:LYS:NZ	2.27	0.67
3:G:172:GLN:HB2	3:G:457:ILE:HG23	1.77	0.67
2:P:91:ARG:CZ	1:A:311:ASP:CG	2.62	0.67
2:P:175:ASP:OD2	3:J:369:ARG:NH2	2.28	0.67
3:D:153:HIS:CE1	3:D:155:PHE:HB2	2.30	0.67
3:D:445:ALA:HA	3:D:448:GLU:HG3	1.77	0.67
3:J:172:GLN:HB2	3:J:457:ILE:HG23	1.77	0.67
1:A:350:SER:OG	3:D:536:GLU:OE1	2.10	0.67
3:D:184:LYS:NZ	3:D:188:THR:OG1	2.26	0.67
3:G:301:LEU:HD11	3:G:354:GLY:HA3	1.77	0.66
1:A:297:ASN:HB3	1:A:329:ILE:HG22	1.77	0.66
3:D:172:GLN:HB2	3:D:457:ILE:HG23	1.77	0.66
3:J:301:LEU:HD11	3:J:354:GLY:HA3	1.77	0.66
1:A:111:ASN:OD1	1:A:177:ARG:NH1	2.21	0.66
3:D:281:ARG:HH11	3:D:320:VAL:HG11	1.61	0.66
1:B:40:HIS:ND1	1:A:171:LEU:HD11	2.09	0.66
1:B:44:MET:HE3	1:A:168:GLY:CA	2.24	0.66
1:B:308:GLY:HA3	2:O:125:ARG:HH22	1.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:301:LEU:HD11	3:D:354:GLY:HA3	1.77	0.66
3:J:153:HIS:CE1	3:J:155:PHE:HB2	2.30	0.66
3:J:281:ARG:HH11	3:J:320:VAL:HG11	1.61	0.66
1:B:350:SER:OG	3:G:536:GLU:OE1	2.10	0.66
3:G:153:HIS:CE1	3:G:155:PHE:HB2	2.30	0.66
3:G:445:ALA:HA	3:G:448:GLU:HG3	1.77	0.66
1:B:297:ASN:HB3	1:B:329:ILE:HG22	1.77	0.66
3:G:293:LYS:HB3	3:G:329:LEU:HD21	1.78	0.66
3:J:293:LYS:HB3	3:J:329:LEU:HD21	1.78	0.66
3:G:184:LYS:NZ	3:G:188:THR:OG1	2.26	0.65
3:J:176:ILE:HG21	3:J:184:LYS:HE3	1.79	0.65
3:G:176:ILE:HG21	3:G:184:LYS:HE3	1.79	0.65
3:D:293:LYS:HB3	3:D:329:LEU:HD21	1.78	0.65
3:D:39:VAL:HG23	3:D:71:VAL:HG11	1.79	0.65
3:D:176:ILE:HG21	3:D:184:LYS:HE3	1.79	0.65
1:C:297:ASN:HB3	1:C:329:ILE:HG22	1.77	0.65
3:J:39:VAL:HG23	3:J:71:VAL:HG11	1.79	0.65
3:J:184:LYS:NZ	3:J:188:THR:OG1	2.26	0.65
1:C:142:LEU:CD1	1:C:165:ILE:HD12	2.24	0.65
3:G:39:VAL:HG23	3:G:71:VAL:HG11	1.79	0.65
2:P:171:ILE:CD1	1:C:311:ASP:OD1	2.29	0.65
3:D:143:ARG:NH1	3:D:159:ASP:OD1	2.29	0.65
3:J:445:ALA:HA	3:J:448:GLU:HG3	1.77	0.65
3:D:486:GLN:HG2	3:D:517:LEU:HD11	1.79	0.65
3:G:143:ARG:NH1	3:G:159:ASP:OD1	2.29	0.65
3:G:281:ARG:HH11	3:G:320:VAL:HG11	1.61	0.65
3:D:709:PHE:O	3:D:711:ASN:N	2.30	0.65
3:J:143:ARG:NH1	3:J:159:ASP:OD1	2.29	0.65
3:J:477:CYS:SG	3:J:651:HIS:NE2	2.70	0.65
3:G:486:GLN:HG2	3:G:517:LEU:HD11	1.79	0.64
1:B:287:ILE:CD1	1:C:205:GLU:OE2	2.36	0.64
1:B:290:ARG:HD2	1:C:244:ASP:OD1	1.97	0.64
3:G:468:PHE:O	3:G:471:ASN:ND2	2.30	0.64
3:G:709:PHE:O	3:G:711:ASN:N	2.30	0.64
1:C:350:SER:OG	3:J:536:GLU:OE1	2.10	0.64
3:J:724:ILE:HD12	3:J:774:GLU:HA	1.79	0.64
1:B:304:THR:O	1:B:335:ARG:NH2	2.29	0.64
3:D:468:PHE:O	3:D:471:ASN:ND2	2.30	0.64
3:G:724:ILE:HD12	3:G:774:GLU:HA	1.79	0.64
3:D:162:TYR:HB2	3:D:195:PHE:CE1	2.33	0.64
3:D:174:ILE:HG13	3:D:668:HIS:CE1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:477:CYS:SG	3:G:651:HIS:NE2	2.70	0.64
3:D:275:PHE:HD2	3:D:596:LYS:HE3	1.62	0.64
3:J:486:GLN:HG2	3:J:517:LEU:HD11	1.79	0.64
1:B:64:ILE:CD1	1:A:169:TYR:HD1	1.99	0.64
3:D:477:CYS:SG	3:D:651:HIS:NE2	2.70	0.64
3:J:723:ARG:NE	3:J:735:PHE:HB2	2.12	0.64
3:J:709:PHE:O	3:J:711:ASN:N	2.30	0.64
1:B:170:ALA:N	1:C:43:VAL:HG22	2.09	0.64
1:B:307:PRO:HB2	2:O:125:ARG:HH12	0.82	0.64
3:J:46:PHE:HD2	3:J:99:PRO:HG3	1.63	0.64
2:O:169:LEU:O	2:O:173:GLU:HG3	1.98	0.64
2:P:171:ILE:HD11	1:C:311:ASP:CG	2.15	0.64
3:D:717:ASP:HB3	3:D:721:ARG:NH1	2.13	0.64
3:D:724:ILE:HD12	3:D:774:GLU:HA	1.79	0.64
3:G:717:ASP:HB3	3:G:721:ARG:NH1	2.13	0.63
1:B:171:LEU:HD11	1:C:40:HIS:CE1	2.32	0.63
3:G:174:ILE:HB	3:G:459:VAL:HA	1.79	0.63
1:A:304:THR:O	1:A:335:ARG:NH2	2.29	0.63
3:G:162:TYR:HB2	3:G:195:PHE:CE1	2.33	0.63
1:B:307:PRO:CA	2:O:125:ARG:HH12	2.11	0.63
3:G:266:TYR:OH	3:G:661:ASN:ND2	2.30	0.63
3:J:266:TYR:OH	3:J:661:ASN:ND2	2.30	0.63
3:G:174:ILE:HG13	3:G:668:HIS:CE1	2.28	0.63
3:G:723:ARG:NE	3:G:735:PHE:HB2	2.12	0.63
1:C:304:THR:O	1:C:335:ARG:NH2	2.29	0.63
3:G:247:PHE:HD1	3:G:460:LEU:HB3	1.63	0.63
3:G:275:PHE:HD2	3:G:596:LYS:HE3	1.62	0.63
3:J:275:PHE:HD2	3:J:596:LYS:HE3	1.62	0.63
1:B:23:GLY:N	1:B:344:SER:OG	2.32	0.63
3:J:162:TYR:HB2	3:J:195:PHE:CE1	2.32	0.63
3:J:717:ASP:HB3	3:J:721:ARG:NH1	2.13	0.63
2:O:169:LEU:HD23	2:O:173:GLU:OE2	1.99	0.63
3:D:266:TYR:OH	3:D:661:ASN:ND2	2.30	0.63
1:C:23:GLY:N	1:C:344:SER:OG	2.32	0.63
3:G:46:PHE:HD2	3:G:99:PRO:HG3	1.62	0.62
3:D:723:ARG:NE	3:D:735:PHE:HB2	2.12	0.62
1:A:23:GLY:N	1:A:344:SER:OG	2.32	0.62
3:D:162:TYR:HB2	3:D:195:PHE:HE1	1.64	0.62
3:D:174:ILE:HB	3:D:459:VAL:HA	1.79	0.62
1:B:64:ILE:HD13	1:A:169:TYR:CG	2.33	0.62
3:J:174:ILE:HB	3:J:459:VAL:HA	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HB2	1:B:134:VAL:HG12	1.82	0.62
1:A:105:LEU:HB2	1:A:134:VAL:HG12	1.82	0.62
3:J:174:ILE:HG13	3:J:668:HIS:CE1	2.28	0.62
3:G:162:TYR:HB2	3:G:195:PHE:HE1	1.64	0.62
3:J:162:TYR:HB2	3:J:195:PHE:HE1	1.64	0.62
1:B:64:ILE:CD1	1:A:169:TYR:CG	2.78	0.62
3:G:470:PHE:HD2	3:G:589:ASN:HD21	1.47	0.62
3:D:46:PHE:HD2	3:D:99:PRO:HG3	1.62	0.62
3:D:470:PHE:HD2	3:D:589:ASN:HD21	1.47	0.61
3:J:247:PHE:HD1	3:J:460:LEU:HB3	1.63	0.61
3:J:470:PHE:HD2	3:J:589:ASN:HD21	1.47	0.61
1:C:105:LEU:HB2	1:C:134:VAL:HG12	1.82	0.61
3:G:406:VAL:HG12	3:G:407:GLY:H	1.66	0.61
3:D:247:PHE:HD1	3:D:460:LEU:HB3	1.63	0.61
3:D:719:ARG:NE	3:D:741:GLY:HA3	2.15	0.61
3:J:406:VAL:HG12	3:J:407:GLY:H	1.66	0.61
3:J:599:ASP:OD1	3:J:646:THR:HA	2.01	0.61
3:J:719:ARG:NE	3:J:741:GLY:HA3	2.15	0.61
2:P:90:ARG:NH1	1:A:221:LEU:CD2	2.63	0.61
3:D:406:VAL:HG12	3:D:407:GLY:H	1.66	0.61
1:A:157:ASP:O	1:A:182:GLY:N	2.32	0.61
3:G:599:ASP:OD1	3:G:646:THR:HA	2.01	0.61
3:G:534:LEU:HD23	3:G:597:ASN:HD22	1.66	0.61
1:B:157:ASP:O	1:B:182:GLY:N	2.32	0.60
1:B:168:GLY:HA2	1:C:44:MET:HE1	1.65	0.60
3:G:719:ARG:NE	3:G:741:GLY:HA3	2.15	0.60
3:G:715:TYR:OH	3:G:719:ARG:NH1	2.34	0.60
3:J:755:GLN:HG3	3:J:756:TYR:HD1	1.66	0.60
2:P:90:ARG:CD	1:A:221:LEU:CD2	2.57	0.60
1:A:189:LEU:HA	1:A:192:ILE:HG22	1.84	0.60
3:J:715:TYR:OH	3:J:719:ARG:NH1	2.34	0.60
3:G:676:ASN:HA	3:G:688:LEU:HD22	1.84	0.60
1:C:98:PRO:HB2	1:C:129:VAL:HG12	1.84	0.60
3:J:534:LEU:HD23	3:J:597:ASN:HD22	1.66	0.60
3:J:676:ASN:HA	3:J:688:LEU:HD22	1.84	0.60
2:O:169:LEU:HD22	2:O:173:GLU:OE2	2.00	0.60
3:D:676:ASN:HA	3:D:688:LEU:HD22	1.84	0.60
3:J:288:GLN:NE2	3:J:329:LEU:HA	2.17	0.60
3:D:715:TYR:OH	3:D:719:ARG:NH1	2.34	0.60
1:A:98:PRO:HB2	1:A:129:VAL:HG12	1.84	0.60
1:A:143:TYR:OH	3:D:540:PHE:CZ	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:375:PRO:HG3	3:J:396:LEU:HD13	1.84	0.60
1:B:189:LEU:HA	1:B:192:ILE:HG22	1.84	0.60
3:G:288:GLN:NE2	3:G:329:LEU:HA	2.17	0.60
3:J:416:ASN:OD1	3:J:417:VAL:N	2.35	0.60
3:G:416:ASN:OD1	3:G:417:VAL:N	2.35	0.59
2:P:175:ASP:HB2	3:J:369:ARG:HH22	1.66	0.59
1:C:189:LEU:HA	1:C:192:ILE:HG22	1.84	0.59
3:J:356:ILE:HD13	3:J:432:TYR:HB2	1.84	0.59
1:B:98:PRO:HB2	1:B:129:VAL:HG12	1.84	0.59
3:G:375:PRO:HG3	3:G:396:LEU:HD13	1.84	0.59
3:D:534:LEU:HD23	3:D:597:ASN:HD22	1.66	0.59
3:D:599:ASP:OD1	3:D:646:THR:HA	2.01	0.59
1:C:157:ASP:O	1:C:182:GLY:N	2.32	0.59
3:G:671:ARG:HG2	3:G:696:ASN:HD21	1.67	0.59
3:G:356:ILE:HD13	3:G:432:TYR:HB2	1.84	0.59
3:G:755:GLN:HG3	3:G:756:TYR:HD1	1.66	0.59
1:A:124:PHE:HZ	1:A:359:LYS:HA	1.67	0.59
3:D:375:PRO:HG3	3:D:396:LEU:HD13	1.84	0.59
3:D:288:GLN:NE2	3:D:329:LEU:HA	2.17	0.59
1:C:124:PHE:HZ	1:C:359:LYS:HA	1.67	0.59
3:J:671:ARG:HG2	3:J:696:ASN:HD21	1.67	0.59
1:B:40:HIS:CG	1:A:171:LEU:CD1	2.86	0.59
1:B:124:PHE:HZ	1:B:359:LYS:HA	1.67	0.59
3:D:188:THR:HA	3:D:191:VAL:HB	1.85	0.59
3:D:671:ARG:HG2	3:D:696:ASN:HD21	1.67	0.59
2:P:91:ARG:NE	1:A:311:ASP:OD1	2.35	0.59
3:D:504:GLU:HG3	3:D:760:HIS:HB2	1.85	0.59
3:J:468:PHE:O	3:J:471:ASN:ND2	2.30	0.59
1:A:50:LYS:HB2	1:A:53:TYR:CZ	2.38	0.59
1:A:209:VAL:O	1:A:212:ILE:HG22	2.02	0.59
3:D:416:ASN:OD1	3:D:417:VAL:N	2.35	0.59
1:B:209:VAL:O	1:B:212:ILE:HG22	2.02	0.59
2:O:169:LEU:HD23	2:O:173:GLU:CD	2.23	0.59
3:J:153:HIS:HE1	3:J:155:PHE:CD2	2.21	0.59
2:O:93:GLN:HB3	3:D:368:GLN:NE2	2.18	0.59
3:G:153:HIS:HE1	3:G:155:PHE:CD2	2.21	0.58
3:G:504:GLU:HG3	3:G:760:HIS:HB2	1.85	0.58
3:D:356:ILE:HD13	3:D:432:TYR:HB2	1.84	0.58
1:C:142:LEU:HD12	1:C:165:ILE:CD1	2.30	0.58
1:C:209:VAL:O	1:C:212:ILE:HG22	2.03	0.58
1:B:44:MET:CE	1:A:168:GLY:CA	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:91:ARG:NH1	1:A:311:ASP:CA	2.66	0.58
1:C:155:SER:HA	1:C:160:THR:HA	1.85	0.58
1:B:155:SER:HA	1:B:160:THR:HA	1.85	0.58
3:D:755:GLN:HG3	3:D:756:TYR:HD1	1.66	0.58
1:B:50:LYS:HB2	1:B:53:TYR:CZ	2.38	0.58
3:G:146:LYS:N	3:G:149:GLU:OE2	2.37	0.58
3:G:188:THR:HA	3:G:191:VAL:HB	1.85	0.58
2:P:91:ARG:CD	1:A:311:ASP:OD1	2.51	0.58
1:A:264:PRO:HG3	1:A:271:SER:O	2.04	0.58
1:C:210:ARG:NH1	1:C:214:GLU:OE2	2.37	0.58
1:A:155:SER:HA	1:A:160:THR:HA	1.85	0.58
1:B:307:PRO:C	2:O:125:ARG:HH12	2.06	0.58
3:J:504:GLU:HG3	3:J:760:HIS:HB2	1.85	0.58
1:B:264:PRO:HG3	1:B:271:SER:O	2.04	0.58
1:A:210:ARG:NH1	1:A:214:GLU:OE2	2.37	0.58
1:C:50:LYS:HB2	1:C:53:TYR:CZ	2.38	0.58
1:B:210:ARG:NH1	1:B:214:GLU:OE2	2.37	0.58
2:P:90:ARG:HH11	1:A:221:LEU:HD23	1.67	0.58
3:D:81:PRO:O	3:D:85:ASP:N	2.36	0.58
3:D:153:HIS:HE1	3:D:155:PHE:CD2	2.21	0.58
3:J:188:THR:HA	3:J:191:VAL:HB	1.85	0.58
1:B:287:ILE:HD11	1:C:205:GLU:OE1	2.03	0.57
3:D:146:LYS:N	3:D:149:GLU:OE2	2.37	0.57
3:J:81:PRO:O	3:J:85:ASP:N	2.36	0.57
1:B:307:PRO:C	2:O:125:ARG:NH2	2.47	0.57
3:G:534:LEU:HA	3:G:548:PHE:HE2	1.70	0.57
3:D:545:ASP:OD1	3:D:546:MET:N	2.37	0.57
1:C:264:PRO:HG3	1:C:271:SER:O	2.04	0.57
3:J:352:LEU:HD21	3:J:616:MET:HG2	1.87	0.57
2:P:91:ARG:HD3	1:A:311:ASP:OD1	2.05	0.57
3:J:545:ASP:OD1	3:J:546:MET:N	2.37	0.57
1:B:168:GLY:HA3	1:C:44:MET:HE3	1.79	0.57
2:P:175:ASP:CB	3:J:369:ARG:NH2	2.65	0.57
3:J:77:LEU:HD12	3:J:99:PRO:HG2	1.87	0.57
3:G:352:LEU:HD21	3:G:616:MET:HG2	1.87	0.57
3:D:352:LEU:HD21	3:D:616:MET:HG2	1.87	0.57
1:B:290:ARG:CD	1:C:244:ASP:OD1	2.53	0.57
3:G:77:LEU:HD12	3:G:99:PRO:HG2	1.86	0.57
3:G:405:LYS:HA	3:G:409:GLU:HG3	1.87	0.56
3:G:713:ILE:HG23	3:G:721:ARG:HH22	1.70	0.56
3:D:154:ILE:HG12	3:D:670:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:405:LYS:HA	3:D:409:GLU:HG3	1.87	0.56
3:D:713:ILE:HG23	3:D:721:ARG:HH22	1.70	0.56
3:J:37:VAL:HG23	3:J:49:ALA:HB3	1.88	0.56
3:J:154:ILE:HG12	3:J:670:VAL:HG22	1.88	0.56
1:B:64:ILE:HD12	1:A:169:TYR:CE1	2.35	0.56
3:G:37:VAL:HG23	3:G:49:ALA:HB3	1.87	0.56
3:G:154:ILE:HG12	3:G:670:VAL:HG22	1.88	0.56
3:J:534:LEU:HA	3:J:548:PHE:HE2	1.70	0.56
3:D:77:LEU:HD12	3:D:99:PRO:HG2	1.86	0.56
3:J:713:ILE:HG23	3:J:721:ARG:HH22	1.70	0.56
3:G:545:ASP:OD1	3:G:546:MET:N	2.37	0.56
1:A:151:ILE:HD11	1:A:293:LEU:HB3	1.87	0.56
3:D:37:VAL:HG23	3:D:49:ALA:HB3	1.87	0.56
1:C:151:ILE:HD11	1:C:293:LEU:HB3	1.87	0.56
1:B:308:GLY:HA2	2:O:125:ARG:HH21	1.64	0.55
2:P:167:ARG:NH2	1:C:308:GLY:HA3	2.21	0.55
3:D:234:LYS:HA	3:D:240:ASN:H	1.71	0.55
3:D:247:PHE:HE2	3:D:249:ARG:HD3	1.71	0.55
3:D:534:LEU:HA	3:D:548:PHE:HE2	1.70	0.55
3:G:232:ASN:HA	3:G:242:SER:HA	1.89	0.55
3:G:234:LYS:HA	3:G:240:ASN:H	1.71	0.55
1:B:82:MET:SD	1:B:86:TRP:NE1	2.80	0.55
3:G:247:PHE:HE2	3:G:249:ARG:HD3	1.71	0.55
2:P:171:ILE:CD1	1:C:311:ASP:OD2	2.54	0.55
3:D:232:ASN:HA	3:D:242:SER:HA	1.89	0.55
1:B:151:ILE:HD11	1:B:293:LEU:HB3	1.87	0.55
3:J:391:ASN:OD1	3:J:392:SER:N	2.40	0.55
1:B:205:GLU:OE2	1:A:287:ILE:HD11	2.01	0.55
3:J:146:LYS:N	3:J:149:GLU:OE2	2.37	0.55
3:J:232:ASN:HA	3:J:242:SER:HA	1.88	0.55
3:J:405:LYS:HA	3:J:409:GLU:HG3	1.87	0.55
1:B:169:TYR:CG	1:C:64:ILE:CD1	2.86	0.55
3:G:325:ASP:HA	3:G:328:GLU:HB2	1.88	0.55
3:D:738:SER:HB2	3:D:739:ARG:NH2	2.22	0.55
1:C:74:GLY:O	1:C:111:ASN:ND2	2.40	0.55
3:J:247:PHE:HE2	3:J:249:ARG:HD3	1.71	0.55
1:B:74:GLY:O	1:B:111:ASN:ND2	2.40	0.55
2:O:176:LEU:CD2	3:J:369:ARG:HH21	2.20	0.55
3:G:81:PRO:O	3:G:85:ASP:N	2.36	0.55
3:G:391:ASN:OD1	3:G:392:SER:N	2.40	0.55
2:P:90:ARG:NH2	1:A:311:ASP:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:184:LYS:HG2	3:G:187:ASN:HD22	1.71	0.55
2:P:90:ARG:CZ	1:A:221:LEU:CD2	2.84	0.55
1:C:82:MET:SD	1:C:86:TRP:NE1	2.80	0.55
3:J:184:LYS:HG2	3:J:187:ASN:HD22	1.71	0.55
3:J:325:ASP:HA	3:J:328:GLU:HB2	1.88	0.55
3:J:738:SER:HB2	3:J:739:ARG:NH2	2.22	0.55
1:B:186:THR:HG23	1:B:209:VAL:HG13	1.89	0.55
1:A:186:THR:HG23	1:A:209:VAL:HG13	1.89	0.55
3:G:347:ASN:O	3:G:351:LYS:HG3	2.07	0.54
3:G:738:SER:HB2	3:G:739:ARG:NH2	2.22	0.54
3:D:391:ASN:OD1	3:D:392:SER:N	2.40	0.54
1:C:186:THR:HG23	1:C:209:VAL:HG13	1.89	0.54
1:A:82:MET:SD	1:A:86:TRP:NE1	2.80	0.54
3:D:39:VAL:HG11	3:D:63:THR:HG22	1.89	0.54
3:D:184:LYS:HG2	3:D:187:ASN:HD22	1.71	0.54
3:D:325:ASP:HA	3:D:328:GLU:HB2	1.88	0.54
3:G:368:GLN:NE2	2:P:135:GLN:HB3	2.16	0.54
3:J:234:LYS:HA	3:J:240:ASN:H	1.71	0.54
1:B:46:GLY:CA	3:D:540:PHE:CZ	2.90	0.54
3:D:287:TYR:HA	3:D:290:LEU:HB2	1.90	0.54
3:J:293:LYS:HG3	3:J:329:LEU:HD11	1.89	0.54
3:J:347:ASN:O	3:J:351:LYS:HG3	2.07	0.54
3:J:447:LEU:HD23	3:J:447:LEU:O	2.08	0.54
1:B:40:HIS:CD2	1:A:171:LEU:HD12	2.41	0.54
1:A:103:THR:O	1:A:132:MET:HA	2.08	0.54
1:C:11:ASP:HB3	1:C:18:LYS:HG2	1.90	0.54
1:C:103:THR:O	1:C:132:MET:HA	2.08	0.54
3:G:447:LEU:HD23	3:G:447:LEU:O	2.08	0.54
1:A:74:GLY:O	1:A:111:ASN:ND2	2.40	0.54
1:A:79:TRP:HH2	1:A:119:MET:HB2	1.73	0.54
1:C:9:VAL:HG13	1:C:340:TRP:NE1	2.23	0.54
1:B:11:ASP:HB3	1:B:18:LYS:HG2	1.90	0.54
1:B:103:THR:O	1:B:132:MET:HA	2.08	0.54
3:G:39:VAL:HG11	3:G:63:THR:HG22	1.89	0.54
3:G:287:TYR:HA	3:G:290:LEU:HB2	1.90	0.54
3:G:293:LYS:HG3	3:G:329:LEU:HD11	1.89	0.54
3:G:671:ARG:HG2	3:G:696:ASN:ND2	2.23	0.54
2:O:169:LEU:HD23	2:O:173:GLU:HG3	1.89	0.54
3:D:192:ILE:HD11	3:D:250:ILE:HD13	1.90	0.54
3:D:447:LEU:O	3:D:447:LEU:HD23	2.08	0.54
3:J:403:ARG:NH1	3:J:409:GLU:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:96:GLU:OE1	3:D:368:GLN:HB3	2.08	0.53
2:O:173:GLU:HB3	3:J:368:GLN:NE2	2.20	0.53
3:G:192:ILE:HD11	3:G:250:ILE:HD13	1.91	0.53
3:D:347:ASN:O	3:D:351:LYS:HG3	2.07	0.53
1:B:43:VAL:HG22	1:A:170:ALA:H	1.72	0.53
3:G:404:VAL:O	3:G:412:THR:OG1	2.25	0.53
1:A:11:ASP:HB3	1:A:18:LYS:HG2	1.90	0.53
3:J:192:ILE:HD11	3:J:250:ILE:HD13	1.90	0.53
3:J:287:TYR:HA	3:J:290:LEU:HB2	1.90	0.53
3:J:422:TYR:HE2	3:J:598:LYS:HD2	1.73	0.53
1:B:79:TRP:HH2	1:B:119:MET:HB2	1.73	0.53
3:G:422:TYR:HE2	3:G:598:LYS:HD2	1.73	0.53
3:G:755:GLN:HG3	3:G:756:TYR:CD1	2.43	0.53
3:D:59:VAL:N	3:D:71:VAL:O	2.34	0.53
3:D:293:LYS:HG3	3:D:329:LEU:HD11	1.89	0.53
3:D:422:TYR:HE2	3:D:598:LYS:HD2	1.73	0.53
3:D:705:CYS:HA	3:D:710:PRO:HG2	1.90	0.53
3:J:39:VAL:HG11	3:J:63:THR:HG22	1.89	0.53
3:J:59:VAL:N	3:J:71:VAL:O	2.34	0.53
3:G:403:ARG:NH1	3:G:409:GLU:O	2.40	0.53
3:D:248:ILE:O	3:D:459:VAL:N	2.42	0.53
3:D:403:ARG:NH1	3:D:409:GLU:O	2.40	0.53
3:D:755:GLN:HG3	3:D:756:TYR:CD1	2.44	0.53
3:J:671:ARG:HG2	3:J:696:ASN:ND2	2.23	0.53
3:J:755:GLN:HG3	3:J:756:TYR:CD1	2.43	0.53
3:D:404:VAL:O	3:D:412:THR:OG1	2.25	0.53
1:C:198:TYR:CZ	1:C:248:ILE:HG13	2.44	0.53
2:O:169:LEU:HD23	2:O:173:GLU:CG	2.39	0.53
3:G:131:LEU:O	3:G:133:VAL:N	2.40	0.53
2:P:175:ASP:OD2	3:J:369:ARG:CZ	2.57	0.53
1:A:9:VAL:HG13	1:A:340:TRP:NE1	2.23	0.53
1:A:198:TYR:CZ	1:A:248:ILE:HG13	2.44	0.53
3:D:88:GLU:HB2	3:D:152:PRO:HG3	1.89	0.53
3:J:406:VAL:HG12	3:J:407:GLY:N	2.23	0.53
1:B:198:TYR:CZ	1:B:248:ILE:HG13	2.44	0.53
3:G:179:GLU:OE2	3:G:241:SER:OG	2.27	0.53
3:D:179:GLU:OE2	3:D:241:SER:OG	2.27	0.53
3:D:671:ARG:HG2	3:D:696:ASN:ND2	2.23	0.53
3:J:88:GLU:HB2	3:J:152:PRO:HG3	1.89	0.53
3:G:406:VAL:HG12	3:G:407:GLY:N	2.24	0.53
3:J:179:GLU:OE2	3:J:241:SER:OG	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:403:ARG:NH1	3:J:409:GLU:HG2	2.24	0.53
3:J:509:GLU:HG3	3:J:510:PHE:H	1.74	0.53
3:J:555:ASN:HB3	3:J:556:HIS:ND1	2.24	0.53
1:B:9:VAL:HG13	1:B:340:TRP:NE1	2.23	0.53
3:G:80:ASN:ND2	3:G:93:LEU:HB3	2.24	0.53
3:G:403:ARG:NH1	3:G:409:GLU:HG2	2.24	0.53
1:A:20:GLY:HA3	1:A:340:TRP:CZ2	2.44	0.53
3:D:509:GLU:HG3	3:D:510:PHE:H	1.74	0.53
1:A:8:LEU:HD23	1:A:9:VAL:N	2.24	0.53
3:D:80:ASN:ND2	3:D:93:LEU:HB3	2.24	0.53
1:C:157:ASP:O	1:C:181:ALA:HB1	2.09	0.53
1:C:326:LYS:HB3	1:C:328:LYS:HZ3	1.74	0.53
1:B:157:ASP:O	1:B:181:ALA:HB1	2.09	0.52
2:P:91:ARG:HH11	1:A:311:ASP:HB2	1.61	0.52
3:D:306:ASN:HB3	3:D:309:ASP:OD2	2.09	0.52
3:D:403:ARG:NH1	3:D:409:GLU:HG2	2.24	0.52
1:C:8:LEU:HD23	1:C:9:VAL:N	2.24	0.52
3:J:306:ASN:HB3	3:J:309:ASP:OD2	2.09	0.52
1:B:20:GLY:HA3	1:B:340:TRP:CZ2	2.44	0.52
1:B:44:MET:HE3	1:A:148:THR:OG1	2.09	0.52
1:B:290:ARG:HD2	1:C:244:ASP:CG	2.29	0.52
3:G:217:GLU:HG2	3:G:218:ASP:N	2.25	0.52
