



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:29 AM UTC

PDB ID : 6FBV / pdb_00006fbv
EMDB ID : EMD-4230
Title : Single particle cryo em structure of Mycobacterium tuberculosis RNA polymerase in complex with Fidaxomicin
Authors : Das, K.; Lin, W.; Ebright, E.
Deposited on : 2017-12-19
Resolution : 3.52 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

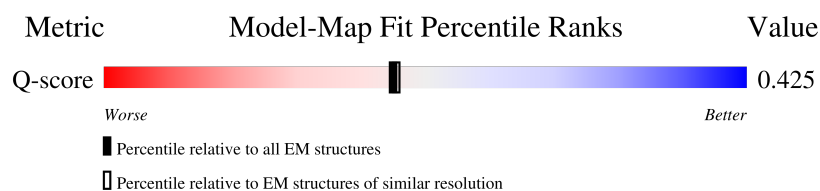
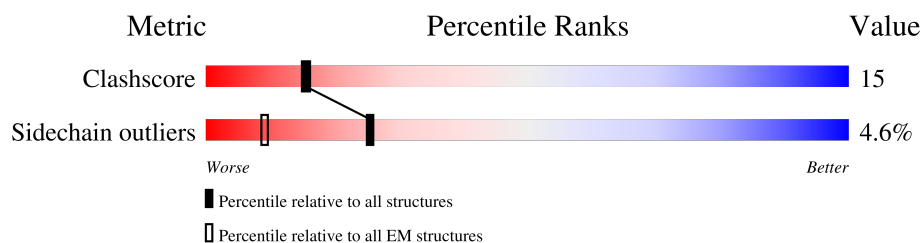
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13017 (3.02 - 4.02)

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	347	
1	B	347	
2	C	1178	
3	D	1316	
4	E	110	

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Mol	Chain	Length	Quality of chain
5	F	528	23%37%17%45%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25146 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	B	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	LEU	ILE	conflict	UNP P9WGZ1
B	3	LEU	ILE	conflict	UNP P9WGZ1

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1118	Total	C	N	O	S	0	0
			8671	5427	1521	1684	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9951	6224	1808	1878	41		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			654	417	108	129		

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	293	Total	C	N	O	S	0	0
			2343	1465	424	445	9		

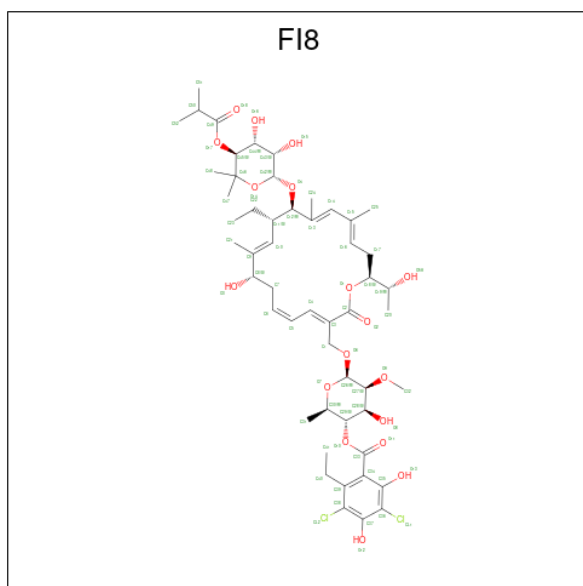
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total	Zn	0
			2	2	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	Mg	0
			1	1	

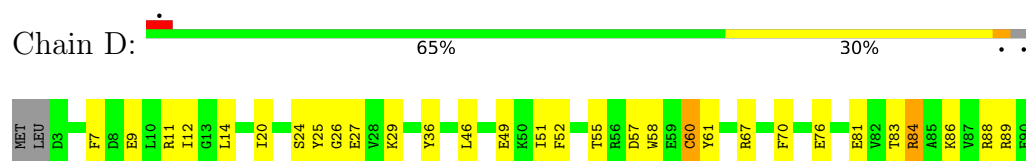
- Molecule 8 is Fidaxomicin (CCD ID: FI8) (formula: C₅₂H₇₄Cl₂O₁₈) (labeled as "Ligand of Interest" by depositor).

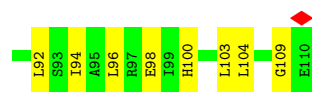


Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	Cl	O	0
			72	52	2	18	

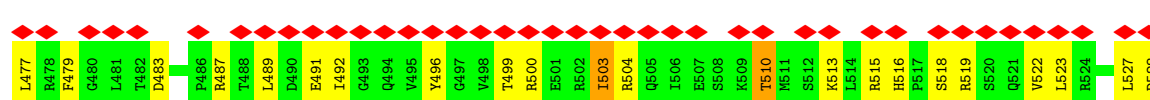
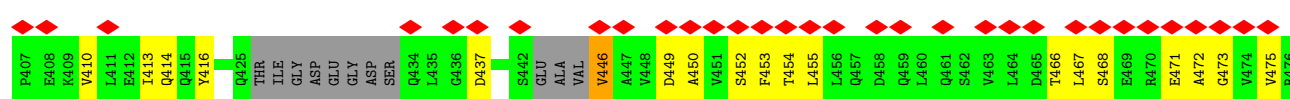
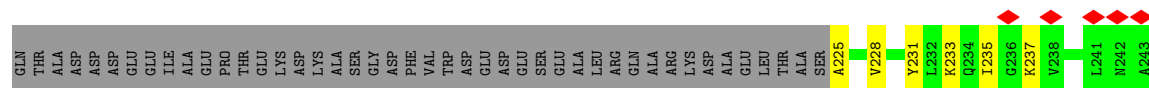
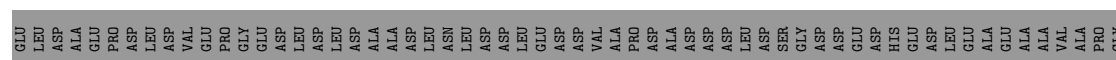
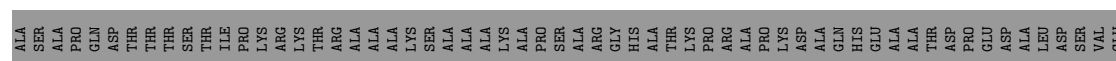
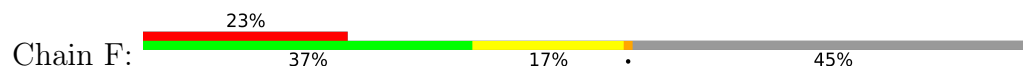
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	D	3	Total	O	0
			3	3	





• Molecule 5: RNA polymerase sigma factor SigA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68895	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 ($e^-/\text{\AA}^2$)	1.4	Depositor
Minimum defocus (nm)	-1.0	Depositor
Maximum defocus (nm)	-2.0	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.255	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	203.712, 203.712, 203.712	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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: MG, FI8, 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	A	0.31	0/1726	0.62	0/2348
1	B	0.26	0/1775	0.61	1/2414 (0.0%)
2	C	0.30	0/8830	0.63	1/11972 (0.0%)
3	D	0.28	1/10116 (0.0%)	0.60	0/13673
4	E	0.26	0/667	0.61	1/908 (0.1%)
5	F	0.20	0/2371	0.54	1/3193 (0.0%)
All	All	0.28	1/25485 (0.0%)	0.61	4/34508 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	592	VAL	CA-C	5.14	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	82	LEU	N-CA-C	7.09	118.90	111.03
5	F	344	SER	N-CA-C	-6.20	104.21	110.97
1	B	57	ASP	N-CA-C	6.20	117.91	111.03
2	C	66	GLY	N-CA-C	-5.19	100.88	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1700	0	1734	48	0
1	B	1749	0	1781	53	0
2	C	8671	0	8610	250	0
3	D	9951	0	10024	338	0
4	E	654	0	648	20	0
5	F	2343	0	2377	86	0
6	D	2	0	0	0	0
7	D	1	0	0	0	0
8	D	72	0	0	7	0
9	D	3	0	0	0	0
All	All	25146	0	25174	736	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 15.

