



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:26 PM UTC

PDB ID : 8B0H / pdb_00008b0h
EMDB ID : EMD-15781
Title : 2C9, C5b9-CD59 cryoEM structure
Authors : Couves, E.C.; Gardner, S.; Bubeck, D.
Deposited on : 2022-09-07
Resolution : 3.30 Å (reported)
Based on initial models : 7NYD, 2J8B

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
MolProbity : 4-5-2 with Phenix2.0
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

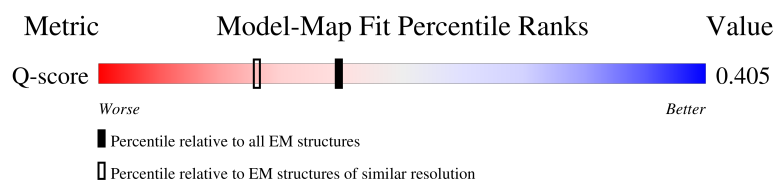
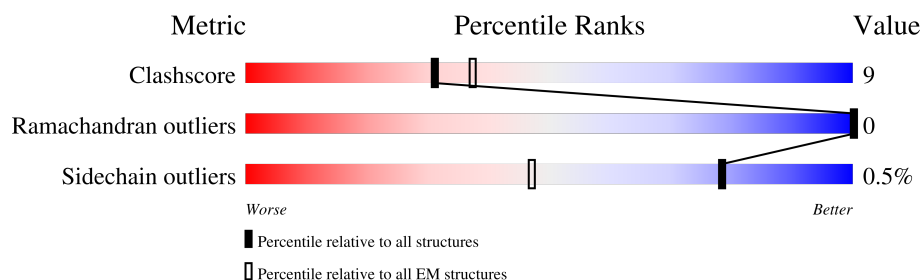
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



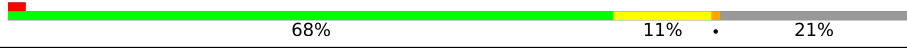
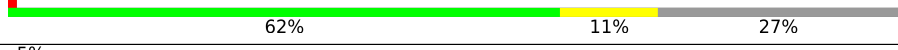
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	G	128	
2	D	591	
3	F	202	
4	E	584	

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Mol	Chain	Length	Quality of chain
5	A	1676	
6	C	843	
7	B	934	
8	H	559	
8	I	559	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 72850 atoms, of which 35735 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 CD59 glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	78	Total	C	H	N	O	S	0	0
			1209	389	580	106	123	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	MET	SER	conflict	UNP P13987

- Molecule 2 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	507	Total	C	H	N	O	S	0	0
			7926	2520	3872	726	771	37		

- Molecule 3 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	168	Total	C	H	N	O	S	0	0
			2602	841	1283	230	244	4		

- Molecule 4 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	513	Total	C	H	N	O	S	0	0
			7866	2503	3814	716	794	39		

- Molecule 5 is a protein called Complement C5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	1245	Total	C	H	N	O	S	0	0
			19678	6330	9829	1617	1874	28		

- Molecule 6 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	646	Total	C	H	N	O	S	0	0
			9762	3133	4727	876	986	40		

- Molecule 7 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	B	737	Total	C	H	N	O	S	0	0
			11267	3570	5491	1021	1135	50		

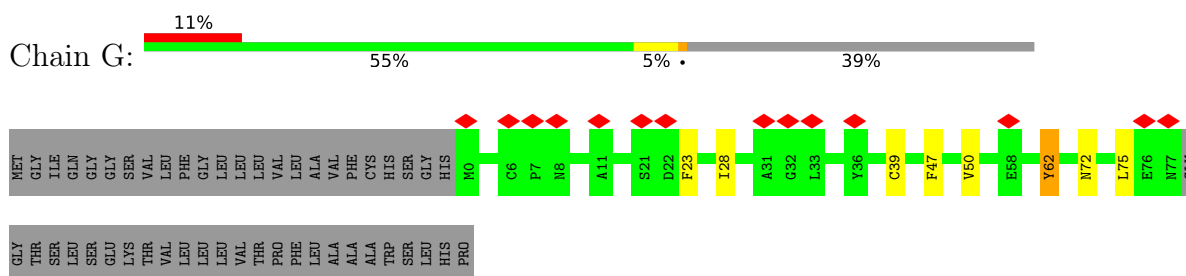
- Molecule 8 is a protein called Complement component C9.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	407	Total	C	H	N	O	S	0	0
			6310	2009	3091	561	620	29		
8	I	402	Total	C	H	N	O	S	0	0
			6230	1981	3048	556	615	30		