3:G:306:ASN:HB3	3:G:309:ASP:OD2	2.09	0.52
3:D:548:PHE:CE1	3:D:552:LEU:HD11	2.45	0.52
3:J:705:CYS:HA	3:J:710:PRO:HG2	1.90	0.52
1:B:8:LEU:HD23	1:B:9:VAL:N	2.24	0.52
3:G:88:GLU:HB2	3:G:152:PRO:HG3	1.89	0.52
3:G:548:PHE:CE1	3:G:552:LEU:HD11	2.45	0.52
2:P:167:ARG:HH21	1:C:308:GLY:HA3	1.75	0.52
3:D:217:GLU:HG2	3:D:218:ASP:N	2.25	0.52
1:C:20:GLY:HA3	1:C:340:TRP:CZ2	2.44	0.52
3:J:80:ASN:ND2	3:J:93:LEU:HB3	2.24	0.52
3:D:406:VAL:HG12	3:D:407:GLY:N	2.23	0.52
3:D:555:ASN:HB3	3:D:556:HIS:ND1	2.24	0.52
3:J:217:GLU:HG2	3:J:218:ASP:N	2.25	0.52
1:B:132:MET:SD	1:B:133:TYR:N	2.82	0.52
3:G:509:GLU:HG3	3:G:510:PHE:H	1.74	0.52
1:A:140:LEU:HD11	1:A:343:GLY:HA2	1.91	0.52
1:C:79:TRP:HH2	1:C:119:MET:HB2	1.73	0.52
3:G:109:TYR:OH	3:G:682:GLY:N	2.34	0.52
3:G:555:ASN:HB3	3:G:556:HIS:ND1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:403:ARG:HE	3:G:411:VAL:HA	1.75	0.52
1:A:157:ASP:O	1:A:181:ALA:HB1	2.09	0.52
3:D:109:TYR:OH	3:D:682:GLY:N	2.34	0.52
3:J:403:ARG:HE	3:J:411:VAL:HA	1.75	0.52
2:P:172:ILE:HG13	3:J:369:ARG:CZ	2.40	0.52
1:C:132:MET:SD	1:C:133:TYR:N	2.82	0.52
1:C:287:ILE:HG13	1:C:290:ARG:NH2	2.25	0.52
2:P:171:ILE:HG21	1:C:311:ASP:OD1	2.09	0.52
2:O:93:GLN:HB3	3:D:368:GLN:HE22	1.75	0.52
3:G:705:CYS:HA	3:G:710:PRO:HG2	1.90	0.52
3:J:277:LEU:HG	3:J:279:ALA:H	1.75	0.52
3:J:548:PHE:CE1	3:J:552:LEU:HD11	2.45	0.52
1:B:46:GLY:CA	3:D:540:PHE:CE1	2.88	0.51
1:B:287:ILE:HG13	1:B:290:ARG:NH2	2.25	0.51
3:D:277:LEU:HG	3:D:279:ALA:H	1.75	0.51
3:G:277:LEU:HG	3:G:279:ALA:H	1.75	0.51
1:A:132:MET:SD	1:A:133:TYR:N	2.82	0.51
1:C:140:LEU:HD11	1:C:343:GLY:HA2	1.91	0.51
1:C:142:LEU:HD22	1:C:147:ARG:O	2.10	0.51
3:J:103:TYR:HA	3:J:106:LYS:HE2	1.91	0.51
3:D:48:LYS:HB3	3:D:64:GLU:OE1	2.10	0.51
1:B:71:ILE:HD11	1:B:82:MET:HG3	1.93	0.51
1:B:90:PHE:CE2	1:B:98:PRO:HB3	2.46	0.51
3:G:48:LYS:HB3	3:G:64:GLU:OE1	2.09	0.51
3:D:103:TYR:HA	3:D:106:LYS:HE2	1.91	0.51
3:J:48:LYS:HB3	3:J:64:GLU:OE1	2.09	0.51
1:A:71:ILE:HD11	1:A:82:MET:HG3	1.93	0.51
3:D:403:ARG:HE	3:D:411:VAL:HA	1.75	0.51
1:C:190:MET:HE1	1:C:206:ARG:HA	1.93	0.51
3:G:103:TYR:HA	3:G:106:LYS:HE2	1.91	0.51
3:G:704:ILE:HD13	3:G:707:LYS:HZ3	1.75	0.51
1:C:71:ILE:HD11	1:C:82:MET:HG3	1.92	0.51
1:C:90:PHE:CE2	1:C:98:PRO:HB3	2.46	0.51
1:B:190:MET:HE1	1:B:206:ARG:HA	1.93	0.51
1:A:90:PHE:CE2	1:A:98:PRO:HB3	2.46	0.51
3:J:528:MET:HG2	3:J:528:MET:O	2.10	0.51
1:B:289:ILE:HG22	1:B:293:LEU:HG	1.93	0.51
3:G:528:MET:O	3:G:528:MET:HG2	2.10	0.51
1:A:287:ILE:HG13	1:A:290:ARG:NH2	2.25	0.51
3:D:337:ASP:OD1	3:D:346:LYS:HG3	2.11	0.51
3:D:381:ALA:O	3:D:384:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD11	1:B:343:GLY:HA2	1.91	0.51
1:A:289:ILE:HG22	1:A:293:LEU:HG	1.93	0.51
3:D:423:ALA:HA	3:D:600:PRO:HD2	1.93	0.51
3:G:423:ALA:HA	3:G:600:PRO:HD2	1.93	0.51
3:G:534:LEU:CD2	3:G:597:ASN:HD22	2.24	0.51
3:D:528:MET:O	3:D:528:MET:HG2	2.10	0.51
3:D:348:SER:HA	3:D:351:LYS:HG3	1.92	0.50
3:D:717:ASP:HB3	3:D:721:ARG:HH12	1.75	0.50
3:J:248:ILE:O	3:J:459:VAL:N	2.41	0.50
1:B:14:SER:OG	1:B:157:ASP:OD1	2.29	0.50
3:G:348:SER:HA	3:G:351:LYS:HG3	1.92	0.50
1:A:116:ARG:HD3	1:A:134:VAL:HG21	1.93	0.50
3:D:534:LEU:CD2	3:D:597:ASN:HD22	2.24	0.50
3:J:534:LEU:CD2	3:J:597:ASN:HD22	2.24	0.50
3:D:93:LEU:O	3:D:96:LEU:HD22	2.11	0.50
3:G:93:LEU:O	3:G:96:LEU:HD22	2.11	0.50
1:A:111:ASN:HB3	1:A:112:PRO:HD3	1.93	0.50
1:A:190:MET:HE1	1:A:206:ARG:HA	1.93	0.50
3:D:131:LEU:O	3:D:133:VAL:N	2.40	0.50
1:C:289:ILE:HG22	1:C:293:LEU:HG	1.93	0.50
3:J:93:LEU:O	3:J:96:LEU:HD22	2.11	0.50
3:J:401:HIS:HD2	3:J:413:LYS:HB3	1.77	0.50
3:J:423:ALA:HA	3:J:600:PRO:HD2	1.93	0.50
3:G:337:ASP:OD1	3:G:346:LYS:HG3	2.11	0.50
3:D:287:TYR:HD1	3:D:290:LEU:HD22	1.77	0.50
3:D:243:ARG:HB3	3:D:269:GLU:OE1	2.11	0.50
3:J:337:ASP:OD1	3:J:346:LYS:HG3	2.11	0.50
3:G:243:ARG:HB3	3:G:269:GLU:OE1	2.11	0.50
3:G:287:TYR:HD1	3:G:290:LEU:HD22	1.77	0.50
3:G:401:HIS:HD2	3:G:413:LYS:HB3	1.77	0.50
3:G:597:ASN:OD1	3:G:647:VAL:N	2.45	0.50
1:C:116:ARG:HD3	1:C:134:VAL:HG21	1.93	0.50
3:J:348:SER:HA	3:J:351:LYS:HG3	1.92	0.50
3:J:597:ASN:OD1	3:J:647:VAL:N	2.45	0.50
3:J:613:SER:HB3	3:J:616:MET:HE3	1.94	0.50
1:B:111:ASN:HB3	1:B:112:PRO:HD3	1.93	0.50
1:B:116:ARG:HD3	1:B:134:VAL:HG21	1.93	0.50
3:G:154:ILE:HD12	3:G:157:ILE:HB	1.94	0.50
1:C:153:LEU:HD13	1:C:162:ASN:OD1	2.12	0.50
3:J:287:TYR:HD1	3:J:290:LEU:HD22	1.77	0.50
1:A:20:GLY:HA3	1:A:340:TRP:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD13	1:A:162:ASN:OD1	2.12	0.50
1:A:227:MET:HA	1:A:255:PHE:CZ	2.47	0.50
3:D:597:ASN:OD1	3:D:647:VAL:N	2.45	0.50
1:C:146:GLY:HA2	3:J:541:PRO:HB3	1.94	0.50
3:J:288:GLN:HE21	3:J:329:LEU:HA	1.76	0.50
3:J:243:ARG:HB3	3:J:269:GLU:OE1	2.11	0.49
3:G:59:VAL:N	3:G:71:VAL:O	2.34	0.49
3:G:613:SER:HB3	3:G:616:MET:HE3	1.93	0.49
1:A:326:LYS:HB3	1:A:328:LYS:HZ3	1.76	0.49
3:D:288:GLN:HE21	3:D:329:LEU:HA	1.76	0.49
3:D:613:SER:HB3	3:D:616:MET:HE3	1.93	0.49
1:C:221:LEU:HD13	1:C:312:ARG:HD2	1.94	0.49
3:J:153:HIS:HE1	3:J:155:PHE:HB2	1.77	0.49
3:G:345:GLU:O	3:G:349:MET:HG2	2.13	0.49
1:C:111:ASN:HB3	1:C:112:PRO:HD3	1.93	0.49
1:B:146:GLY:HA2	3:G:541:PRO:HB3	1.94	0.49
1:A:146:GLY:HA2	3:D:541:PRO:HB3	1.94	0.49
3:J:720:GLN:HA	3:J:723:ARG:NH1	2.27	0.49
1:B:227:MET:HA	1:B:255:PHE:CZ	2.47	0.49
3:G:717:ASP:HB3	3:G:721:ARG:HH12	1.75	0.49
3:D:401:HIS:HD2	3:D:413:LYS:HB3	1.77	0.49
3:D:720:GLN:HA	3:D:723:ARG:NH1	2.27	0.49
1:C:227:MET:HA	1:C:255:PHE:HZ	1.78	0.49
1:B:221:LEU:HD13	1:B:312:ARG:HD2	1.94	0.49
3:G:720:GLN:HA	3:G:723:ARG:NH1	2.27	0.49
1:A:227:MET:HA	1:A:255:PHE:HZ	1.78	0.49
1:C:20:GLY:HA3	1:C:340:TRP:HZ2	1.76	0.49
1:C:227:MET:HA	1:C:255:PHE:CZ	2.47	0.49
1:A:221:LEU:HD13	1:A:312:ARG:HD2	1.94	0.49
3:D:345:GLU:O	3:D:349:MET:HG2	2.13	0.49
3:J:154:ILE:HD12	3:J:157:ILE:HB	1.94	0.49
1:B:64:ILE:HD12	1:A:169:TYR:CG	2.47	0.49
3:D:128:TYR:CD2	3:D:681:PRO:HG3	2.43	0.49
3:D:296:GLU:O	3:D:300:MET:HG2	2.13	0.49
3:D:509:GLU:HG3	3:D:510:PHE:N	2.28	0.49
1:C:14:SER:OG	1:C:157:ASP:OD1	2.29	0.49
3:J:193:GLN:O	3:J:197:VAL:HG23	2.12	0.49
1:B:49:GLN:OE1	1:B:49:GLN:N	2.46	0.49
3:G:509:GLU:HG3	3:G:510:PHE:N	2.28	0.49
3:G:741:GLY:O	3:G:743:GLU:HG3	2.13	0.49
3:D:741:GLY:O	3:D:743:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:HA3	1:B:340:TRP:HZ2	1.76	0.48
1:B:63:GLY:HA3	1:A:289:ILE:CG1	2.41	0.48
3:D:62:GLU:HA	3:D:68:THR:HA	1.95	0.48
3:J:131:LEU:O	3:J:133:VAL:N	2.40	0.48
3:J:345:GLU:O	3:J:349:MET:HG2	2.13	0.48
3:J:509:GLU:HG3	3:J:510:PHE:N	2.28	0.48
1:B:153:LEU:HD13	1:B:162:ASN:OD1	2.12	0.48
1:A:7:ALA:O	1:A:8:LEU:HB2	2.13	0.48
3:D:154:ILE:HD12	3:D:157:ILE:HB	1.94	0.48
3:D:540:PHE:CG	3:D:541:PRO:HD2	2.49	0.48
3:J:717:ASP:HB3	3:J:721:ARG:HH12	1.75	0.48
3:G:193:GLN:O	3:G:197:VAL:HG23	2.12	0.48
3:G:540:PHE:CG	3:G:541:PRO:HD2	2.48	0.48
3:D:193:GLN:O	3:D:197:VAL:HG23	2.12	0.48
3:D:469:ASP:HA	3:D:572:LYS:HE3	1.94	0.48
2:P:132:SER:O	2:P:135:GLN:CG	2.61	0.48
3:D:722:TYR:OH	3:D:770:LEU:HA	2.14	0.48
3:J:741:GLY:O	3:J:743:GLU:HG3	2.13	0.48
2:O:173:GLU:HG2	2:P:172:ILE:HD11	1.91	0.48
3:G:62:GLU:HA	3:G:68:THR:HA	1.95	0.48
1:C:142:LEU:HD11	1:C:165:ILE:HB	1.94	0.48
1:C:349:LEU:HD22	3:J:536:GLU:HG3	1.95	0.48
3:J:296:GLU:O	3:J:300:MET:HG2	2.13	0.48
1:B:256:ARG:HG2	1:B:256:ARG:O	2.14	0.48
1:B:349:LEU:HD22	3:G:536:GLU:HG3	1.95	0.48
3:G:381:ALA:O	3:G:384:SER:OG	2.28	0.48
3:J:62:GLU:HA	3:J:68:THR:HA	1.95	0.48
3:J:281:ARG:NH1	3:J:320:VAL:HG11	2.28	0.48
3:G:610:LYS:HD2	3:G:610:LYS:N	2.29	0.48
3:G:711:ASN:HD22	3:G:767:ALA:HB2	1.79	0.48
3:D:690:MET:SD	3:D:691:HIS:N	2.87	0.48
3:D:722:TYR:OH	3:D:773:LEU:HD12	2.14	0.48
3:J:540:PHE:CG	3:J:541:PRO:HD2	2.48	0.48
3:G:248:ILE:HB	3:G:459:VAL:HG13	1.96	0.48
3:G:296:GLU:O	3:G:300:MET:HG2	2.13	0.48
1:C:256:ARG:O	1:C:256:ARG:HG2	2.14	0.48
3:J:548:PHE:HE1	3:J:552:LEU:HD11	1.79	0.48
3:J:690:MET:SD	3:J:691:HIS:N	2.87	0.48
1:B:200:PHE:HD1	1:B:205:GLU:HB3	1.79	0.48
3:G:248:ILE:O	3:G:459:VAL:N	2.42	0.48
3:G:690:MET:SD	3:G:691:HIS:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:HD22	3:D:536:GLU:HG3	1.95	0.48
3:J:469:ASP:HA	3:J:572:LYS:HE3	1.94	0.48
1:B:7:ALA:O	1:B:8:LEU:HB2	2.14	0.47
3:G:722:TYR:OH	3:G:770:LEU:HA	2.14	0.47
1:A:14:SER:OG	1:A:157:ASP:OD1	2.29	0.47
3:D:248:ILE:HB	3:D:459:VAL:HG13	1.96	0.47
1:C:7:ALA:O	1:C:8:LEU:HB2	2.14	0.47
1:C:49:GLN:N	1:C:49:GLN:OE1	2.46	0.47
3:G:288:GLN:HE21	3:G:329:LEU:HA	1.77	0.47
1:A:71:ILE:CD1	1:A:76:ILE:HG12	2.44	0.47
1:A:71:ILE:HD12	1:A:76:ILE:HG12	1.96	0.47
1:A:256:ARG:O	1:A:256:ARG:HG2	2.14	0.47
1:A:351:THR:HG23	3:D:536:GLU:OE1	2.14	0.47
3:D:669:PHE:HB3	3:D:671:ARG:NH1	2.29	0.47
3:D:704:ILE:HD13	3:D:707:LYS:NZ	2.28	0.47
1:C:120:THR:O	1:C:124:PHE:CB	2.62	0.47
1:C:333:PRO:HG2	3:J:413:LYS:O	2.15	0.47
3:J:404:VAL:O	3:J:412:THR:OG1	2.25	0.47
1:B:120:THR:O	1:B:124:PHE:CB	2.63	0.47
1:B:333:PRO:HG2	3:G:413:LYS:O	2.15	0.47
3:G:184:LYS:O	3:G:186:VAL:N	2.47	0.47
3:G:230:PHE:HE1	3:G:285:ILE:HG12	1.80	0.47
3:G:469:ASP:HA	3:G:572:LYS:HE3	1.94	0.47
1:A:120:THR:O	1:A:124:PHE:CB	2.63	0.47
1:A:361:GLU:OE2	1:A:373:LYS:NZ	2.47	0.47
3:D:358:HIS:HE1	3:D:380:GLU:O	1.98	0.47
3:D:711:ASN:HD22	3:D:767:ALA:HB2	1.79	0.47
3:J:248:ILE:HB	3:J:459:VAL:HG13	1.96	0.47
3:J:704:ILE:HD13	3:J:707:LYS:NZ	2.28	0.47
3:J:722:TYR:OH	3:J:770:LEU:HA	2.14	0.47
1:B:71:ILE:HD12	1:B:76:ILE:HG12	1.96	0.47
1:B:227:MET:HA	1:B:255:PHE:HZ	1.78	0.47
3:G:669:PHE:HB3	3:G:671:ARG:NH1	2.29	0.47
3:G:704:ILE:HD13	3:G:707:LYS:NZ	2.28	0.47
1:A:49:GLN:N	1:A:49:GLN:OE1	2.46	0.47
3:D:128:TYR:H	3:D:681:PRO:HB3	1.80	0.47
3:D:184:LYS:HG2	3:D:187:ASN:ND2	2.29	0.47
3:D:610:LYS:N	3:D:610:LYS:HD2	2.29	0.47
1:C:79:TRP:CH2	1:C:119:MET:HB2	2.50	0.47
1:C:96:VAL:HG21	1:C:101:HIS:NE2	2.30	0.47
1:C:154:ASP:OD1	1:C:155:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:GLU:OE2	1:C:373:LYS:NZ	2.47	0.47
3:J:128:TYR:H	3:J:681:PRO:HB3	1.80	0.47
3:J:610:LYS:HD2	3:J:610:LYS:N	2.29	0.47
3:G:548:PHE:HE1	3:G:552:LEU:HD11	1.79	0.47
3:G:722:TYR:OH	3:G:773:LEU:HD12	2.14	0.47
1:C:288:ASP:OD1	1:C:289:ILE:HG12	2.14	0.47
1:B:71:ILE:CD1	1:B:76:ILE:HG12	2.44	0.47
1:B:96:VAL:HG21	1:B:101:HIS:NE2	2.30	0.47
1:B:361:GLU:OE2	1:B:373:LYS:NZ	2.47	0.47
2:O:176:LEU:HD22	3:J:369:ARG:HH21	1.80	0.47
3:D:570:LYS:HE2	3:D:570:LYS:HA	1.96	0.47
1:C:209:VAL:HA	1:C:212:ILE:HG22	1.95	0.47
3:J:128:TYR:CD2	3:J:681:PRO:HG3	2.43	0.47
1:B:79:TRP:CH2	1:B:119:MET:HB2	2.50	0.47
1:B:154:ASP:OD1	1:B:155:SER:N	2.47	0.47
1:B:205:GLU:OE1	1:A:287:ILE:HD12	2.07	0.47
1:B:209:VAL:HA	1:B:212:ILE:HG22	1.95	0.47
1:B:351:THR:HG23	3:G:536:GLU:OE1	2.14	0.47
3:G:184:LYS:HG2	3:G:187:ASN:ND2	2.29	0.47
3:G:709:PHE:O	3:G:764:PHE:HB3	2.15	0.47
2:P:79:THR:HG21	1:A:238:LYS:NZ	2.30	0.47
3:D:184:LYS:O	3:D:186:VAL:N	2.47	0.47
3:D:546:MET:O	3:D:549:LYS:HG2	2.14	0.47
3:D:548:PHE:HE1	3:D:552:LEU:HD11	1.79	0.47
3:J:275:PHE:HA	3:J:315:GLN:HE22	1.80	0.47
3:J:546:MET:O	3:J:549:LYS:HG2	2.14	0.47
3:J:669:PHE:HB3	3:J:671:ARG:NH1	2.29	0.47
3:J:709:PHE:O	3:J:764:PHE:HB3	2.15	0.47
3:G:275:PHE:HA	3:G:315:GLN:HE22	1.80	0.47
3:G:281:ARG:NH1	3:G:320:VAL:HG11	2.28	0.47
3:D:230:PHE:HE1	3:D:285:ILE:HG12	1.79	0.47
3:D:248:ILE:HG23	3:D:263:ILE:HG22	1.96	0.47
1:C:71:ILE:CD1	1:C:76:ILE:HG12	2.44	0.47
3:J:184:LYS:HG2	3:J:187:ASN:ND2	2.29	0.47
3:J:381:ALA:O	3:J:384:SER:OG	2.28	0.47
3:J:711:ASN:HD22	3:J:767:ALA:HB2	1.79	0.47
3:G:546:MET:O	3:G:549:LYS:HG2	2.14	0.47
1:A:288:ASP:OD1	1:A:289:ILE:HG12	2.15	0.47
3:J:230:PHE:HE1	3:J:285:ILE:HG12	1.80	0.47
3:J:249:ARG:HG2	3:J:262:ASP:O	2.15	0.47
3:J:722:TYR:OH	3:J:773:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLY:HA3	1:A:322:PRO:HG2	1.93	0.47
3:G:176:ILE:CG2	3:G:184:LYS:HE3	2.45	0.47
3:G:358:HIS:HE1	3:G:380:GLU:O	1.98	0.47
1:A:96:VAL:HG21	1:A:101:HIS:NE2	2.30	0.47
3:D:709:PHE:O	3:D:764:PHE:HB3	2.15	0.47
1:B:322:PRO:HG3	1:C:245:GLY:HA3	1.97	0.46
3:G:517:LEU:O	3:G:521:ILE:HG12	2.15	0.46
1:A:209:VAL:HA	1:A:212:ILE:HG22	1.96	0.46
1:A:333:PRO:HG2	3:D:413:LYS:O	2.15	0.46
3:D:275:PHE:HA	3:D:315:GLN:HE22	1.80	0.46
3:D:282:ASP:HB2	3:D:287:TYR:OH	2.15	0.46
3:J:477:CYS:SG	3:J:651:HIS:CD2	3.08	0.46
1:B:288:ASP:OD1	1:B:289:ILE:HG12	2.15	0.46
3:G:570:LYS:HE2	3:G:570:LYS:HA	1.96	0.46
1:A:136:ILE:HG13	1:A:139:VAL:HG22	1.98	0.46
1:A:164:PRO:HG2	1:A:174:ALA:HB3	1.97	0.46
1:A:200:PHE:HD1	1:A:205:GLU:HB3	1.79	0.46
3:D:176:ILE:CG2	3:D:184:LYS:HE3	2.45	0.46
3:D:273:VAL:HB	3:D:429:LYS:HG2	1.97	0.46
1:C:351:THR:HG23	3:J:536:GLU:OE1	2.15	0.46
1:C:362:TYR:CE1	1:C:367:PRO:HA	2.50	0.46
3:J:176:ILE:CG2	3:J:184:LYS:HE3	2.45	0.46
3:J:451:GLN:OE1	3:J:451:GLN:N	2.49	0.46
3:G:451:GLN:OE1	3:G:451:GLN:N	2.49	0.46
3:G:544:THR:OG1	3:G:547:THR:OG1	2.29	0.46
3:D:423:ALA:HB2	3:D:600:PRO:HG2	1.97	0.46
3:J:184:LYS:O	3:J:186:VAL:N	2.47	0.46
1:B:136:ILE:HG13	1:B:139:VAL:HG22	1.98	0.46
1:B:164:PRO:HG2	1:B:174:ALA:HB3	1.97	0.46
1:B:332:PRO:O	1:B:335:ARG:HG3	2.16	0.46
3:G:273:VAL:HB	3:G:429:LYS:HG2	1.97	0.46
1:A:332:PRO:O	1:A:335:ARG:HG3	2.16	0.46
3:J:570:LYS:HA	3:J:570:LYS:HE2	1.96	0.46
1:B:177:ARG:HG2	1:B:178:LEU:N	2.31	0.46
1:B:362:TYR:CE1	1:B:367:PRO:HA	2.50	0.46
3:G:248:ILE:HG23	3:G:263:ILE:HG22	1.96	0.46
3:G:282:ASP:HB2	3:G:287:TYR:OH	2.15	0.46
1:A:154:ASP:OD1	1:A:155:SER:N	2.47	0.46
1:A:177:ARG:HG2	1:A:178:LEU:N	2.31	0.46
1:B:287:ILE:HD11	1:C:205:GLU:CD	2.24	0.46
3:G:249:ARG:HG2	3:G:262:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:CD2	1:A:289:ILE:HG23	2.51	0.46
1:A:362:TYR:CE1	1:A:367:PRO:HA	2.51	0.46
3:D:100:ALA:HA	3:D:103:TYR:HE1	1.79	0.46
1:C:136:ILE:HG13	1:C:139:VAL:HG22	1.98	0.46
1:C:191:LYS:O	1:C:194:THR:HG22	2.16	0.46
1:C:200:PHE:HD1	1:C:205:GLU:HB3	1.79	0.46
3:J:248:ILE:HG23	3:J:263:ILE:HG22	1.96	0.46
3:J:335:ALA:HA	3:J:338:VAL:HG22	1.98	0.46
3:J:704:ILE:HD13	3:J:707:LYS:HZ3	1.81	0.46
3:G:153:HIS:HE1	3:G:155:PHE:HB2	1.77	0.46
3:G:335:ALA:HA	3:G:338:VAL:HG22	1.98	0.46
2:P:91:ARG:NE	1:A:311:ASP:HB2	2.29	0.46
3:J:385:ALA:HB1	3:J:390:LEU:O	2.16	0.46
3:J:423:ALA:HB2	3:J:600:PRO:HG2	1.97	0.46
3:G:128:TYR:H	3:G:681:PRO:HB3	1.80	0.46
3:G:232:ASN:O	3:G:284:HIS:HD2	1.99	0.46
3:G:262:ASP:OD1	3:G:444:ASN:ND2	2.49	0.46
1:A:107:GLU:OE1	1:A:111:ASN:ND2	2.49	0.46
3:D:288:GLN:HG3	3:D:329:LEU:HB3	1.98	0.46
1:C:164:PRO:HG2	1:C:174:ALA:HB3	1.97	0.46
1:C:166:TYR:CD2	1:C:289:ILE:HG23	2.51	0.46
1:C:332:PRO:O	1:C:335:ARG:HG3	2.16	0.46
3:J:282:ASP:HB2	3:J:287:TYR:OH	2.15	0.46
3:J:358:HIS:HE1	3:J:380:GLU:O	1.98	0.46
1:B:107:GLU:OE1	1:B:111:ASN:ND2	2.49	0.46
1:B:166:TYR:CD2	1:B:289:ILE:HG23	2.51	0.46
1:B:191:LYS:O	1:B:194:THR:HG22	2.16	0.46
3:G:423:ALA:HB2	3:G:600:PRO:HG2	1.97	0.46
3:G:477:CYS:SG	3:G:651:HIS:CD2	3.08	0.46
1:A:79:TRP:CH2	1:A:119:MET:HB2	2.50	0.46
3:D:335:ALA:HA	3:D:338:VAL:HG22	1.98	0.46
1:C:177:ARG:HG2	1:C:178:LEU:N	2.31	0.46
3:J:273:VAL:HB	3:J:429:LYS:HG2	1.97	0.46
3:D:38:PHE:O	3:D:76:VAL:HG13	2.16	0.46
3:D:81:PRO:HD2	3:D:84:PHE:HB2	1.98	0.46
3:D:385:ALA:HB1	3:D:390:LEU:O	2.16	0.46
3:D:451:GLN:OE1	3:D:451:GLN:N	2.49	0.46
3:D:517:LEU:O	3:D:521:ILE:HG12	2.15	0.46
1:C:107:GLU:OE1	1:C:111:ASN:ND2	2.49	0.46
3:J:232:ASN:O	3:J:284:HIS:HD2	1.99	0.46
3:J:288:GLN:HG3	3:J:329:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:700:GLU:O	3:J:704:ILE:HG12	2.16	0.46
3:G:81:PRO:HD2	3:G:84:PHE:HB2	1.98	0.45
3:G:288:GLN:HG3	3:G:329:LEU:HB3	1.98	0.45
3:D:700:GLU:O	3:D:704:ILE:HG12	2.16	0.45
1:C:71:ILE:HD12	1:C:76:ILE:HG12	1.96	0.45
3:J:517:LEU:O	3:J:521:ILE:HG12	2.15	0.45
3:J:549:LYS:HB3	3:J:590:ILE:HD11	1.97	0.45
3:J:262:ASP:OD1	3:J:444:ASN:ND2	2.49	0.45
3:G:549:LYS:HB3	3:G:590:ILE:HD11	1.97	0.45
1:A:166:TYR:O	1:A:169:TYR:N	2.48	0.45
3:D:90:MET:HG2	3:D:117:TYR:O	2.17	0.45
3:D:249:ARG:HG2	3:D:262:ASP:O	2.15	0.45
3:D:477:CYS:SG	3:D:651:HIS:CD2	3.08	0.45
3:J:81:PRO:HD2	3:J:84:PHE:HB2	1.98	0.45
3:J:90:MET:HG2	3:J:117:TYR:O	2.17	0.45
3:J:402:PRO:HG3	3:J:415:GLN:HE21	1.82	0.45
3:G:38:PHE:O	3:G:76:VAL:HG13	2.16	0.45
3:D:262:ASP:OD1	3:D:444:ASN:ND2	2.49	0.45
1:B:335:ARG:C	1:B:337:TYR:H	2.20	0.45
3:G:83:LYS:HD3	3:G:721:ARG:HG2	1.99	0.45
3:D:402:PRO:HG3	3:D:415:GLN:HE21	1.82	0.45
3:D:549:LYS:HB3	3:D:590:ILE:HD11	1.97	0.45
1:A:335:ARG:C	1:A:337:TYR:H	2.20	0.45
3:D:83:LYS:HD3	3:D:721:ARG:HG2	1.99	0.45
