



Full wwPDB EM Validation Report ⓘ

Jan 7, 2023 – 09:59 AM EST

PDB ID : 8F5O
EMDB ID : EMD-28866
Title : Structure of Leishmania tarentolae IFT-A (state 1)
Authors : Zhou, H.; Brown, A.
Deposited on : 2022-11-14
Resolution : 3.50 Å (reported)

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

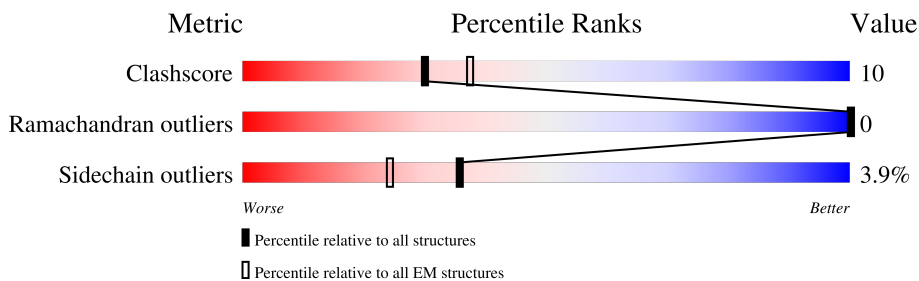
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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	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	B	1247	
2	C	1292	
3	E	1654	
4	A	368	
5	F	1376	
6	D	1642	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43398 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 Intraflagellar transport protein 122B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1134	8965	5674	1570	1658	63	0	0

- Molecule 2 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1179	9354	5929	1622	1735	68	0	0

- Molecule 3 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	1076	8380	5291	1451	1588	50	0	0

- Molecule 4 is a protein called NET domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	53	427	264	69	87	7	0	0

- Molecule 5 is a protein called WD_REPEATS_REGION domain-containing protein.

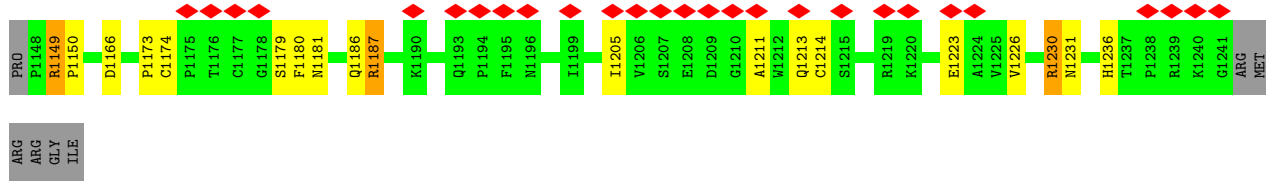
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	911	7045	4431	1231	1349	34	0	0

- Molecule 6 is a protein called TPR_REGION domain-containing protein.

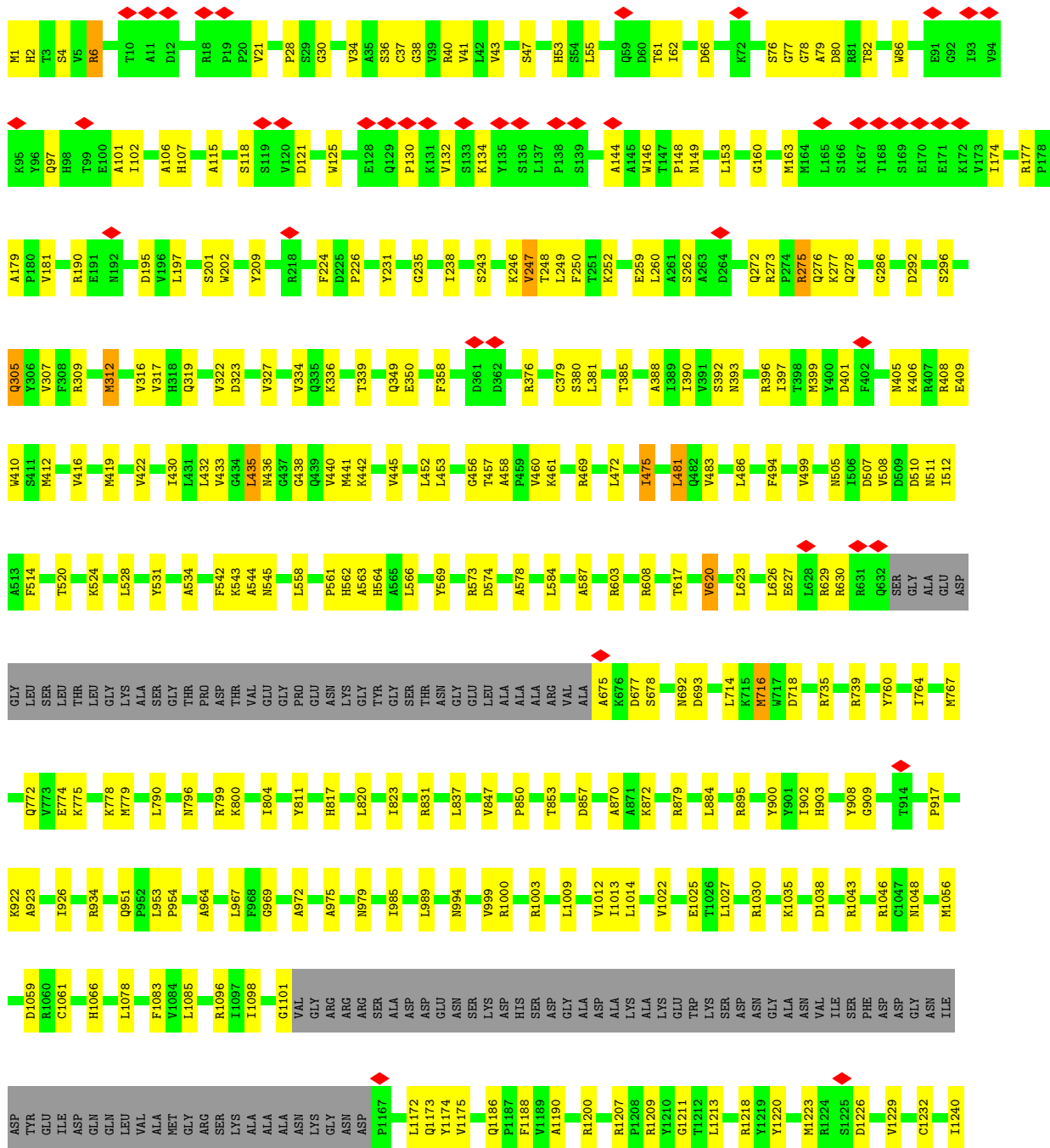
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	1180	9223	5796	1638	1738	51	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	B	2	Total 2	Zn 2	0
7	C	2	Total 2	Zn 2	0



• Molecule 2: Intraflagellar transport protein 122 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	239280	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 ($e^-/\text{\AA}^2$)	57.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	86.420	Depositor
Minimum map value	-36.983	Depositor
Average map value	0.020	Depositor
Map value standard deviation	1.359	Depositor
Recommended contour level	9.0	Depositor
Map size (\AA)	514.6, 514.6, 514.6	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	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:
ZN

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	B	0.28	0/9156	0.51	0/12403
2	C	0.28	0/9548	0.52	0/12921
3	E	0.29	0/8546	0.52	0/11608
4	A	0.25	0/432	0.56	0/584
5	F	0.28	0/7173	0.51	0/9746
6	D	0.30	0/9377	0.54	1/12718 (0.0%)
All	All	0.29	0/44232	0.52	1/59980 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1003	LEU	CA-CB-CG	5.09	127.02	115.30

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	B	8965	0	8873	170	0
2	C	9354	0	9301	185	0
3	E	8380	0	8309	173	0
4	A	427	0	413	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	7045	0	7054	101	0
6	D	9223	0	9265	253	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
All	All	43398	0	43215	868	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 10.