All (736) 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:D:282:ARG:HH21	3:D:282:ARG:CB	1.28	1.43
3:D:282:ARG:HB2	3:D:282:ARG:NH2	1.08	1.40
3:D:285:LYS:HE3	3:D:285:LYS:HA	1.29	1.10
3:D:282:ARG:CB	3:D:282:ARG:NH2	2.04	0.96
3:D:277:LEU:O	3:D:281:ILE:HG13	1.67	0.95
1:B:98:ARG:HG2	1:B:135:GLU:HG2	1.53	0.91
2:C:1106:ILE:HG13	2:C:1112:ILE:HD11	1.59	0.84
3:D:762:ARG:NH1	3:D:762:ARG:HB2	1.93	0.84
5:F:471:GLU:HB3	5:F:510:THR:HG21	1.57	0.84
2:C:232:GLN:HE22	2:C:277:ILE:HG12	1.42	0.83
2:C:819:ARG:O	2:C:823:ALA:HB2	1.79	0.83
3:D:281:ILE:CD1	3:D:296:LEU:HD22	2.09	0.83
3:D:282:ARG:HB2	3:D:282:ARG:CZ	2.08	0.81
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.13	0.80
2:C:226:ILE:HD12	2:C:229:LYS:HZ3	1.44	0.80
1:B:170:PRO:HB2	1:B:202:ILE:HG21	1.64	0.79
3:D:899:VAL:HG11	3:D:920:ALA:HB2	1.64	0.79
2:C:850:ILE:HG22	2:C:871:VAL:HG22	1.63	0.78
3:D:101:VAL:HG21	3:D:378:VAL:HG11	1.65	0.78
3:D:285:LYS:HA	3:D:285:LYS:CE	2.12	0.78
3:D:430:ILE:HD13	3:D:541:MET:HE3	1.66	0.77
5:F:379:LEU:HD23	5:F:413:ILE:HG21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:THR:HG22	3:D:375:GLN:HE22	1.47	0.77
3:D:302:PHE:HZ	3:D:312:MET:HE3	1.49	0.76
3:D:877:LEU:HD22	3:D:1157:ILE:HD13	1.66	0.76
3:D:278:ARG:HA	3:D:281:ILE:HD12	1.66	0.75
2:C:628:THR:HG23	2:C:975:PRO:HA	1.68	0.75
3:D:356:ARG:NH1	5:F:330:ARG:HH22	1.84	0.75
5:F:235:ILE:HD12	5:F:300:LEU:HD13	1.68	0.75
1:A:71:GLU:HG2	1:A:75:GLU:HG2	1.70	0.74
2:C:116:LYS:HE2	2:C:132:PRO:HD3	1.68	0.74
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.53	0.74
3:D:457:MET:SD	3:D:473:LYS:HB2	2.28	0.73
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.69	0.73
3:D:556:ARG:HG3	4:E:35:ILE:HD11	1.71	0.73
3:D:366:ILE:HD13	5:F:325:ASN:HB3	1.69	0.73
3:D:286:GLY:HA2	3:D:289:LYS:HB3	1.69	0.73
3:D:924:THR:HG23	3:D:980:GLY:HA2	1.69	0.72
1:A:175:THR:HG22	2:C:910:GLY:HA3	1.71	0.72
2:C:1007:LYS:HB3	2:C:1022:PRO:HB2	1.70	0.72
1:A:33:THR:HG21	1:B:37:SER:HA	1.72	0.72
3:D:762:ARG:CB	3:D:762:ARG:HH11	2.03	0.72
3:D:746:LEU:HD21	3:D:820:MET:HE1	1.71	0.72
2:C:486:ILE:HD11	3:D:849:TYR:CE2	2.25	0.72
1:B:14:LEU:HD23	1:B:19:SER:HB3	1.72	0.70
1:B:95:MET:HE1	1:B:116:VAL:HG11	1.72	0.70
3:D:463:LEU:HD11	3:D:486:VAL:HG22	1.70	0.70
2:C:1087:GLU:OE2	3:D:547:LEU:HB2	1.91	0.70
3:D:290:LEU:HD23	3:D:290:LEU:C	2.17	0.70
2:C:547:PRO:HB2	2:C:555:VAL:HB	1.74	0.70
3:D:469:ILE:HD13	3:D:469:ILE:C	2.16	0.70
3:D:469:ILE:HD13	3:D:469:ILE:O	1.92	0.70
2:C:919:THR:HG21	3:D:729:VAL:HG12	1.73	0.70
3:D:981:ARG:O	3:D:1152:LYS:NZ	2.25	0.70
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.74	0.69
3:D:1222:SER:HB2	3:D:1250:GLU:HG3	1.73	0.69
2:C:191:ILE:HG13	2:C:198:THR:HG22	1.74	0.69
2:C:1094:ASP:OD2	3:D:420:LYS:NZ	2.24	0.69
5:F:344:SER:O	5:F:348:THR:HB	1.93	0.69
1:A:53:SER:OG	1:A:161:ARG:NH2	2.26	0.69
3:D:762:ARG:NH1	3:D:762:ARG:CB	2.55	0.69
2:C:807:THR:HG23	2:C:835:THR:HG21	1.74	0.68
2:C:1119:GLU:OE1	2:C:1119:GLU:HA	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:281:ILE:HD11	3:D:296:LEU:HD22	1.75	0.68
5:F:299:ASN:HB2	5:F:328:LEU:HD21	1.76	0.68
3:D:384:ASN:HB2	3:D:401:SER:HB3	1.75	0.68
3:D:285:LYS:HE3	3:D:285:LYS:CA	2.17	0.68
5:F:515:ARG:HD3	5:F:518:SER:HB3	1.76	0.67
3:D:459:ARG:O	3:D:463:LEU:HG	1.95	0.67
3:D:892:GLN:HG3	3:D:892:GLN:O	1.94	0.67
3:D:102:THR:HG21	3:D:129:ILE:HD13	1.77	0.67
2:C:446:LEU:HB2	2:C:713:MET:HE2	1.76	0.67
5:F:336:ASP:OD1	5:F:336:ASP:N	2.28	0.67
2:C:232:GLN:NE2	2:C:277:ILE:HG12	2.11	0.66
3:D:1227:GLN:HG3	3:D:1228:GLU:HG3	1.76	0.66
2:C:259:ARG:NH1	2:C:259:ARG:HG2	2.11	0.66
3:D:248:TYR:HB3	3:D:251:TYR:HB2	1.78	0.66
3:D:1053:VAL:HG11	3:D:1099:LEU:HD11	1.78	0.66
2:C:226:ILE:HD12	2:C:229:LYS:NZ	2.11	0.66
2:C:797:ARG:H	2:C:797:ARG:HD2	1.59	0.66
2:C:981:GLN:HG2	2:C:982:GLU:H	1.60	0.66
3:D:463:LEU:O	3:D:464:ASN:HB2	1.94	0.66
3:D:876:ARG:HD2	3:D:1211:THR:HG22	1.78	0.65
2:C:465:ARG:HH11	2:C:492:PRO:HB2	1.60	0.65
3:D:278:ARG:HA	3:D:281:ILE:CD1	2.25	0.65
3:D:567:SER:HB2	3:D:574:LEU:HG	1.78	0.65
5:F:290:ARG:O	5:F:294:HIS:HB3	1.97	0.65
3:D:286:GLY:HA2	3:D:289:LYS:HD3	1.78	0.65
3:D:60:CYS:SG	3:D:61:TYR:N	2.70	0.65
5:F:452:SER:HA	5:F:455:LEU:HD12	1.78	0.64
2:C:259:ARG:HG2	2:C:259:ARG:HH11	1.61	0.64
2:C:311:VAL:HG11	2:C:377:ARG:HD2	1.78	0.64
2:C:611:MET:SD	2:C:892:LYS:HG2	2.37	0.64
3:D:89:ARG:HB3	3:D:323:GLU:HB2	1.79	0.64
3:D:356:ARG:CZ	5:F:330:ARG:NH2	2.60	0.64
1:A:10:SER:HB3	1:A:23:ILE:HG12	1.79	0.64
1:B:15:THR:HG22	1:B:16:ASP:H	1.62	0.64
3:D:589:THR:HG23	3:D:670:ARG:HG2	1.80	0.63
2:C:915:ILE:HD11	2:C:917:LEU:HD21	1.80	0.63
2:C:764:LEU:HD13	2:C:810:GLY:HA2	1.81	0.63
1:A:68:GLY:HA3	1:A:132:GLY:HA3	1.80	0.63
3:D:666:THR:OG1	3:D:667:THR:N	2.32	0.63
3:D:1088:VAL:HB	3:D:1099:LEU:HA	1.80	0.63
1:A:40:ARG:NH1	2:C:903:ASP:OD1	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:800:ILE:O	3:D:804:ASP:HB2	1.99	0.62
5:F:350:TRP:CE3	5:F:350:TRP:HA	2.34	0.62
5:F:249:LEU:HD11	5:F:343:PHE:HZ	1.64	0.62
3:D:1034:LEU:HD11	3:D:1137:GLU:HB3	1.81	0.62
2:C:83:VAL:HG21	2:C:310:ARG:HH22	1.65	0.62
1:B:104:GLU:OE2	1:B:124:HIS:ND1	2.32	0.61
2:C:294:THR:O	2:C:298:ASN:HB2	2.00	0.61
3:D:118:LEU:HD11	3:D:265:ILE:HG13	1.82	0.61
3:D:357:LEU:HD21	3:D:366:ILE:HG22	1.82	0.61
2:C:95:PRO:HB3	2:C:106:SER:HB3	1.83	0.61
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.36	0.61
2:C:1097:VAL:HG22	8:D:1904:FI8:C31	2.31	0.60
2:C:746:VAL:HG12	2:C:747:LEU:HG	1.83	0.60
3:D:177:LEU:HD13	3:D:201:GLY:HA3	1.83	0.60
3:D:598:GLU:HB2	3:D:631:ALA:HB1	1.82	0.60
2:C:1072:GLU:N	2:C:1072:GLU:OE1	2.33	0.60
2:C:525:SER:OG	2:C:527:GLU:HG2	2.01	0.60
2:C:1067:ARG:HA	3:D:421:ARG:HA	1.82	0.60
1:B:10:SER:HA	1:B:22:VAL:O	2.01	0.60
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.84	0.60
3:D:876:ARG:HD2	3:D:1211:THR:CG2	2.32	0.60
2:C:134:PHE:CE1	2:C:153:PHE:HD1	2.20	0.60
3:D:27:GLU:HB2	3:D:94:HIS:CE1	2.36	0.60
3:D:1108:GLY:HA3	3:D:1125:GLN:NE2	2.16	0.60
5:F:306:LEU:HD12	5:F:351:ILE:HD11	1.84	0.60
2:C:1136:GLU:OE1	3:D:11:ARG:NE	2.35	0.59
3:D:463:LEU:CD1	3:D:486:VAL:HG22	2.30	0.59
3:D:965:VAL:O	3:D:1159:ARG:HD2	2.02	0.59
2:C:1133:LEU:HD13	3:D:12:ILE:HD11	1.83	0.59
3:D:765:LEU:HD22	3:D:769:GLU:HB3	1.84	0.59
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.84	0.59
1:B:8:THR:HG21	1:B:26:LEU:HD23	1.85	0.59
2:C:157:PHE:CE1	2:C:389:ILE:HD11	2.38	0.59
2:C:815:THR:HB	2:C:818:GLU:HB3	1.83	0.59
3:D:169:GLU:HB3	3:D:208:ILE:HD13	1.85	0.59
2:C:653:VAL:HG13	2:C:658:ILE:HD11	1.85	0.59
2:C:884:LYS:HD3	2:C:1033:LEU:HD12	1.85	0.59
3:D:1083:ARG:HH11	3:D:1112:MET:HE1	1.68	0.59
4:E:87:LEU:HG	4:E:88:GLN:HG3	1.84	0.59
2:C:732:GLU:HB3	3:D:536:PHE:HD2	1.68	0.59
2:C:760:ARG:HB3	2:C:865:VAL:HG22	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:290:LEU:HD23	3:D:290:LEU:O	2.03	0.58
2:C:157:PHE:HE1	2:C:389:ILE:HD11	1.68	0.58
5:F:231:TYR:CZ	5:F:235:ILE:HD11	2.38	0.58
5:F:489:LEU:HD13	5:F:504:ARG:HH21	1.69	0.58
2:C:658:ILE:HG12	2:C:672:MET:HE3	1.85	0.58
2:C:741:LEU:HD22	2:C:746:VAL:HG11	1.86	0.58
2:C:188:ASP:OD1	2:C:189:GLU:N	2.35	0.58
2:C:775:ASN:HB3	5:F:528:ASP:O	2.02	0.58
3:D:444:PRO:HD2	3:D:447:MET:HE2	1.84	0.58
3:D:925:LEU:HD11	3:D:960:VAL:HG21	1.84	0.58
3:D:95:ILE:HB	3:D:317:VAL:HG22	1.86	0.58
1:A:79:ASN:ND2	1:A:125:ILE:O	2.37	0.58
2:C:882:GLY:O	2:C:1037:VAL:HG13	2.04	0.58
1:B:202:ILE:HD13	1:B:207:ALA:HB2	1.86	0.58
2:C:115:VAL:HG11	2:C:129:TYR:CE2	2.39	0.58
2:C:233:PRO:HB2	2:C:236:VAL:HG23	1.86	0.58
2:C:833:ARG:HG3	2:C:833:ARG:HH11	1.69	0.57
3:D:232:LYS:HG2	3:D:264:LEU:HD21	1.86	0.57
3:D:356:ARG:CZ	5:F:330:ARG:HH22	2.17	0.57
3:D:454:PRO:HA	3:D:457:MET:HE2	1.86	0.57
5:F:317:PHE:HE1	5:F:321:ILE:HD11	1.69	0.57
3:D:327:MET:HG3	3:D:337:THR:HB	1.86	0.57
1:A:119:HIS:ND1	1:A:201:SER:HA	2.19	0.57
2:C:540:VAL:HG22	2:C:563:ARG:HG3	1.85	0.57
3:D:420:LYS:HD2	3:D:420:LYS:N	2.19	0.57
3:D:963:ARG:HG2	3:D:978:CYS:HB2	1.85	0.57
5:F:249:LEU:O	5:F:253:ILE:HG12	2.05	0.57
1:B:50:ALA:HB2	1:B:167:ILE:O	2.03	0.57
2:C:819:ARG:O	2:C:823:ALA:CB	2.51	0.57
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.86	0.57
2:C:187:PHE:HB3	2:C:348:LEU:HD22	1.87	0.57
3:D:156:ALA:O	3:D:160:LYS:CB	2.53	0.57
3:D:872:TYR:HE2	3:D:876:ARG:HH21	1.52	0.57
2:C:855:ARG:HD3	2:C:861:LEU:HD12	1.87	0.57
1:A:153:ARG:HA	1:A:153:ARG:NE	2.20	0.57
1:A:213:LYS:HD2	1:B:223:ARG:HG3	1.87	0.57
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.87	0.57
2:C:833:ARG:HG2	2:C:834:ASP:H	1.68	0.57
2:C:921:GLY:O	2:C:925:ARG:HG2	2.05	0.57
3:D:762:ARG:HH11	3:D:762:ARG:HB3	1.69	0.57
2:C:721:VAL:HG21	2:C:917:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:226:ILE:HD11	2:C:237:LEU:HD22	1.86	0.56
2:C:464:SER:HB3	2:C:467:ARG:HB2	1.87	0.56
5:F:326:LEU:O	5:F:330:ARG:HG3	2.06	0.56
3:D:513:GLU:HB2	4:E:35:ILE:HG21	1.86	0.56
3:D:530:GLU:HB2	3:D:578:ARG:HD2	1.87	0.56
2:C:141:ASN:HD21	2:C:409:VAL:HG13	1.70	0.56
3:D:832:ILE:HG22	3:D:834:ARG:H	1.69	0.56
3:D:427:ARG:HA	3:D:541:MET:O	2.05	0.56
2:C:851:ARG:HH11	2:C:851:ARG:HG2	1.71	0.56
2:C:413:THR:HG22	2:C:415:GLN:H	1.71	0.56
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.88	0.56
2:C:884:LYS:HE2	2:C:892:LYS:HB3	1.88	0.56
3:D:778:TRP:HB2	3:D:823:LEU:HD21	1.88	0.56
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.88	0.56
2:C:226:ILE:H	2:C:229:LYS:HG2	1.70	0.55
2:C:625:LEU:HG	2:C:718:ASN:ND2	2.21	0.55
2:C:853:PHE:O	2:C:867:GLU:HA	2.05	0.55
5:F:331:ALA:CB	5:F:350:TRP:HD1	2.19	0.55
2:C:922:VAL:HB	2:C:923:PRO:HD3	1.87	0.55
8:D:1904:FI8:C24	8:D:1904:FI8:C25	2.84	0.55
1:B:149:ALA:HB2	1:B:164:VAL:C	2.32	0.55
2:C:918:ASN:OD1	2:C:919:THR:N	2.40	0.55
3:D:173:ARG:HD3	3:D:204:GLU:HB3	1.87	0.55
3:D:554:GLU:O	3:D:558:LEU:HB2	2.06	0.55
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.89	0.55
2:C:1128:LEU:HD22	2:C:1133:LEU:HD12	1.89	0.55
3:D:1164:ARG:HD2	3:D:1208:MET:HE1	1.88	0.55
3:D:1246:ASN:OD1	3:D:1246:ASN:N	2.40	0.55
2:C:251:ARG:HG3	2:C:251:ARG:HH11	1.71	0.55
3:D:428:SER:O	3:D:540:GLN:HA	2.07	0.55
5:F:235:ILE:HG23	5:F:300:LEU:HB2	1.88	0.55
2:C:105:LEU:HD12	2:C:138:GLU:O	2.07	0.55
2:C:93:LEU:HD22	2:C:393:MET:HG3	1.89	0.55
2:C:502:VAL:HG23	2:C:587:VAL:O	2.07	0.55
3:D:889:HIS:HB2	3:D:991:ILE:HD11	1.88	0.55
5:F:293:ASN:O	5:F:297:GLU:HG2	2.07	0.55
2:C:400:VAL:HG13	2:C:417:LEU:HB3	1.88	0.55
3:D:507:LEU:HD12	3:D:574:LEU:HD12	1.88	0.54
3:D:992:GLY:O	3:D:1261:GLY:N	2.36	0.54
2:C:1043:ALA:HB2	3:D:447:MET:HG3	1.90	0.54
3:D:1050:THR:HB	3:D:1107:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:297:GLU:HA	5:F:300:LEU:HD12	1.89	0.54
1:A:107:ALA:HB2	1:A:123:MET:HE2	1.88	0.54
2:C:731:TYR:CE1	3:D:579:LEU:HB3	2.42	0.54
5:F:410:VAL:O	5:F:414:GLN:HG2	2.08	0.54
3:D:151:LEU:HD13	3:D:248:TYR:HE2	1.72	0.54
3:D:156:ALA:O	3:D:160:LYS:HB3	2.07	0.54
3:D:184:LEU:HD11	3:D:197:VAL:HG11	1.90	0.54
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.29	0.54
3:D:162:VAL:HG21	3:D:219:LEU:HD11	1.90	0.54
3:D:676:LEU:HD22	3:D:715:LYS:HB3	1.89	0.54
2:C:185:VAL:HG23	2:C:316:VAL:HG22	1.88	0.54
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.90	0.54
3:D:1003:ILE:HD11	3:D:1154:ILE:HG13	1.88	0.54
1:B:171:VAL:HA	1:B:198:THR:HG22	1.90	0.54
2:C:767:GLU:HG2	2:C:807:THR:HA	1.90	0.54
8:D:1904:FI8:C33	8:D:1904:FI8:C41	2.86	0.54
2:C:240:ALA:O	2:C:274:LEU:HD21	2.09	0.53
2:C:53:LEU:HD12	2:C:637:ASP:HB2	1.90	0.53
2:C:611:MET:HE2	2:C:890:GLY:HA2	1.90	0.53
3:D:106:TYR:CD1	3:D:312:MET:HE2	2.42	0.53
3:D:1245:LEU:O	3:D:1251:ASN:ND2	2.41	0.53
5:F:381:ARG:NH1	5:F:385:GLU:OE2	2.41	0.53
3:D:889:HIS:O	3:D:977:THR:OG1	2.21	0.53
3:D:1180:LEU:HD13	3:D:1208:MET:HE2	1.90	0.53
2:C:348:LEU:HD11	2:C:367:THR:HG22	1.89	0.53
1:A:197:GLU:OE2	2:C:996:ARG:NH2	2.41	0.53
3:D:173:ARG:HE	3:D:173:ARG:HA	1.74	0.53
3:D:239:ASN:OD1	3:D:239:ASN:N	2.41	0.53
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.90	0.53
3:D:111:PRO:HB2	3:D:116:TYR:CE2	2.44	0.53
3:D:1269:ASN:O	4:E:109:GLY:HA2	2.09	0.53
1:A:210:SER:HB2	1:B:228:GLU:HG2	1.90	0.53
1:B:183:VAL:HG12	1:B:184:GLU:HG3	1.89	0.53
3:D:461:VAL:HG21	3:D:469:ILE:HA	1.91	0.53
5:F:228:VAL:HA	5:F:318:LEU:HD21	1.91	0.53
1:A:15:THR:HB	1:A:18:ARG:O	2.09	0.52
3:D:789:LEU:HD21	3:D:818:ALA:HB3	1.90	0.52
8:D:1904:FI8:C21	8:D:1904:FI8:C22	2.85	0.52
2:C:102:SER:HA	2:C:142:ASN:HB2	1.90	0.52
2:C:756:GLU:HB3	2:C:870:ARG:HG2	1.92	0.52
3:D:530:GLU:HG3	3:D:574:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:739:ASN:HB2	2:C:899:LEU:O	2.09	0.52
2:C:758:ASP:N	2:C:758:ASP:OD1	2.40	0.52
3:D:116:TYR:HE1	3:D:294:LYS:HB3	1.73	0.52
3:D:52:PHE:CD1	3:D:322:PRO:HD3	2.44	0.52
3:D:356:ARG:NH1	5:F:330:ARG:NH2	2.54	0.52
3:D:778:TRP:CE2	3:D:835:PRO:HG3	2.44	0.52
3:D:387:ARG:NH2	5:F:225:ALA:O	2.43	0.52
3:D:965:VAL:HG11	3:D:1156:VAL:HG22	1.91	0.52
1:A:152:ASN:HB3	1:A:163:PRO:HG3	1.92	0.52
2:C:217:ASP:HB2	2:C:231:ARG:HH12	1.74	0.52
3:D:762:ARG:HB2	3:D:762:ARG:CZ	2.39	0.52
3:D:360:LEU:HD21	5:F:329:ILE:CG2	2.40	0.52
5:F:231:TYR:O	5:F:235:ILE:HG12	2.10	0.52
2:C:449:LEU:HD23	2:C:589:VAL:HG11	1.92	0.51
2:C:820:LEU:HD11	5:F:475:VAL:HG13	1.93	0.51
1:A:191:LYS:HE2	1:A:193:ILE:HD11	1.91	0.51
2:C:56:VAL:HG21	2:C:500:LEU:HD21	1.91	0.51
5:F:446:VAL:HG22	5:F:449:ASP:H	1.75	0.51
5:F:477:LEU:HD11	5:F:496:TYR:HB2	1.92	0.51
2:C:974:THR:OG1	2:C:979:GLY:HA3	2.10	0.51
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.43	0.51
2:C:39:VAL:HG12	2:C:963:LEU:HG	1.91	0.51
3:D:602:ALA:HB1	3:D:606:HIS:O	2.11	0.51
3:D:925:LEU:HD11	3:D:960:VAL:CG2	2.40	0.51
1:A:10:SER:HA	1:A:22:VAL:O	2.10	0.51
2:C:507:ASN:HB3	2:C:513:GLU:CD	2.36	0.51
2:C:822:ARG:CZ	2:C:829:ALA:HB2	2.40	0.51
3:D:1275:THR:HG22	3:D:1277:GLU:H	1.76	0.51
5:F:317:PHE:CE1	5:F:321:ILE:HD11	2.46	0.51
2:C:54:LEU:HD21	2:C:449:LEU:HD12	1.92	0.51
2:C:604:ARG:CZ	2:C:925:ARG:HD2	2.41	0.51
2:C:107:PHE:HB3	2:C:137:ALA:HA	1.92	0.51
3:D:285:LYS:CE	3:D:285:LYS:CA	2.86	0.51
3:D:926:GLY:O	3:D:940:ARG:NH1	2.44	0.51
5:F:468:SER:HB3	5:F:471:GLU:HG2	1.93	0.51
2:C:56:VAL:HG21	2:C:500:LEU:CD2	2.41	0.51
2:C:389:ILE:O	2:C:393:MET:HB2	2.10	0.51
2:C:628:THR:C	2:C:630:MET:H	2.19	0.51
2:C:731:TYR:HE1	3:D:579:LEU:HB3	1.75	0.51
3:D:938:VAL:HG23	3:D:952:LEU:HD13	1.93	0.51
5:F:262:LEU:HD12	5:F:263:MET:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:477:LEU:HD11	5:F:496:TYR:CG	2.46	0.51
2:C:821:LEU:HD12	5:F:523:LEU:HD23	1.93	0.50
2:C:981:GLN:HG2	2:C:982:GLU:N	2.26	0.50
2:C:1077:GLN:HE21	2:C:1085:LEU:HD21	1.76	0.50
3:D:84:ARG:HB3	3:D:86:LYS:HG2	1.92	0.50
3:D:525:HIS:CE1	3:D:527:LEU:HB2	2.45	0.50
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.46	0.50
3:D:1182:ASP:OD1	3:D:1183:ARG:N	2.44	0.50
5:F:510:THR:HG22	5:F:513:LYS:HB2	1.94	0.50
1:B:182:ARG:NH1	3:D:488:GLU:HG2	2.26	0.50
2:C:507:ASN:HB2	2:C:508:PRO:HD2	1.94	0.50
1:A:18:ARG:HB3	1:A:197:GLU:HG3	1.93	0.50
3:D:124:ASP:HB3	3:D:234:LEU:HD11	1.92	0.50
3:D:170:LEU:HD21	3:D:209:ARG:HB2	1.93	0.50
3:D:12:ILE:O	3:D:1240:CYS:HA	2.11	0.50
2:C:689:ILE:CD1	2:C:710:ASP:HA	2.42	0.50
3:D:1003:ILE:HD11	3:D:1154:ILE:HA	1.93	0.50
5:F:350:TRP:HA	5:F:350:TRP:HE3	1.76	0.50
3:D:400:LYS:HD2	3:D:404:ASP:CG	2.36	0.50
3:D:701:ALA:HA	3:D:709:VAL:HG21	1.94	0.50
5:F:334:LYS:HD2	5:F:350:TRP:HE1	1.75	0.50
1:A:8:THR:O	1:B:221:LEU:HD11	2.11	0.50
2:C:224:VAL:HG12	2:C:234:VAL:HA	1.93	0.50
5:F:344:SER:O	5:F:348:THR:CB	2.60	0.50
2:C:226:ILE:HG23	2:C:300:PHE:HZ	1.77	0.50
2:C:107:PHE:N	2:C:107:PHE:CD2	2.77	0.49
3:D:328:VAL:HG21	8:D:1904:FI8:C20	2.42	0.49
3:D:579:LEU:HD11	3:D:808:THR:HB	1.94	0.49
2:C:744:GLU:O	2:C:745:ASP:HB2	2.11	0.49
2:C:936:LEU:HB2	2:C:985:LEU:HD11	1.94	0.49
3:D:1003:ILE:CD1	3:D:1154:ILE:HG13	2.41	0.49
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.94	0.49
3:D:27:GLU:HB2	3:D:94:HIS:HE1	1.77	0.49
3:D:554:GLU:HB3	4:E:54:VAL:HG11	1.94	0.49
3:D:1124:VAL:HG12	3:D:1125:GLN:HG3	1.93	0.49
2:C:928:ILE:CG2	3:D:817:LEU:HD11	2.43	0.49
2:C:239:LYS:HE3	2:C:262:LEU:HD11	1.95	0.49
2:C:252:PHE:CD1	2:C:258:MET:HG2	2.48	0.49
5:F:331:ALA:HA	5:F:350:TRP:HD1	1.78	0.49
5:F:489:LEU:H	5:F:489:LEU:HD23	1.77	0.49
2:C:48:LEU:HD22	2:C:528:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:24:SER:HB2	3:D:94:HIS:HB3	1.95	0.49
3:D:576:MET:HB2	3:D:697:ILE:HD12	1.93	0.49
5:F:291:ALA:O	5:F:295:LEU:HB3	2.12	0.49
1:B:11:GLU:HG2	1:B:12:ASP:N	2.28	0.49
1:B:129:ASN:C	1:B:129:ASN:HD22	2.21	0.49
5:F:473:GLY:HA3	5:F:496:TYR:OH	2.13	0.49
2:C:1127:GLU:HG2	3:D:320:ILE:HD11	1.95	0.49
3:D:904:ARG:HA	3:D:910:LEU:HA	1.95	0.49
5:F:489:LEU:HD13	5:F:504:ARG:NH2	2.27	0.49
1:A:96:TYR:CE2	1:A:137:GLU:HB3	2.48	0.49
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.95	0.49
3:D:1190:ASN:ND2	3:D:1201:ALA:H	2.11	0.49
5:F:355:ILE:O	5:F:359:MET:HB3	2.13	0.49
2:C:104:SER:HB3	2:C:140:ILE:HB	1.94	0.48
2:C:264:LYS:HB3	2:C:264:LYS:HE3	1.64	0.48
2:C:63:TRP:HD1	2:C:70:TRP:CE2	2.31	0.48