3:D:281:ARG:NH1	3:D:320:VAL:HG11	2.28	0.45
1:A:191:LYS:O	1:A:194:THR:HG22	2.16	0.45
1:C:256:ARG:HH11	1:C:256:ARG:HG3	1.81	0.45
1:B:18:LYS:HD2	1:B:340:TRP:HB2	1.99	0.45
3:G:385:ALA:HB1	3:G:390:LEU:O	2.16	0.45
3:G:700:GLU:O	3:G:704:ILE:HG12	2.16	0.45
1:A:287:ILE:O	1:A:287:ILE:HG22	2.17	0.45
3:D:232:ASN:O	3:D:284:HIS:HD2	1.99	0.45
3:D:301:LEU:HG	3:D:303:ILE:HG12	1.99	0.45
3:D:402:PRO:HA	3:D:604:THR:HG21	1.99	0.45
1:C:7:ALA:HA	1:C:102:PRO:HD2	1.99	0.45
3:J:567:ARG:HD2	3:J:567:ARG:HA	1.74	0.45
1:B:7:ALA:HA	1:B:102:PRO:HD2	1.99	0.45
1:B:244:ASP:OD1	1:A:287:ILE:C	2.54	0.45
3:J:38:PHE:O	3:J:76:VAL:HG13	2.16	0.45
1:B:62:ARG:CG	1:A:288:ASP:OD2	2.27	0.45
3:G:435:MET:HG3	3:G:615:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:155:PHE:HE1	3:J:191:VAL:HG22	1.82	0.45
3:J:555:ASN:HB3	3:J:556:HIS:CE1	2.52	0.45
1:B:46:GLY:O	3:D:540:PHE:CZ	2.70	0.44
1:B:287:ILE:CG2	1:C:244:ASP:HB2	2.47	0.44
3:G:155:PHE:HE1	3:G:191:VAL:HG22	1.82	0.44
3:G:251:HIS:HB3	3:G:453:ARG:HB2	1.99	0.44
3:D:555:ASN:HB3	3:D:556:HIS:CE1	2.52	0.44
3:D:659:MET:O	3:D:663:ARG:N	2.45	0.44
3:J:153:HIS:O	3:J:156:SER:OG	2.19	0.44
1:B:351:THR:H	3:G:536:GLU:CD	2.21	0.44
3:G:402:PRO:HA	3:G:604:THR:HG21	1.99	0.44
2:P:171:ILE:HD11	1:C:311:ASP:OD2	2.16	0.44
1:A:7:ALA:HA	1:A:102:PRO:HD2	1.99	0.44
1:C:107:GLU:HG3	1:C:108:ALA:O	2.18	0.44
3:J:402:PRO:HA	3:J:604:THR:HG21	1.99	0.44
1:B:99:GLU:HB2	1:B:100:GLU:OE1	2.17	0.44
3:G:248:ILE:N	3:G:459:VAL:O	2.41	0.44
3:G:555:ASN:HB3	3:G:556:HIS:CE1	2.52	0.44
1:A:351:THR:H	3:D:536:GLU:CD	2.21	0.44
3:D:77:LEU:HD23	3:D:77:LEU:HA	1.83	0.44
3:D:155:PHE:HE1	3:D:191:VAL:HG22	1.82	0.44
3:D:251:HIS:HB3	3:D:453:ARG:HB2	1.99	0.44
3:D:704:ILE:HD13	3:D:707:LYS:HZ3	1.81	0.44
1:C:99:GLU:HB2	1:C:100:GLU:OE1	2.17	0.44
1:C:189:LEU:HD12	1:C:257:CYS:SG	2.58	0.44
3:J:251:HIS:HB3	3:J:453:ARG:HB2	1.99	0.44
1:B:46:GLY:HA3	3:D:540:PHE:CZ	2.48	0.44
1:B:107:GLU:HG3	1:B:108:ALA:O	2.17	0.44
1:B:287:ILE:HG22	1:B:287:ILE:O	2.17	0.44
3:G:301:LEU:HG	3:G:303:ILE:HG12	1.99	0.44
3:G:567:ARG:HD2	3:G:567:ARG:HA	1.74	0.44
1:A:99:GLU:HB2	1:A:100:GLU:OE1	2.17	0.44
1:A:107:GLU:HG3	1:A:108:ALA:O	2.17	0.44
3:J:100:ALA:HA	3:J:103:TYR:HE1	1.79	0.44
3:J:217:GLU:HG2	3:J:218:ASP:H	1.82	0.44
3:J:301:LEU:HG	3:J:303:ILE:HG12	1.99	0.44
3:J:676:ASN:HB3	3:J:685:ASP:HB2	2.00	0.44
3:D:269:GLU:HG2	3:D:269:GLU:O	2.17	0.44
3:D:435:MET:HG3	3:D:615:LYS:NZ	2.32	0.44
1:C:351:THR:H	3:J:536:GLU:CD	2.21	0.44
1:B:189:LEU:HD12	1:B:257:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:90:MET:HG2	3:G:117:TYR:O	2.17	0.44
1:A:7:ALA:HB1	1:A:102:PRO:HB2	2.00	0.44
1:A:18:LYS:HD2	1:A:340:TRP:HB2	1.99	0.44
3:D:219:GLN:HG3	3:D:447:LEU:HD12	2.00	0.44
3:D:594:LEU:HD12	3:D:595:GLN:N	2.33	0.44
3:D:698:VAL:O	3:D:702:ILE:HG12	2.18	0.44
3:J:115:TYR:CE1	3:J:154:ILE:HG22	2.53	0.44
1:B:45:VAL:O	3:D:540:PHE:CZ	2.70	0.44
3:G:269:GLU:O	3:G:269:GLU:HG2	2.17	0.44
3:J:435:MET:HG3	3:J:615:LYS:NZ	2.32	0.44
1:B:10:CYS:SG	1:B:86:TRP:HZ3	2.41	0.44
1:B:256:ARG:HG3	1:B:256:ARG:HH11	1.81	0.44
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.86	0.44
3:J:83:LYS:HD3	3:J:721:ARG:HG2	1.99	0.44
3:J:281:ARG:HH22	3:J:284:HIS:CD2	2.36	0.44
1:B:7:ALA:HB1	1:B:102:PRO:HB2	2.00	0.44
1:B:151:ILE:HD11	1:B:293:LEU:HD22	1.99	0.44
3:G:217:GLU:HG2	3:G:218:ASP:H	1.82	0.44
3:G:594:LEU:HD12	3:G:595:GLN:N	2.33	0.44
1:A:286:ASP:O	1:A:290:ARG:NE	2.51	0.44
1:C:287:ILE:O	1:C:287:ILE:HG22	2.17	0.44
3:J:219:GLN:HG3	3:J:447:LEU:HD12	2.00	0.44
3:J:540:PHE:CD2	3:J:541:PRO:HD2	2.53	0.44
3:J:617:LEU:O	3:J:621:PHE:HB2	2.18	0.44
3:G:115:TYR:CE1	3:G:154:ILE:HG22	2.53	0.43
3:G:219:GLN:HG3	3:G:447:LEU:HD12	2.00	0.43
3:G:376:ASP:OD1	3:G:377:GLY:N	2.51	0.43
3:G:402:PRO:HG3	3:G:415:GLN:HE21	1.82	0.43
3:G:540:PHE:CD2	3:G:541:PRO:HD2	2.53	0.43
1:A:189:LEU:HD12	1:A:257:CYS:SG	2.58	0.43
3:D:217:GLU:HG2	3:D:218:ASP:H	1.82	0.43
1:C:166:TYR:O	1:C:169:TYR:N	2.48	0.43
3:J:376:ASP:OD1	3:J:377:GLY:N	2.51	0.43
3:G:676:ASN:HB3	3:G:685:ASP:HB2	2.00	0.43
1:A:10:CYS:SG	1:A:86:TRP:HZ3	2.41	0.43
1:A:147:ARG:NE	1:A:330:ILE:HG21	2.33	0.43
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.81	0.43
3:D:260:SER:HB2	3:D:449:THR:HB	2.00	0.43
3:D:281:ARG:HH22	3:D:284:HIS:CD2	2.36	0.43
3:D:746:LEU:HD12	3:D:751:ILE:O	2.19	0.43
1:C:120:THR:O	1:C:124:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ARG:NE	1:B:330:ILE:HG21	2.34	0.43
3:G:128:TYR:CD2	3:G:681:PRO:HG3	2.43	0.43
3:G:617:LEU:O	3:G:621:PHE:HB2	2.18	0.43
1:A:84:LYS:HE3	1:A:84:LYS:HB2	1.82	0.43
3:D:376:ASP:OD1	3:D:377:GLY:N	2.51	0.43
3:J:223:ALA:HB1	3:J:227:LEU:HD23	2.00	0.43
3:J:230:PHE:CE1	3:J:285:ILE:HG12	2.54	0.43
3:J:260:SER:HB2	3:J:449:THR:HB	2.00	0.43
3:J:594:LEU:HD12	3:J:595:GLN:N	2.33	0.43
1:B:12:ASN:O	1:B:12:ASN:ND2	2.51	0.43
1:B:166:TYR:O	1:B:169:TYR:N	2.48	0.43
1:B:289:ILE:CD1	1:C:63:GLY:HA3	2.23	0.43
1:B:322:PRO:CG	1:C:245:GLY:HA3	2.48	0.43
1:C:18:LYS:HD2	1:C:340:TRP:HB2	1.99	0.43
1:C:159:VAL:HG21	1:C:177:ARG:CZ	2.48	0.43
3:J:269:GLU:O	3:J:269:GLU:HG2	2.17	0.43
3:J:698:VAL:O	3:J:702:ILE:HG12	2.17	0.43
3:J:709:PHE:N	3:J:710:PRO:HD2	2.34	0.43
1:B:33:SER:O	1:B:33:SER:OG	2.34	0.43
3:G:260:SER:HB2	3:G:449:THR:HB	2.01	0.43
3:D:676:ASN:HB3	3:D:685:ASP:HB2	2.00	0.43
1:C:147:ARG:NE	1:C:330:ILE:HG21	2.33	0.43
1:C:286:ASP:O	1:C:290:ARG:NE	2.51	0.43
3:J:277:LEU:HB3	3:J:280:GLU:HG2	2.01	0.43
1:B:120:THR:O	1:B:124:PHE:HB2	2.18	0.43
1:B:159:VAL:HG21	1:B:177:ARG:CZ	2.48	0.43
1:B:286:ASP:O	1:B:290:ARG:NE	2.51	0.43
3:G:267:LEU:HD21	3:G:655:LEU:HB2	2.00	0.43
3:G:746:LEU:HD12	3:G:751:ILE:O	2.19	0.43
2:P:90:ARG:NE	1:A:221:LEU:CD2	2.79	0.43
3:D:230:PHE:CE1	3:D:285:ILE:HG12	2.53	0.43
1:C:7:ALA:HB1	1:C:102:PRO:HB2	2.00	0.43
1:C:10:CYS:SG	1:C:86:TRP:HZ3	2.41	0.43
1:C:335:ARG:C	1:C:337:TYR:H	2.20	0.43
3:J:192:ILE:CD1	3:J:250:ILE:HD13	2.48	0.43
3:G:277:LEU:HB3	3:G:280:GLU:HG2	2.01	0.43
1:A:159:VAL:HG21	1:A:177:ARG:CZ	2.48	0.43
1:A:346:LEU:HG	1:A:352:PHE:CE2	2.54	0.43
3:D:115:TYR:CE1	3:D:154:ILE:HG22	2.53	0.43
3:D:267:LEU:HD21	3:D:655:LEU:HB2	2.00	0.43
3:J:269:GLU:OE2	3:J:269:GLU:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:223:ALA:HB1	3:G:227:LEU:HD23	2.00	0.43
3:G:709:PHE:N	3:G:710:PRO:HD2	2.34	0.43
3:D:277:LEU:HB3	3:D:280:GLU:HG2	2.01	0.43
3:D:540:PHE:CD2	3:D:541:PRO:HD2	2.53	0.43
3:D:617:LEU:O	3:D:621:PHE:HB2	2.18	0.43
1:C:151:ILE:HD11	1:C:293:LEU:HD22	1.99	0.43
1:C:346:LEU:HG	1:C:352:PHE:CE2	2.54	0.43
3:J:428:ALA:O	3:J:431:VAL:HG12	2.19	0.43
1:B:346:LEU:HG	1:B:352:PHE:CE2	2.54	0.43
3:G:230:PHE:CE1	3:G:285:ILE:HG12	2.54	0.43
1:A:12:ASN:O	1:A:12:ASN:ND2	2.51	0.43
3:D:192:ILE:CD1	3:D:250:ILE:HD13	2.48	0.43
3:D:223:ALA:HB1	3:D:227:LEU:HD23	2.00	0.43
3:D:709:PHE:N	3:D:710:PRO:HD2	2.34	0.43
1:C:36:GLY:HA2	1:C:66:THR:O	2.19	0.43
3:G:525:GLU:CD	3:G:652:ARG:HE	2.21	0.43
3:G:698:VAL:O	3:G:702:ILE:HG12	2.18	0.43
3:D:173:SER:OG	3:D:667:PRO:HA	2.19	0.43
3:J:525:GLU:CD	3:J:652:ARG:HE	2.21	0.43
1:B:36:GLY:HA2	1:B:66:THR:O	2.19	0.42
3:G:428:ALA:O	3:G:431:VAL:HG12	2.19	0.42
1:A:151:ILE:HD11	1:A:293:LEU:HD22	1.99	0.42
3:D:567:ARG:HD2	3:D:567:ARG:HA	1.74	0.42
3:G:443:ILE:HD13	3:G:443:ILE:HA	1.89	0.42
3:G:659:MET:O	3:G:663:ARG:N	2.45	0.42
1:A:198:TYR:CE1	1:A:248:ILE:HG13	2.55	0.42
3:D:249:ARG:HH12	3:D:264:GLU:N	2.18	0.42
3:D:269:GLU:OE2	3:D:269:GLU:N	2.37	0.42
3:J:141:ALA:O	3:J:143:ARG:N	2.52	0.42
3:J:267:LEU:HD21	3:J:655:LEU:HB2	2.00	0.42
1:B:151:ILE:HG23	1:B:163:VAL:O	2.20	0.42
3:G:281:ARG:HH22	3:G:284:HIS:CD2	2.36	0.42
3:G:372:GLN:OE1	3:G:401:HIS:NE2	2.51	0.42
1:A:120:THR:O	1:A:124:PHE:HB2	2.18	0.42
3:D:141:ALA:O	3:D:143:ARG:N	2.52	0.42
3:D:522:ASP:HA	3:D:526:LYS:HB2	2.01	0.42
1:C:12:ASN:O	1:C:12:ASN:ND2	2.51	0.42
3:J:659:MET:O	3:J:663:ARG:N	2.45	0.42
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.87	0.42
3:D:246:LYS:O	3:D:248:ILE:HG12	2.19	0.42
3:D:428:ALA:O	3:D:431:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:173:SER:OG	3:J:667:PRO:HA	2.19	0.42
3:J:372:GLN:OE1	3:J:401:HIS:NE2	2.52	0.42
3:J:477:CYS:HG	3:J:651:HIS:CE1	2.37	0.42
1:B:108:ALA:HB3	1:B:111:ASN:HD21	1.85	0.42
1:B:198:TYR:CE1	1:B:248:ILE:HG13	2.55	0.42
3:G:37:VAL:HG21	3:G:51:ILE:CG2	2.46	0.42
3:G:272:ARG:HB3	3:G:283:TYR:OH	2.19	0.42
1:A:36:GLY:HA2	1:A:66:THR:O	2.19	0.42
3:D:272:ARG:HB3	3:D:283:TYR:OH	2.20	0.42
3:D:372:GLN:OE1	3:D:401:HIS:NE2	2.51	0.42
3:D:525:GLU:CD	3:D:652:ARG:HE	2.21	0.42
3:J:249:ARG:HH12	3:J:264:GLU:N	2.17	0.42
3:J:522:ASP:HA	3:J:526:LYS:HB2	2.01	0.42
3:J:746:LEU:HD12	3:J:751:ILE:O	2.19	0.42
1:B:193:LEU:HD12	1:B:193:LEU:HA	1.86	0.42
3:G:173:SER:OG	3:G:667:PRO:HA	2.19	0.42
3:G:192:ILE:CD1	3:G:250:ILE:HD13	2.49	0.42
3:G:269:GLU:OE2	3:G:269:GLU:N	2.37	0.42
1:C:198:TYR:CE1	1:C:248:ILE:HG13	2.55	0.42
3:J:272:ARG:HB3	3:J:283:TYR:OH	2.20	0.42
3:G:246:LYS:O	3:G:248:ILE:HG12	2.19	0.42
2:P:79:THR:HG21	1:A:238:LYS:HZ2	1.85	0.42
3:D:59:VAL:HG21	3:D:76:VAL:HG21	2.01	0.42
3:D:725:LEU:HB3	3:D:748:SER:OG	2.19	0.42
1:C:108:ALA:HB3	1:C:111:ASN:HD21	1.85	0.42
3:J:59:VAL:O	3:J:70:THR:HA	2.20	0.42
3:J:262:ASP:OD1	3:J:263:ILE:N	2.53	0.42
3:J:761:THR:HG22	3:J:761:THR:O	2.20	0.42
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.75	0.42
1:B:327:ILE:HG22	1:B:327:ILE:O	2.20	0.42
3:G:249:ARG:HH12	3:G:264:GLU:N	2.17	0.42
3:D:224:ASN:N	3:D:225:PRO:HD2	2.35	0.42
1:C:213:LYS:HZ2	1:C:213:LYS:HG2	1.59	0.42
3:J:569:ILE:CD1	3:J:572:LYS:HG3	2.40	0.42
3:G:59:VAL:HG21	3:G:76:VAL:HG21	2.01	0.42
3:G:141:ALA:O	3:G:143:ARG:N	2.52	0.42
3:G:725:LEU:HB3	3:G:748:SER:OG	2.19	0.42
1:A:76:ILE:HG21	1:A:82:MET:HE2	2.02	0.42
1:A:104:LEU:O	1:A:105:LEU:HD23	2.20	0.42
1:A:200:PHE:CD1	1:A:205:GLU:HB3	2.55	0.42
1:C:76:ILE:HG21	1:C:82:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:320:VAL:HG13	3:J:320:VAL:O	2.20	0.42
1:B:104:LEU:O	1:B:105:LEU:HD23	2.20	0.42
1:B:210:ARG:HG3	1:B:211:ASP:N	2.35	0.42
3:G:761:THR:HG22	3:G:761:THR:O	2.20	0.42
1:A:151:ILE:HG23	1:A:163:VAL:O	2.19	0.42
1:A:206:ARG:O	1:A:209:VAL:HG12	2.20	0.42
3:D:335:ALA:O	3:D:339:LEU:HG	2.20	0.42
1:C:327:ILE:O	1:C:327:ILE:HG22	2.20	0.42
1:B:298:VAL:HG22	1:B:299:MET:O	2.20	0.41
3:G:320:VAL:HG13	3:G:320:VAL:O	2.20	0.41
3:G:662:LEU:HA	3:G:665:THR:OG1	2.20	0.41
2:P:167:ARG:HH21	1:C:308:GLY:CA	2.32	0.41
1:A:327:ILE:HG22	1:A:327:ILE:O	2.20	0.41
3:D:663:ARG:HD3	3:D:663:ARG:HA	1.85	0.41
3:J:662:LEU:HA	3:J:665:THR:OG1	2.20	0.41
1:B:200:PHE:CD1	1:B:205:GLU:HB3	2.55	0.41
3:G:179:GLU:CD	3:G:463:ALA:HA	2.41	0.41
3:G:262:ASP:OD1	3:G:263:ILE:N	2.53	0.41
1:A:108:ALA:HB3	1:A:111:ASN:HD21	1.85	0.41
3:D:40:PRO:HA	3:D:45:GLU:HA	2.03	0.41
3:D:320:VAL:O	3:D:320:VAL:HG13	2.20	0.41
3:D:477:CYS:O	3:D:481:THR:HG23	2.21	0.41
1:C:298:VAL:HG22	1:C:299:MET:O	2.20	0.41
3:J:246:LYS:HA	3:J:265:THR:HA	2.02	0.41
3:J:335:ALA:O	3:J:339:LEU:HG	2.20	0.41
1:B:213:LYS:HZ2	1:B:213:LYS:HG2	1.59	0.41
3:G:477:CYS:HG	3:G:651:HIS:CE1	2.38	0.41
3:D:153:HIS:O	3:D:156:SER:OG	2.19	0.41
3:D:179:GLU:CD	3:D:463:ALA:HA	2.41	0.41
3:D:537:GLU:HG2	3:D:548:PHE:HD2	1.85	0.41
3:J:59:VAL:HG21	3:J:76:VAL:HG21	2.01	0.41
3:J:224:ASN:N	3:J:225:PRO:HD2	2.35	0.41
3:J:246:LYS:O	3:J:248:ILE:HG12	2.19	0.41
3:J:477:CYS:O	3:J:481:THR:HG23	2.20	0.41
1:B:76:ILE:HG21	1:B:82:MET:HE2	2.02	0.41
3:G:59:VAL:O	3:G:70:THR:HA	2.20	0.41
3:G:77:LEU:HD23	3:G:77:LEU:HA	1.83	0.41
3:G:224:ASN:N	3:G:225:PRO:HD2	2.35	0.41
1:A:298:VAL:HG22	1:A:299:MET:O	2.20	0.41
3:D:422:TYR:CE2	3:D:598:LYS:HD2	2.53	0.41
3:J:537:GLU:HG2	3:J:548:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:725:LEU:HB3	3:J:748:SER:OG	2.20	0.41
1:B:206:ARG:O	1:B:209:VAL:HG12	2.20	0.41
3:G:40:PRO:HA	3:G:45:GLU:HA	2.03	0.41
3:G:247:PHE:HA	3:G:460:LEU:HA	2.03	0.41
1:A:108:ALA:HB3	1:A:111:ASN:ND2	2.36	0.41
1:A:133:TYR:CD2	1:A:352:PHE:HZ	2.38	0.41
3:D:43:LYS:HB3	3:D:44:GLU:OE1	2.20	0.41
3:D:153:HIS:CE1	3:D:155:PHE:CD2	3.06	0.41
3:D:184:LYS:HD3	3:D:184:LYS:C	2.41	0.41
3:D:662:LEU:HA	3:D:665:THR:OG1	2.20	0.41
1:C:200:PHE:CD1	1:C:205:GLU:HB3	2.55	0.41
3:J:40:PRO:HA	3:J:45:GLU:HA	2.02	0.41
3:J:109:TYR:OH	3:J:682:GLY:N	2.34	0.41
3:J:184:LYS:HD3	3:J:184:LYS:C	2.41	0.41
3:J:481:THR:HG22	3:J:655:LEU:HD12	2.02	0.41
3:J:544:THR:OG1	3:J:547:THR:OG1	2.29	0.41
1:B:326:LYS:HD3	1:B:328:LYS:HZ1	1.84	0.41
3:G:335:ALA:O	3:G:339:LEU:HG	2.20	0.41
3:G:422:TYR:CE2	3:G:598:LYS:HD2	2.53	0.41
3:D:481:THR:HG22	3:D:655:LEU:HD12	2.02	0.41
3:D:761:THR:O	3:D:761:THR:HG22	2.20	0.41
1:C:104:LEU:O	1:C:105:LEU:HD23	2.20	0.41
1:C:151:ILE:HG23	1:C:163:VAL:O	2.19	0.41
3:J:317:GLU:O	3:J:318:THR:HG22	2.21	0.41
1:B:133:TYR:CD2	1:B:352:PHE:HZ	2.38	0.41
1:B:326:LYS:HB3	1:B:328:LYS:HZ3	1.86	0.41
3:G:184:LYS:C	3:G:184:LYS:HD3	2.41	0.41
3:G:522:ASP:HA	3:G:526:LYS:HB2	2.01	0.41
1:A:210:ARG:HG3	1:A:211:ASP:N	2.35	0.41
3:D:262:ASP:OD1	3:D:263:ILE:N	2.53	0.41
3:D:403:ARG:CZ	3:D:411:VAL:HG22	2.51	0.41
1:C:206:ARG:O	1:C:209:VAL:HG12	2.20	0.41
3:J:179:GLU:CD	3:J:463:ALA:HA	2.41	0.41
1:B:84:LYS:HE3	1:B:84:LYS:HB2	1.82	0.41
1:B:302:GLY:O	1:B:303:THR:HG22	2.21	0.41
3:G:317:GLU:O	3:G:318:THR:HG22	2.21	0.41
3:D:246:LYS:HA	3:D:265:THR:HA	2.03	0.41
3:D:544:THR:OG1	3:D:547:THR:OG1	2.29	0.41
1:C:210:ARG:HG3	1:C:211:ASP:N	2.35	0.41
3:J:77:LEU:HD23	3:J:77:LEU:HA	1.83	0.41
3:J:247:PHE:HA	3:J:460:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:341:PHE:CE1	3:J:442:ARG:HG2	2.56	0.41
3:G:43:LYS:HB3	3:G:44:GLU:OE1	2.20	0.41
3:G:341:PHE:CE1	3:G:442:ARG:HG2	2.56	0.41
3:G:400:CYS:SG	3:G:401:HIS:ND1	2.73	0.41
2:P:175:ASP:CG	3:J:369:ARG:NH2	2.74	0.41
1:A:302:GLY:O	1:A:303:THR:HG22	2.21	0.41
3:D:59:VAL:O	3:D:70:THR:HA	2.20	0.41
3:D:115:TYR:CD1	3:D:153:HIS:HA	2.56	0.41
3:D:153:HIS:HE1	3:D:155:PHE:HB2	1.77	0.41
3:D:281:ARG:HH22	3:D:284:HIS:CG	2.39	0.41
3:D:341:PHE:CE1	3:D:442:ARG:HG2	2.56	0.41
3:D:489:PHE:HD1	3:D:669:PHE:CZ	2.39	0.41
3:D:590:ILE:HA	3:D:593:TRP:NE1	2.36	0.41
1:C:108:ALA:HB3	1:C:111:ASN:ND2	2.36	0.41
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.86	0.41
3:J:715:TYR:CZ	3:J:719:ARG:NH1	2.89	0.41
3:G:281:ARG:HH22	3:G:284:HIS:CG	2.39	0.41
3:G:403:ARG:CZ	3:G:411:VAL:HG22	2.51	0.41
3:G:489:PHE:HD1	3:G:669:PHE:CZ	2.39	0.41
3:G:590:ILE:HA	3:G:593:TRP:NE1	2.36	0.41
3:D:92:MET:O	3:D:93:LEU:HG	2.21	0.41
1:C:302:GLY:O	1:C:303:THR:HG22	2.21	0.41
3:J:281:ARG:HH22	3:J:284:HIS:CG	2.39	0.41
3:J:590:ILE:HA	3:J:593:TRP:NE1	2.36	0.41
3:G:92:MET:O	3:G:93:LEU:HG	2.21	0.40
3:G:246:LYS:HA	3:G:265:THR:HA	2.03	0.40
3:G:537:GLU:HG2	3:G:548:PHE:HD2	1.85	0.40
3:D:247:PHE:HA	3:D:460:LEU:HA	2.03	0.40
3:D:522:ASP:OD2	3:D:523:LEU:N	2.54	0.40
3:D:708:GLY:C	3:D:710:PRO:HD2	2.42	0.40
1:C:223:PHE:HB2	1:C:259:GLU:OE2	2.21	0.40
3:J:422:TYR:CE2	3:J:598:LYS:HD2	2.53	0.40
3:J:582:TYR:CG	3:J:583:ALA:N	2.89	0.40
3:G:477:CYS:O	3:G:481:THR:HG23	2.20	0.40
3:G:481:THR:HG22	3:G:655:LEU:HD12	2.02	0.40
3:G:522:ASP:OD2	3:G:523:LEU:N	2.54	0.40
3:G:708:GLY:C	3:G:710:PRO:HD2	2.42	0.40
3:D:248:ILE:N	3:D:459:VAL:O	2.41	0.40
3:J:115:TYR:HB3	3:J:152:PRO:O	2.22	0.40
3:G:39:VAL:HB	3:G:49:ALA:HB2	2.03	0.40
3:G:115:TYR:CD1	3:G:153:HIS:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:HB2	1:A:259:GLU:OE2	2.21	0.40
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.94	0.40
1:C:133:TYR:CD2	1:C:352:PHE:HZ	2.38	0.40
3:J:325:ASP:O	3:J:329:LEU:N	2.54	0.40
3:J:412:THR:C	3:J:413:LYS:HG3	2.42	0.40
3:J:478:ILE:O	3:J:481:THR:OG1	2.33	0.40
3:J:489:PHE:HD1	3:J:669:PHE:CZ	2.39	0.40
3:G:154:ILE:HD12	3:G:154:ILE:HA	1.91	0.40
1:A:24:ASP:OD1	1:A:25:ASP:N	2.55	0.40
3:D:317:GLU:O	3:D:318:THR:HG22	2.21	0.40
3:J:39:VAL:HB	3:J:49:ALA:HB2	2.03	0.40
3:J:708:GLY:C	3:J:710:PRO:HD2	2.42	0.40
1:B:108:ALA:HB3	1:B:111:ASN:ND2	2.36	0.40
3:G:412:THR:C	3:G:413:LYS:HG3	2.42	0.40
3:G:582:TYR:CG	3:G:583:ALA:N	2.89	0.40
2:P:90:ARG:HH22	1:A:308:GLY:HA2	1.87	0.40
3:D:39:VAL:HB	3:D:49:ALA:HB2	2.03	0.40
3:D:412:THR:C	3:D:413:LYS:HG3	2.42	0.40
1:C:327:ILE:O	1:C:329:ILE:HG23	2.22	0.40
3:J:43:LYS:HB3	3:J:44:GLU:OE1	2.21	0.40
3:J:403:ARG:CZ	3:J:411:VAL:HG22	2.51	0.40
3:J:738:SER:HB2	3:J:739:ARG:HH21	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 PDB entries followed by that with respect to all EM entries.