All (868) 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)
3:E:441:CYS:O	3:E:445:GLU:HB3	1.71	0.89
2:C:76:SER:HG	2:C:86:TRP:HE1	1.25	0.80
5:F:446:SER:HB3	5:F:462:TYR:HB2	1.66	0.78
2:C:197:LEU:HB3	2:C:209:TYR:O	1.84	0.76
5:F:789:SER:HB3	5:F:808:MET:HB2	1.66	0.76
3:E:499:ASN:N	3:E:499:ASN:OD1	2.22	0.73
6:D:1034:MET:SD	6:D:1034:MET:N	2.60	0.72
6:D:682:LEU:HD11	6:D:738:GLN:HB3	1.71	0.72
3:E:570:PRO:HA	3:E:584:SER:HA	1.70	0.72
2:C:4:SER:HB3	2:C:292:ASP:O	1.90	0.71
6:D:569:ILE:HD13	6:D:614:LYS:HD2	1.73	0.71
1:B:462:ILE:HD13	1:B:514:LEU:HD21	1.74	0.69
1:B:116:ALA:HB3	1:B:125:CYS:HB3	1.73	0.69
3:E:514:ASP:O	3:E:518:SER:N	2.26	0.69
6:D:1236:PRO:O	6:D:1239:ASN:ND2	2.25	0.69
6:D:1010:GLN:NE2	6:D:1030:GLN:OE1	2.27	0.68
6:D:799:TYR:O	6:D:802:ALA:HB3	1.93	0.68
3:E:1208:ARG:O	3:E:1212:LYS:NZ	2.27	0.67
5:F:321:LEU:HB3	5:F:334:GLY:O	1.95	0.67
6:D:1308:HIS:HA	6:D:1311:ILE:HD12	1.76	0.67
1:B:353:TRP:HE1	1:B:358:ASN:HA	1.60	0.67
1:B:1063:ARG:HA	1:B:1149:ARG:HH12	1.60	0.66
1:B:266:THR:O	1:B:274:PRO:HA	1.96	0.66
1:B:846:VAL:HA	2:C:430:ILE:HD11	1.78	0.66
6:D:651:CYS:HB3	6:D:656:ASP:HB2	1.78	0.66
6:D:1135:ALA:HB2	6:D:1168:HIS:HE1	1.59	0.66
6:D:1123:THR:HA	6:D:1126:ARG:HE	1.60	0.65
5:F:23:LEU:HD13	5:F:326:ARG:HH22	1.61	0.65
6:D:1591:ASP:OD2	6:D:1594:VAL:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:ND2	1:B:120:SER:OG	2.30	0.65
2:C:442:LYS:HG3	2:C:453:LEU:HD11	1.79	0.65
2:C:336:LYS:NZ	2:C:379:CYS:SG	2.70	0.65
2:C:735:ARG:HG3	2:C:739:ARG:HH22	1.62	0.64
4:A:162:SER:OG	4:A:185:ARG:NH2	2.31	0.64
3:E:656:LEU:HB2	3:E:671:TRP:HB2	1.80	0.64
2:C:41:VAL:HB	2:C:55:LEU:HB2	1.80	0.64
6:D:803:HIS:HA	6:D:806:LEU:HB3	1.79	0.64
2:C:1078:LEU:HD21	2:C:1240:ILE:HG12	1.80	0.64
3:E:20:ILE:HG22	3:E:31:THR:HG22	1.78	0.64
2:C:272:GLN:NE2	2:C:276:GLN:O	2.32	0.63
3:E:454:ARG:NH2	3:E:822:CYS:SG	2.66	0.63
6:D:632:THR:O	6:D:636:GLN:NE2	2.32	0.63
2:C:524:LYS:NZ	2:C:528:LEU:O	2.30	0.63
3:E:454:ARG:O	3:E:456:ARG:NH1	2.31	0.63
2:C:505:ASN:HB2	2:C:511:ASN:HB2	1.81	0.63
2:C:902:ILE:HD13	2:C:1257:CYS:HB3	1.81	0.63
2:C:1000:ARG:O	2:C:1000:ARG:NH1	2.31	0.63
5:F:324:TRP:O	5:F:326:ARG:NH2	2.29	0.63
1:B:646:GLU:HB3	1:B:650:LEU:HB3	1.80	0.62
6:D:1443:PHE:HB3	6:D:1465:ARG:HH22	1.64	0.62
5:F:784:GLU:HG3	5:F:788:ILE:HD11	1.80	0.62
6:D:1263:VAL:O	6:D:1340:ARG:NH2	2.32	0.62
5:F:266:LEU:HD21	5:F:303:ILE:HD12	1.82	0.62
5:F:364:ASN:OD1	5:F:365:ARG:NH1	2.32	0.62
1:B:254:ASN:ND2	1:B:256:SER:OG	2.33	0.62
3:E:26:ARG:HG3	3:E:75:GLU:HG2	1.82	0.62
5:F:223:PHE:HB3	5:F:227:LEU:HD12	1.82	0.62
6:D:1475:LYS:NZ	6:D:1508:SER:O	2.33	0.62
2:C:1207:ARG:HB3	2:C:1209:ARG:HH21	1.65	0.61
2:C:1269:MET:SD	2:C:1269:MET:N	2.70	0.61
3:E:15:LEU:HD22	3:E:446:LEU:HB2	1.82	0.61
6:D:1466:LEU:O	6:D:1469:SER:OG	2.18	0.61
1:B:433:TRP:HE1	1:B:457:SER:HB2	1.66	0.61
3:E:972:ASP:N	3:E:972:ASP:OD1	2.34	0.61
6:D:536:GLU:O	6:D:540:GLN:NE2	2.33	0.61
1:B:200:LEU:HA	1:B:223:TYR:HA	1.83	0.61
5:F:122:LEU:HB2	5:F:131:VAL:HB	1.83	0.61
1:B:532:ASN:ND2	1:B:534:ASN:OD1	2.34	0.61
6:D:1159:GLU:O	6:D:1163:ARG:N	2.33	0.61
2:C:316:VAL:HG12	2:C:327:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:ALA:HB2	1:B:812:ILE:HG21	1.83	0.61
2:C:545:ASN:OD1	2:C:562:HIS:NE2	2.33	0.61
5:F:350:VAL:HG11	5:F:389:PHE:HA	1.81	0.61
6:D:789:LEU:HD13	6:D:806:LEU:HD13	1.82	0.61
1:B:735:GLU:HB2	1:B:738:ARG:HH21	1.65	0.61
2:C:1046:ARG:NH2	2:C:1186:GLN:O	2.33	0.61
5:F:12:ALA:O	5:F:36:LYS:NZ	2.34	0.61
1:B:827:SER:OG	1:B:828:MET:SD	2.58	0.61
6:D:567:ALA:O	6:D:571:HIS:ND1	2.34	0.61
6:D:508:SER:HA	6:D:511:ASN:HD22	1.66	0.60
6:D:666:GLN:O	6:D:669:THR:OG1	2.19	0.60
1:B:74:ASN:ND2	1:B:76:GLN:OE1	2.35	0.60
6:D:537:ALA:O	6:D:541:ASP:N	2.26	0.60
6:D:1336:THR:O	6:D:1339:THR:OG1	2.17	0.60
6:D:1557:SER:HA	6:D:1560:TRP:HD1	1.66	0.60
2:C:62:ILE:HG22	2:C:78:GLY:HA3	1.84	0.60
5:F:358:VAL:HG23	5:F:372:LEU:HD21	1.83	0.60
3:E:333:ARG:HG2	3:E:344:VAL:HG22	1.83	0.60
6:D:1573:HIS:O	6:D:1601:ASN:ND2	2.34	0.60
6:D:798:PHE:O	6:D:802:ALA:N	2.33	0.59
6:D:447:TYR:OH	6:D:557:ASN:OD1	2.20	0.59
6:D:1002:ALA:O	6:D:1005:THR:OG1	2.19	0.59
6:D:1225:GLU:OE2	6:D:1228:ARG:NH1	2.34	0.59
1:B:943:LYS:HE2	1:B:1001:LEU:HD22	1.83	0.59
1:B:946:TYR:HB3	1:B:994:ALA:HA	1.83	0.59
2:C:319:GLN:O	2:C:323:ASP:HA	2.03	0.59
6:D:327:VAL:O	6:D:331:ARG:N	2.33	0.59
1:B:1:MET:N	1:B:326:ASN:OD1	2.32	0.59
2:C:148:PRO:HD2	2:C:190:ARG:HH21	1.67	0.59
3:E:190:ARG:NH1	3:E:257:VAL:O	2.36	0.59
4:A:171:ARG:HH12	6:D:1323:VAL:HG23	1.68	0.59
2:C:627:GLU:HG3	2:C:630:ARG:HH12	1.68	0.59
6:D:867:SER:O	6:D:871:SER:N	2.35	0.59
6:D:1584:TRP:HE1	6:D:1589:GLU:HG3	1.67	0.59
1:B:42:LYS:HB3	1:B:57:SER:HB3	1.84	0.59
6:D:327:VAL:HG12	6:D:331:ARG:HE	1.68	0.59
6:D:1115:GLU:OE2	6:D:1119:GLN:NE2	2.35	0.59
2:C:1098:ILE:O	2:C:1200:ARG:NH1	2.35	0.59
5:F:460:VAL:O	5:F:466:VAL:HA	2.01	0.59
6:D:1211:TYR:HE1	6:D:1248:ARG:HG3	1.68	0.58
6:D:1301:THR:OG1	6:D:1302:THR:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG13	1:B:102:GLU:HB3	1.85	0.58
3:E:829:PRO:HG2	3:E:854:ARG:HH11	1.68	0.58
1:B:83:SER:OG	1:B:84:ASP:N	2.35	0.58
3:E:365:THR:HA	3:E:378:PHE:O	2.03	0.58
1:B:633:ASP:OD2	1:B:636:ARG:NH2	2.37	0.58
2:C:406:LYS:HZ1	2:C:409:GLU:HB2	1.67	0.58
6:D:333:LEU:O	6:D:338:ASP:N	2.35	0.58
6:D:1573:HIS:HD2	6:D:1601:ASN:HA	1.69	0.58
6:D:849:GLU:OE1	6:D:852:GLN:NE2	2.37	0.58
6:D:972:LEU:HA	6:D:975:GLN:HG2	1.85	0.58
1:B:578:LEU:O	1:B:579:ARG:NH1	2.35	0.57
5:F:706:ILE:HD13	5:F:722:GLU:HG2	1.86	0.57
2:C:870:ALA:O	2:C:872:LYS:NZ	2.37	0.57
3:E:459:ASP:HB3	3:E:495:ILE:HG23	1.86	0.57
2:C:30:GLY:HA3	2:C:275:ARG:HH12	1.68	0.57
6:D:1034:MET:HA	6:D:1037:ILE:HD12	1.86	0.57
6:D:1509:PRO:HB2	6:D:1514:LEU:HD21	1.87	0.57
1:B:716:LEU:O	1:B:722:GLN:NE2	2.37	0.57
2:C:442:LYS:HE2	2:C:453:LEU:HD21	1.86	0.57
6:D:410:ALA:O	6:D:413:ARG:NH1	2.37	0.57
6:D:773:GLN:O	6:D:777:ALA:N	2.37	0.57
3:E:194:VAL:HG12	3:E:259:TYR:CZ	2.40	0.57
3:E:458:TRP:NE1	3:E:827:THR:OG1	2.36	0.57
1:B:1057:ARG:NH1	1:B:1060:GLN:OE1	2.35	0.57
2:C:179:ALA:HB3	2:C:201:SER:HB2	1.87	0.57
3:E:15:LEU:H	3:E:444:SER:HA	1.70	0.57
3:E:156:ARG:HE	3:E:183:GLN:HE21	1.53	0.57
5:F:635:GLY:HA2	5:F:651:LEU:HD12	1.85	0.57
6:D:1015:GLU:HA	6:D:1018:LEU:HD12	1.87	0.57
1:B:228:LEU:O	1:B:241:ASN:ND2	2.36	0.56
2:C:224:PHE:HB2	2:C:243:SER:H	1.70	0.56
2:C:1003:ARG:NH2	2:C:1030:ARG:O	2.38	0.56
2:C:1085:LEU:HA	2:C:1190:ALA:HB3	1.87	0.56
2:C:1223:MET:SD	2:C:1223:MET:N	2.78	0.56
5:F:396:MET:HE1	5:F:472:ARG:HH12	1.70	0.56
5:F:794:GLN:O	5:F:797:GLU:HB3	2.05	0.56
2:C:235:GLY:O	2:C:252:LYS:NZ	2.39	0.56
5:F:656:ASN:ND2	5:F:665:GLU:OE1	2.37	0.56
5:F:754:SER:OG	5:F:755:SER:N	2.38	0.56
6:D:1479:MET:HG3	6:D:1544:PHE:HE1	1.70	0.56
2:C:82:THR:HA	2:C:97:GLN:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:422:VAL:HG12	2:C:469:ARG:HH11	1.70	0.56
2:C:79:ALA:HA	2:C:101:ALA:HB1	1.87	0.56
5:F:20:VAL:HG11	5:F:59:ALA:HA	1.88	0.56
5:F:732:LEU:HD21	5:F:756:GLN:HB2	1.87	0.56
6:D:606:MET:SD	6:D:636:GLN:NE2	2.75	0.56
2:C:857:ASP:O	3:E:996:ARG:NH1	2.39	0.56
5:F:573:VAL:HG22	5:F:585:THR:HG22	1.86	0.56
6:D:1161:LEU:HA	6:D:1164:LYS:HE2	1.87	0.56
2:C:37:CYS:SG	2:C:40:ARG:NH2	2.76	0.56
2:C:796:ASN:OD1	2:C:811:TYR:OH	2.23	0.56
5:F:163:LEU:HB3	5:F:176:ILE:HB	1.88	0.56
5:F:582:VAL:HG22	5:F:595:VAL:HG12	1.87	0.56
6:D:442:GLY:O	6:D:446:LEU:N	2.38	0.56
6:D:616:TRP:O	6:D:619:THR:OG1	2.23	0.56
1:B:1186:GLN:HE21	1:B:1187:ARG:HE	1.54	0.56
6:D:334:MET:SD	6:D:335:GLN:NE2	2.79	0.56
1:B:190:LYS:NZ	1:B:237:GLU:O	2.38	0.56
2:C:520:THR:HA	2:C:534:ALA:HA	1.87	0.56
5:F:531:ARG:HH22	5:F:571:LYS:HD3	1.71	0.55
1:B:251:ILE:HB	1:B:260:LEU:HD11	1.87	0.55
2:C:349:GLN:OE1	2:C:376:ARG:NH2	2.39	0.55
2:C:416:VAL:HA	2:C:435:LEU:HA	1.87	0.55
3:E:14:GLN:N	3:E:34:VAL:O	2.34	0.55
3:E:650:GLN:OE1	3:E:653:ARG:NH2	2.40	0.55
6:D:1045:CYS:HB3	6:D:1083:ALA:HB2	1.87	0.55
1:B:606:GLU:OE2	1:B:651:ARG:NH2	2.40	0.55
1:B:819:TYR:HA	1:B:822:LEU:HB3	1.87	0.55
2:C:118:SER:OG	2:C:121:ASP:OD1	2.23	0.55
3:E:1204:ARG:HD2	3:E:1231:LEU:HD11	1.87	0.55
6:D:1455:GLN:OE1	6:D:1457:THR:N	2.39	0.55
3:E:1185:GLU:OE1	3:E:1197:TYR:OH	2.24	0.55
1:B:406:ARG:NH2	1:B:457:SER:OG	2.40	0.55
2:C:248:THR:HA	2:C:259:GLU:HA	1.87	0.55
2:C:1043:ARG:NH2	2:C:1048:ASN:OD1	2.40	0.55
3:E:1018:ALA:HA	3:E:1021:MET:HG2	1.88	0.55
6:D:800:ILE:O	6:D:804:SER:N	2.35	0.55
6:D:1475:LYS:NZ	6:D:1508:SER:OG	2.35	0.55
3:E:470:ASP:OD1	3:E:470:ASP:N	2.36	0.55
6:D:907:ASP:OD1	6:D:907:ASP:N	2.40	0.55
1:B:685:THR:O	1:B:690:ASP:N	2.37	0.55
6:D:1147:GLU:HA	6:D:1514:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:349:GLN:O	2:C:376:ARG:NE	2.39	0.54
6:D:957:THR:O	6:D:961:ARG:NH1	2.39	0.54
3:E:471:MET:HB3	3:E:483:LEU:HD11	1.90	0.54
6:D:445:GLN:HA	6:D:448:ARG:HB2	1.90	0.54
6:D:839:GLU:O	6:D:842:GLU:HB3	2.07	0.54
2:C:307:VAL:HG22	2:C:317:VAL:HG13	1.89	0.54
2:C:1013:ILE:HG22	5:F:730:LYS:HD3	1.89	0.54
3:E:547:ARG:HE	3:E:560:GLN:HA	1.71	0.54
1:B:529:MET:HG2	1:B:540:VAL:HG22	1.89	0.54
2:C:831:ARG:NH1	2:C:1277:GLU:OE2	2.40	0.54
2:C:1101:GLY:HA2	2:C:1200:ARG:HH22	1.73	0.54
3:E:260:ASP:O	3:E:264:ARG:N	2.40	0.54
3:E:711:GLU:OE1	3:E:870:ARG:NH1	2.41	0.54
3:E:886:ASP:O	5:F:798:TYR:OH	2.25	0.54
1:B:229:GLN:HG3	1:B:241:ASN:HB2	1.90	0.54
2:C:273:ARG:NH1	2:C:278:GLN:OE1	2.40	0.54
3:E:646:ARG:O	3:E:697:TRP:NE1	2.38	0.54
6:D:642:ASP:N	6:D:642:ASP:OD1	2.41	0.54
1:B:691:PHE:HB3	1:B:714:ARG:HD3	1.89	0.54
2:C:934:ARG:NH2	2:C:975:ALA:O	2.41	0.54
3:E:672:VAL:HG21	3:E:808:LEU:HD21	1.88	0.54
3:E:1020:ILE:HD12	3:E:1033:VAL:HG13	1.89	0.54
3:E:536:HIS:NE2	3:E:577:ASN:O	2.39	0.54
6:D:1084:ARG:HA	6:D:1087:LEU:HD23	1.89	0.54
2:C:160:GLY:HA2	2:C:181:VAL:HG23	1.89	0.54
2:C:510:ASP:OD1	2:C:510:ASP:N	2.40	0.54
6:D:408:ARG:NH1	6:D:554:VAL:O	2.41	0.54
1:B:165:LEU:HG	1:B:175:VAL:HG22	1.90	0.53
1:B:605:GLU:OE1	1:B:651:ARG:NH2	2.41	0.53
1:B:624:THR:HG23	1:B:643:VAL:HG23	1.89	0.53
1:B:753:ARG:NH2	1:B:758:ASP:OD2	2.40	0.53
2:C:1012:VAL:HG22	5:F:729:GLU:HA	1.89	0.53
3:E:375:LEU:HD11	3:E:439:LEU:HD11	1.90	0.53
5:F:163:LEU:HD23	5:F:176:ILE:HD12	1.89	0.53
1:B:824:GLN:NE2	1:B:827:SER:OG	2.42	0.53
2:C:28:PRO:O	2:C:275:ARG:NH2	2.40	0.53
2:C:412:MET:SD	2:C:412:MET:N	2.81	0.53
2:C:972:ALA:O	5:F:755:SER:OG	2.26	0.53
2:C:979:ASN:OD1	5:F:725:ARG:NH1	2.40	0.53
3:E:343:ASP:OD1	3:E:343:ASP:N	2.41	0.53
5:F:655:ASN:ND2	5:F:665:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:GLN:NE2	1:B:1009:ASP:OD2	2.41	0.53
6:D:824:PHE:HB3	6:D:840:LEU:HD13	1.91	0.53
3:E:547:ARG:NH1	3:E:561:MET:O	2.42	0.53
5:F:161:PRO:HB2	5:F:178:LEU:HB2	1.90	0.53
5:F:611:VAL:HG21	5:F:619:LEU:HB2	1.89	0.53
5:F:677:ARG:NH1	5:F:701:ASP:OD2	2.41	0.53
6:D:1032:VAL:O	6:D:1035:SER:OG	2.16	0.53
1:B:659:ASP:OD1	1:B:659:ASP:N	2.41	0.53
3:E:674:ASP:O	3:E:678:ASP:CA	2.57	0.53
5:F:409:GLU:HB2	5:F:439:LEU:HD11	1.90	0.53
3:E:985:GLU:OE1	3:E:988:GLN:NE2	2.42	0.53
6:D:399:LEU:HA	6:D:402:PHE:HB2	1.89	0.53
6:D:515:ARG:O	6:D:520:GLY:N	2.42	0.53
6:D:1475:LYS:HB3	6:D:1544:PHE:HZ	1.73	0.53
6:D:1540:LYS:O	6:D:1543:ARG:NH2	2.42	0.53
2:C:144:ALA:HB1	2:C:153:LEU:HD11	1.89	0.53
2:C:408:ARG:NH1	2:C:445:VAL:O	2.42	0.53
5:F:288:VAL:HG22	5:F:293:VAL:HG22	1.90	0.53
6:D:1352:PHE:HB3	6:D:1446:LEU:HD23	1.91	0.53
6:D:1533:ASP:HB3	6:D:1542:ALA:HB2	1.90	0.53
1:B:47:PRO:HA	1:B:50:GLN:HB2	1.91	0.53
6:D:1264:ARG:NE	6:D:1531:TYR:OH	2.38	0.53
1:B:310:VAL:HG13	1:B:321:ALA:HB3	1.90	0.53
1:B:493:SER:HB2	1:B:531:VAL:HG11	1.91	0.53
6:D:545:ARG:HB3	6:D:551:GLU:HB3	1.90	0.53
2:C:804:ILE:HD12	2:C:823:ILE:HD11	1.90	0.52
3:E:1157:ALA:HA	3:E:1160:SER:HB3	1.89	0.52
3:E:1208:ARG:HA	3:E:1211:TRP:CD1	2.44	0.52
2:C:34:VAL:HG22	2:C:43:VAL:HG22	1.90	0.52
3:E:572:ILE:HB	3:E:583:VAL:HB	1.91	0.52
3:E:674:ASP:O	3:E:678:ASP:HA	2.08	0.52
6:D:974:ASP:OD1	6:D:974:ASP:N	2.35	0.52
6:D:977:TRP:NE1	6:D:997:ASP:OD2	2.42	0.52
6:D:1574:LYS:O	6:D:1577:SER:OG	2.27	0.52
1:B:72:THR:HG22	1:B:81:THR:HB	1.91	0.52
1:B:906:ARG:NH2	1:B:908:THR:OG1	2.42	0.52
2:C:994:ASN:ND2	2:C:1025:GLU:OE2	2.43	0.52
2:C:1218:ARG:NH2	2:C:1220:TYR:OH	2.38	0.52
6:D:954:ALA:N	6:D:957:THR:OG1	2.43	0.52
6:D:1342:PRO:HA	6:D:1345:LEU:HD13	1.92	0.52
2:C:309:ARG:HD2	2:C:312:MET:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:693:ASP:N	2:C:693:ASP:OD1	2.41	0.52
3:E:657:MET:HG2	3:E:670:ILE:HD11	1.90	0.52
5:F:387:PRO:HA	5:F:401:VAL:HG13	1.90	0.52
5:F:350:VAL:HG12	5:F:390:ILE:HG12	1.91	0.52
6:D:589:GLU:O	6:D:593:ARG:N	2.42	0.52
1:B:372:ASN:OD1	1:B:373:ALA:N	2.41	0.52
3:E:65:PRO:HA	3:E:81:TRP:HA	1.91	0.52
3:E:466:GLN:NE2	3:E:468:SER:O	2.42	0.52
3:E:481:GLN:NE2	3:E:848:TYR:O	2.43	0.52
3:E:595:SER:OG	3:E:598:ASP:OD1	2.27	0.52
6:D:789:LEU:HD22	6:D:806:LEU:HB2	1.92	0.52
6:D:1567:TYR:HB2	6:D:1576:ALA:HB2	1.91	0.52
6:D:1462:VAL:HG22	6:D:1465:ARG:HH21	1.75	0.52
5:F:848:ILE:HG21	5:F:875:LEU:HB2	1.92	0.52
6:D:1613:ASP:OD1	6:D:1613:ASP:N	2.42	0.52
3:E:1185:GLU:OE2	3:E:1208:ARG:NH1	2.42	0.52
6:D:1148:GLN:N	6:D:1148:GLN:OE1	2.42	0.52
1:B:370:TYR:OH	1:B:372:ASN:ND2	2.36	0.52
2:C:608:ARG:HG2	2:C:623:LEU:HD23	1.91	0.52
6:D:304:LEU:HA	6:D:307:ALA:HB3	1.92	0.52