2:C:396:MET:HE3	2:C:400:VAL:HG21	1.95	0.48
3:D:554:GLU:HB2	3:D:558:LEU:HD12	1.95	0.48
3:D:456:VAL:O	3:D:460:LEU:HB2	2.12	0.48
3:D:1250:GLU:CD	3:D:1250:GLU:H	2.21	0.48
3:D:131:PHE:HB3	3:D:256:MET:HE3	1.95	0.48
3:D:576:MET:HE1	3:D:694:ALA:HA	1.94	0.48
3:D:826:ASN:HD22	3:D:830:GLU:HG3	1.78	0.48
4:E:43:LEU:HD13	4:E:53:LEU:HD11	1.95	0.48
3:D:352:ASN:O	3:D:355:LYS:HG2	2.14	0.48
4:E:92:LEU:HD23	4:E:96:LEU:HD13	1.94	0.48
3:D:897:ILE:HG23	3:D:1128:ARG:NH2	2.28	0.48
1:A:33:THR:CG2	1:B:37:SER:HA	2.43	0.48
3:D:290:LEU:C	3:D:290:LEU:CD2	2.85	0.48
3:D:302:PHE:CZ	3:D:312:MET:HE3	2.40	0.48
2:C:220:ASP:HB3	2:C:257:ILE:HD12	1.96	0.48
3:D:460:LEU:HD21	3:D:475:MET:SD	2.53	0.48
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.94	0.48
2:C:277:ILE:HD12	2:C:296:LEU:HD11	1.96	0.48
2:C:909:ASP:OD1	2:C:1001:LEU:HD11	2.14	0.48
3:D:1166:THR:OG1	3:D:1206:VAL:HG21	2.13	0.48
3:D:1167:ILE:HD13	3:D:1175:PHE:CD2	2.49	0.48
8:D:1904:FI8:C47	8:D:1904:FI8:C49	2.92	0.48
2:C:191:ILE:HA	2:C:198:THR:HA	1.95	0.47
3:D:1244:LYS:HD2	3:D:1244:LYS:N	2.29	0.47
4:E:82:LEU:HB3	4:E:103:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:272:LYS:HD3	5:F:278:ARG:HH22	1.78	0.47
2:C:805:LYS:HE3	2:C:835:THR:HG23	1.96	0.47
3:D:457:MET:SD	3:D:473:LYS:CB	3.00	0.47
2:C:905:PRO:O	2:C:913:VAL:HG13	2.15	0.47
3:D:26:GLY:HA3	3:D:51:ILE:HG12	1.96	0.47
3:D:491:ILE:HD11	3:D:516:LEU:HG	1.97	0.47
3:D:1010:LEU:HA	3:D:1145:GLN:HG3	1.96	0.47
1:A:68:GLY:HA3	1:A:132:GLY:CA	2.44	0.47
5:F:294:HIS:HA	5:F:297:GLU:HG2	1.96	0.47
5:F:331:ALA:HA	5:F:350:TRP:CD1	2.49	0.47
5:F:499:THR:OG1	5:F:500:ARG:N	2.47	0.47
3:D:400:LYS:HD2	3:D:404:ASP:OD1	2.14	0.47
1:A:13:VAL:O	1:A:19:SER:HB3	2.14	0.47
1:A:162:ILE:HG22	1:A:163:PRO:O	2.15	0.47
2:C:523:VAL:HA	2:C:552:GLY:O	2.15	0.47
3:D:118:LEU:HD21	3:D:265:ILE:HG12	1.97	0.47
2:C:653:VAL:HG13	2:C:658:ILE:CD1	2.45	0.47
2:C:708:THR:HA	2:C:712:GLU:O	2.15	0.47
2:C:1131:LEU:HD13	3:D:105:TRP:CH2	2.50	0.47
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.70	0.47
2:C:177:SER:HB3	2:C:378:LEU:HD21	1.97	0.47
2:C:493:ASN:HA	2:C:496:LEU:HD12	1.97	0.47
3:D:88:ARG:HG3	3:D:323:GLU:HG2	1.95	0.47
3:D:588:LEU:HD13	3:D:723:TRP:CE2	2.50	0.47
1:B:97:LEU:HB2	1:B:110:ILE:HG12	1.96	0.47
3:D:110:VAL:HA	3:D:111:PRO:HA	1.77	0.47
3:D:133:ALA:O	3:D:256:MET:HG3	2.15	0.47
3:D:363:PRO:HG3	5:F:296:LEU:HD22	1.97	0.47
3:D:466:ALA:HB3	3:D:472:ALA:HB2	1.97	0.47
3:D:1120:GLU:OE1	3:D:1123:ARG:NH1	2.48	0.47
3:D:741:ARG:HE	3:D:741:ARG:HB2	1.40	0.46
3:D:821:LYS:HD3	3:D:840:PHE:HE1	1.81	0.46
3:D:923:ARG:NH2	3:D:1155:GLU:OE2	2.48	0.46
1:B:72:ASP:H	1:B:75:GLU:HB2	1.80	0.46
1:B:158:GLU:HB3	1:B:161:ARG:HB2	1.97	0.46
2:C:934:THR:HA	2:C:1027:TYR:O	2.15	0.46
3:D:67:ARG:CZ	5:F:483:ASP:HB3	2.45	0.46
3:D:463:LEU:CD1	3:D:486:VAL:CG2	2.93	0.46
3:D:469:ILE:C	3:D:469:ILE:CD1	2.85	0.46
2:C:251:ARG:HG3	2:C:251:ARG:NH1	2.30	0.46
2:C:473:ARG:HG2	2:C:496:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:29:LYS:O	3:D:352:ASN:ND2	2.32	0.46
3:D:229:LEU:HD12	3:D:233:GLN:OE1	2.15	0.46
3:D:637:LEU:HD11	3:D:671:VAL:HG22	1.97	0.46
3:D:901:LEU:N	3:D:958:THR:O	2.46	0.46
3:D:963:ARG:HG2	3:D:978:CYS:CB	2.45	0.46
2:C:314:TYR:HE2	2:C:318:LYS:HZ3	1.63	0.46
3:D:877:LEU:HD23	3:D:1210:ILE:HD13	1.97	0.46
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.48	0.46
5:F:358:ALA:O	5:F:362:GLN:HG2	2.15	0.46
2:C:1128:LEU:HD23	2:C:1128:LEU:HA	1.74	0.46
3:D:259:GLU:HG3	3:D:260:SER:N	2.30	0.46
3:D:360:LEU:HD21	5:F:329:ILE:HG22	1.96	0.46
5:F:499:THR:HG21	5:F:500:ARG:HH11	1.81	0.46
1:A:209:ALA:HA	1:B:222:ALA:O	2.16	0.46
3:D:9:GLU:OE1	3:D:1244:LYS:NZ	2.42	0.46
3:D:14:LEU:HD23	3:D:14:LEU:HA	1.60	0.46
3:D:793:TYR:CD1	3:D:800:ILE:HG12	2.51	0.46
5:F:449:ASP:O	5:F:453:PHE:HB2	2.16	0.46
2:C:571:VAL:CG1	2:C:575:GLU:HB2	2.46	0.46
3:D:170:LEU:HD22	3:D:205:MET:HE3	1.98	0.46
3:D:331:ASP:OD1	3:D:331:ASP:N	2.48	0.46
2:C:296:LEU:HD23	2:C:296:LEU:HA	1.78	0.46
3:D:52:PHE:O	3:D:91:ARG:HD2	2.16	0.46
3:D:438:LEU:O	3:D:561:SER:OG	2.32	0.46
3:D:616:ALA:O	3:D:620:MET:HG3	2.16	0.46
5:F:296:LEU:O	5:F:300:LEU:HG	2.16	0.46
2:C:129:TYR:CE1	2:C:161:THR:HG22	2.51	0.46
2:C:445:PRO:HB2	2:C:713:MET:SD	2.55	0.46
2:C:529:VAL:HG11	2:C:578:TYR:HE2	1.81	0.46
2:C:1137:VAL:HG11	3:D:7:PHE:CD1	2.51	0.46
5:F:257:LEU:CD2	5:F:337:TYR:CE1	2.99	0.46
1:B:78:LEU:HD21	3:D:611:VAL:HG12	1.98	0.45
2:C:213:GLU:HG2	2:C:225:ARG:O	2.16	0.45
2:C:68:PRO:O	2:C:72:GLU:HG2	2.15	0.45
8:D:1904:FI8:C10	8:D:1904:FI8:C6	2.95	0.45
5:F:299:ASN:HB2	5:F:328:LEU:CD2	2.45	0.45
1:A:55:ARG:HB3	1:A:137:GLU:HG3	1.97	0.45
2:C:689:ILE:HD11	2:C:710:ASP:HA	1.96	0.45
2:C:752:ILE:HG12	2:C:874:ALA:HB2	1.97	0.45
3:D:424:TYR:CE2	3:D:547:LEU:HD11	2.51	0.45
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:189:GLU:HB3	2:C:200:HIS:ND1	2.30	0.45
2:C:514:THR:OG1	2:C:585:GLN:NE2	2.48	0.45
3:D:36:TYR:CD1	5:F:416:TYR:HE1	2.34	0.45
3:D:86:LYS:O	3:D:89:ARG:HG2	2.17	0.45
3:D:579:LEU:CD1	3:D:808:THR:HB	2.47	0.45
1:B:38:LEU:HA	1:B:38:LEU:HD12	1.69	0.45
2:C:200:HIS:HB3	2:C:348:LEU:HD23	1.98	0.45
2:C:223:GLY:HA3	2:C:231:ARG:NE	2.32	0.45
2:C:592:ALA:HB3	2:C:630:MET:HG2	1.97	0.45
3:D:14:LEU:HD21	3:D:106:TYR:OH	2.16	0.45
4:E:71:LEU:HA	4:E:76:LEU:HD21	1.99	0.45
4:E:85:PRO:HB3	4:E:94:ILE:HD13	1.99	0.45
3:D:25:TYR:CD2	3:D:91:ARG:HD3	2.52	0.45
3:D:222:ILE:HD13	3:D:247:ARG:NH2	2.32	0.45
3:D:785:VAL:HG21	3:D:820:MET:HE3	1.99	0.45
2:C:335:GLU:HG3	2:C:336:GLU:H	1.82	0.45
2:C:378:LEU:HD13	2:C:512:ILE:HD11	1.99	0.45
3:D:1244:LYS:HD2	3:D:1244:LYS:H	1.82	0.45
1:B:27:GLU:HB3	1:B:30:PHE:CD1	2.52	0.45
3:D:36:TYR:CE2	5:F:369:PRO:HD3	2.51	0.45
1:B:215:LEU:HA	1:B:215:LEU:HD23	1.73	0.45
3:D:639:GLN:O	3:D:640:LEU:HD23	2.17	0.45
3:D:880:VAL:O	3:D:1160:GLN:HG2	2.17	0.45
5:F:472:ALA:HA	5:F:475:VAL:HB	1.99	0.45
2:C:519:VAL:HG22	2:C:524:VAL:HA	1.98	0.44
2:C:1108:LYS:HD3	2:C:1108:LYS:HA	1.72	0.44
2:C:152:VAL:HG21	2:C:418:ILE:HD12	1.99	0.44
2:C:440:MET:HE3	2:C:452:LYS:HE3	1.99	0.44
2:C:608:GLY:O	2:C:612:GLN:HG3	2.17	0.44
3:D:605:ASP:OD1	3:D:606:HIS:N	2.51	0.44
3:D:817:LEU:HD12	3:D:817:LEU:HA	1.65	0.44
3:D:985:THR:HG22	3:D:987:LYS:HG3	1.98	0.44
3:D:1038:ARG:HE	3:D:1038:ARG:HB2	1.57	0.44
3:D:1117:ASP:O	3:D:1121:VAL:HG23	2.18	0.44
1:A:23:ILE:HD12	1:A:192:LEU:HD23	1.98	0.44
1:A:33:THR:HG21	1:B:37:SER:CA	2.46	0.44
1:B:78:LEU:HD22	3:D:613:SER:HA	1.99	0.44
1:B:99:LYS:HG2	1:B:100:GLN:H	1.83	0.44
1:B:220:GLY:O	1:B:224:GLU:HG3	2.18	0.44
2:C:67:SER:OG	2:C:68:PRO:HD2	2.17	0.44
2:C:809:LYS:H	2:C:832:VAL:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:934:THR:HG1	2:C:1028:MET:HE3	1.82	0.44
3:D:926:GLY:H	3:D:962:VAL:HA	1.81	0.44
3:D:1034:LEU:HD13	3:D:1138:VAL:HG23	1.99	0.44
3:D:1086:LEU:HB2	3:D:1112:MET:C	2.43	0.44
4:E:46:ARG:HE	4:E:100:HIS:HA	1.82	0.44
4:E:47:VAL:HG21	4:E:53:LEU:N	2.32	0.44
3:D:445:LYS:HA	3:D:516:LEU:HD22	1.99	0.44
4:E:47:VAL:HG23	4:E:56:TYR:HD1	1.83	0.44
1:A:171:VAL:HG12	1:A:172:LEU:H	1.83	0.44
2:C:217:ASP:HB3	2:C:221:THR:H	1.82	0.44
2:C:449:LEU:HB2	2:C:638:ALA:HB2	1.98	0.44
2:C:449:LEU:CD2	2:C:589:VAL:HG11	2.47	0.44
2:C:604:ARG:NH1	2:C:925:ARG:HD2	2.32	0.44
2:C:752:ILE:HG12	2:C:874:ALA:CB	2.47	0.44
3:D:443:LEU:HD12	3:D:443:LEU:HA	1.77	0.44
3:D:1190:ASN:HD21	3:D:1201:ALA:H	1.66	0.44
1:A:61:HIS:HB2	2:C:846:LYS:HD2	2.00	0.44
1:A:144:ARG:HG3	1:A:144:ARG:HH11	1.83	0.44
2:C:882:GLY:HA2	2:C:894:VAL:CG1	2.47	0.44
3:D:194:ARG:HD2	3:D:194:ARG:C	2.42	0.44
3:D:739:PRO:HG2	3:D:742:LYS:HB2	2.00	0.44
3:D:913:ASP:CG	3:D:914:PRO:HD2	2.43	0.44
3:D:1023:ASP:OD1	3:D:1023:ASP:N	2.50	0.44
3:D:1033:GLU:HB2	3:D:1038:ARG:NH2	2.32	0.44
2:C:732:GLU:HB3	3:D:536:PHE:CD2	2.49	0.44
3:D:136:ILE:HD13	3:D:229:LEU:HD11	1.99	0.44
3:D:827:PRO:HD3	3:D:854:HIS:CD2	2.53	0.44
3:D:1096:GLU:H	3:D:1096:GLU:CD	2.26	0.44
5:F:292:LYS:HB3	5:F:292:LYS:HE2	1.71	0.44
2:C:247:GLN:HA	2:C:250:GLU:HG2	2.00	0.44
2:C:854:SER:HA	2:C:867:GLU:HG3	2.00	0.44
2:C:1038:ASP:OD1	2:C:1038:ASP:N	2.51	0.44
2:C:1125:LEU:HD23	2:C:1125:LEU:HA	1.66	0.44
3:D:131:PHE:CB	3:D:256:MET:HE3	2.48	0.44
3:D:151:LEU:HD13	3:D:248:TYR:CE2	2.52	0.44
3:D:459:ARG:HD2	3:D:459:ARG:HA	1.83	0.44
3:D:880:VAL:HA	3:D:1214:SER:HB3	1.99	0.44
1:A:119:HIS:CE1	1:A:201:SER:HA	2.52	0.44
3:D:120:LEU:HD12	3:D:125:LEU:HD13	1.99	0.44
3:D:988:LEU:HD23	3:D:988:LEU:HA	1.73	0.44
3:D:1108:GLY:HA3	3:D:1125:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:445:PRO:HD2	2:C:707:CYS:HB2	1.99	0.43
2:C:631:GLU:HB3	2:C:713:MET:HB2	1.99	0.43
3:D:629:VAL:HG11	3:D:723:TRP:CH2	2.53	0.43
3:D:820:MET:HE2	3:D:820:MET:HB3	1.70	0.43
3:D:874:THR:OG1	3:D:1004:GLY:HA3	2.18	0.43
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.80	0.43
1:B:96:TYR:O	1:B:110:ILE:HG23	2.18	0.43
2:C:39:VAL:CG1	2:C:963:LEU:HG	2.48	0.43
2:C:378:LEU:HD11	2:C:455:LEU:HG	2.00	0.43
3:D:250:GLU:O	3:D:250:GLU:HG2	2.17	0.43
3:D:1267:TYR:O	3:D:1270:ILE:HG13	2.18	0.43
2:C:485:PRO:HB2	3:D:853:THR:HG21	1.99	0.43
2:C:773:ILE:CG2	2:C:776:ILE:HD12	2.49	0.43
2:C:820:LEU:HD12	5:F:479:PHE:CB	2.48	0.43
2:C:1118:PRO:HG2	3:D:1255:GLY:HA3	1.99	0.43
3:D:946:ASP:N	3:D:947:PRO:HD2	2.34	0.43
4:E:103:LEU:HA	4:E:103:LEU:HD23	1.57	0.43
5:F:231:TYR:CE1	5:F:235:ILE:HD11	2.53	0.43
1:A:8:THR:O	1:A:9:LEU:HD23	2.17	0.43
2:C:413:THR:HG23	2:C:414:PRO:HD2	2.00	0.43
2:C:490:GLU:OE2	2:C:607:MET:HE2	2.17	0.43
3:D:256:MET:HE2	3:D:256:MET:HB3	1.96	0.43
3:D:454:PRO:HA	3:D:457:MET:CE	2.48	0.43
5:F:349:TRP:CZ3	5:F:350:TRP:CZ3	3.07	0.43
1:B:85:VAL:HG11	1:B:140:VAL:HG11	2.01	0.43
2:C:240:ALA:HB1	2:C:274:LEU:HD23	1.99	0.43
2:C:525:SER:OG	2:C:526:ASP:N	2.52	0.43
2:C:925:ARG:HB2	2:C:927:ASN:OD1	2.18	0.43
3:D:425:SER:HA	3:D:543:VAL:O	2.19	0.43
3:D:730:THR:HG22	3:D:731:VAL:N	2.33	0.43
3:D:925:LEU:HA	3:D:925:LEU:HD12	1.63	0.43
5:F:249:LEU:HD11	5:F:343:PHE:CZ	2.49	0.43
1:A:51:VAL:HG11	1:A:138:LEU:HD23	2.00	0.43
2:C:965:GLU:O	2:C:965:GLU:HG3	2.18	0.43
3:D:118:LEU:O	3:D:120:LEU:HG	2.19	0.43
2:C:485:PRO:O	3:D:857:ARG:NH2	2.52	0.43
2:C:613:ARG:HB2	2:C:613:ARG:CZ	2.49	0.43
2:C:632:LEU:HD12	2:C:711:GLY:O	2.18	0.43
2:C:944:TRP:CE2	2:C:988:LEU:HD22	2.54	0.43
3:D:363:PRO:HG2	3:D:366:ILE:HG13	2.00	0.43
3:D:931:ASP:OD1	3:D:932:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	2.00	0.43
5:F:503:ILE:HD12	5:F:503:ILE:HA	1.85	0.43
5:F:292:LYS:O	5:F:296:LEU:HB2	2.19	0.43
1:A:12:ASP:OD1	1:A:13:VAL:N	2.52	0.43
1:B:18:ARG:HG2	1:B:197:GLU:HG3	2.01	0.43
1:B:40:ARG:O	1:B:44:SER:HB3	2.19	0.43
1:B:146:TYR:O	3:D:624:ARG:NE	2.49	0.43
2:C:150:GLN:HG2	2:C:151:THR:H	1.84	0.43
2:C:412:ILE:HD12	2:C:412:ILE:HA	1.89	0.43
3:D:1005:GLU:C	3:D:1007:GLY:H	2.27	0.43
1:B:97:LEU:HD13	1:B:110:ILE:HG12	2.01	0.43
2:C:627:GLY:O	2:C:973:SER:HA	2.19	0.43
2:C:846:LYS:O	2:C:873:VAL:HA	2.18	0.43
3:D:244:LEU:HG	3:D:252:PHE:CZ	2.54	0.43
3:D:463:LEU:HB3	3:D:465:HIS:CE1	2.54	0.43
3:D:716:LEU:HD23	3:D:716:LEU:HA	1.77	0.43
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.84	0.43
3:D:746:LEU:HD23	3:D:746:LEU:HA	1.70	0.42
3:D:1034:LEU:HD11	3:D:1137:GLU:CB	2.47	0.42
5:F:466:THR:HG21	5:F:516:HIS:CE1	2.54	0.42
2:C:213:GLU:CG	2:C:225:ARG:HB2	2.49	0.42
3:D:939:GLU:OE1	3:D:939:GLU:N	2.47	0.42
3:D:1055:LEU:HD12	3:D:1064:ILE:HG12	2.00	0.42
2:C:400:VAL:HG22	2:C:417:LEU:O	2.19	0.42
3:D:527:LEU:HD23	3:D:527:LEU:HA	1.65	0.42
1:B:98:ARG:HB3	1:B:133:LYS:NZ	2.34	0.42
2:C:107:PHE:HB3	2:C:137:ALA:CB	2.49	0.42
2:C:116:LYS:HA	2:C:116:LYS:HD3	1.82	0.42
2:C:140:ILE:HA	2:C:147:ILE:HG12	2.02	0.42
2:C:224:VAL:HG21	2:C:237:LEU:HD23	2.00	0.42
2:C:279:ARG:HH21	2:C:287:PRO:HB2	1.85	0.42
2:C:348:LEU:HD21	2:C:367:THR:HG22	2.00	0.42
3:D:1245:LEU:HD23	3:D:1245:LEU:HA	1.79	0.42
2:C:479:HIS:O	2:C:480:TYR:C	2.62	0.42
3:D:480:ARG:O	3:D:483:VAL:HG22	2.20	0.42
5:F:331:ALA:CA	5:F:350:TRP:HD1	2.32	0.42
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.67	0.42
2:C:98:ASP:OD1	2:C:99:PHE:N	2.52	0.42
2:C:202:VAL:HG21	2:C:345:LEU:HB2	2.02	0.42
2:C:218:LYS:H	2:C:218:LYS:HG2	1.71	0.42
2:C:689:ILE:HG22	2:C:702:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:276:SER:O	3:D:280:VAL:HG23	2.19	0.42
3:D:731:VAL:HG22	3:D:799:ILE:HD11	2.01	0.42
1:A:65:THR:HG22	1:A:72:ASP:HB3	2.02	0.42
1:B:98:ARG:HG2	1:B:135:GLU:CG	2.38	0.42
2:C:1101:LYS:HD3	2:C:1101:LYS:HA	1.75	0.42
3:D:1274:PRO:HA	4:E:104:LEU:HD23	2.00	0.42
2:C:134:PHE:HE1	2:C:153:PHE:HD1	1.65	0.42
3:D:451:LEU:HD23	3:D:451:LEU:HA	1.65	0.42
2:C:934:THR:OG1	2:C:1028:MET:HE3	2.19	0.42
3:D:624:ARG:HG2	3:D:626:VAL:HG23	2.02	0.42
2:C:401:ARG:O	2:C:404:MET:HG2	2.20	0.42
2:C:483:MET:HE3	2:C:498:GLY:HA3	2.01	0.42
2:C:785:ASP:HA	2:C:791:ARG:NH2	2.34	0.42
3:D:76:GLU:CD	3:D:76:GLU:H	2.28	0.42
3:D:642:PRO:HB3	3:D:662:TRP:CD2	2.55	0.42
3:D:1276:GLU:H	3:D:1276:GLU:CD	2.28	0.42
1:A:223:ARG:HD2	1:B:213:LYS:HG3	2.01	0.41
2:C:809:LYS:N	2:C:831:GLU:O	2.53	0.41
2:C:905:PRO:HB2	2:C:1010:LEU:HD13	2.02	0.41
3:D:49:GLU:OE2	3:D:55:THR:OG1	2.29	0.41
3:D:778:TRP:CB	3:D:823:LEU:HD21	2.49	0.41
1:A:9:LEU:HA	1:B:221:LEU:HD13	2.02	0.41
1:A:89:GLU:HG2	1:A:90:ASP:N	2.36	0.41
1:B:71:GLU:HG3	1:B:75:GLU:OE1	2.20	0.41
3:D:468:ASN:OD1	3:D:468:ASN:N	2.51	0.41
1:A:129:ASN:OD1	1:A:130:ASP:N	2.52	0.41
2:C:384:LEU:HD23	2:C:384:LEU:HA	1.80	0.41
2:C:631:GLU:H	2:C:631:GLU:HG3	1.70	0.41
2:C:1091:ILE:CD1	2:C:1102:VAL:HG21	2.49	0.41
3:D:57:ASP:HB3	3:D:58:TRP:HE3	1.82	0.41
3:D:156:ALA:O	3:D:160:LYS:HB2	2.20	0.41
3:D:234:LEU:HA	3:D:234:LEU:HD23	1.78	0.41
3:D:573:PRO:HG2	3:D:576:MET:HE2	2.02	0.41
3:D:816:THR:HG23	3:D:821:LYS:HA	2.01	0.41
5:F:387:LEU:HD13	5:F:393:GLU:HA	2.01	0.41
2:C:450:THR:HG21	2:C:613:ARG:HD2	2.02	0.41
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	2.02	0.41
5:F:487:ARG:HH21	5:F:491:GLU:HG2	1.85	0.41
3:D:104:ILE:HD11	3:D:386:ARG:HB3	2.02	0.41
3:D:471:SER:O	3:D:474:ARG:HB3	2.21	0.41
3:D:1063:LYS:HG3	3:D:1077:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:O	1:A:8:THR:HG23	2.20	0.41
1:B:226:ASN:CG	1:B:227:VAL:H	2.29	0.41
2:C:455:LEU:HD11	2:C:500:LEU:HB2	2.03	0.41
2:C:775:ASN:ND2	5:F:527:LEU:O	2.54	0.41
3:D:46:LEU:HD21	3:D:348:ILE:HD11	2.02	0.41
3:D:99:ALA:HA	3:D:100:PRO:HD3	1.91	0.41
3:D:1170:SER:O	3:D:1173:THR:OG1	2.37	0.41
3:D:1248:LEU:O	3:D:1252:VAL:HG23	2.21	0.41
2:C:277:ILE:HG21	2:C:296:LEU:HD21	2.02	0.41
3:D:24:SER:CB	3:D:94:HIS:HB3	2.49	0.41
3:D:203:ARG:HD3	3:D:206:ARG:HH21	1.86	0.41
3:D:237:ASP:HB3	3:D:239:ASN:OD1	2.21	0.41
3:D:739:PRO:HD3	3:D:789:LEU:HD13	2.03	0.41
3:D:1031:VAL:HG23	3:D:1141:VAL:HG11	2.02	0.41
5:F:450:ALA:O	5:F:454:THR:HG23	2.20	0.41
1:B:182:ARG:HH12	3:D:488:GLU:HG2	1.85	0.41
2:C:388:GLN:HG3	2:C:430:PHE:CD1	2.55	0.41
2:C:720:LEU:HD13	2:C:1027:TYR:CE1	2.55	0.41
3:D:244:LEU:HG	3:D:252:PHE:HZ	1.84	0.41
3:D:1033:GLU:O	3:D:1033:GLU:HG2	2.15	0.41
1:A:89:GLU:HG2	1:A:91:GLU:H	1.85	0.41
1:B:5:GLN:NE2	1:B:6:ARG:O	2.54	0.41
1:B:56:ILE:HG21	1:B:66:VAL:HG21	2.03	0.41
2:C:197:LYS:HD2	2:C:198:THR:H	1.86	0.41
2:C:248:ILE:CG2	2:C:262:LEU:HD22	2.51	0.41
2:C:611:MET:CE	2:C:890:GLY:HA2	2.51	0.41
2:C:663:ASP:CG	2:C:695:ARG:HH12	2.29	0.41
3:D:131:PHE:CZ	3:D:371:LYS:HB3	2.55	0.41
3:D:1011:THR:HG22	3:D:1012:MET:N	2.36	0.41
3:D:1034:LEU:HD11	3:D:1137:GLU:CG	2.51	0.41
5:F:233:LYS:HG2	5:F:237:LYS:HE3	2.03	0.41
2:C:728:GLY:HA3	3:D:721:PHE:CD2	2.57	0.41
3:D:320:ILE:HG12	3:D:321:PRO:HD2	2.02	0.41
3:D:886:VAL:HA	3:D:974:VAL:O	2.21	0.41
5:F:323:GLU:HG2	5:F:358:ALA:HB3	2.03	0.41
1:A:119:HIS:C	1:A:121:PRO:HD3	2.46	0.40
1:B:148:PRO:HG3	3:D:626:VAL:HG21	2.03	0.40
2:C:484:CYS:HB2	2:C:588:SER:HB3	2.02	0.40
2:C:548:ILE:HD11	2:C:579:MET:HE1	2.03	0.40
3:D:557:ILE:HD13	4:E:53:LEU:HG	2.03	0.40
3:D:1074:GLU:H	3:D:1074:GLU:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:325:ASN:O	5:F:329:ILE:HG13	2.20	0.40
1:B:96:TYR:HB2	1:B:98:ARG:HH12	1.87	0.40
2:C:760:ARG:CB	2:C:865:VAL:HG22	2.51	0.40
3:D:81:GLU:HG2	3:D:83:THR:HG23	2.02	0.40
3:D:203:ARG:HA	3:D:203:ARG:HD2	1.92	0.40
3:D:297:LYS:HB2	3:D:297:LYS:HE2	1.86	0.40
3:D:1054:ARG:HD3	3:D:1065:THR:HB	2.03	0.40
2:C:1106:ILE:HG13	2:C:1112:ILE:CD1	2.41	0.40
3:D:793:TYR:HD1	3:D:800:ILE:HG12	1.86	0.40
4:E:63:GLN:O	4:E:66:ASP:N	2.54	0.40
5:F:477:LEU:HB3	5:F:492:ILE:HG23	2.04	0.40
5:F:515:ARG:HG3	5:F:519:ARG:HG3	2.04	0.40
1:B:34:LEU:O	1:B:38:LEU:HB2	2.20	0.40
2:C:1106:ILE:HG21	3:D:454:PRO:HB2	2.03	0.40
1:A:54:ILE:HG22	1:A:138:LEU:HD23	2.02	0.40
3:D:463:LEU:HD12	3:D:486:VAL:CG2	2.52	0.40
3:D:965:VAL:HG22	3:D:974:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	192/297 (65%)	188 (98%)	4 (2%)	47 66
1	B	197/297 (66%)	190 (96%)	7 (4%)	31 57
2	C	947/998 (95%)	896 (95%)	51 (5%)	20 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1058/1095 (97%)	1008 (95%)	50 (5%)	23	50
4	E	70/90 (78%)	68 (97%)	2 (3%)	37	61
5	F	249/427 (58%)	238 (96%)	11 (4%)	25	51
All	All	2713/3204 (85%)	2588 (95%)	125 (5%)	25	50