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	367/377 (97%)	324 (88%)	41 (11%)	2 (0%)	29	68
1	B	367/377 (97%)	324 (88%)	41 (11%)	2 (0%)	29	68
1	C	367/377 (97%)	324 (88%)	41 (11%)	2 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	164/284 (58%)	164 (100%)	0	0	100	100
2	P	164/284 (58%)	164 (100%)	0	0	100	100
3	D	699/850 (82%)	618 (88%)	80 (11%)	1 (0%)	51	85
3	G	699/850 (82%)	618 (88%)	80 (11%)	1 (0%)	51	85
3	J	699/850 (82%)	618 (88%)	80 (11%)	1 (0%)	51	85
All	All	3526/4249 (83%)	3154 (89%)	363 (10%)	9 (0%)	44	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
3	G	710	PRO
1	A	111	ASN
3	D	710	PRO
1	C	111	ASN
3	J	710	PRO
1	B	112	PRO
1	A	112	PRO
1	C	112	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 PDB entries followed by that with respect to all EM entries.

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	312/320 (98%)	310 (99%)	2 (1%)	86	92
1	B	312/320 (98%)	310 (99%)	2 (1%)	86	92
1	C	312/320 (98%)	311 (100%)	1 (0%)	92	95
2	O	141/245 (58%)	138 (98%)	3 (2%)	53	72
2	P	141/245 (58%)	141 (100%)	0	100	100
3	D	616/736 (84%)	611 (99%)	5 (1%)	81	89
3	G	616/736 (84%)	611 (99%)	5 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	616/736 (84%)	611 (99%)	5 (1%)	81	89
All	All	3066/3658 (84%)	3043 (99%)	23 (1%)	82	89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	ASN
1	B	143	TYR
2	O	51	LYS
2	O	101	ARG
2	O	207	LEU
3	G	424	LYS
3	G	453	ARG
3	G	479	ASN
3	G	706	ARG
3	G	739	ARG
1	A	12	ASN
1	A	143	TYR
3	D	424	LYS
3	D	453	ARG
3	D	479	ASN
3	D	706	ARG
3	D	739	ARG
1	C	12	ASN
3	J	424	LYS
3	J	453	ARG
3	J	479	ASN
3	J	706	ARG
3	J	739	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	GLN
3	G	126	ASN
3	G	153	HIS
3	G	187	ASN
3	G	284	HIS
3	G	288	GLN
3	G	358	HIS
3	G	368	GLN