6:D:962:ILE:HD12	6:D:962:ILE:H	1.75	0.52
6:D:1534:THR:OG1	6:D:1535:GLN:NE2	2.42	0.52
1:B:23:ASN:HB2	1:B:73:TRP:CD2	2.44	0.51
2:C:505:ASN:ND2	2:C:543:LYS:O	2.43	0.51
3:E:674:ASP:O	3:E:678:ASP:N	2.43	0.51
3:E:1036:ILE:O	3:E:1040:THR:OG1	2.19	0.51
6:D:745:ASP:N	6:D:745:ASP:OD1	2.38	0.51
6:D:854:ILE:HG21	6:D:886:LYS:HZ2	1.75	0.51
6:D:1010:GLN:HG2	6:D:1034:MET:HB3	1.92	0.51
1:B:212:ARG:NH1	1:B:345:LYS:O	2.44	0.51
1:B:547:THR:HG21	1:B:575:VAL:HB	1.92	0.51
6:D:883:ASP:HB2	6:D:886:LYS:HG2	1.92	0.51
1:B:1230:ARG:NE	1:B:1231:ASN:OD1	2.43	0.51
3:E:813:PHE:O	3:E:856:ARG:NH1	2.44	0.51
3:E:869:VAL:HG13	3:E:895:ILE:HG23	1.93	0.51
5:F:202:VAL:HB	5:F:209:LEU:HB3	1.92	0.51
5:F:224:ASN:HB3	5:F:227:LEU:HG	1.92	0.51
6:D:439:CYS:SG	6:D:440:GLY:N	2.83	0.51
3:E:71:HIS:HB2	3:E:76:LEU:HB3	1.92	0.51
6:D:515:ARG:HG2	6:D:519:ARG:HD2	1.92	0.51
5:F:404:GLN:HB3	5:F:443:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1513:ILE:HD11	6:D:1526:MET:HE1	1.92	0.51
1:B:264:ALA:HB3	1:B:277:VAL:HG13	1.92	0.51
6:D:753:LEU:HD13	6:D:773:GLN:HG2	1.92	0.51
1:B:106:ASN:O	1:B:108:ASN:ND2	2.43	0.51
2:C:272:GLN:NE2	2:C:273:ARG:O	2.36	0.51
1:B:943:LYS:HZ3	1:B:944:LYS:HE3	1.76	0.51
3:E:943:ASP:O	3:E:947:GLN:NE2	2.44	0.51
3:E:1228:ASP:HB3	3:E:1231:LEU:HD23	1.92	0.51
5:F:595:VAL:HG11	5:F:673:LEU:HA	1.91	0.51
1:B:107:ARG:NH1	1:B:109:SER:OG	2.44	0.50
1:B:340:PHE:HE1	1:B:351:MET:HB2	1.76	0.50
1:B:460:ARG:HG2	1:B:474:PRO:HB3	1.93	0.50
2:C:507:ASP:HB2	2:C:544:ALA:HB2	1.92	0.50
2:C:1260:ARG:O	2:C:1267:ARG:NH2	2.45	0.50
3:E:155:GLN:O	3:E:183:GLN:NE2	2.44	0.50
3:E:507:GLN:HB3	3:E:527:LEU:HD23	1.92	0.50
5:F:745:LYS:NZ	5:F:749:ASN:OD1	2.44	0.50
6:D:1217:GLU:HB3	6:D:1222:ASN:HB3	1.92	0.50
1:B:106:ASN:ND2	1:B:108:ASN:OD1	2.45	0.50
1:B:638:ARG:NH1	1:B:640:ASP:OD2	2.44	0.50
1:B:806:TYR:HA	1:B:809:LEU:HD12	1.93	0.50
1:B:842:MET:O	1:B:845:THR:OG1	2.25	0.50
2:C:38:GLY:HA2	2:C:61:THR:HG23	1.94	0.50
2:C:923:ALA:HB2	5:F:827:VAL:HG11	1.91	0.50
6:D:498:GLN:NE2	6:D:499:PRO:O	2.44	0.50
6:D:923:GLU:HA	6:D:926:VAL:HG22	1.93	0.50
6:D:506:GLU:HA	6:D:509:MET:HG2	1.93	0.50
6:D:1123:THR:HA	6:D:1126:ARG:NE	2.26	0.50
1:B:366:ARG:NH1	1:B:384:PRO:O	2.44	0.50
2:C:617:THR:HA	2:C:620:VAL:HG12	1.94	0.50
3:E:695:VAL:HB	3:E:715:LEU:HD11	1.93	0.50
6:D:633:LEU:HD11	6:D:643:ALA:HB3	1.94	0.50
6:D:979:VAL:HG11	6:D:1072:VAL:HG22	1.92	0.50
1:B:699:ILE:HD11	2:C:714:LEU:HA	1.92	0.50
2:C:764:ILE:HD12	2:C:790:LEU:HD23	1.92	0.50
3:E:934:ARG:NH1	5:F:766:ASP:OD2	2.42	0.50
5:F:677:ARG:O	5:F:680:SER:OG	2.29	0.50
1:B:1230:ARG:NH1	4:A:190:ASP:OD1	2.44	0.50
6:D:311:LEU:HD13	6:D:329:LYS:HA	1.93	0.50
6:D:969:TYR:O	6:D:973:ARG:N	2.45	0.50
3:E:149:LEU:HB3	3:E:161:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:645:ALA:HA	3:E:655:ALA:O	2.11	0.50
3:E:698:ASN:ND2	3:E:711:GLU:O	2.43	0.50
3:E:1017:ASP:N	3:E:1017:ASP:OD1	2.44	0.50
3:E:1205:SER:OG	3:E:1208:ARG:NH2	2.44	0.50
5:F:660:ARG:NH1	5:F:681:ASN:OD1	2.44	0.50
6:D:857:TYR:HB3	6:D:874:VAL:HG22	1.94	0.50
6:D:1140:LEU:O	6:D:1144:LEU:N	2.44	0.50
6:D:1257:THR:OG1	6:D:1258:THR:N	2.44	0.50
6:D:507:LEU:O	6:D:511:ASN:ND2	2.45	0.50
6:D:1460:ARG:HH12	6:D:1538:ARG:HH22	1.60	0.50
6:D:1539:LEU:HD12	6:D:1540:LYS:HD3	1.93	0.50
2:C:461:LYS:HE2	2:C:475:ILE:HD11	1.93	0.49
2:C:677:ASP:OD1	2:C:677:ASP:N	2.44	0.49
2:C:1281:ALA:HA	2:C:1284:LYS:HG2	1.92	0.49
3:E:417:MET:HA	3:E:794:ARG:HE	1.77	0.49
2:C:163:MET:HA	2:C:174:ILE:HG12	1.93	0.49
3:E:1190:ASP:N	3:E:1190:ASP:OD1	2.41	0.49
3:E:422:VAL:HG13	3:E:424:LYS:H	1.78	0.49
6:D:1333:ALA:O	6:D:1337:MET:HG2	2.12	0.49
6:D:1624:THR:O	6:D:1624:THR:OG1	2.28	0.49
5:F:599:HIS:O	5:F:599:HIS:ND1	2.41	0.49
6:D:1081:THR:HB	6:D:1084:ARG:HH21	1.76	0.49
1:B:747:ASP:OD1	1:B:747:ASP:N	2.43	0.49
2:C:675:ALA:N	2:C:678:SER:HG	2.09	0.49
3:E:260:ASP:O	3:E:264:ARG:CA	2.60	0.49
5:F:769:GLN:HB3	5:F:772:ARG:HG2	1.95	0.49
3:E:1047:ARG:HE	3:E:1093:TRP:HZ2	1.60	0.49
1:B:401:SER:HB2	2:C:561:PRO:HA	1.93	0.49
1:B:1026:ASP:HB2	1:B:1031:PRO:HG3	1.95	0.49
2:C:66:ASP:OD2	2:C:107:HIS:ND1	2.43	0.49
2:C:850:PRO:HA	2:C:853:THR:HG22	1.95	0.49
3:E:1217:GLY:O	3:E:1221:ASN:ND2	2.45	0.49
5:F:786:PRO:O	5:F:789:SER:HB2	2.12	0.49
6:D:851:GLU:HA	6:D:854:ILE:HD12	1.95	0.49
1:B:26:GLN:OE1	1:B:28:TRP:NE1	2.40	0.49
2:C:1046:ARG:HD2	2:C:1066:HIS:HB2	1.94	0.49
3:E:245:PHE:HD2	3:E:285:LYS:HZ1	1.60	0.49
5:F:659:LEU:HD13	5:F:661:THR:HG22	1.93	0.49
6:D:1070:LEU:O	6:D:1073:GLN:NE2	2.38	0.49
3:E:331:ARG:HE	3:E:344:VAL:HG11	1.77	0.49
3:E:493:VAL:HG22	3:E:502:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1077:SER:O	3:E:1081:THR:OG1	2.22	0.49
1:B:716:LEU:HD21	1:B:721:LYS:HB3	1.93	0.49
2:C:1245:GLU:OE1	3:E:1205:SER:OG	2.30	0.49
3:E:1202:ALA:HB1	3:E:1205:SER:HB2	1.95	0.49
5:F:116:LYS:HG2	5:F:140:ARG:HG3	1.94	0.49
6:D:1158:PHE:O	6:D:1161:LEU:HB3	2.13	0.49
1:B:1173:PRO:HA	1:B:1180:PHE:HA	1.95	0.48
2:C:438:GLY:O	2:C:456:GLY:N	2.46	0.48
5:F:745:LYS:NZ	5:F:745:LYS:O	2.39	0.48
1:B:649:LEU:HD21	1:B:677:LEU:HD11	1.95	0.48
1:B:863:ARG:NH2	1:B:889:ASP:OD2	2.46	0.48
1:B:917:ALA:HB1	1:B:919:LYS:HE2	1.94	0.48
6:D:1194:ARG:O	6:D:1198:ALA:N	2.46	0.48
1:B:420:SER:HB2	1:B:436:ARG:HH21	1.78	0.48
5:F:770:TRP:HE3	5:F:788:ILE:HG22	1.77	0.48
6:D:327:VAL:HB	6:D:331:ARG:HH21	1.79	0.48
1:B:1:MET:HB3	1:B:325:PRO:HA	1.93	0.48
2:C:132:VAL:HB	2:C:134:LYS:HE3	1.94	0.48
2:C:767:MET:HE1	2:C:772:GLN:H	1.79	0.48
3:E:140:SER:HA	3:E:150:VAL:O	2.12	0.48
3:E:641:SER:OG	3:E:659:THR:OG1	2.31	0.48
5:F:837:GLU:OE2	5:F:840:ARG:NH1	2.46	0.48
1:B:493:SER:OG	1:B:494:GLU:N	2.46	0.48
1:B:577:ASN:OD1	1:B:578:LEU:N	2.46	0.48
1:B:1049:GLY:HA3	1:B:1166:ASP:HB2	1.95	0.48
3:E:495:ILE:HB	3:E:500:ILE:HD12	1.96	0.48
4:A:171:ARG:NE	6:D:1319:LEU:O	2.46	0.48
5:F:903:ILE:HD13	5:F:924:ILE:HG23	1.94	0.48
6:D:509:MET:SD	6:D:509:MET:N	2.86	0.48
2:C:817:HIS:HA	2:C:820:LEU:HD12	1.95	0.48
3:E:6:VAL:HG22	3:E:449:LEU:HG	1.95	0.48
3:E:855:LEU:HB2	3:E:858:PHE:HB2	1.94	0.48
6:D:389:ARG:HH22	6:D:422:GLN:HB3	1.78	0.48
1:B:1002:MET:HA	1:B:1005:GLN:HG3	1.95	0.48
2:C:969:GLY:O	2:C:1059:ASP:N	2.45	0.48
6:D:315:PHE:HB3	6:D:325:PRO:HG2	1.94	0.48
6:D:456:GLU:HA	6:D:459:ARG:HD2	1.96	0.48
6:D:1122:THR:O	6:D:1126:ARG:HG3	2.13	0.48
2:C:80:ASP:OD2	2:C:82:THR:OG1	2.31	0.48
3:E:669:ARG:HA	3:E:684:ASP:HA	1.96	0.48
6:D:798:PHE:O	6:D:801:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASN:O	1:B:358:ASN:N	2.47	0.48
2:C:926:ILE:HG13	2:C:1213:LEU:HD13	1.94	0.48
2:C:1061:CYS:HB3	2:C:1066:HIS:H	1.79	0.48
6:D:1155:ARG:NH2	6:D:1159:GLU:OE2	2.46	0.48
1:B:934:ALA:HB1	1:B:941:LYS:HE3	1.95	0.48
2:C:202:TRP:NE1	2:C:226:PRO:O	2.42	0.48
5:F:469:SER:HB3	5:F:480:PRO:HB3	1.96	0.48
6:D:766:ILE:O	6:D:769:VAL:HB	2.13	0.48
2:C:36:SER:HB2	2:C:62:ILE:HG13	1.94	0.47
2:C:385:THR:OG1	2:C:388:ALA:O	2.31	0.47
2:C:433:VAL:O	2:C:440:VAL:HA	2.14	0.47
3:E:547:ARG:CZ	3:E:561:MET:H	2.27	0.47
3:E:604:PRO:O	3:E:606:ARG:NE	2.46	0.47
3:E:658:SER:OG	3:E:667:ASP:OD2	2.27	0.47
3:E:667:ASP:OD2	3:E:669:ARG:NH1	2.46	0.47
5:F:700:LEU:HD21	5:F:734:LEU:HD23	1.95	0.47
5:F:706:ILE:HG23	5:F:718:VAL:HG13	1.96	0.47
1:B:717:ASP:OD1	1:B:717:ASP:N	2.47	0.47
3:E:539:GLY:HA3	3:E:551:GLU:O	2.14	0.47
3:E:670:ILE:HG12	3:E:695:VAL:HG11	1.95	0.47
5:F:629:PRO:HB3	5:F:637:VAL:HG11	1.95	0.47
1:B:217:ALA:HB1	1:B:230:LEU:HB3	1.96	0.47
2:C:569:TYR:HD1	2:C:574:ASP:HB3	1.79	0.47
3:E:18:GLN:HG2	3:E:19:LEU:HG	1.96	0.47
5:F:614:SER:OG	5:F:617:ASP:OD1	2.32	0.47
6:D:1264:ARG:NH2	6:D:1535:GLN:OE1	2.46	0.47
1:B:620:LEU:HD12	1:B:676:LYS:HB3	1.97	0.47
1:B:849:ALA:HB2	1:B:872:VAL:HG11	1.95	0.47
6:D:525:THR:O	6:D:529:ARG:HG2	2.15	0.47
6:D:994:ASN:HB2	6:D:1000:LEU:HD22	1.96	0.47
6:D:1181:HIS:HA	6:D:1553:ASN:OD1	2.14	0.47
6:D:1257:THR:OG1	6:D:1259:GLN:OE1	2.25	0.47
1:B:116:ALA:HB1	1:B:157:TRP:HD1	1.79	0.47
3:E:69:THR:HG1	3:E:142:TRP:HD1	1.60	0.47
6:D:767:GLY:O	6:D:770:ILE:HG12	2.15	0.47
6:D:854:ILE:HD13	6:D:886:LYS:HZ1	1.78	0.47
6:D:1567:TYR:HD1	6:D:1572:LYS:HZ1	1.63	0.47
2:C:249:LEU:HD22	2:C:260:LEU:HD11	1.96	0.47
6:D:1437:VAL:HG22	6:D:1465:ARG:HH11	1.78	0.47
6:D:1633:MET:SD	6:D:1633:MET:N	2.87	0.47
5:F:331:LEU:HD21	5:F:345:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1000:LEU:HA	6:D:1003:LEU:HD23	1.96	0.47
6:D:1011:ARG:HA	6:D:1014:LEU:HD12	1.95	0.47
1:B:191:CYS:SG	1:B:229:GLN:NE2	2.88	0.47
3:E:650:GLN:HE21	3:E:712:TYR:HB2	1.80	0.47
5:F:388:ALA:N	5:F:400:GLY:O	2.47	0.47
3:E:962:VAL:HG12	3:E:966:ARG:HG3	1.97	0.47
6:D:802:ALA:O	6:D:805:GLN:HG3	2.15	0.47
2:C:247:VAL:O	2:C:260:LEU:N	2.44	0.47
1:B:26:GLN:HB2	1:B:28:TRP:CD1	2.49	0.46
1:B:1035:TYR:HD1	1:B:1038:ILE:HD12	1.80	0.46
2:C:77:GLY:HA3	2:C:102:ILE:HD11	1.97	0.46
3:E:693:ASN:HB2	3:E:720:TYR:HE2	1.80	0.46
3:E:897:ASN:HD21	3:E:899:ALA:HB3	1.80	0.46
3:E:1107:LEU:O	3:E:1111:ASN:ND2	2.33	0.46
6:D:374:HIS:O	6:D:377:ALA:N	2.37	0.46
6:D:1250:ILE:HD11	6:D:1317:LEU:HB3	1.96	0.46
1:B:469:ARG:HA	1:B:515:GLN:HG2	1.97	0.46
2:C:718:ASP:OD1	2:C:718:ASP:N	2.48	0.46
3:E:28:LEU:HD23	3:E:41:ILE:HD11	1.97	0.46
6:D:671:ASP:OD1	6:D:672:PHE:N	2.48	0.46
6:D:1123:THR:O	6:D:1127:MET:HG3	2.15	0.46
1:B:899:LYS:O	1:B:899:LYS:NZ	2.38	0.46
2:C:438:GLY:HA2	2:C:460:VAL:HG23	1.97	0.46
2:C:895:ARG:NH2	2:C:1255:PRO:O	2.42	0.46
6:D:529:ARG:O	6:D:533:GLN:N	2.48	0.46
2:C:106:ALA:HB3	2:C:115:ALA:HB3	1.96	0.46
2:C:246:LYS:HG2	2:C:262:SER:HA	1.98	0.46
2:C:441:MET:SD	2:C:452:LEU:HA	2.55	0.46
2:C:505:ASN:OD1	2:C:508:VAL:N	2.36	0.46
3:E:541:ILE:HB	3:E:573:MET:HE1	1.98	0.46
5:F:387:PRO:HB3	5:F:399:ALA:HB1	1.97	0.46
6:D:374:HIS:O	6:D:376:ALA:N	2.48	0.46
1:B:869:CYS:HA	1:B:872:VAL:HG12	1.96	0.46
1:B:882:ALA:HA	1:B:887:LEU:HD12	1.97	0.46
2:C:573:ARG:HB3	2:C:603:ARG:HH12	1.81	0.46
2:C:1083:PHE:HD2	2:C:1190:ALA:HB2	1.80	0.46
1:B:168:THR:HG1	1:B:172:GLU:H	1.63	0.46
1:B:794:SER:OG	1:B:795:LYS:NZ	2.49	0.46
2:C:125:TRP:HZ3	2:C:130:PRO:HA	1.81	0.46
5:F:160:ASP:OD1	5:F:160:ASP:N	2.38	0.46
5:F:533:PHE:CD1	5:F:573:VAL:HB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:645:LEU:HD21	6:D:664:LEU:HA	1.97	0.46
6:D:1094:ASP:OD1	6:D:1096:SER:OG	2.34	0.46
1:B:106:ASN:N	1:B:106:ASN:OD1	2.48	0.46
1:B:997:TYR:CZ	1:B:1000:LEU:HD23	2.51	0.46
2:C:1218:ARG:HH21	2:C:1220:TYR:HH	1.61	0.46
3:E:1:MET:O	3:E:693:ASN:ND2	2.44	0.46
3:E:470:ASP:HA	3:E:490:VAL:HG23	1.97	0.46
5:F:788:ILE:H	5:F:788:ILE:HG13	1.52	0.46
6:D:770:ILE:O	6:D:773:GLN:HB2	2.15	0.46
6:D:1462:VAL:O	6:D:1465:ARG:NH2	2.49	0.46
1:B:1231:ASN:HB3	1:B:1236:HIS:HA	1.98	0.46
2:C:774:GLU:O	2:C:778:LYS:NZ	2.44	0.46
2:C:1009:LEU:HD11	2:C:1014:LEU:HD11	1.98	0.46
2:C:1241:ALA:HB1	3:E:1204:ARG:HD3	1.97	0.46
5:F:570:GLN:HA	5:F:587:ASP:HB3	1.98	0.46
1:B:466:ASP:OD2	1:B:479:ARG:NH1	2.47	0.46
1:B:768:GLU:N	1:B:768:GLU:OE1	2.49	0.46
2:C:190:ARG:NH1	2:C:195:ASP:OD1	2.49	0.46
3:E:254:ILE:HD11	3:E:268:THR:HB	1.98	0.46
3:E:832:LEU:HD23	3:E:850:ILE:HD11	1.98	0.46
5:F:535:ASN:OD1	5:F:539:THR:N	2.45	0.46
6:D:321:CYS:O	6:D:323:ILE:N	2.43	0.46
6:D:997:ASP:OD1	6:D:1000:LEU:N	2.46	0.46
2:C:1078:LEU:HD13	2:C:1229:VAL:HG13	1.98	0.46
3:E:1223:ALA:O	3:E:1226:SER:OG	2.26	0.46
5:F:633:PHE:O	5:F:636:THR:OG1	2.32	0.46
6:D:452:LYS:HE2	6:D:481:GLN:HG2	1.96	0.46
1:B:614:LEU:HD12	1:B:624:THR:HB	1.98	0.45
1:B:684:HIS:O	1:B:688:GLN:HG3	2.16	0.45
1:B:1205:ILE:HG21	1:B:1211:ALA:HB2	1.98	0.45
5:F:449:THR:OG1	5:F:461:VAL:O	2.31	0.45
1:B:808:LYS:O	1:B:812:ILE:HG12	2.16	0.45
1:B:1004:GLN:NE2	4:A:182:CYS:O	2.49	0.45
2:C:837:LEU:HG	2:C:847:VAL:HG21	1.98	0.45
1:B:483:THR:OG1	1:B:485:ASP:OD1	2.33	0.45
2:C:43:VAL:HB	2:C:53:HIS:HB2	1.97	0.45
2:C:231:TYR:HB3	2:C:235:GLY:HA2	1.97	0.45
6:D:753:LEU:HD22	6:D:773:GLN:HG2	1.98	0.45
1:B:114:ASP:HB3	1:B:155:VAL:HG12	1.97	0.45
2:C:967:LEU:HB3	2:C:985:ILE:HD13	1.97	0.45
3:E:33:TRP:HE1	3:E:40:LEU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1229:GLU:O	3:E:1233:LEU:HB2	2.17	0.45
6:D:1634:ASP:OD1	6:D:1634:ASP:N	2.50	0.45
3:E:879:TYR:CZ	3:E:887:GLU:HB3	2.51	0.45
5:F:100:CYS:SG	5:F:101:PHE:N	2.90	0.45
5:F:473:ASP:N	5:F:473:ASP:OD1	2.47	0.45
6:D:967:LEU:O	6:D:971:VAL:HG13	2.17	0.45
1:B:664:GLU:O	1:B:667:GLU:HG3	2.16	0.45
1:B:835:LEU:HD12	1:B:835:LEU:H	1.82	0.45
2:C:149:ASN:OD1	2:C:190:ARG:NH2	2.49	0.45
2:C:401:ASP:OD1	2:C:405:ASN:N	2.50	0.45
2:C:799:ARG:HE	2:C:800:LYS:HZ3	1.65	0.45
3:E:4:PHE:CD1	3:E:449:LEU:HB3	2.52	0.45
3:E:1215:GLN:OE1	3:E:1218:VAL:N	2.43	0.45
1:B:18:THR:OG1	1:B:68:VAL:O	2.32	0.45
1:B:105:ASN:OD1	1:B:106:ASN:N	2.50	0.45
1:B:940:LEU:O	1:B:943:LYS:NZ	2.47	0.45
2:C:508:VAL:HB	2:C:511:ASN:ND2	2.31	0.45
3:E:456:ARG:HD2	3:E:824:VAL:HG22	1.99	0.45
3:E:551:GLU:HB3	3:E:555:LEU:HA	1.98	0.45
3:E:844:ASN:HD22	3:E:847:ASP:HB2	1.82	0.45
3:E:863:SER:HB3	3:E:866:ASP:HB2	1.98	0.45
6:D:755:GLU:HG2	6:D:759:LYS:HE2	1.97	0.45
6:D:1308:HIS:O	6:D:1312:ARG:HG2	2.17	0.45
2:C:1172:LEU:HD12	2:C:1173:GLN:HG3	1.99	0.45
6:D:516:TRP:HA	6:D:520:GLY:HA3	1.97	0.45
6:D:527:VAL:O	6:D:531:LEU:N	2.41	0.45
3:E:815:PRO:HD2	3:E:856:ARG:HH22	1.82	0.45
5:F:36:LYS:HD2	5:F:38:ARG:HE	1.81	0.45
6:D:451:ASP:O	6:D:455:THR:OG1	2.25	0.45