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	139	VAL
1	A	164	VAL
1	A	168	TYR
1	B	69	VAL
1	B	105	VAL
1	B	129	ASN
1	B	131	LYS
1	B	166	SER
1	B	169	SER
1	B	202	ILE
2	C	39	VAL
2	C	58	THR
2	C	80	VAL
2	C	83	VAL
2	C	89	VAL
2	C	107	PHE
2	C	133	LEU
2	C	159	MET
2	C	168	ILE
2	C	204	VAL
2	C	235	THR
2	C	268	VAL
2	C	373	PHE
2	C	389	ILE
2	C	397	GLU
2	C	399	VAL
2	C	518	LYS
2	C	528	ILE
2	C	529	VAL
2	C	551	ASP
2	C	672	MET
2	C	689	ILE

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Mol	Chain	Res	Type
2	C	702	ILE
2	C	704	ASP
2	C	721	VAL
2	C	737	LEU
2	C	746	VAL
2	C	749	SER
2	C	772	ASP
2	C	786	GLU
2	C	790	VAL
2	C	797	ARG
2	C	888	ARG
2	C	913	VAL
2	C	915	ILE
2	C	919	THR
2	C	928	ILE
2	C	972	VAL
2	C	974	THR
2	C	976	VAL
2	C	1002	VAL
2	C	1003	ASP
2	C	1036	LEU
2	C	1037	VAL
2	C	1038	ASP
2	C	1042	HIS
2	C	1045	SER
2	C	1084	THR
2	C	1106	ILE
2	C	1111	ASN
2	C	1145	ILE
3	D	60	CYS
3	D	70	PHE
3	D	84	ARG
3	D	97	LEU
3	D	165	GLN
3	D	173	ARG
3	D	221	ASP
3	D	239	ASN
3	D	265	ILE
3	D	275	GLU
3	D	282	ARG
3	D	285	LYS
3	D	345	ARG