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Mol	Chain	Res	Type
3	G	372	GLN
3	G	492	HIS
3	G	661	ASN
3	G	668	HIS
1	A	354	GLN
3	D	126	ASN
3	D	153	HIS
3	D	187	ASN
3	D	251	HIS
3	D	284	HIS
3	D	288	GLN
3	D	358	HIS
3	D	368	GLN
3	D	372	GLN
3	D	492	HIS
3	D	661	ASN
3	D	668	HIS
1	C	246	GLN
1	C	354	GLN
3	J	126	ASN
3	J	153	HIS
3	J	187	ASN
3	J	251	HIS
3	J	284	HIS
3	J	288	GLN
3	J	358	HIS
3	J	372	GLN
3	J	492	HIS
3	J	661	ASN
3	J	668	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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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
4	ADP	C	401	5	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
4	ADP	B	401	5	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
4	ADP	A	401	5	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)

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
4	ADP	C	401	5	-	7/12/32/32	0/3/3/3
4	ADP	B	401	5	-	7/12/32/32	0/3/3/3
4	ADP	A	401	5	-	7/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ADP	C5-C4	2.17	1.46	1.40
4	A	401	ADP	C5-C4	2.15	1.46	1.40
4	B	401	ADP	C5-C4	2.14	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ADP	PA-O3A-PB	-4.04	118.97	132.83