6:D:1085:GLU:HA	6:D:1088:ARG:NH2	2.32	0.45
2:C:481:LEU:HD12	2:C:499:VAL:HG11	1.98	0.45
2:C:1232:CYS:SG	2:C:1244:TYR:OH	2.64	0.45
3:E:933:LEU:HD21	3:E:951:LEU:HA	1.98	0.45
4:A:167:LEU:HA	4:A:170:MET:HG2	1.99	0.45
5:F:721:LEU:HD23	5:F:724:ILE:HD11	1.98	0.45
6:D:1106:GLN:HB3	6:D:1110:ARG:NH2	2.32	0.45
6:D:1135:ALA:O	6:D:1139:ILE:HG22	2.16	0.45
6:D:1541:ASP:HA	6:D:1544:PHE:HB3	1.98	0.45
1:B:578:LEU:HG	1:B:590:VAL:HG22	1.98	0.44
3:E:501:ALA:HA	3:E:510:PHE:HA	1.99	0.44
6:D:1038:CYS:SG	6:D:1090:ALA:HA	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HB3	1:B:320:PHE:HB2	1.98	0.44
1:B:146:ARG:NH2	1:B:180:SER:O	2.50	0.44
1:B:378:CYS:SG	1:B:379:VAL:N	2.89	0.44
1:B:1179:SER:O	1:B:1181:ASN:ND2	2.50	0.44
3:E:536:HIS:HB2	3:E:575:ILE:HD13	1.99	0.44
5:F:36:LYS:HG3	5:F:38:ARG:HG2	1.97	0.44
6:D:812:THR:O	6:D:815:HIS:NE2	2.50	0.44
6:D:1109:TYR:CG	6:D:1140:LEU:HD11	2.53	0.44
6:D:1309:ASP:HA	6:D:1312:ARG:HG2	1.98	0.44
6:D:1531:TYR:O	6:D:1534:THR:OG1	2.28	0.44
1:B:897:TYR:OH	1:B:909:GLU:OE2	2.29	0.44
2:C:177:ARG:NH1	2:C:209:TYR:OH	2.49	0.44
3:E:1213:MET:HB2	3:E:1215:GLN:HB2	1.99	0.44
6:D:587:VAL:HA	6:D:590:LYS:HB3	1.99	0.44
6:D:769:VAL:O	6:D:772:ALA:HB3	2.18	0.44
6:D:1239:ASN:OD1	6:D:1242:CYS:N	2.50	0.44
2:C:379:CYS:HA	2:C:393:ASN:HB2	2.00	0.44
3:E:568:GLY:HA3	3:E:586:LYS:NZ	2.31	0.44
3:E:1076:GLN:HA	3:E:1079:PHE:HD2	1.83	0.44
1:B:363:LYS:NZ	1:B:400:GLY:O	2.33	0.44
2:C:884:LEU:HB3	2:C:900:TYR:CE2	2.53	0.44
6:D:1311:ILE:HD13	6:D:1339:THR:HA	1.99	0.44
1:B:408:ILE:HG22	1:B:410:MET:HG3	2.00	0.44
1:B:675:LYS:NZ	1:B:701:CYS:O	2.51	0.44
1:B:710:VAL:HA	1:B:713:VAL:HG22	2.00	0.44
1:B:1213:GLN:NE2	1:B:1214:CYS:O	2.42	0.44
2:C:319:GLN:O	2:C:323:ASP:CA	2.65	0.44
2:C:472:LEU:HB2	2:C:486:LEU:HD11	1.99	0.44
2:C:872:LYS:HA	2:C:872:LYS:HD3	1.90	0.44
3:E:258:LEU:HD23	3:E:258:LEU:HA	1.87	0.44
3:E:1020:ILE:HD11	3:E:1036:ILE:HB	1.99	0.44
6:D:590:LYS:O	6:D:590:LYS:NZ	2.40	0.44
6:D:878:LEU:HD21	6:D:890:TYR:CD2	2.53	0.44
6:D:1059:MET:SD	6:D:1059:MET:N	2.91	0.44
2:C:380:SER:N	2:C:392:SER:O	2.49	0.44
3:E:254:ILE:HD12	3:E:254:ILE:HA	1.78	0.44
6:D:354:LYS:HE3	6:D:383:ARG:HD2	2.00	0.44
6:D:413:ARG:H	6:D:413:ARG:HD2	1.83	0.44
6:D:962:ILE:HA	6:D:965:TYR:HD2	1.83	0.44
1:B:502:GLU:HB2	1:B:525:ARG:HH21	1.82	0.43
1:B:720:LYS:HB3	1:B:720:LYS:HE3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:LYS:HA	2:C:277:LYS:HD3	1.88	0.43
2:C:531:TYR:HB2	2:C:564:HIS:CD2	2.53	0.43
3:E:248:VAL:HG12	3:E:286:GLY:HA3	1.98	0.43
5:F:687:GLN:OE1	5:F:687:GLN:N	2.44	0.43
6:D:840:LEU:O	6:D:843:ALA:HB3	2.18	0.43
1:B:114:ASP:OD1	1:B:115:PHE:N	2.50	0.43
1:B:600:ASN:OD1	1:B:601:HIS:ND1	2.43	0.43
3:E:546:ASN:ND2	3:E:568:GLY:O	2.51	0.43
6:D:870:LEU:O	6:D:874:VAL:HG23	2.18	0.43
1:B:443:ASP:OD1	1:B:446:ASP:N	2.43	0.43
2:C:21:VAL:HG23	2:C:286:GLY:HA2	2.00	0.43
2:C:390:ILE:HG13	2:C:399:MET:HG3	2.00	0.43
6:D:356:ASN:HD21	6:D:358:GLU:HB3	1.83	0.43
6:D:606:MET:HA	6:D:609:GLN:HB3	2.00	0.43
6:D:1594:VAL:HA	6:D:1597:LYS:HB2	2.00	0.43
1:B:251:ILE:HA	1:B:261:ALA:O	2.19	0.43
1:B:475:THR:OG1	1:B:476:MET:N	2.51	0.43
2:C:1:MET:SD	2:C:296:SER:OG	2.71	0.43
3:E:260:ASP:O	3:E:264:ARG:HA	2.17	0.43
6:D:475:VAL:HG13	6:D:487:ALA:HA	2.00	0.43
1:B:685:THR:HB	1:B:690:ASP:HB3	1.99	0.43
3:E:330:ASP:HA	3:E:352:LEU:O	2.17	0.43
6:D:765:GLN:HA	6:D:798:PHE:CE2	2.54	0.43
2:C:917:PRO:HG2	2:C:922:LYS:HE3	2.00	0.43
2:C:1175:VAL:HG11	2:C:1188:PHE:HE1	1.84	0.43
3:E:1093:TRP:NE1	3:E:1105:GLU:OE2	2.43	0.43
3:E:1103:VAL:HG11	3:E:1126:LEU:HD21	2.01	0.43
5:F:925:ILE:HA	5:F:928:TYR:HB3	2.00	0.43
6:D:292:LEU:HA	6:D:295:VAL:HB	1.98	0.43
6:D:306:LYS:O	6:D:306:LYS:NZ	2.52	0.43
6:D:777:ALA:HB3	6:D:785:SER:HB2	2.01	0.43
6:D:1523:GLU:O	6:D:1527:LEU:HG	2.18	0.43
6:D:1579:CYS:HA	6:D:1582:LYS:HD2	2.00	0.43
1:B:22:TRP:CZ2	1:B:304:GLU:HG3	2.53	0.43
3:E:1107:LEU:HG	3:E:1122:ILE:HG21	2.00	0.43
6:D:1145:TYR:CD2	6:D:1154:ALA:HB2	2.54	0.43
1:B:928:ALA:O	1:B:932:LYS:HG2	2.19	0.43
2:C:884:LEU:HD23	2:C:884:LEU:HA	1.86	0.43
3:E:252:GLU:N	3:E:252:GLU:OE1	2.52	0.43
3:E:885:MET:HE1	3:E:908:CYS:HA	2.00	0.43
3:E:1179:PHE:O	3:E:1182:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:757:ALA:HA	6:D:766:ILE:HD11	2.00	0.43
6:D:805:GLN:HA	6:D:808:LYS:HD2	2.01	0.43
4:A:171:ARG:HH11	6:D:1322:PRO:HA	1.84	0.43
5:F:161:PRO:HD3	5:F:181:VAL:HG22	1.99	0.43
6:D:1617:ARG:O	6:D:1617:ARG:NE	2.52	0.43
3:E:246:PRO:O	3:E:285:LYS:NZ	2.50	0.43
3:E:837:LYS:HB3	3:E:840:GLY:HA3	2.01	0.43
5:F:348:LEU:HD11	5:F:386:ASP:HB3	2.01	0.43
5:F:822:SER:O	5:F:826:SER:OG	2.26	0.43
1:B:5:LEU:HD23	1:B:5:LEU:HA	1.89	0.42
1:B:376:ASP:OD1	1:B:376:ASP:N	2.52	0.42
1:B:1016:LEU:HD11	1:B:1045:VAL:HG11	2.01	0.42
2:C:569:TYR:HB3	2:C:578:ALA:HB2	1.99	0.42
5:F:574:LEU:HD23	5:F:574:LEU:HA	1.73	0.42
1:B:835:LEU:O	1:B:839:LEU:HG	2.19	0.42
2:C:381:LEU:HD13	2:C:419:MET:HB2	2.01	0.42
2:C:393:ASN:O	2:C:396:ARG:HG3	2.18	0.42
5:F:533:PHE:CG	5:F:573:VAL:HB	2.53	0.42
6:D:836:SER:HA	6:D:839:GLU:HG2	2.00	0.42
6:D:1135:ALA:HB2	6:D:1168:HIS:CE1	2.47	0.42
6:D:1193:GLU:O	6:D:1197:ALA:N	2.44	0.42
1:B:353:TRP:NE1	1:B:358:ASN:HA	2.28	0.42
1:B:532:ASN:OD1	1:B:537:GLN:N	2.39	0.42
1:B:577:ASN:ND2	1:B:614:LEU:H	2.17	0.42
2:C:350:GLU:OE2	2:C:376:ARG:NH2	2.53	0.42
2:C:909:GLY:HA3	2:C:1211:GLY:HA3	2.01	0.42
2:C:951:GLN:NE2	3:E:1031:THR:O	2.53	0.42
3:E:456:ARG:HB2	3:E:824:VAL:HG13	2.00	0.42
5:F:25:PRO:HG3	5:F:106:GLN:HE22	1.84	0.42
6:D:586:VAL:O	6:D:590:LYS:N	2.38	0.42
1:B:212:ARG:CZ	1:B:346:VAL:HA	2.50	0.42
2:C:121:ASP:OD1	2:C:121:ASP:N	2.51	0.42
2:C:1226:ASP:OD1	2:C:1226:ASP:N	2.51	0.42
3:E:165:LYS:HE3	3:E:172:VAL:HG11	2.01	0.42
4:A:199:LEU:HA	4:A:202:LEU:HG	2.00	0.42
5:F:372:LEU:HD13	5:F:372:LEU:HA	1.83	0.42
5:F:600:SER:HA	5:F:699:MET:HA	2.02	0.42
6:D:508:SER:HB2	6:D:534:ALA:HB2	2.02	0.42
1:B:80:LEU:HB3	1:B:92:TRP:HB2	2.00	0.42
1:B:614:LEU:HD12	1:B:614:LEU:HA	1.87	0.42
1:B:1027:ASP:OD1	1:B:1027:ASP:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:304:SER:HG	3:E:307:THR:HG1	1.57	0.42
3:E:357:LEU:HD12	3:E:368:VAL:HA	2.00	0.42
3:E:911:SER:OG	3:E:912:GLY:N	2.52	0.42
3:E:1011:GLU:OE2	3:E:1035:ARG:NH1	2.37	0.42
6:D:1150:ARG:O	6:D:1150:ARG:NH1	2.46	0.42
2:C:238:ILE:HG23	2:C:250:PHE:HB2	2.02	0.42
2:C:954:PRO:HB2	3:E:1099:ARG:HH11	1.84	0.42
3:E:346:LEU:HD23	3:E:346:LEU:H	1.85	0.42
6:D:1562:GLU:HA	6:D:1565:LEU:HD12	2.00	0.42
2:C:2:HIS:HE1	2:C:4:SER:HB2	1.84	0.42
3:E:1081:THR:O	3:E:1085:GLN:NE2	2.35	0.42
6:D:534:ALA:HA	6:D:537:ALA:HB3	2.02	0.42
1:B:3:VAL:HG21	1:B:280:PHE:CE1	2.54	0.42
1:B:168:THR:OG1	1:B:172:GLU:N	2.50	0.42
2:C:146:TRP:CE2	2:C:153:LEU:HD13	2.54	0.42
2:C:309:ARG:HD3	2:C:334:VAL:HG13	2.02	0.42
3:E:541:ILE:HG12	3:E:550:PHE:CD1	2.54	0.42
3:E:547:ARG:NE	3:E:560:GLN:HA	2.32	0.42
3:E:574:ASP:O	3:E:580:LEU:HA	2.20	0.42
6:D:1012:ARG:HH21	6:D:1016:HIS:CD2	2.37	0.42
6:D:1345:LEU:HD21	6:D:1452:ILE:HG13	2.02	0.42
1:B:699:ILE:HD12	1:B:699:ILE:HA	1.93	0.42
1:B:1059:GLU:OE2	1:B:1149:ARG:NH2	2.53	0.42
2:C:909:GLY:HA2	2:C:1213:LEU:HG	2.02	0.42
3:E:112:VAL:HA	3:E:115:ILE:HG12	2.01	0.42
3:E:510:PHE:HE1	3:E:526:VAL:HG23	1.85	0.42
3:E:808:LEU:HD23	3:E:808:LEU:HA	1.82	0.42
3:E:1231:LEU:HD13	3:E:1231:LEU:HA	1.86	0.42
6:D:558:ALA:HA	6:D:561:ALA:HB3	2.02	0.42
6:D:972:LEU:HB2	6:D:999:ALA:HB2	2.01	0.42
6:D:1221:ASN:N	6:D:1221:ASN:OD1	2.52	0.42
1:B:118:ASN:HD21	1:B:122:THR:H	1.67	0.42
2:C:305:GLN:NE2	2:C:339:THR:HG21	2.34	0.42
6:D:404:LEU:HD13	6:D:440:GLY:HA2	2.02	0.42
6:D:523:GLU:HB3	6:D:526:ALA:HB3	2.02	0.42
6:D:1005:THR:O	6:D:1009:LEU:HG	2.19	0.42
6:D:1573:HIS:CD2	6:D:1601:ASN:HA	2.51	0.42
1:B:1174:CYS:N	1:B:1179:SER:O	2.50	0.41
2:C:626:LEU:O	2:C:629:ARG:NH2	2.53	0.41
5:F:116:LYS:HA	5:F:140:ARG:HA	2.02	0.41
5:F:796:LEU:HD12	5:F:805:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1511:ILE:HA	6:D:1514:LEU:HD12	2.01	0.41
2:C:249:LEU:HD12	2:C:249:LEU:HA	1.90	0.41
3:E:501:ALA:HB2	3:E:535:ILE:HD12	2.02	0.41
1:B:484:ASN:OD1	1:B:484:ASN:N	2.53	0.41
1:B:596:MET:HE1	1:B:645:PHE:CD2	2.55	0.41
3:E:711:GLU:HG3	3:E:828:ILE:HD12	2.00	0.41
6:D:331:ARG:O	6:D:335:GLN:HG2	2.20	0.41
6:D:607:GLU:HA	6:D:610:LEU:HD23	2.02	0.41
6:D:777:ALA:O	6:D:781:ASP:N	2.47	0.41
3:E:1030:SER:HB2	3:E:1088:GLU:HB2	2.02	0.41
5:F:707:ARG:O	5:F:707:ARG:NH1	2.53	0.41
6:D:1235:LEU:HD12	6:D:1236:PRO:HA	2.02	0.41
3:E:467:ILE:HD12	3:E:845:ALA:HB1	2.02	0.41
5:F:502:LEU:HD12	5:F:511:VAL:HG22	2.03	0.41
5:F:799:ARG:HA	5:F:799:ARG:HD3	1.84	0.41
6:D:1433:LEU:HD22	6:D:1434:GLN:HE21	1.86	0.41
6:D:1625:TYR:HA	6:D:1626:PRO:HD3	1.94	0.41
1:B:1149:ARG:HA	1:B:1150:PRO:HD3	1.95	0.41
6:D:1353:LEU:HD23	6:D:1353:LEU:HA	1.83	0.41
6:D:510:LEU:HD13	6:D:510:LEU:HA	1.91	0.41
1:B:872:VAL:HG13	1:B:874:MET:HG2	2.01	0.41
2:C:397:ILE:HD13	2:C:410:TRP:HB2	2.03	0.41
3:E:222:ASP:HB3	3:E:223:ASP:H	1.65	0.41
3:E:638:LEU:HB3	3:E:639:GLU:H	1.61	0.41
3:E:668:THR:O	3:E:685:PHE:N	2.37	0.41
6:D:376:ALA:O	6:D:380:ARG:HG2	2.21	0.41
6:D:1189:LYS:HZ3	6:D:1189:LYS:HG2	1.79	0.41
6:D:1228:ARG:H	6:D:1228:ARG:HG3	1.68	0.41
6:D:1260:ASP:OD1	6:D:1261:LEU:N	2.41	0.41
1:B:538:LEU:HD21	1:B:540:VAL:HG23	2.03	0.41
1:B:688:GLN:HG3	1:B:688:GLN:H	1.77	0.41
1:B:763:VAL:HA	1:B:766:VAL:HG12	2.03	0.41
1:B:1049:GLY:O	1:B:1052:SER:OG	2.29	0.41
2:C:483:VAL:HG13	2:C:494:PHE:H	1.86	0.41
2:C:714:LEU:HB3	2:C:716:MET:SD	2.61	0.41
2:C:837:LEU:HD23	2:C:837:LEU:HA	1.93	0.41
2:C:964:ALA:HB1	2:C:989:LEU:HB2	2.03	0.41
2:C:1038:ASP:OD1	2:C:1038:ASP:N	2.54	0.41
3:E:528:THR:OG1	3:E:543:VAL:O	2.32	0.41
3:E:971:TYR:CE2	3:E:994:PHE:HB3	2.56	0.41
4:A:198:LEU:O	4:A:201:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:491:LEU:HA	5:F:505:THR:HA	2.02	0.41
6:D:1612:ILE:O	6:D:1616:LYS:HG2	2.21	0.41
2:C:350:GLU:HG3	2:C:376:ARG:HE	1.86	0.41
2:C:879:ARG:HH12	3:E:969:LYS:HE2	1.86	0.41
2:C:1035:LYS:HA	2:C:1035:LYS:HD2	1.86	0.41
3:E:188:VAL:HG21	3:E:228:LEU:HD23	2.02	0.41
3:E:1212:LYS:HE3	3:E:1212:LYS:HB3	1.76	0.41
6:D:405:VAL:HG13	6:D:553:TYR:HD2	1.86	0.41
6:D:1141:LEU:HD23	6:D:1141:LEU:HA	1.76	0.41
6:D:1169:TYR:O	6:D:1173:VAL:HG23	2.20	0.41
2:C:82:THR:HG22	2:C:97:GLN:HB3	2.03	0.40
2:C:903:HIS:NE2	2:C:1257:CYS:O	2.41	0.40
2:C:951:GLN:HB3	2:C:953:LEU:HD13	2.02	0.40
2:C:1270:LYS:H	2:C:1270:LYS:HG3	1.66	0.40
3:E:1051:MET:HG2	3:E:1109:PHE:HZ	1.86	0.40
5:F:501:PHE:HB2	5:F:514:LEU:HD21	2.04	0.40
6:D:740:GLN:HB2	6:D:749:ALA:HB2	2.03	0.40
6:D:960:GLU:O	6:D:963:ASN:HB2	2.21	0.40
6:D:1106:GLN:HB3	6:D:1110:ARG:CZ	2.50	0.40
1:B:45:GLY:O	1:B:50:GLN:NE2	2.37	0.40
2:C:692:ASN:OD1	2:C:693:ASP:N	2.54	0.40
3:E:940:TYR:HD2	3:E:946:VAL:HG21	1.86	0.40
6:D:415:ASP:OD1	6:D:415:ASP:N	2.53	0.40
6:D:438:LEU:HD23	6:D:438:LEU:HA	1.94	0.40
6:D:641:PRO:HD3	6:D:670:LEU:HD21	2.03	0.40
6:D:811:LEU:HG	6:D:812:THR:HG23	2.04	0.40
6:D:1440:PRO:HB3	6:D:1466:LEU:HD11	2.03	0.40
1:B:175:VAL:HG21	1:B:234:ILE:HD12	2.03	0.40
1:B:399:ILE:HG23	2:C:587:ALA:HA	2.03	0.40
2:C:6:ARG:NH1	2:C:47:SER:O	2.37	0.40
2:C:1027:LEU:HD21	5:F:556:VAL:HA	2.04	0.40
3:E:564:THR:N	3:E:567:GLU:OE1	2.44	0.40
6:D:312:ASP:OD1	6:D:329:LYS:NZ	2.45	0.40
6:D:493:LEU:HD13	6:D:493:LEU:HA	1.97	0.40
6:D:891:TYR:HD1	6:D:891:TYR:HA	1.74	0.40
6:D:1628:ILE:HD13	6:D:1628:ILE:HA	1.96	0.40
1:B:177:ASP:HB2	1:B:184:LEU:HD11	2.02	0.40
1:B:276:ILE:HD12	1:B:298:CYS:HB3	2.03	0.40
1:B:1223:GLU:HA	1:B:1226:VAL:HG12	2.03	0.40
2:C:563:ALA:HA	2:C:566:LEU:HB3	2.04	0.40
2:C:1014:LEU:HD13	2:C:1022:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:314:SER:OG	3:E:326:GLY:O	2.39	0.40
5:F:594:PHE:CZ	5:F:608:SER:HB3	2.57	0.40
5:F:764:ARG:HD3	5:F:764:ARG:HA	1.94	0.40
5:F:766:ASP:N	5:F:766:ASP:OD1	2.52	0.40
6:D:594:HIS:CE1	6:D:595:LEU:HG	2.57	0.40
6:D:761:ARG:HD2	6:D:761:ARG:HA	1.90	0.40
6:D:1162:LEU:HD23	6:D:1162:LEU:HA	1.89	0.40
6:D:1607:GLN:HB2	6:D:1610:LYS:NZ	2.36	0.40
1:B:73:TRP:CH2	1:B:80:LEU:HD12	2.57	0.40
1:B:856:PHE:HA	1:B:859:ALA:HB3	2.04	0.40
2:C:457:THR:OG1	2:C:458:ALA:N	2.55	0.40
2:C:800:LYS:HA	2:C:800:LYS:HD3	1.89	0.40
2:C:1232:CYS:SG	2:C:1254:CYS:HB2	2.61	0.40
3:E:3:LEU:HG	3:E:454:ARG:HG2	2.04	0.40
3:E:1194:LEU:HD21	3:E:1218:VAL:HG11	2.03	0.40
5:F:841:GLN:HG2	5:F:868:PHE:CD1	2.57	0.40
6:D:733:TYR:OH	6:D:753:LEU:HA	2.22	0.40
6:D:835:GLN:H	6:D:835:GLN:HG3	1.69	0.40
6:D:1591:ASP:OD2	6:D:1593:ASP:N	2.55	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	B	1126/1247 (90%)	1091 (97%)	35 (3%)	0	100	100
2	C	1173/1292 (91%)	1119 (95%)	54 (5%)	0	100	100
3	E	1064/1654 (64%)	1023 (96%)	41 (4%)	0	100	100
4	A	51/368 (14%)	45 (88%)	6 (12%)	0	100	100
5	F	907/1376 (66%)	865 (95%)	42 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	1164/1642 (71%)	1118 (96%)	46 (4%)	0	100	100
All	All	5485/7579 (72%)	5261 (96%)	224 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	B	960/1046 (92%)	926 (96%)	34 (4%)	36	67
2	C	1014/1094 (93%)	986 (97%)	28 (3%)	43	72
3	E	903/1373 (66%)	862 (96%)	41 (4%)	27	61
4	A	50/288 (17%)	47 (94%)	3 (6%)	19	52
5	F	779/1177 (66%)	763 (98%)	16 (2%)	53	79
6	D	971/1320 (74%)	910 (94%)	61 (6%)	18	51
All	All	4677/6298 (74%)	4494 (96%)	183 (4%)	36	64