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Mol	Chain	Res	Type
3	D	420	LYS
3	D	428	SER
3	D	431	VAL
3	D	440	GLN
3	D	469	ILE
3	D	485	ASP
3	D	509	ILE
3	D	581	MET
3	D	635	VAL
3	D	663	MET
3	D	687	GLN
3	D	714	ASP
3	D	721	PHE
3	D	782	THR
3	D	785	VAL
3	D	801	THR
3	D	824	VAL
3	D	851	ILE
3	D	874	THR
3	D	899	VAL
3	D	918	THR
3	D	921	TYR
3	D	964	SER
3	D	974	VAL
3	D	1033	GLU
3	D	1053	VAL
3	D	1123	ARG
3	D	1154	ILE
3	D	1156	VAL
3	D	1158	VAL
3	D	1169	ASP
3	D	1175	PHE
3	D	1181	ILE
3	D	1194	VAL
3	D	1234	THR
3	D	1243	ASP
3	D	1246	ASN
4	E	31	THR
4	E	43	LEU
5	F	252	ARG
5	F	285	CYS
5	F	294	HIS

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Mol	Chain	Res	Type
5	F	336	ASP
5	F	350	TRP
5	F	392	ARG
5	F	437	ASP
5	F	446	VAL
5	F	467	LEU
5	F	503	ILE
5	F	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	GLN
2	C	141	ASN
2	C	232	GLN
2	C	247	GLN
2	C	407	GLN
2	C	585	GLN
2	C	680	HIS
2	C	1035	HIS
2	C	1054	GLN
2	C	1062	GLN
3	D	415	GLN
3	D	439	HIS
3	D	540	GLN
3	D	544	HIS
3	D	639	GLN
3	D	687	GLN
3	D	1125	GLN
3	D	1133	HIS
3	D	1251	ASN
5	F	299	ASN
5	F	353	GLN
5	F	516	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
8	FI8	D	1904	-	74,75,75	1.24	7 (9%)	96,109,109	1.87	14 (14%)

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
8	FI8	D	1904	-	-	16/75/118/118	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1904	FI8	O17-C49	4.29	1.44	1.34
8	D	1904	FI8	C14-C15	4.04	1.53	1.45
8	D	1904	FI8	C44-C45	-3.32	1.46	1.53
8	D	1904	FI8	C5-C4	3.05	1.52	1.43
8	D	1904	FI8	C4-C3	2.92	1.44	1.36
8	D	1904	FI8	C2-C3	2.20	1.53	1.49
8	D	1904	FI8	C1-C3	2.11	1.53	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	1904	FI8	C5-C4-C3	-10.76	114.05	126.92
8	D	1904	FI8	O1-C2-C3	5.12	119.22	112.11
8	D	1904	FI8	O17-C49-C50	4.57	119.57	111.14
8	D	1904	FI8	C17-C16-C15	-4.46	117.74	127.50
8	D	1904	FI8	C7-C6-C5	-4.03	120.31	125.44
8	D	1904	FI8	C1-C3-C4	-3.22	121.23	125.03
8	D	1904	FI8	C31-C30-C29	-3.14	108.71	113.39
8	D	1904	FI8	O14-C46-C45	2.93	112.38	107.67
8	D	1904	FI8	O2-C2-C3	-2.59	120.26	124.09
8	D	1904	FI8	O10-C33-C34	2.48	119.76	113.53
8	D	1904	FI8	C29-O10-C33	2.24	120.82	117.24
8	D	1904	FI8	C38-C37-C36	2.11	120.04	117.78
8	D	1904	FI8	O10-C33-O11	-2.05	120.22	123.55
8	D	1904	FI8	C29-C28-C27	2.03	113.23	109.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