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	ADP	PA-O3A-PB	-4.03	118.99	132.83
4	A	401	ADP	PA-O3A-PB	-4.03	119.00	132.83
4	A	401	ADP	N3-C2-N1	-3.14	123.77	128.68
4	B	401	ADP	N3-C2-N1	-3.12	123.80	128.68
4	C	401	ADP	N3-C2-N1	-3.08	123.86	128.68
4	A	401	ADP	C4-C5-N7	-2.97	106.30	109.40
4	B	401	ADP	C4-C5-N7	-2.95	106.32	109.40
4	C	401	ADP	C4-C5-N7	-2.94	106.34	109.40
4	A	401	ADP	C3'-C2'-C1'	2.55	104.82	100.98
4	B	401	ADP	C3'-C2'-C1'	2.55	104.82	100.98
4	C	401	ADP	C3'-C2'-C1'	2.55	104.81	100.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

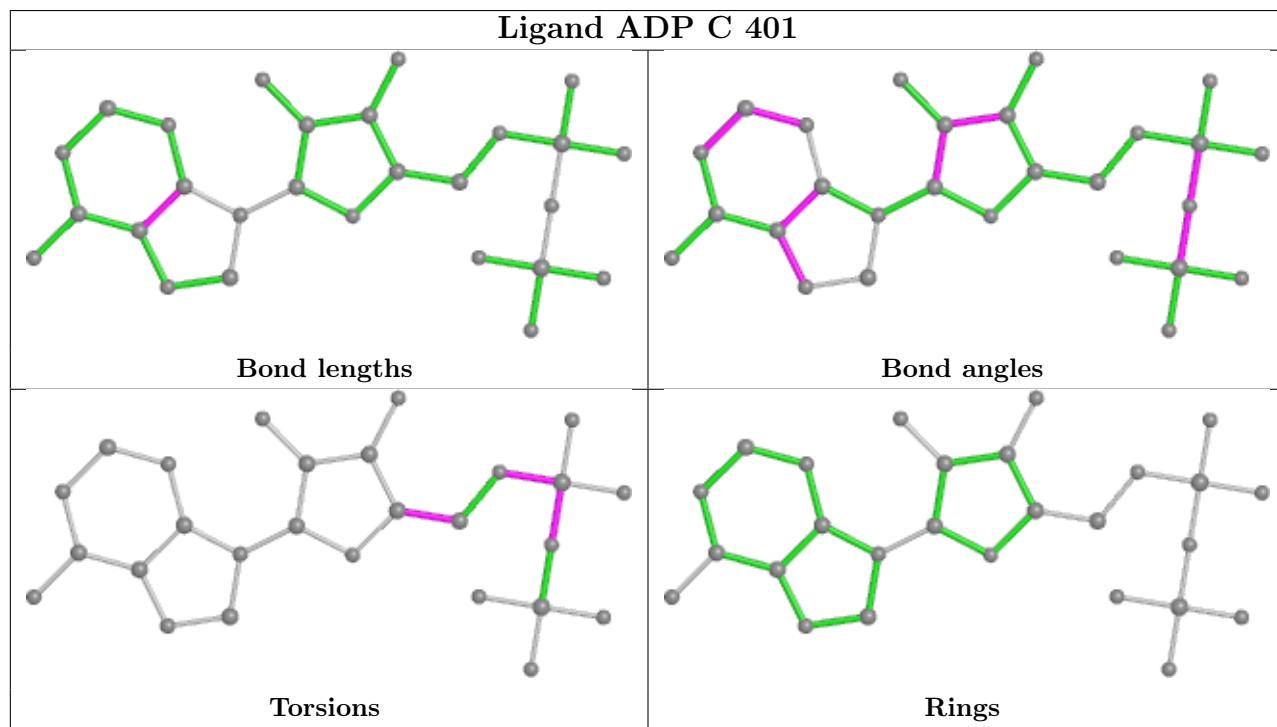
Mol	Chain	Res	Type	Atoms
4	B	401	ADP	C5'-O5'-PA-O1A
4	B	401	ADP	C3'-C4'-C5'-O5'
4	A	401	ADP	C5'-O5'-PA-O1A
4	A	401	ADP	C3'-C4'-C5'-O5'
4	C	401	ADP	C5'-O5'-PA-O1A
4	C	401	ADP	C3'-C4'-C5'-O5'
4	B	401	ADP	O4'-C4'-C5'-O5'
4	A	401	ADP	O4'-C4'-C5'-O5'
4	C	401	ADP	O4'-C4'-C5'-O5'
4	B	401	ADP	C5'-O5'-PA-O3A
4	A	401	ADP	C5'-O5'-PA-O3A
4	C	401	ADP	C5'-O5'-PA-O3A
4	B	401	ADP	C5'-O5'-PA-O2A
4	A	401	ADP	C5'-O5'-PA-O2A
4	C	401	ADP	C5'-O5'-PA-O2A
4	B	401	ADP	PB-O3A-PA-O1A
4	A	401	ADP	PB-O3A-PA-O1A
4	C	401	ADP	PB-O3A-PA-O1A
4	B	401	ADP	PB-O3A-PA-O2A
4	A	401	ADP	PB-O3A-PA-O2A
4	C	401	ADP	PB-O3A-PA-O2A