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	SER
1	B	111	ARG
1	B	163	SER
1	B	211	GLU
1	B	356	ASN
1	B	382	SER
1	B	388	GLN
1	B	415	TYR
1	B	469	ARG
1	B	483	THR
1	B	511	LEU
1	B	533	CYS
1	B	595	ARG

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Mol	Chain	Res	Type
1	B	617	PHE
1	B	624	THR
1	B	668	PHE
1	B	680	LEU
1	B	687	PHE
1	B	688	GLN
1	B	693	TYR
1	B	695	GLU
1	B	720	LYS
1	B	839	LEU
1	B	874	MET
1	B	907	LEU
1	B	927	LEU
1	B	999	PHE
1	B	1002	MET
1	B	1044	LEU
1	B	1047	ASN
1	B	1055	PHE
1	B	1149	ARG
1	B	1187	ARG
1	B	1230	ARG
2	C	6	ARG
2	C	247	VAL
2	C	275	ARG
2	C	305	GLN
2	C	312	MET
2	C	322	VAL
2	C	358	PHE
2	C	432	LEU
2	C	435	LEU
2	C	436	ASN
2	C	475	ILE
2	C	481	LEU
2	C	512	ILE
2	C	514	PHE
2	C	542	PHE
2	C	558	LEU
2	C	584	LEU
2	C	620	VAL
2	C	716	MET
2	C	760	TYR
2	C	775	LYS