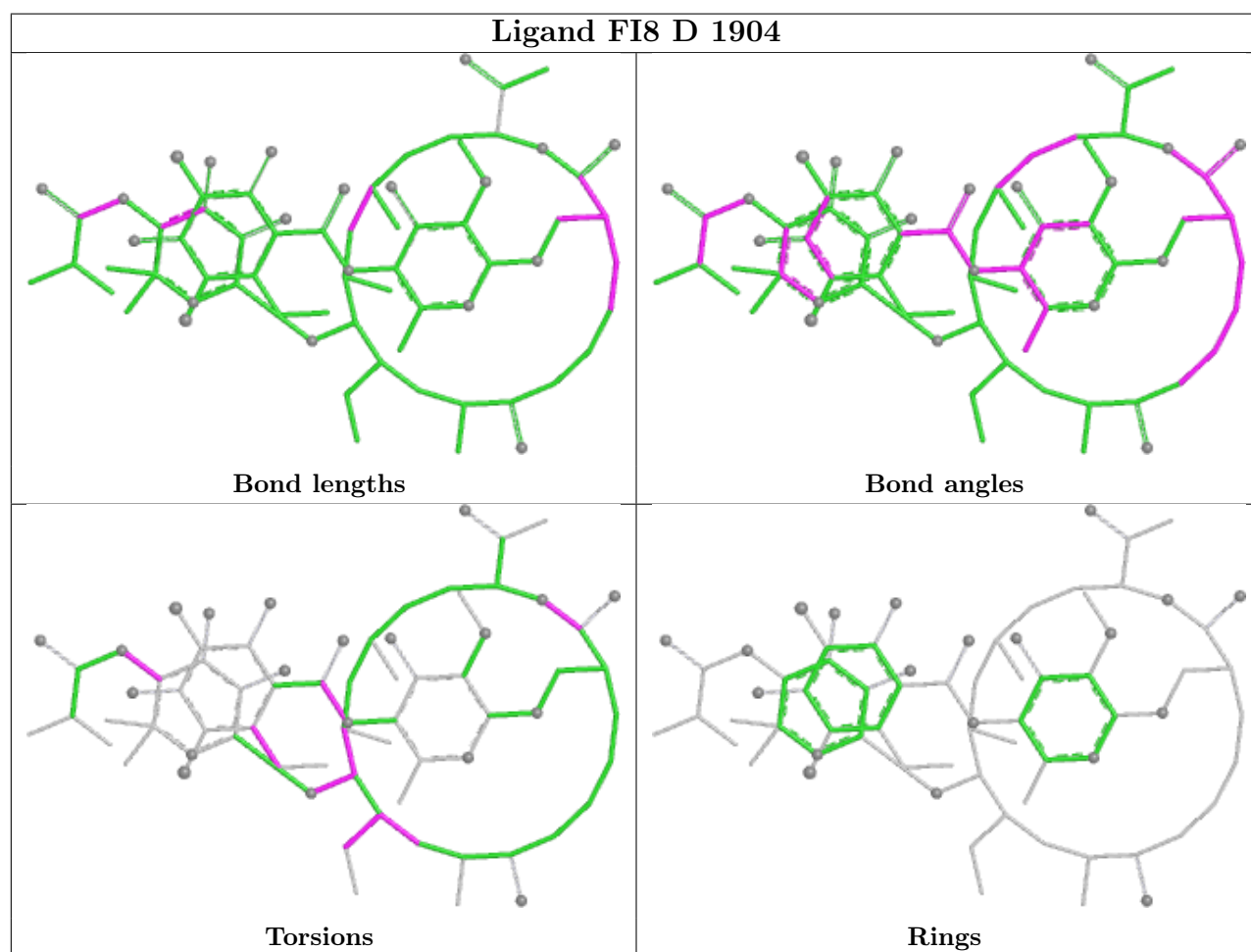
Mol	Chain	Res	Type	Atoms
8	D	1904	FI8	C9-C10-C11-C12
8	D	1904	FI8	C9-C10-C11-C22
8	D	1904	FI8	C11-C12-C13-C14
8	D	1904	FI8	C11-C12-C13-C24
8	D	1904	FI8	O4-C12-C13-C14
8	D	1904	FI8	O4-C12-C13-C24
8	D	1904	FI8	C3-C2-O1-C18
8	D	1904	FI8	C34-C33-O10-C29
8	D	1904	FI8	C38-C39-C40-C41
8	D	1904	FI8	C34-C39-C40-C41
8	D	1904	FI8	O2-C2-O1-C18
8	D	1904	FI8	O11-C33-O10-C29
8	D	1904	FI8	C44-C45-O17-C49
8	D	1904	FI8	C11-C12-O4-C42
8	D	1904	FI8	C10-C11-C22-C23
8	D	1904	FI8	C46-C45-O17-C49

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1904	FI8	7	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

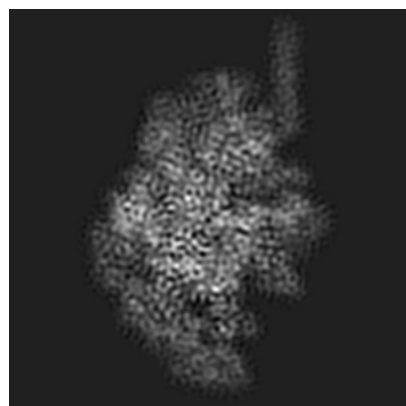
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4230. These allow visual inspection of the internal detail of the map and identification of artifacts.

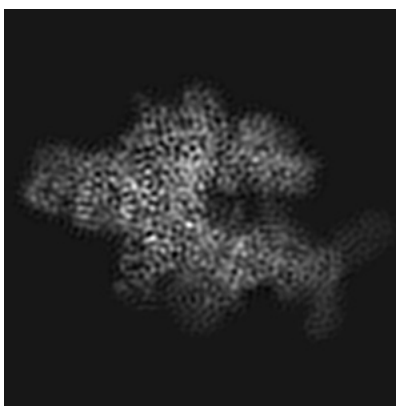
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

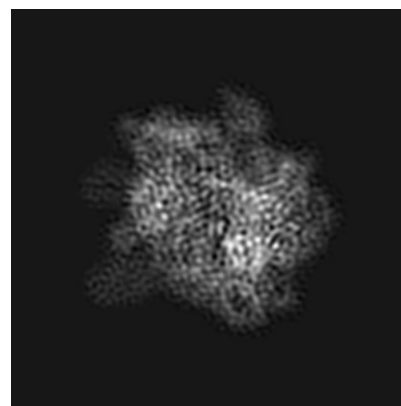
6.1.1 Primary map



X

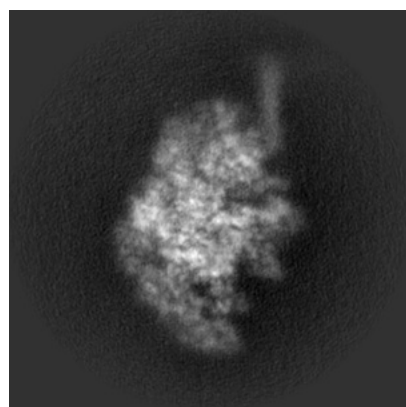


Y

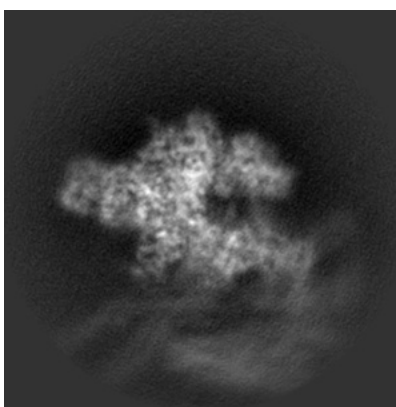


Z

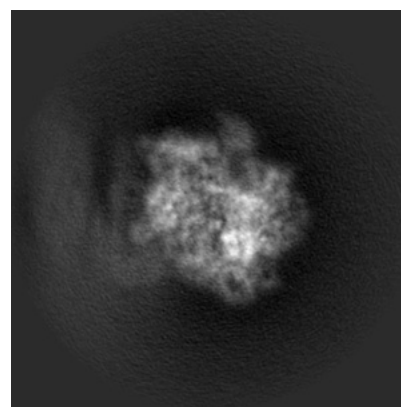
6.1.2 Raw map



X



Y

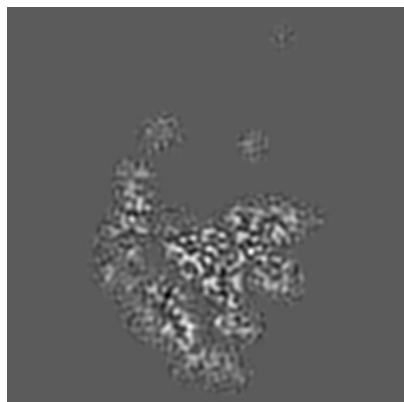


Z

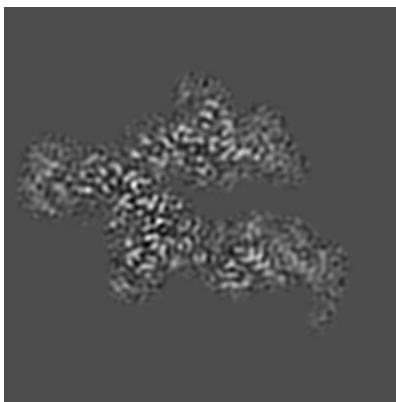
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

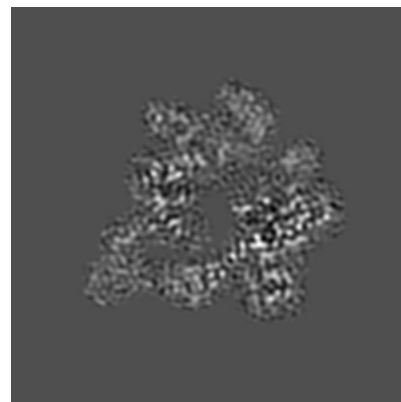
6.2.1 Primary map



X Index: 96

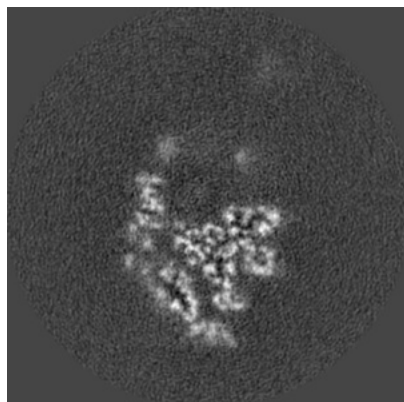


Y Index: 96

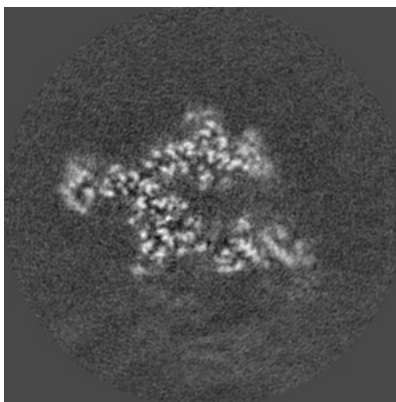


Z Index: 96

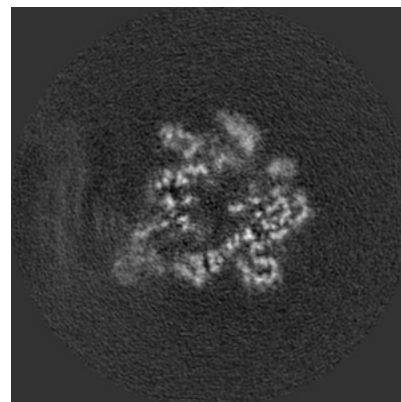
6.2.2 Raw map



X Index: 120



Y Index: 120

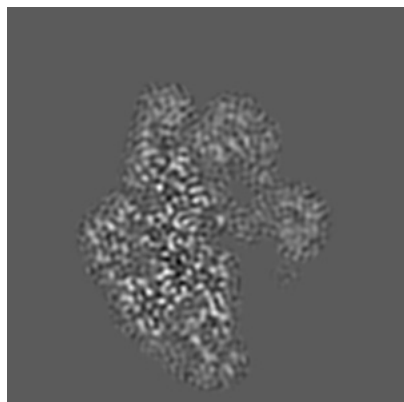


Z Index: 120

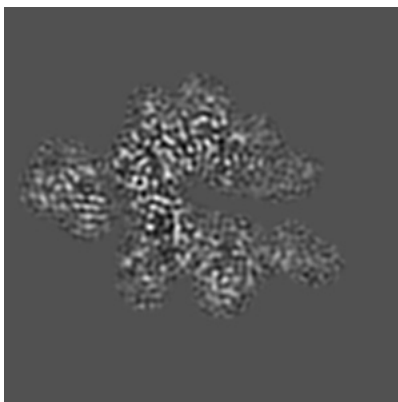
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

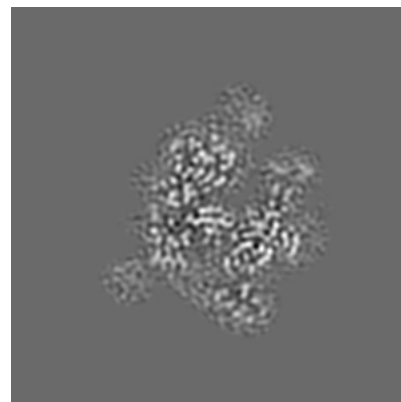
6.3.1 Primary map



X Index: 115

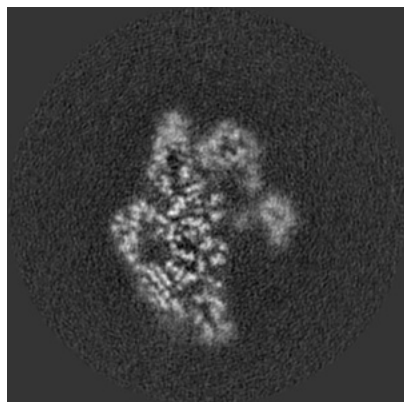


Y Index: 86

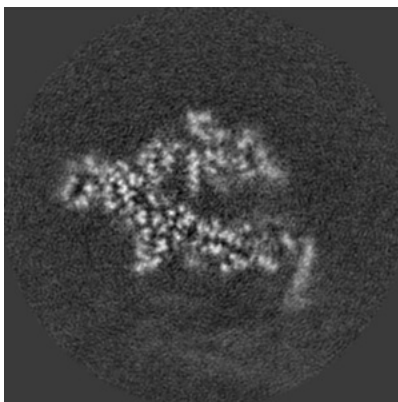


Z Index: 80

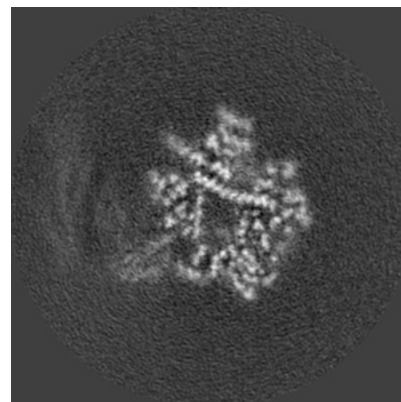
6.3.2 Raw map



X Index: 141



Y Index: 125

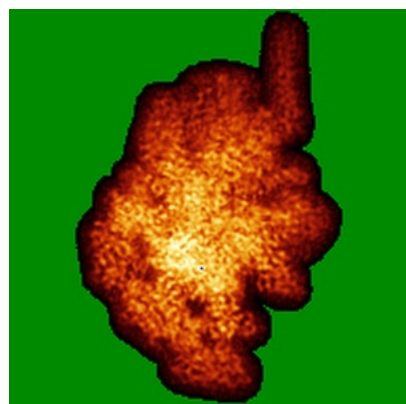


Z Index: 113

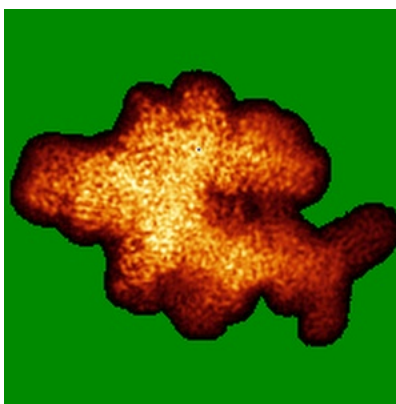
The images above show the largest variance slices of the map in three orthogonal directions.