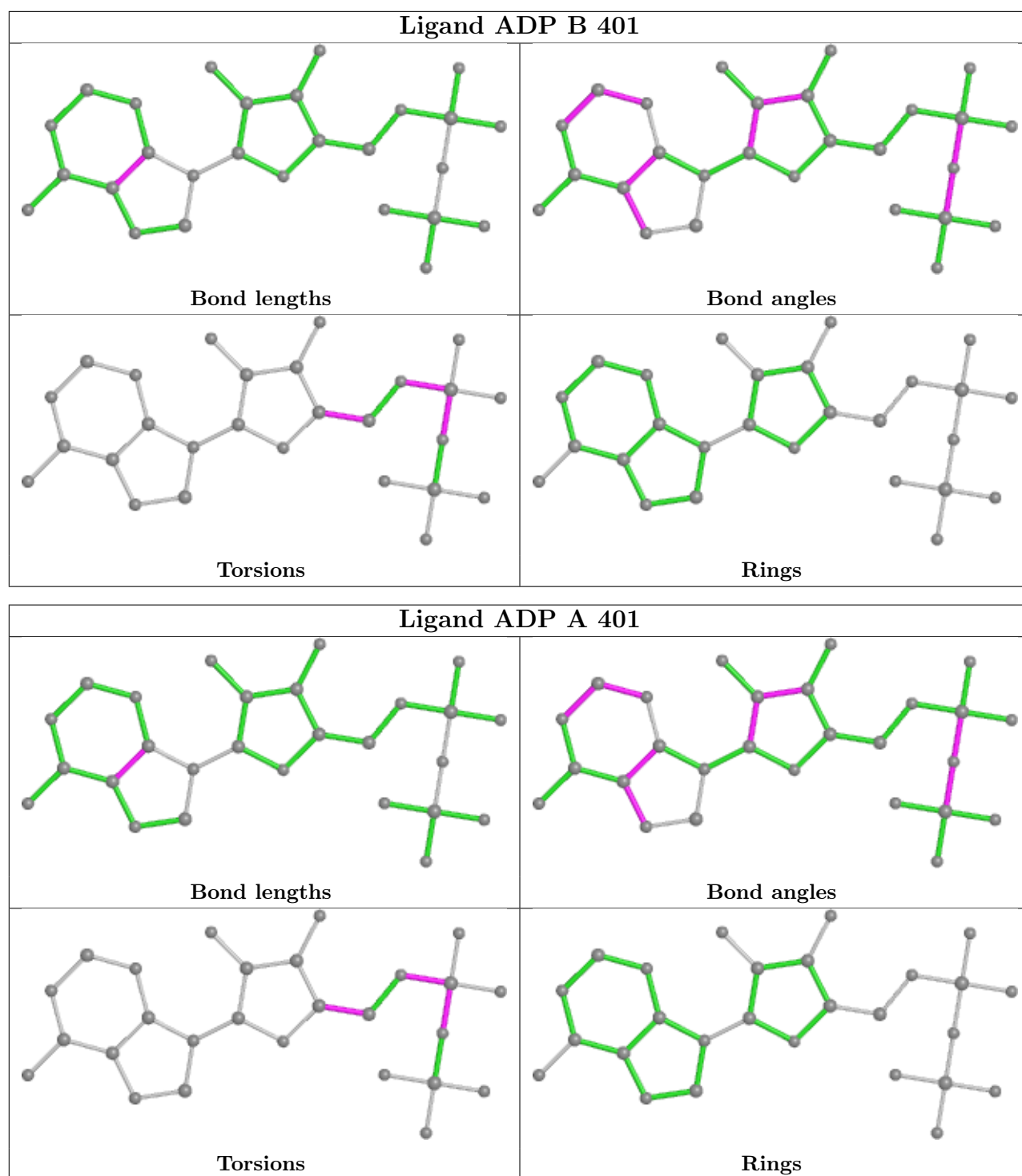
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for 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

There are no chain breaks in this entry.

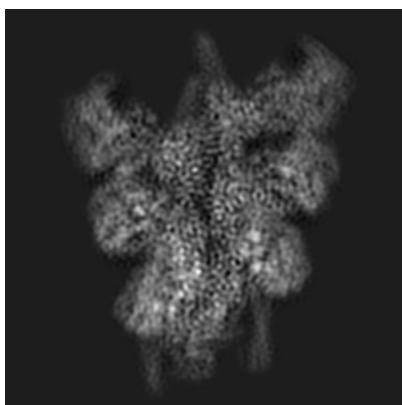
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22067. These allow visual inspection of the internal detail of the map and identification of artifacts.

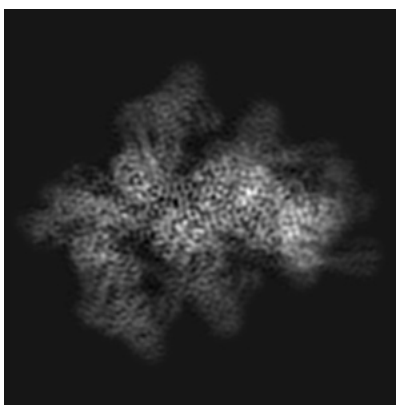
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

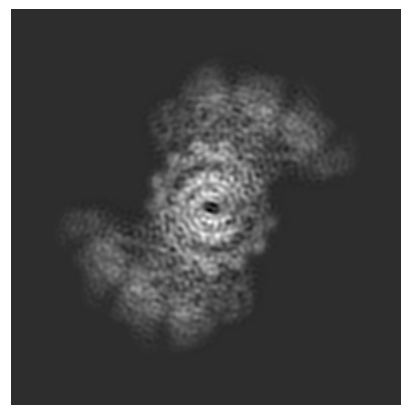
6.1.1 Primary map



X



Y



Z

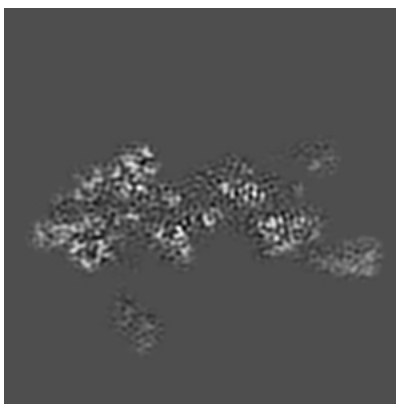
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

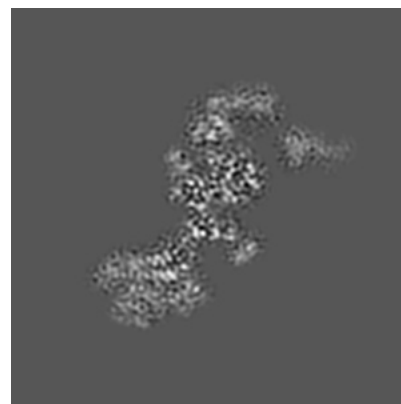
6.2.1 Primary map



X Index: 128



Y Index: 128

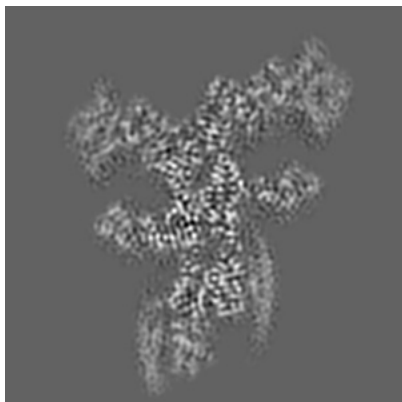


Z Index: 128

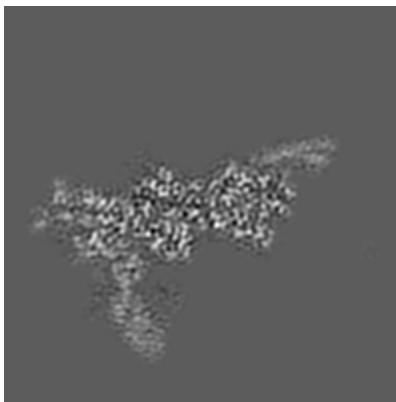
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

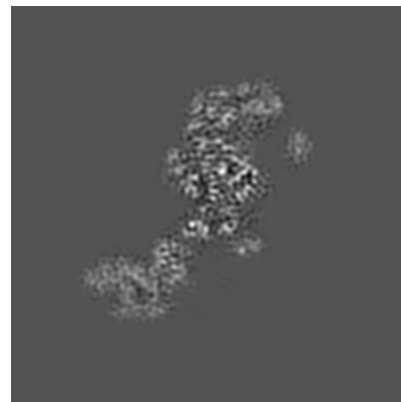
6.3.1 Primary map



X Index: 122



Y Index: 116

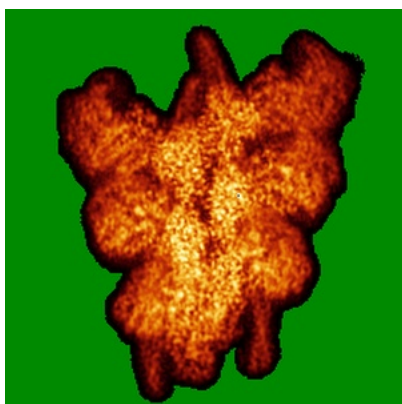


Z Index: 136

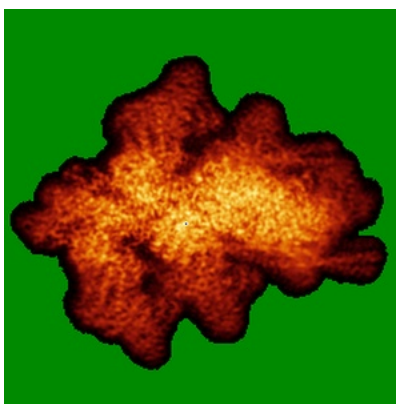
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

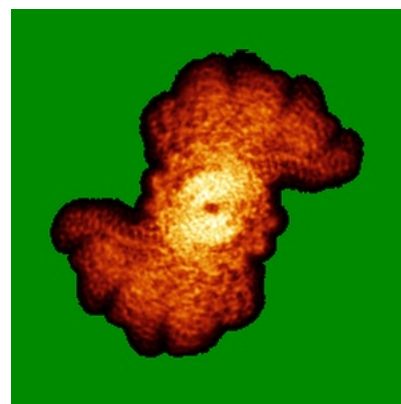
6.4.1 Primary map



X



Y

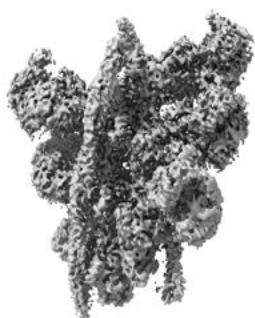


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

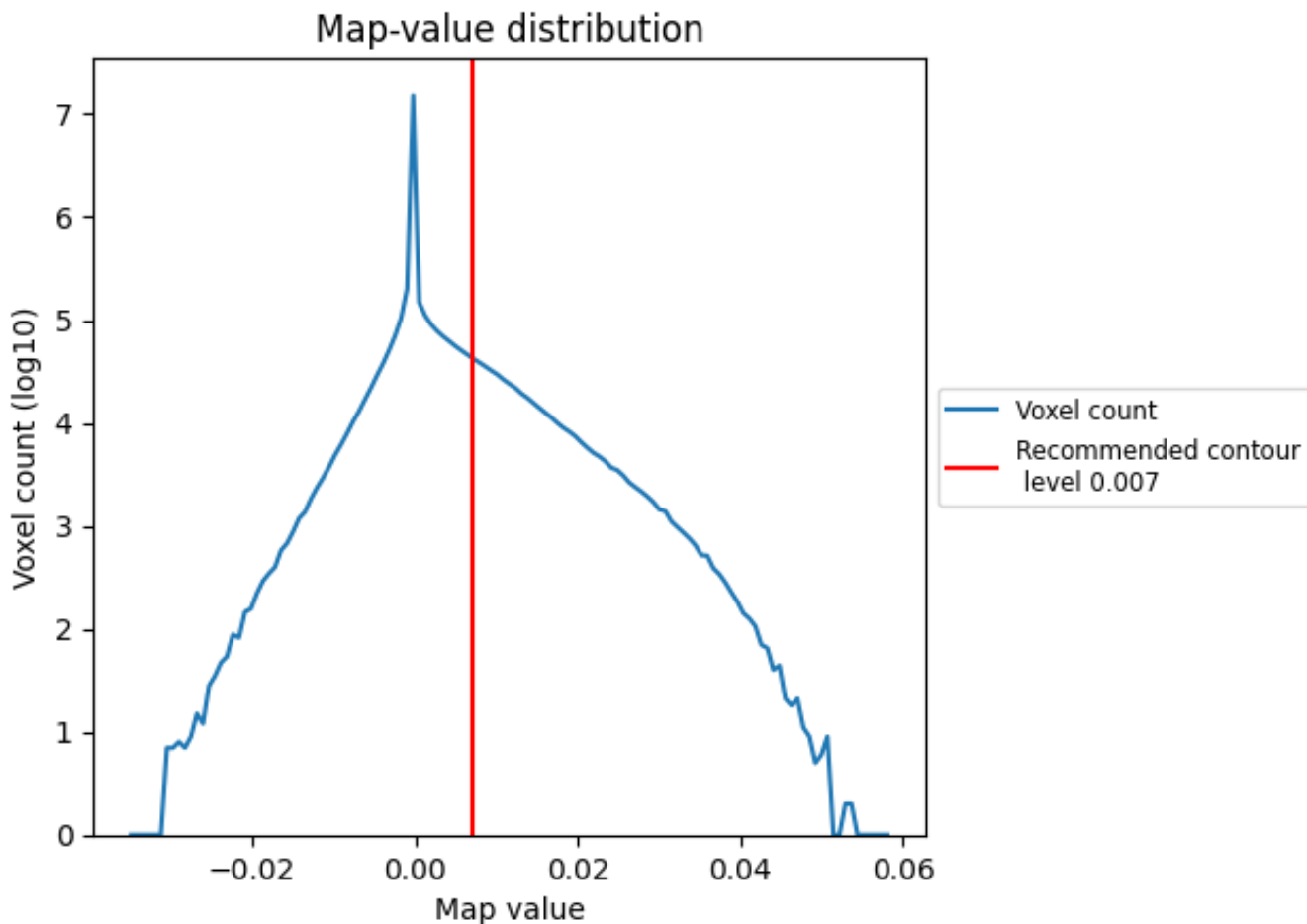
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

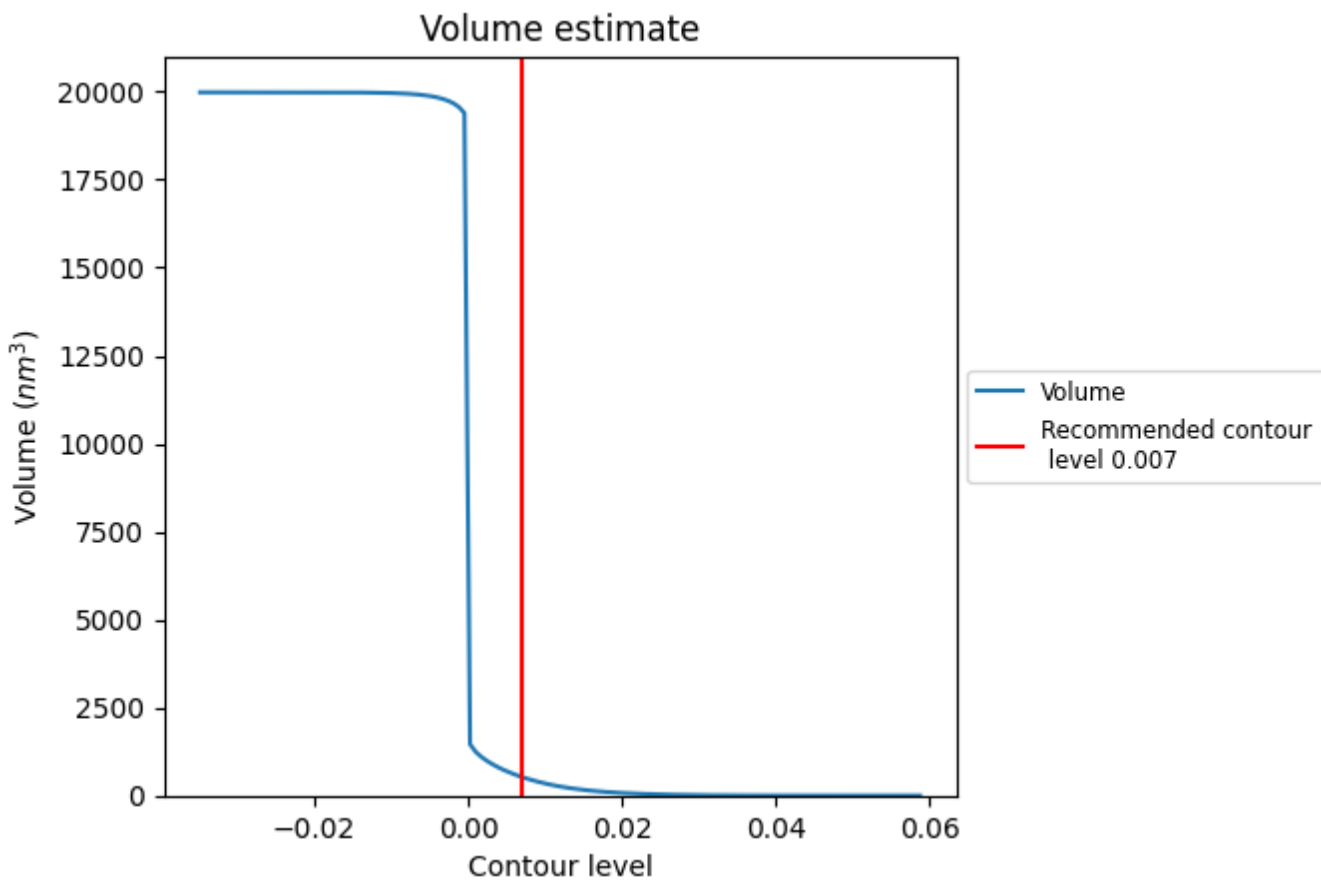
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