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Mol	Chain	Res	Type
2	C	779	MET
2	C	908	TYR
2	C	999	VAL
2	C	1056	MET
2	C	1096	ARG
2	C	1174	TYR
2	C	1269	MET
3	E	7	ASN
3	E	41	ILE
3	E	50	THR
3	E	66	THR
3	E	68	LEU
3	E	150	VAL
3	E	277	VAL
3	E	322	VAL
3	E	325	PHE
3	E	380	HIS
3	E	381	HIS
3	E	437	VAL
3	E	446	LEU
3	E	482	CYS
3	E	499	ASN
3	E	500	ILE
3	E	546	ASN
3	E	591	LEU
3	E	600	GLN
3	E	606	ARG
3	E	841	ASP
3	E	874	MET
3	E	878	TYR
3	E	879	TYR
3	E	889	TYR
3	E	942	ASP
3	E	967	LYS
3	E	970	ARG
3	E	989	ARG
3	E	990	HIS
3	E	1040	THR
3	E	1086	ASN
3	E	1090	LEU
3	E	1165	ASP
3	E	1174	VAL

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Mol	Chain	Res	Type
3	E	1197	TYR
3	E	1212	LYS
3	E	1224	MET
3	E	1232	MET
3	E	1234	GLU
3	E	1237	MET
4	A	191	VAL
4	A	193	TRP
4	A	200	VAL
5	F	266	LEU
5	F	361	PHE
5	F	394	MET
5	F	401	VAL
5	F	450	ASP
5	F	522	THR
5	F	678	TRP
5	F	690	GLU
5	F	702	VAL
5	F	707	ARG
5	F	749	ASN
5	F	806	LEU
5	F	814	ARG
5	F	833	GLU
5	F	839	CYS
5	F	849	ARG
6	D	339	TRP
6	D	400	HIS
6	D	423	PHE
6	D	439	CYS
6	D	469	ASP
6	D	474	THR
6	D	510	LEU
6	D	517	HIS
6	D	518	ARG
6	D	568	TYR
6	D	573	ARG
6	D	593	ARG
6	D	597	PHE
6	D	612	LEU
6	D	617	PHE
6	D	644	PHE
6	D	657	THR