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

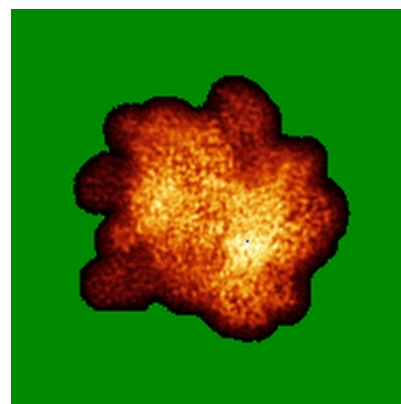
6.4.1 Primary map



X

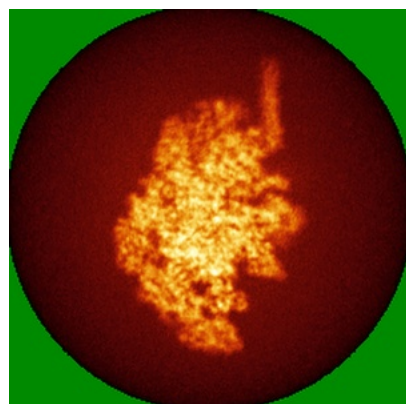


Y

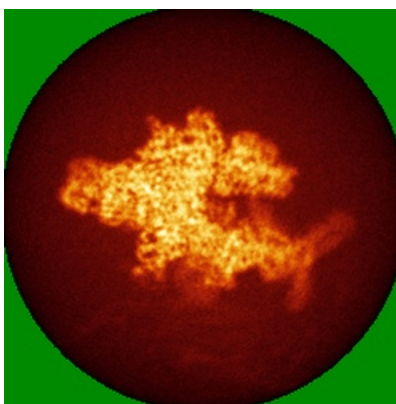


Z

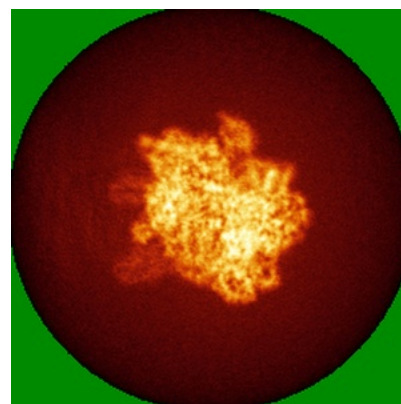
6.4.2 Raw map



X



Y

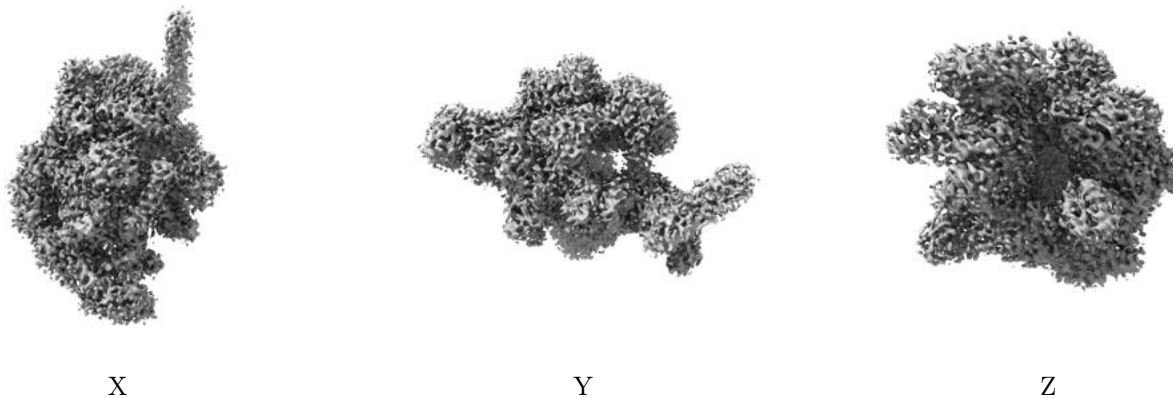


Z

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.

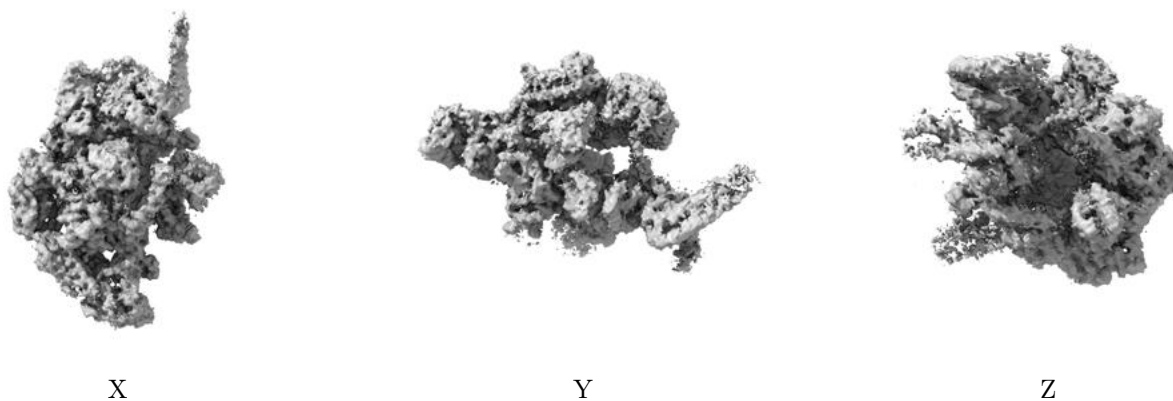
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

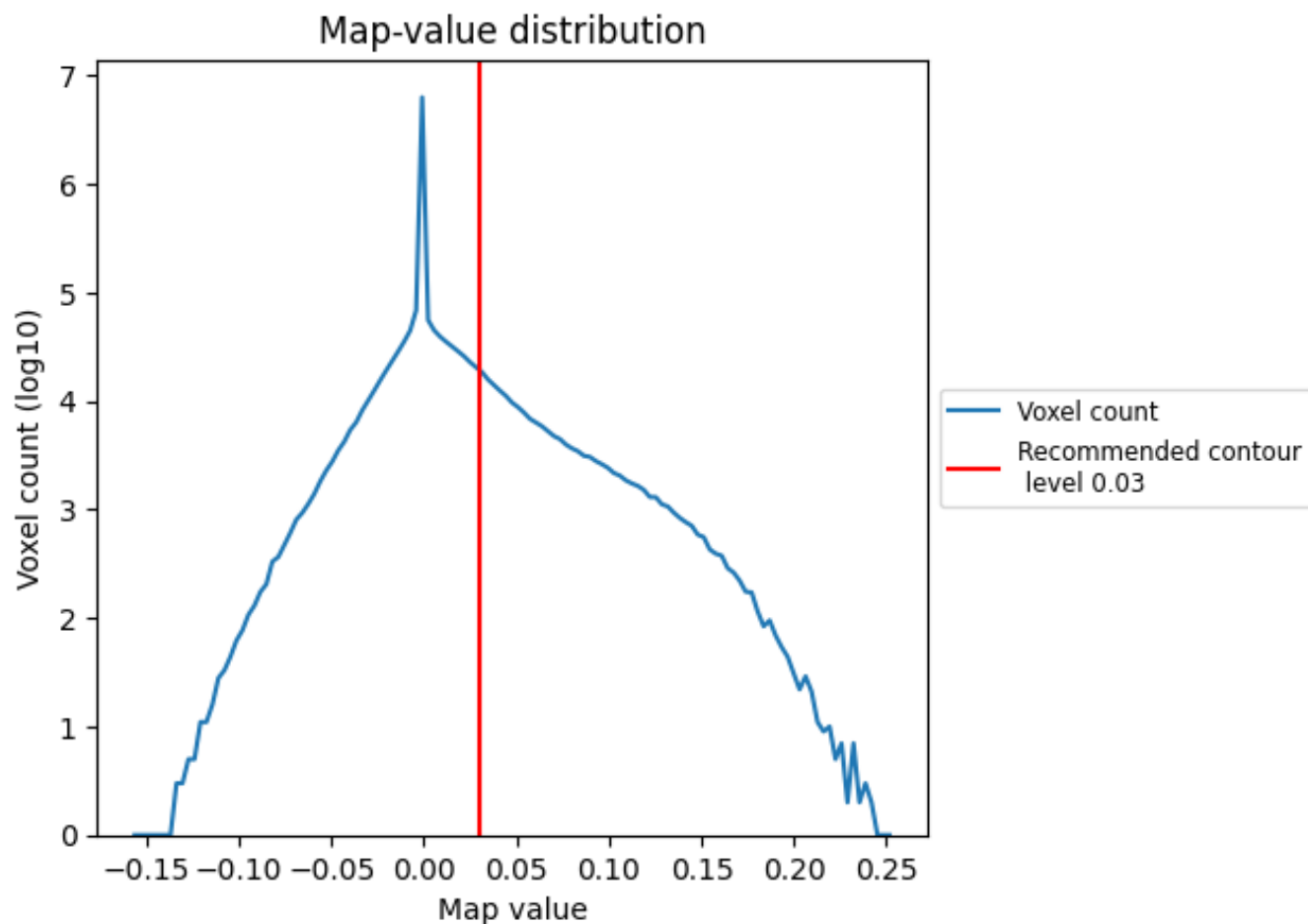
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

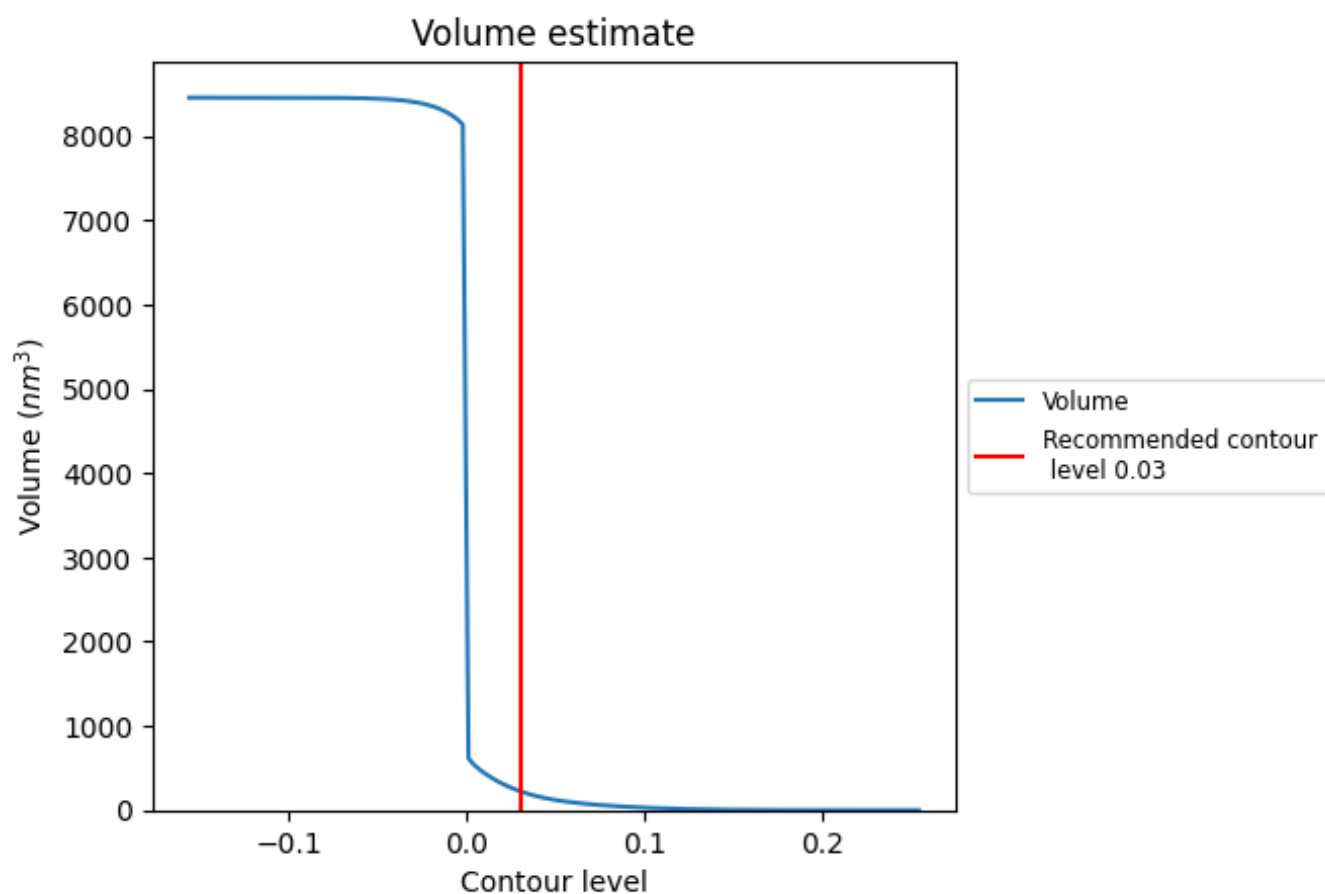
This section contains the results of statistical analysis of the map.

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.