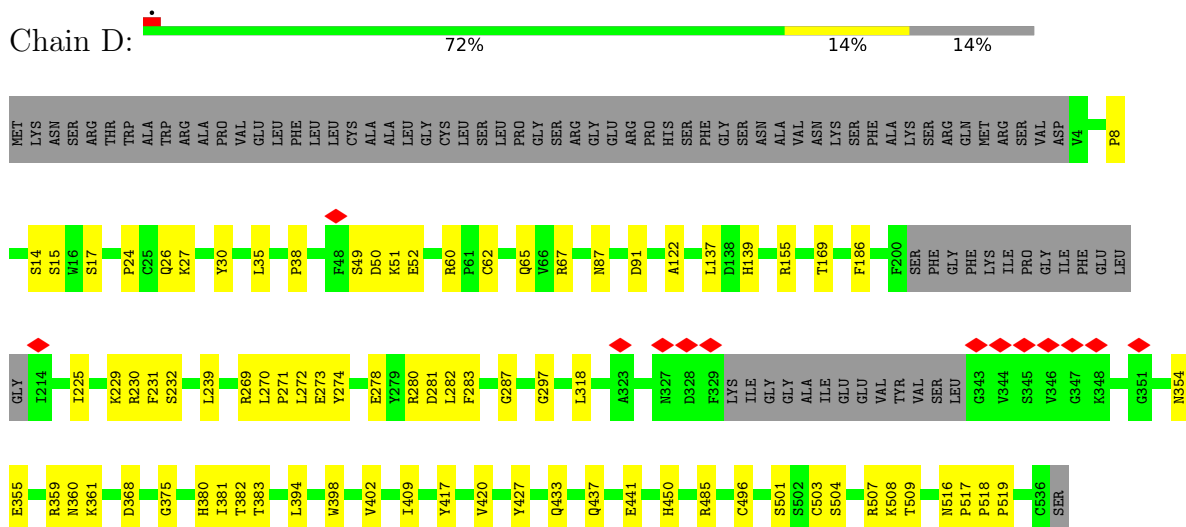
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

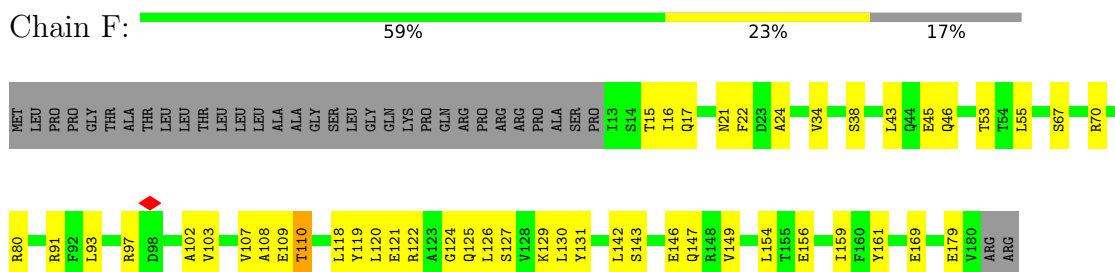
- Molecule 1: CD59 glycoprotein



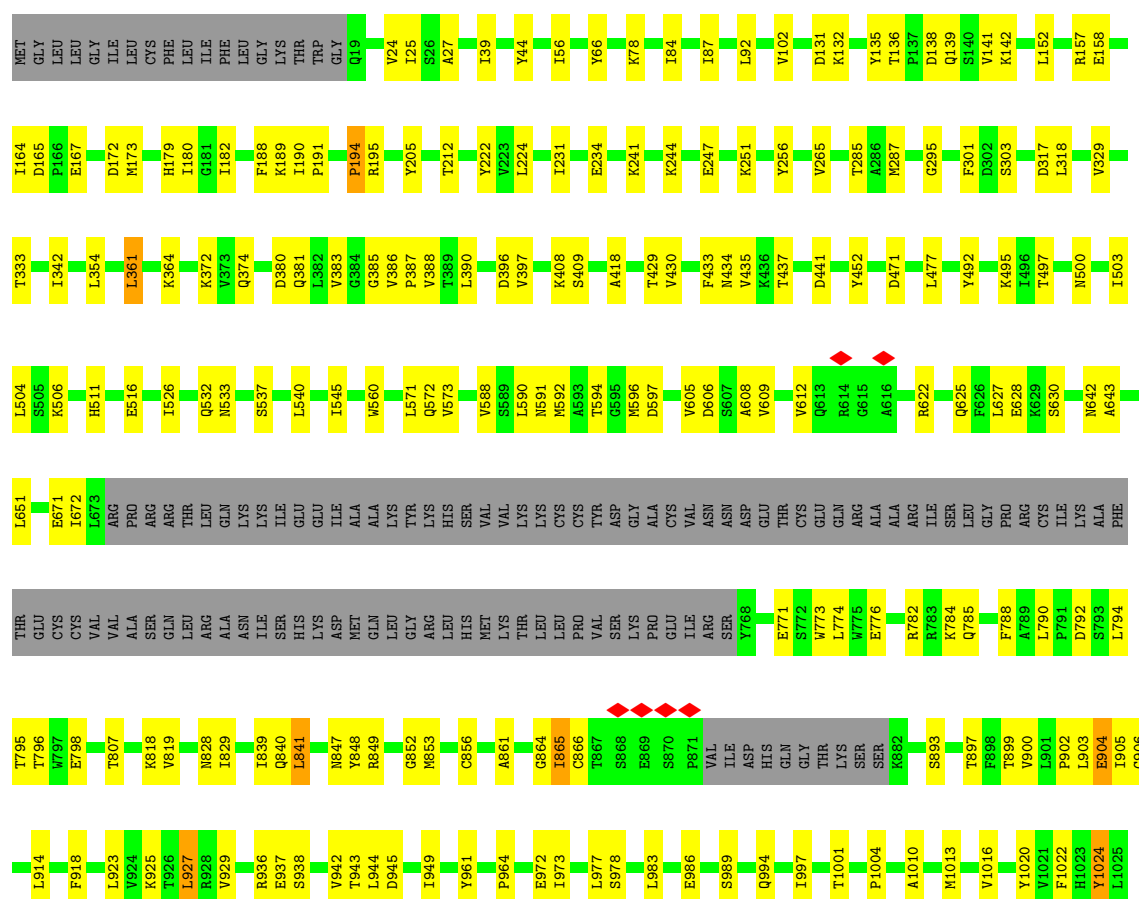
- Molecule 2: Complement component C8 beta chain