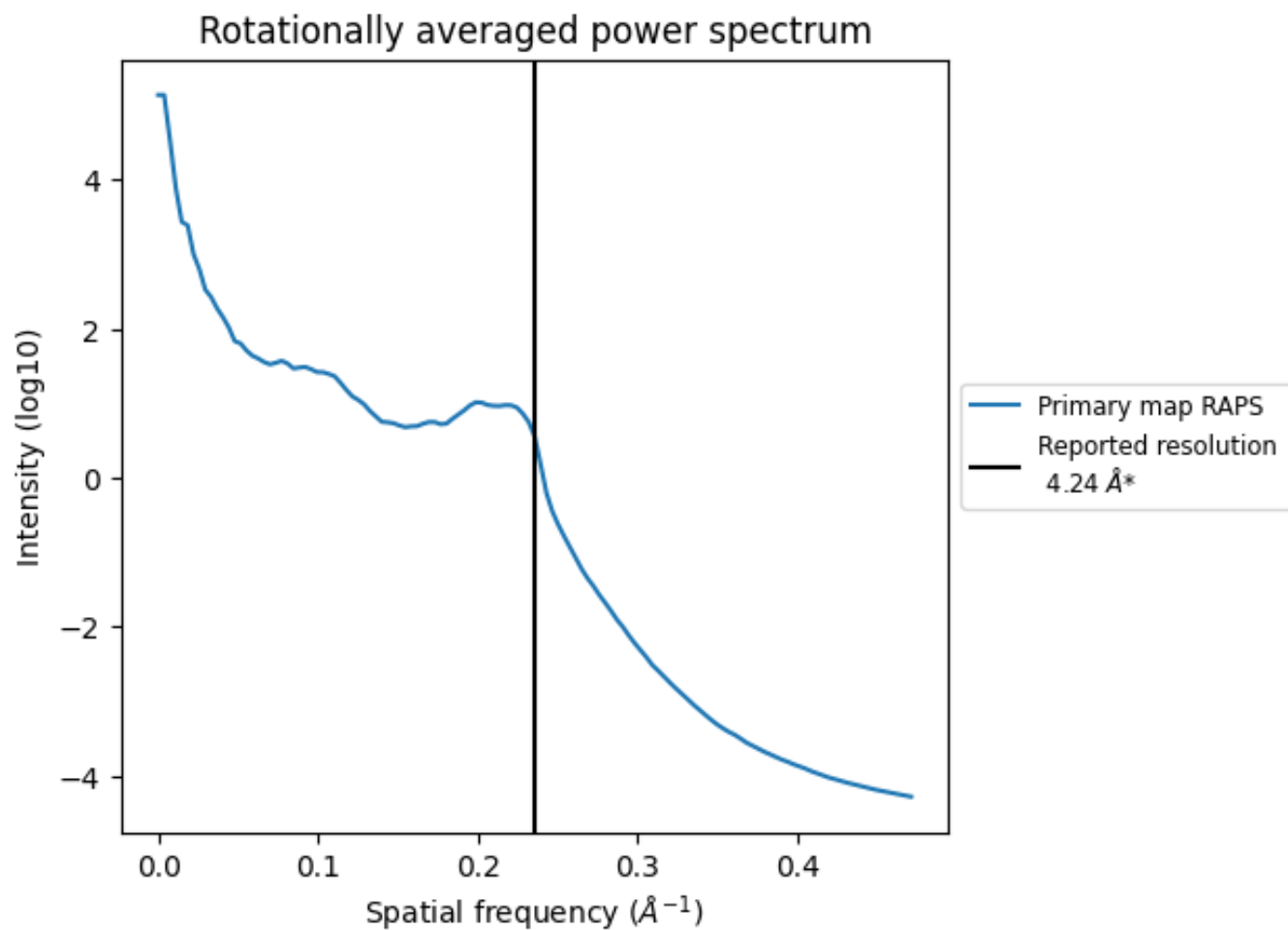
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 528 nm³; this corresponds to an approximate mass of 477 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

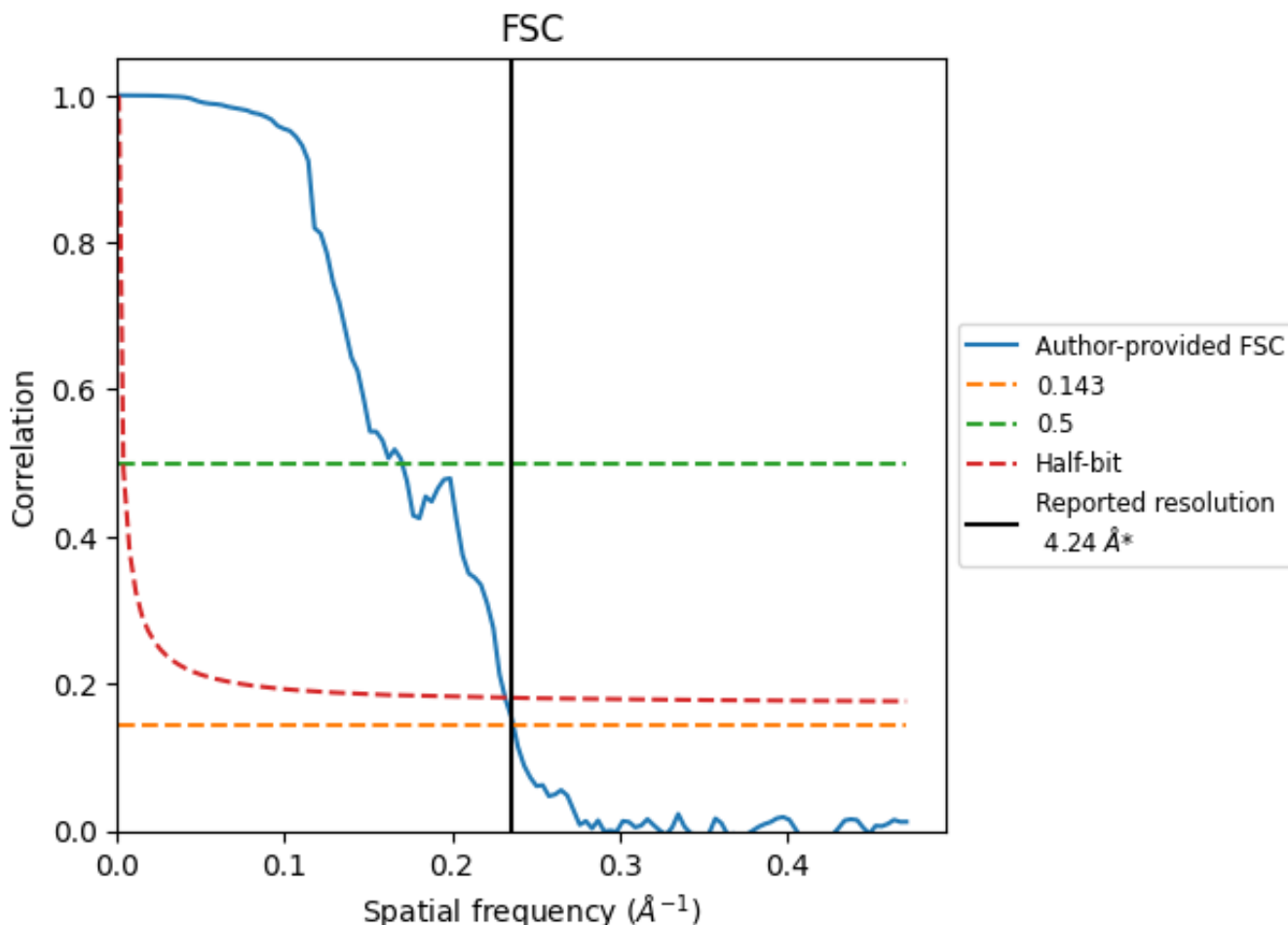


*Reported resolution corresponds to spatial frequency of 0.236\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

8.2 Resolution estimates [i](#)

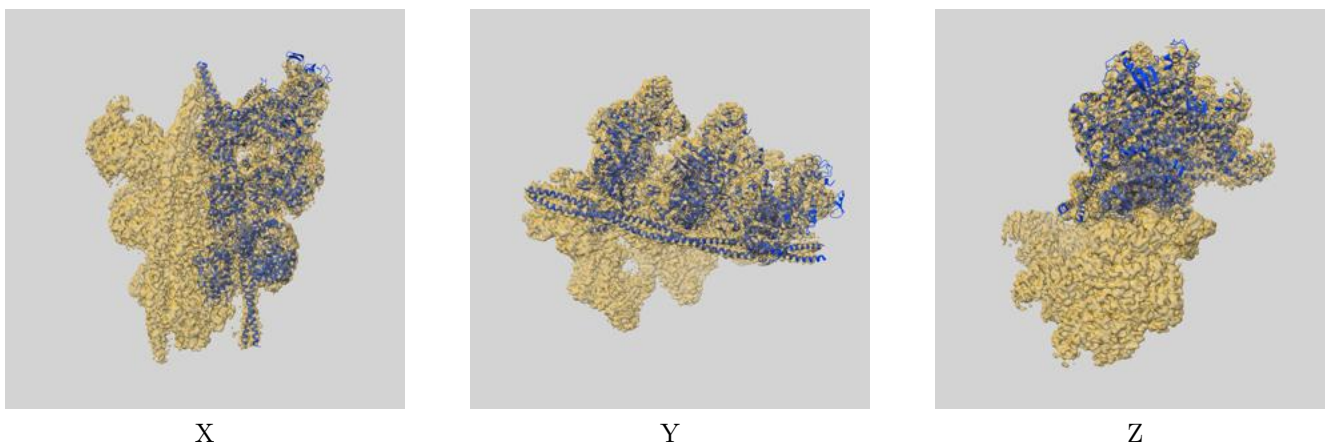
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.24	-	-
Author-provided FSC curve	4.22	5.88	4.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

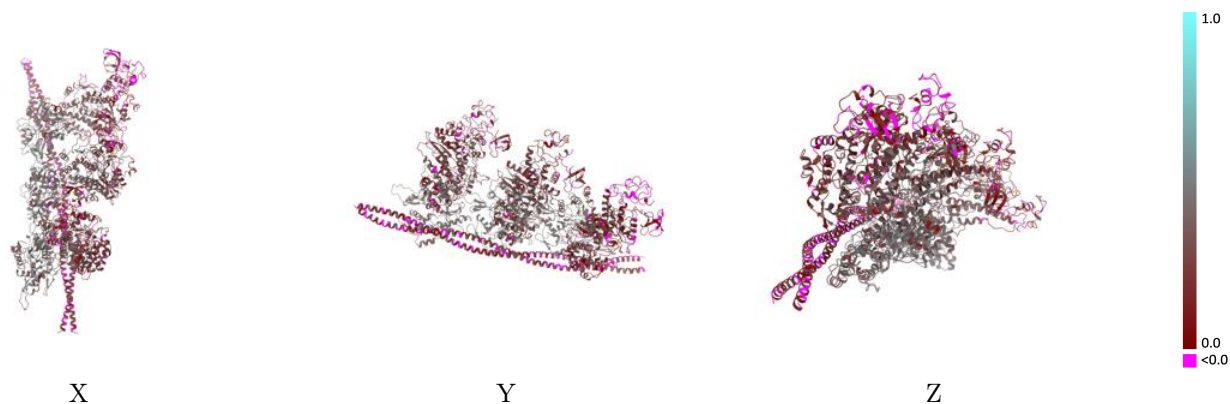
This section contains information regarding the fit between EMDB map EMD-22067 and PDB model 6X5Z. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



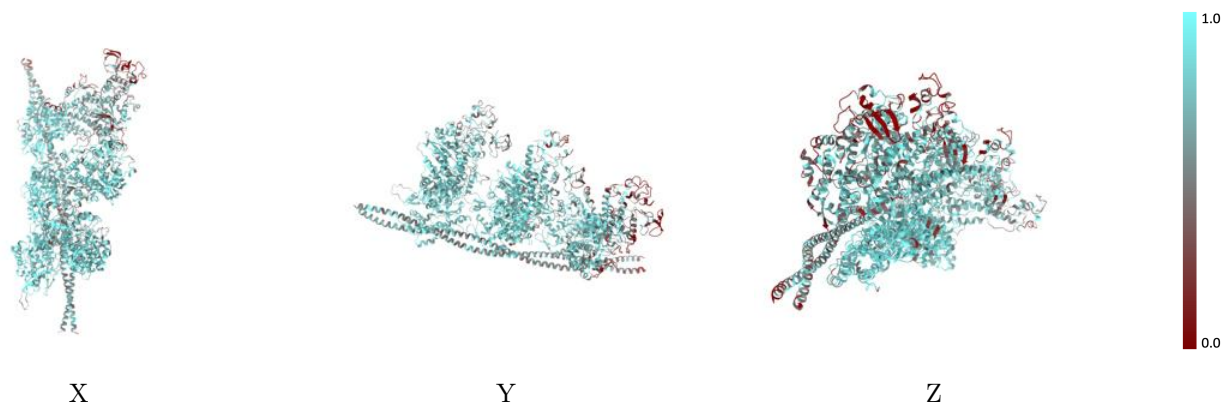
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



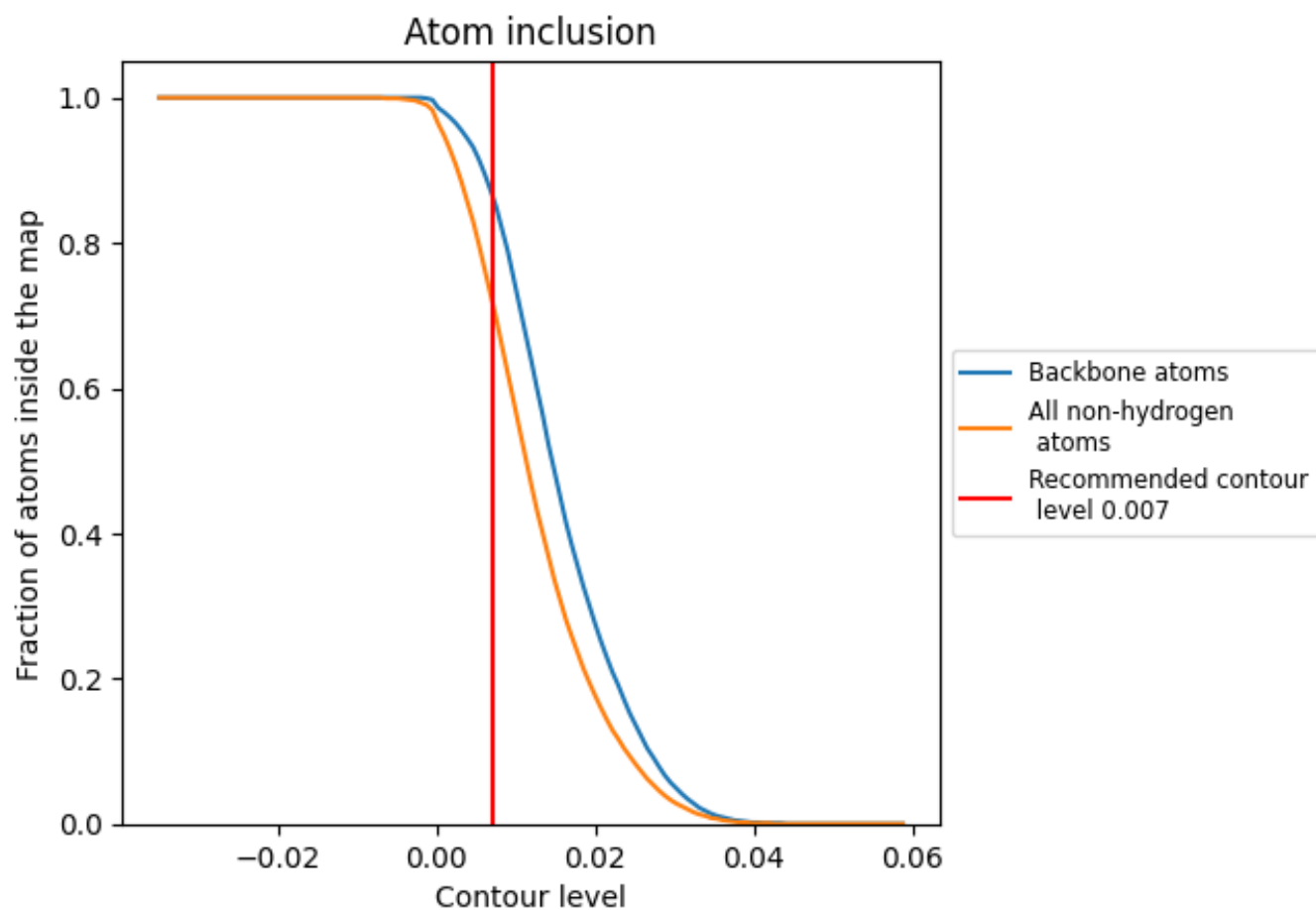
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7230	 0.2870
A	 0.8630	 0.4140
B	 0.8990	 0.4410
C	 0.8200	 0.3960
D	 0.7200	 0.2510
G	 0.7340	 0.3010
J	 0.5660	 0.2000
O	 0.5790	 0.0850
P	 0.5970	 0.1040