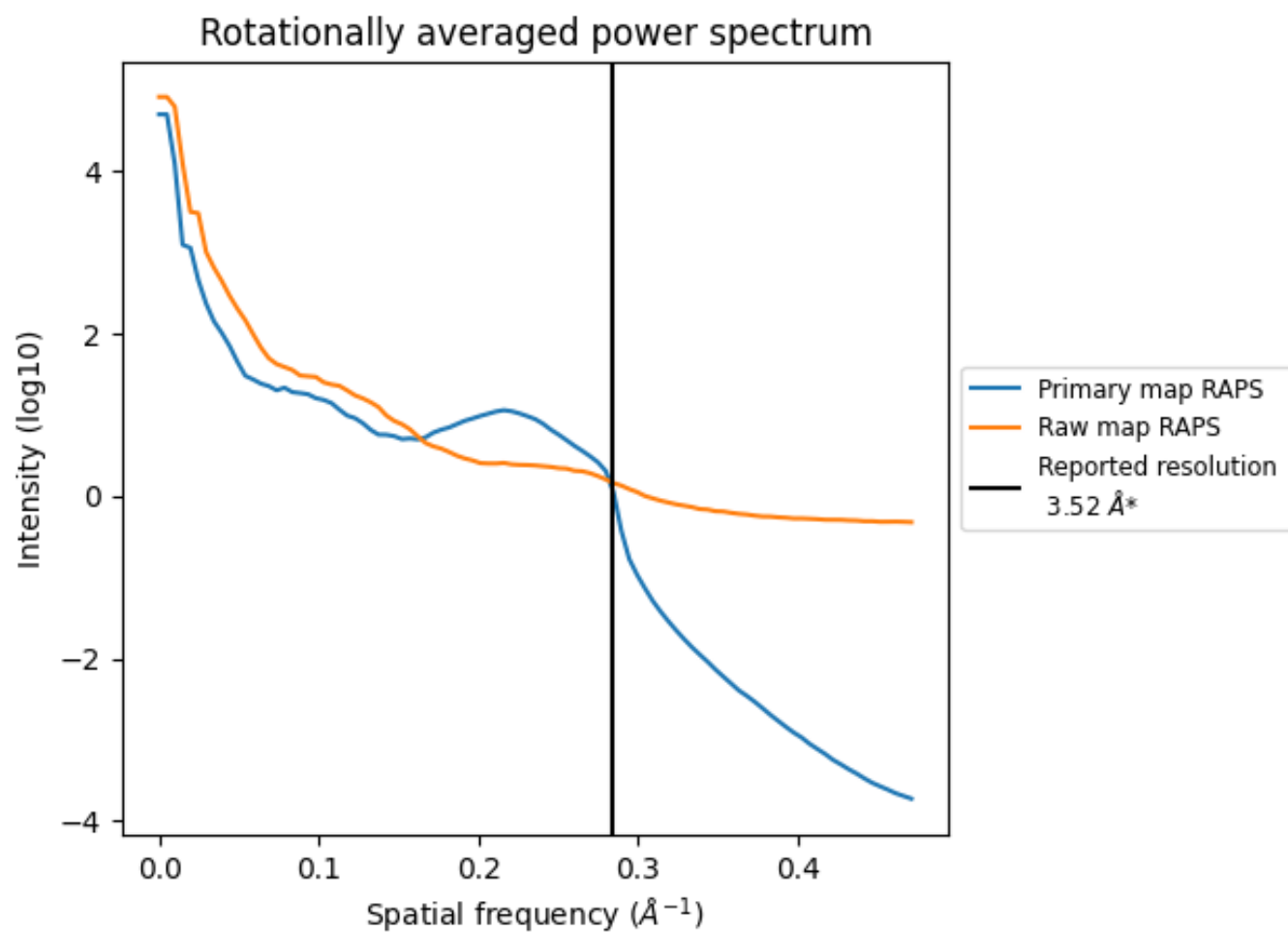
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm^3 ; this corresponds to an approximate mass of 204 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 ⓘ

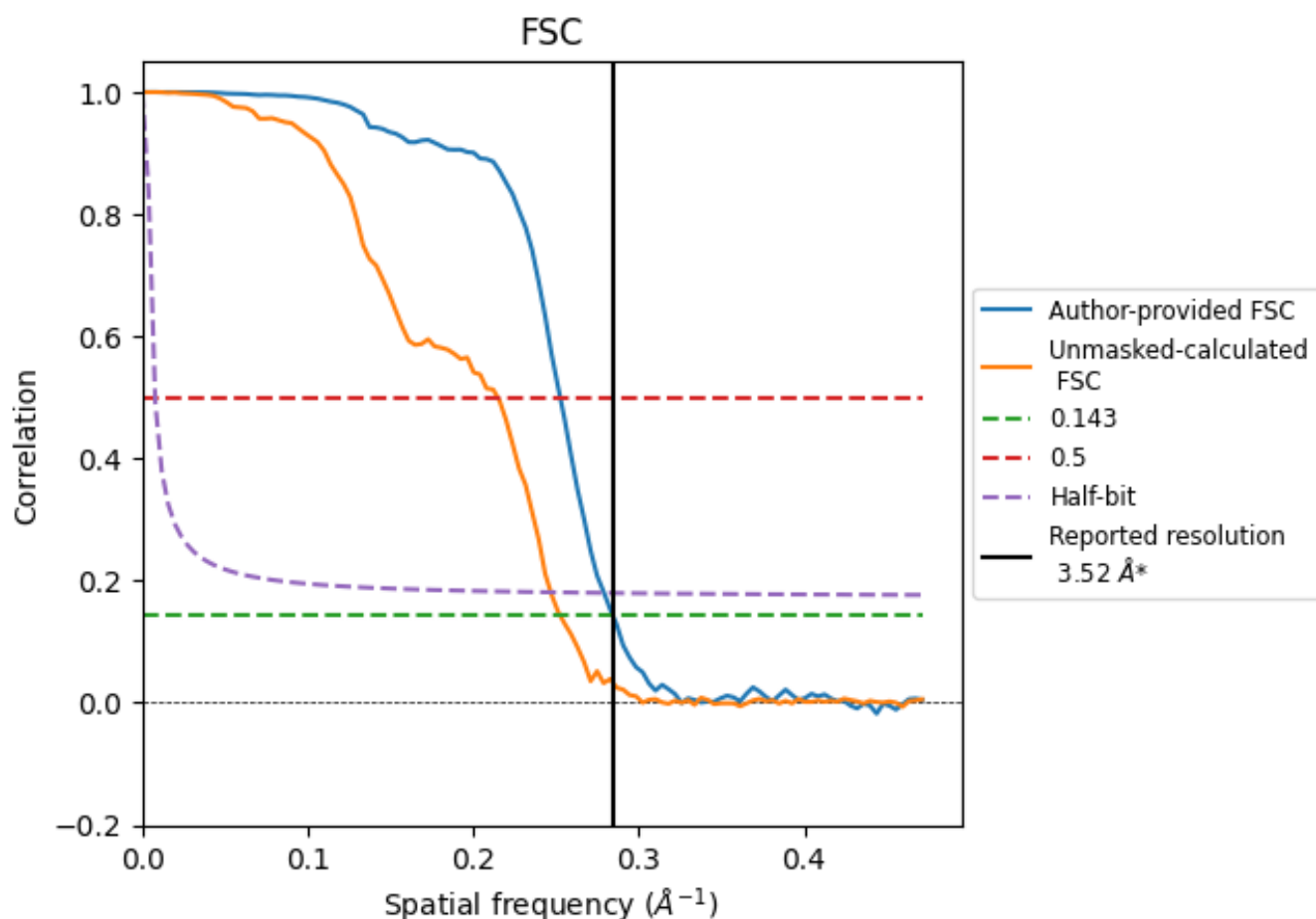


*Reported resolution corresponds to spatial frequency of $0.284 \text{ \AA}^{-1}$

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 0.284 Å⁻¹

8.2 Resolution estimates [i](#)

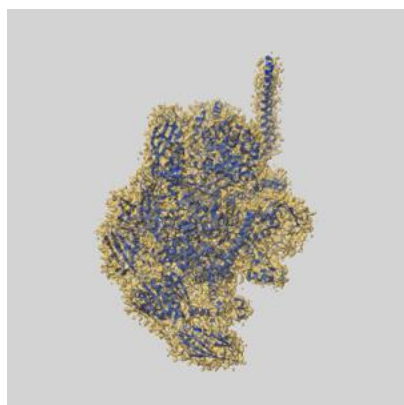
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.52	3.96	3.58
Unmasked-calculated*	3.96	4.66	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.52 by more than 10 %

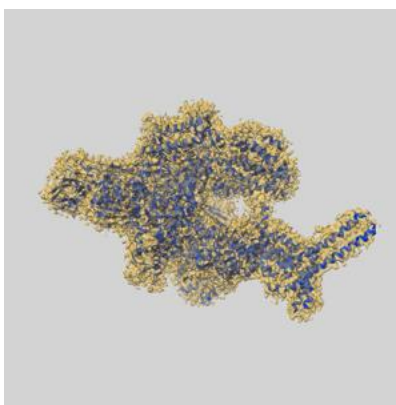
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4230 and PDB model 6FBV. Per-residue inclusion information can be found in section 3 on page 6.

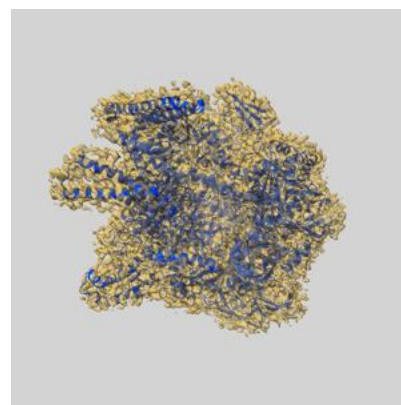
9.1 Map-model overlay [i](#)



X



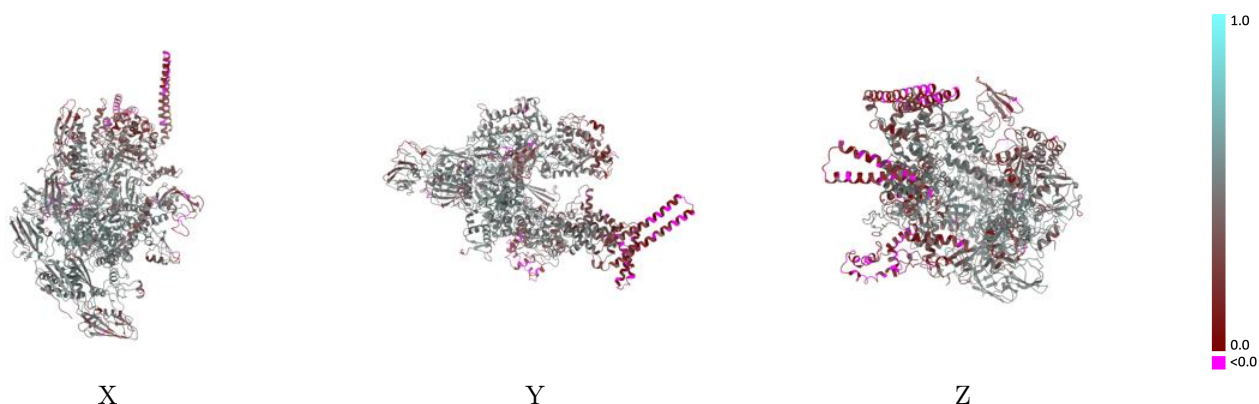
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)

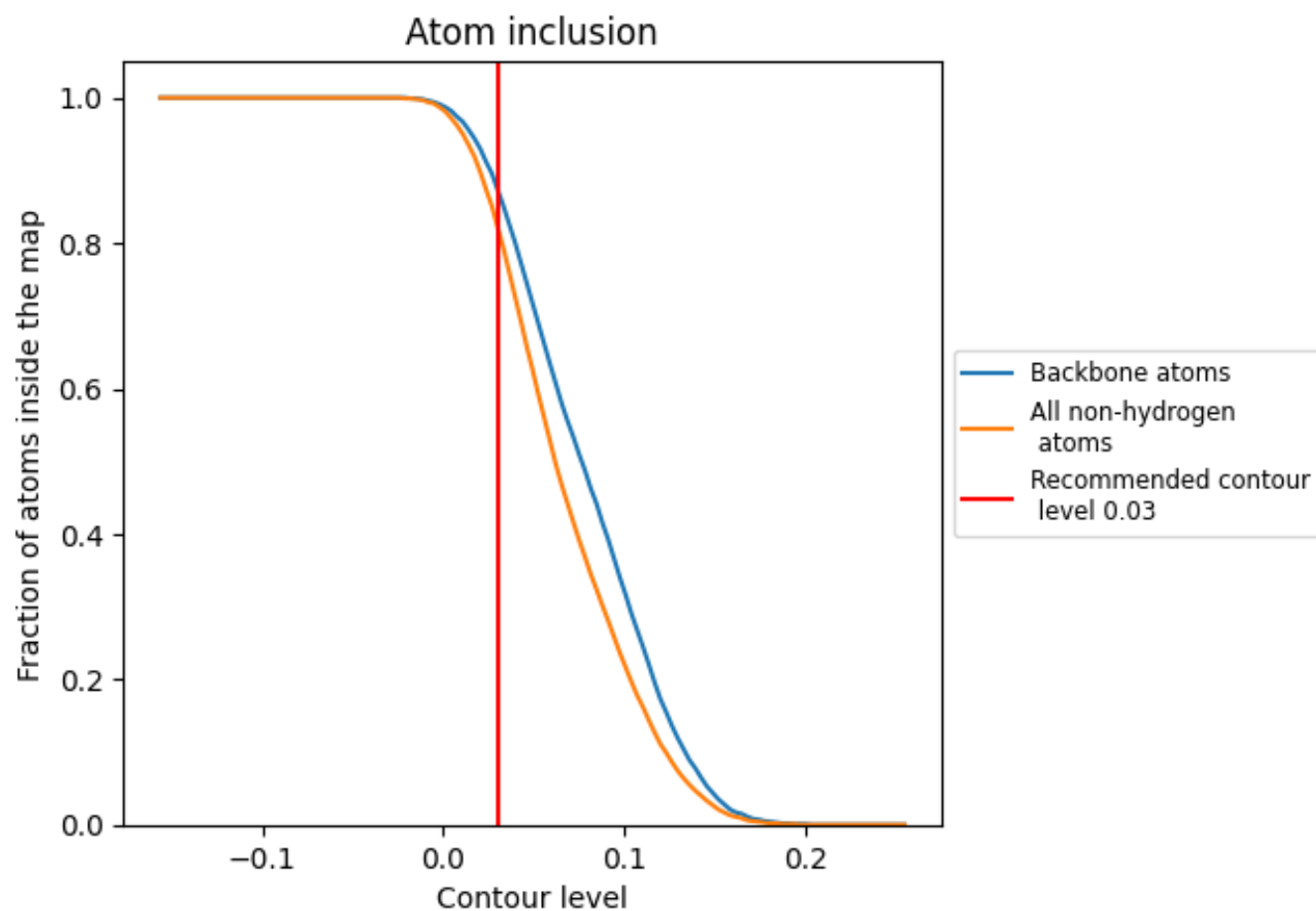


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.4250
A	0.8640	0.4720
B	0.8210	0.4220
C	0.8650	0.4540
D	0.8520	0.4410
E	0.8840	0.4790
F	0.5050	0.1980

1.0

0.0

<0.0