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Mol	Chain	Res	Type
6	D	670	LEU
6	D	679	LEU
6	D	682	LEU
6	D	688	LYS
6	D	733	TYR
6	D	835	GLN
6	D	893	ASP
6	D	905	ARG
6	D	918	ILE
6	D	957	THR
6	D	969	TYR
6	D	974	ASP
6	D	994	ASN
6	D	1003	LEU
6	D	1008	SER
6	D	1017	GLN
6	D	1029	GLU
6	D	1034	MET
6	D	1045	CYS
6	D	1059	MET
6	D	1110	ARG
6	D	1156	ASN
6	D	1158	PHE
6	D	1165	THR
6	D	1172	LEU
6	D	1189	LYS
6	D	1221	ASN
6	D	1227	LEU
6	D	1253	TYR
6	D	1257	THR
6	D	1264	ARG
6	D	1307	LEU
6	D	1327	GLU
6	D	1356	ILE
6	D	1431	PHE
6	D	1435	CYS
6	D	1472	ILE
6	D	1473	THR
6	D	1538	ARG
6	D	1539	LEU
6	D	1578	GLN
6	D	1591	ASP

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Mol	Chain	Res	Type
6	D	1610	LYS
6	D	1624	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	ASN
1	B	108	ASN
1	B	229	GLN
1	B	824	GLN
3	E	183	GLN
3	E	600	GLN
6	D	511	ASN
6	D	540	GLN
6	D	1578	GLN

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

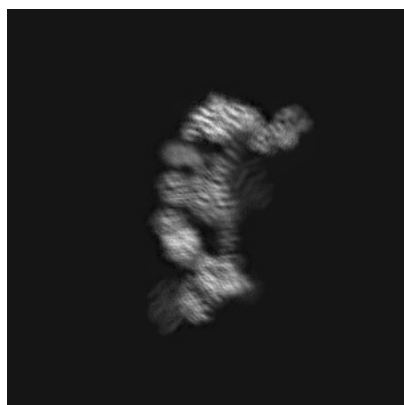
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28866. These allow visual inspection of the internal detail of the map and identification of artifacts.

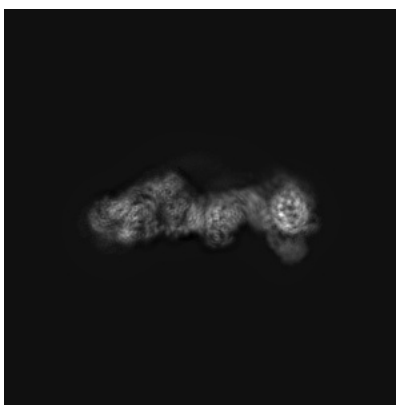
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

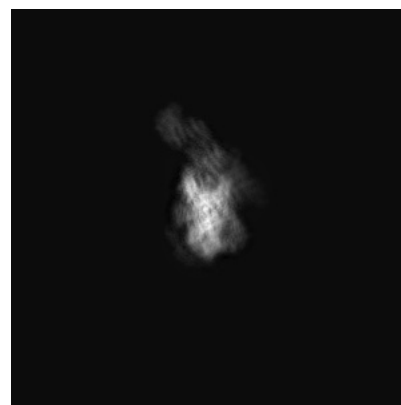
6.1.1 Primary map



X



Y

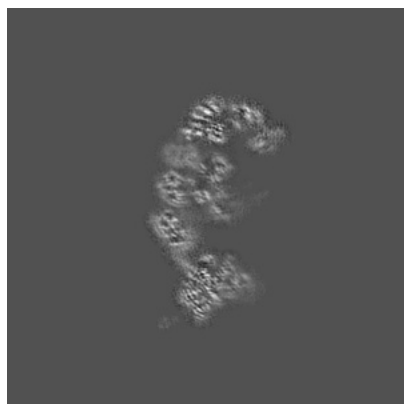


Z

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

6.2 Central slices [i](#)

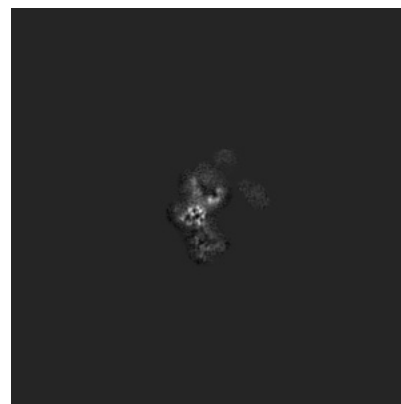
6.2.1 Primary map



X Index: 310



Y Index: 310

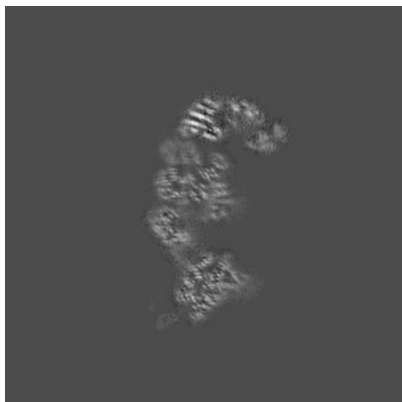


Z Index: 310

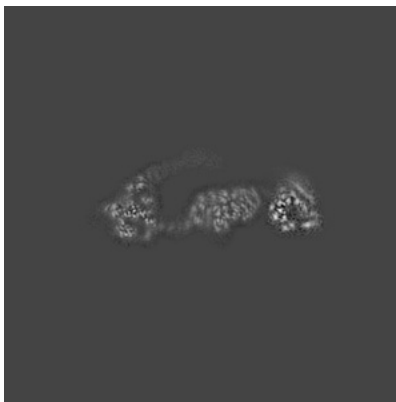
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 305



Y Index: 325



Z Index: 429

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

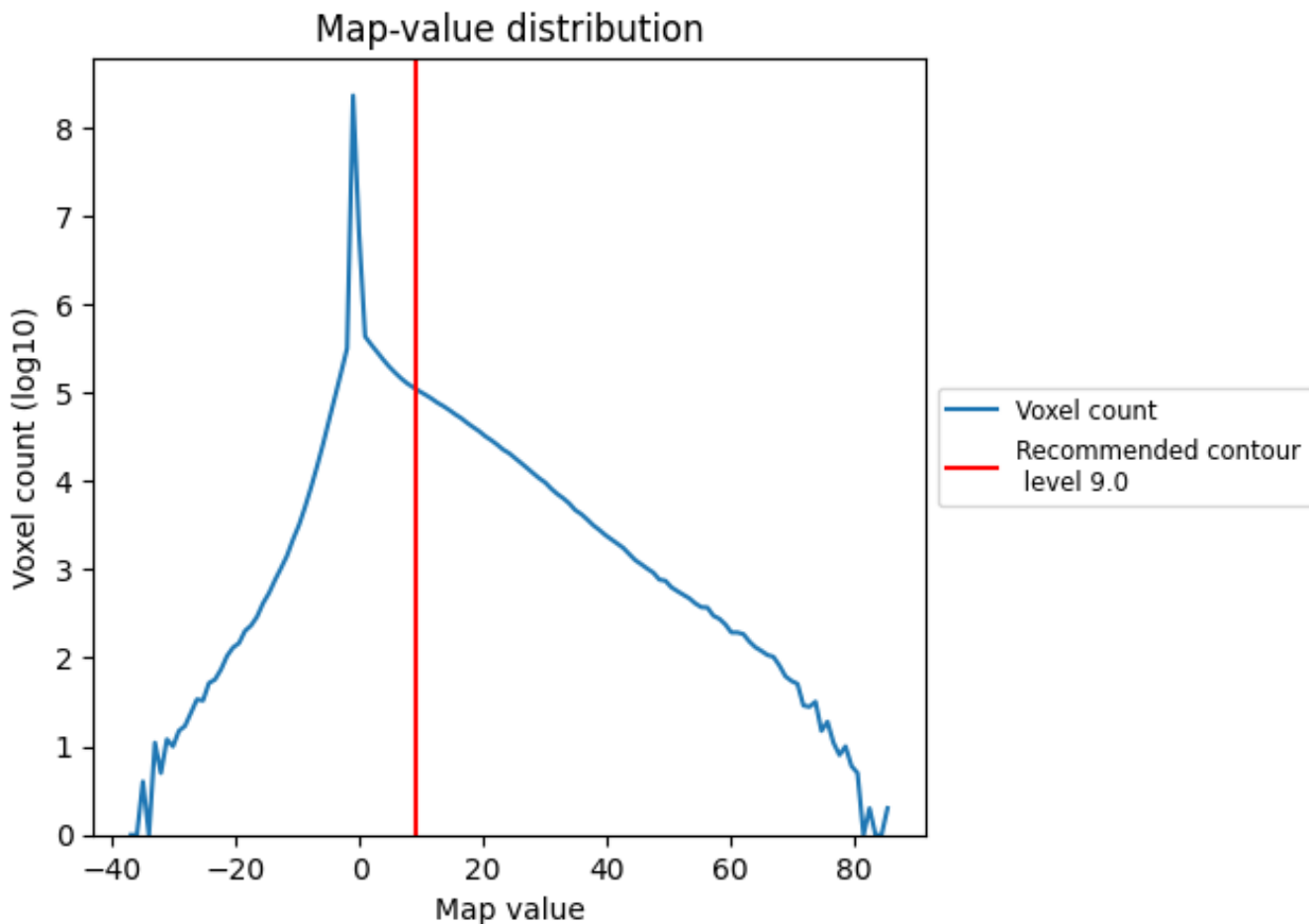
6.5 Mask visualisation

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

7 Map analysis [i](#)

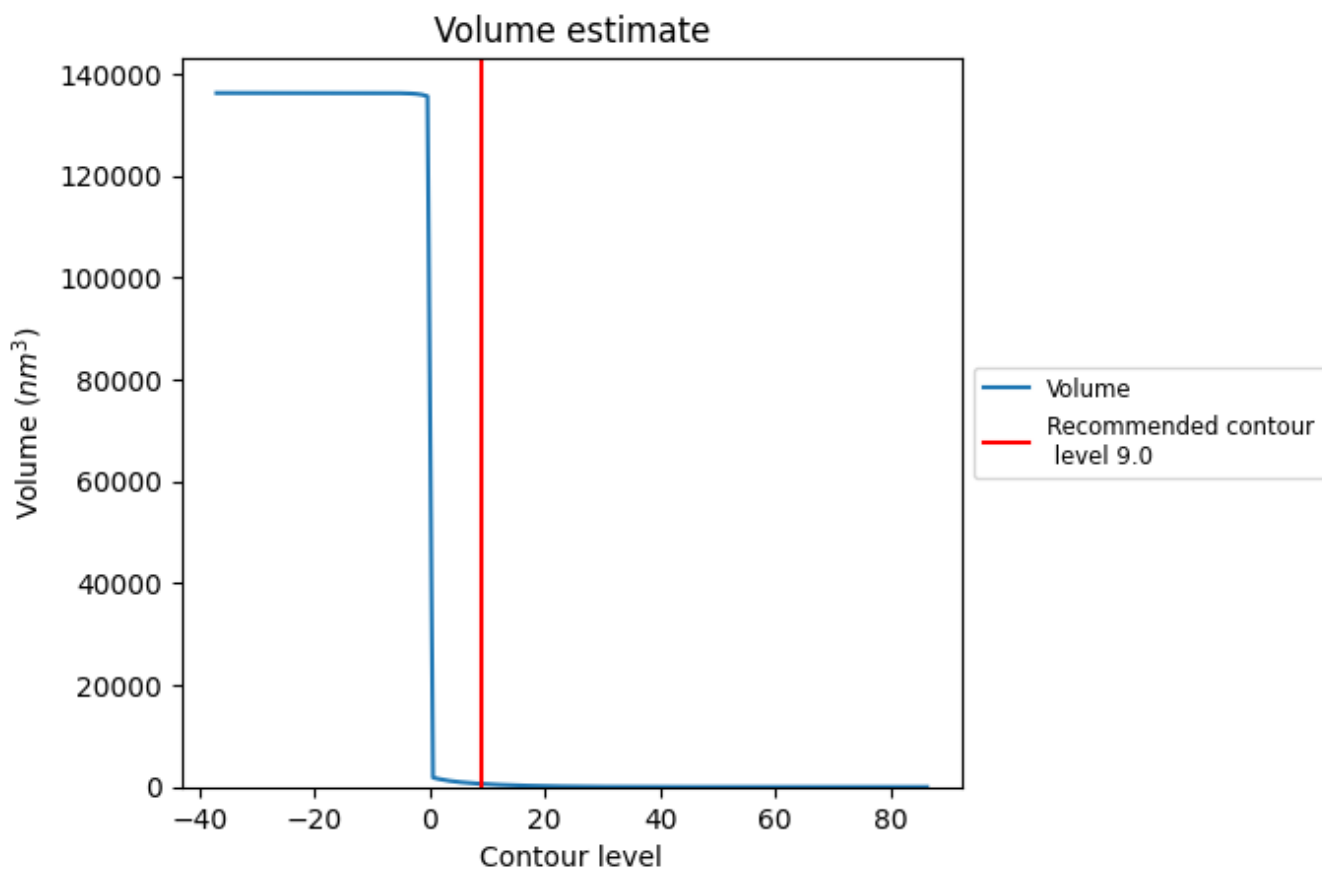
This section contains the results of statistical analysis of the map.

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.

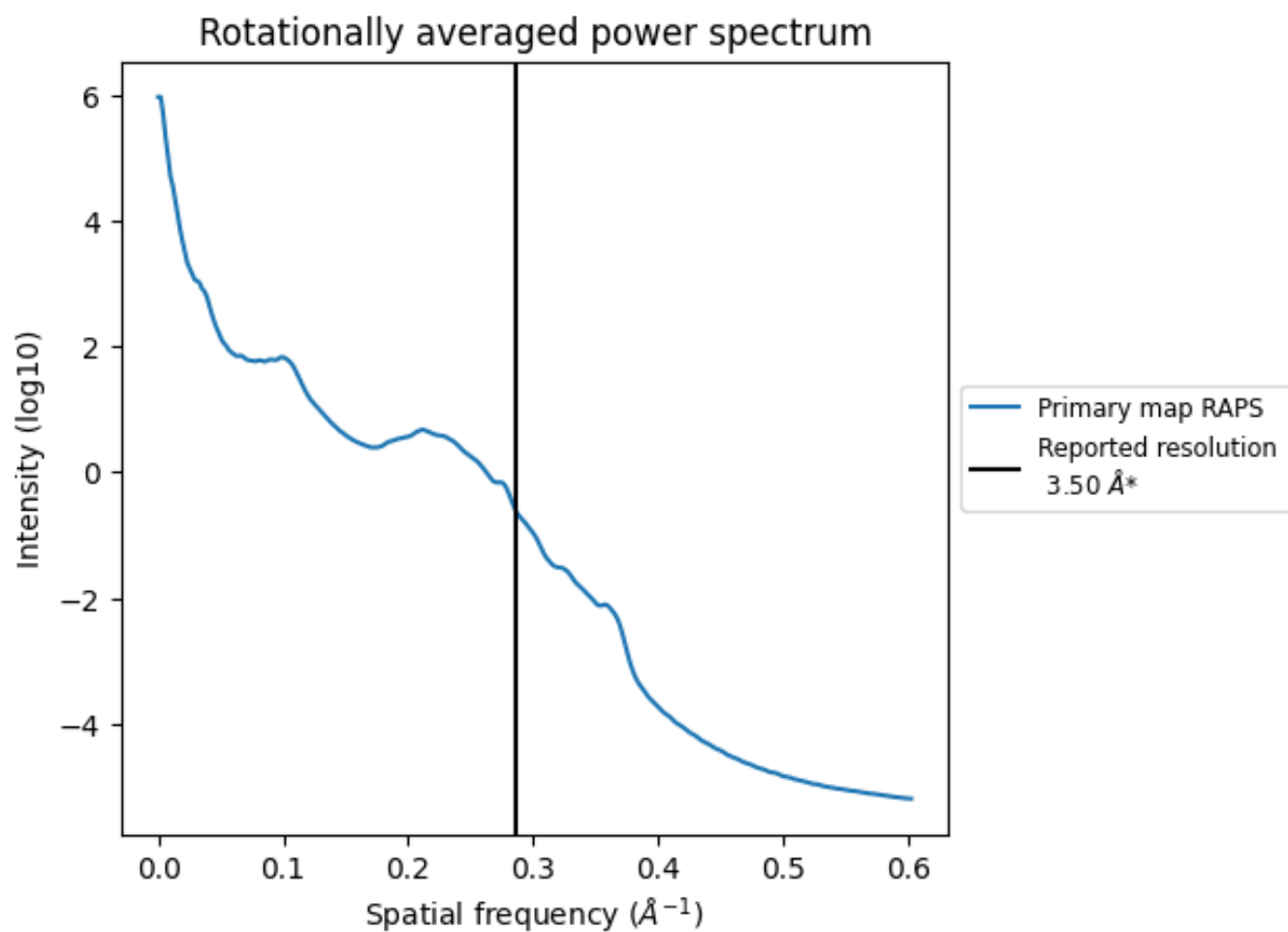
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 619 nm³; this corresponds to an approximate mass of 559 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 0.286\AA^{-1}

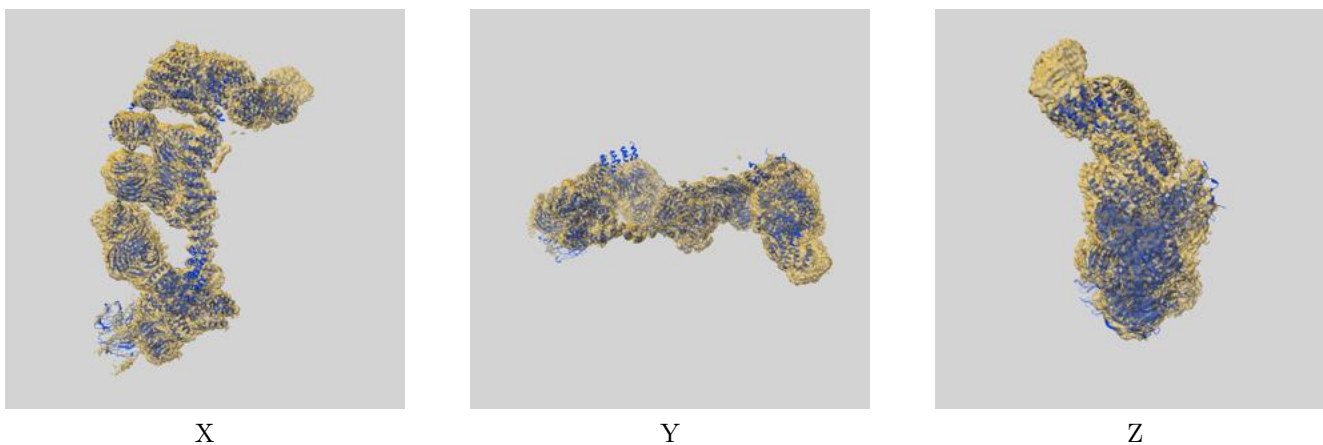
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

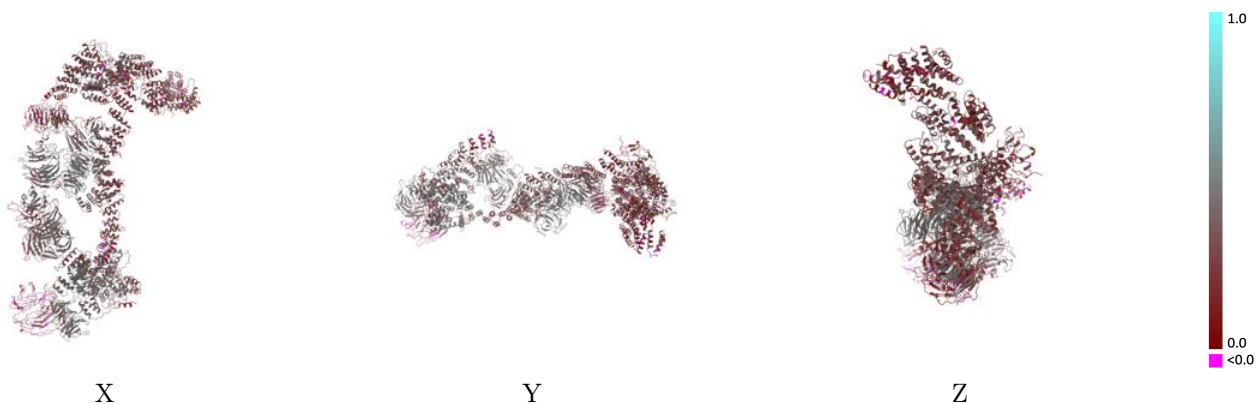
This section contains information regarding the fit between EMDB map EMD-28866 and PDB model 8F5O. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



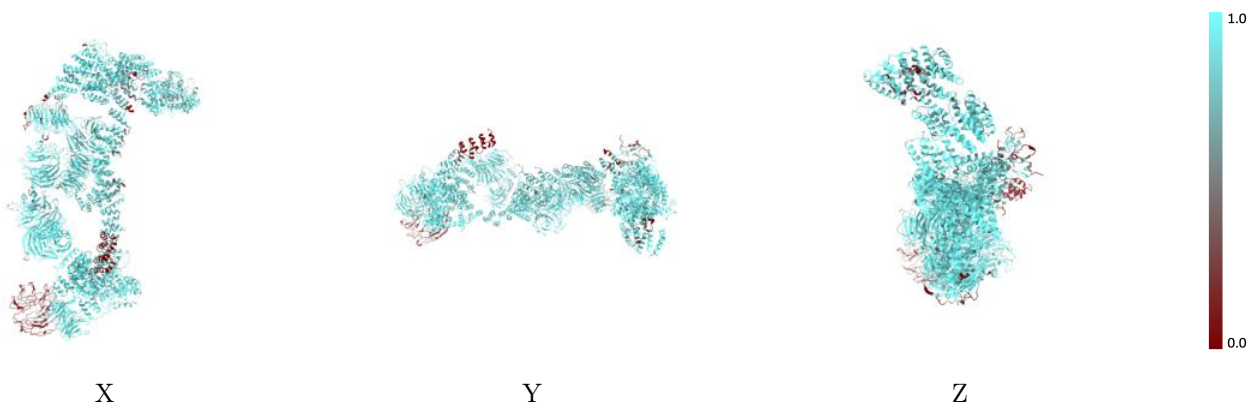
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



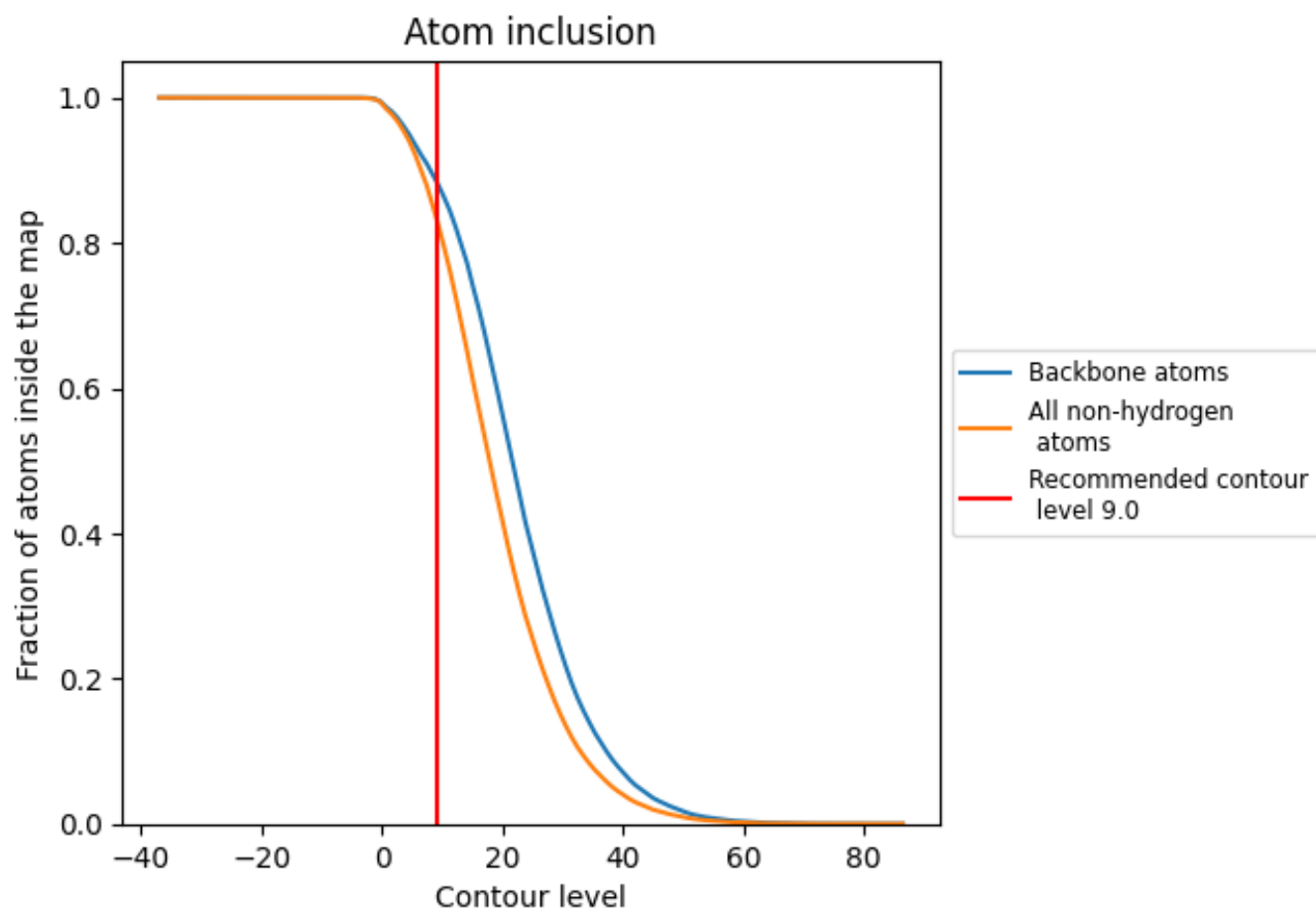
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9.0).















9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (9.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8342	 0.3350
A	 0.8158	 0.2460
B	 0.8775	 0.3710
C	 0.8765	 0.3370
D	 0.8970	 0.2880
E	 0.9351	 0.3800
F	 0.5228	 0.2970