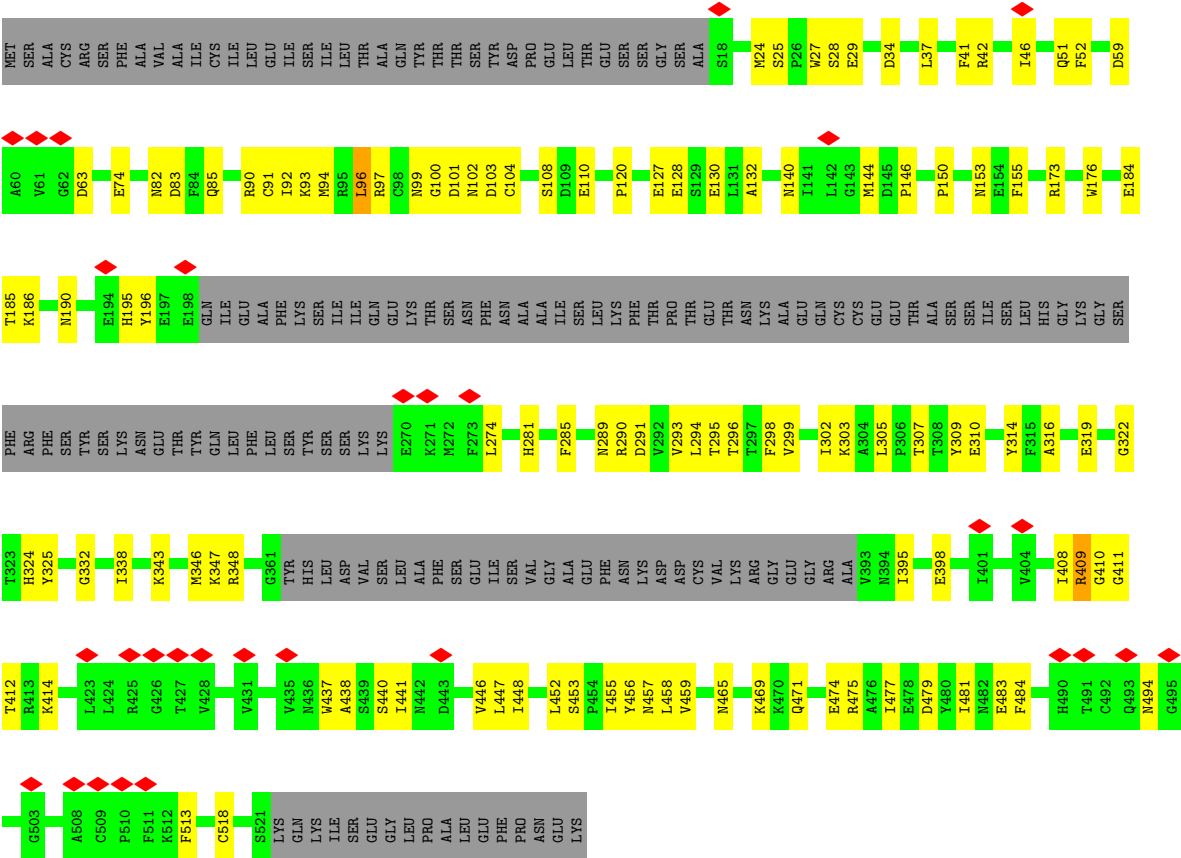


- Molecule 3: Complement component C8 gamma chain



Chain E: 76% 11% 12%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47244	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00481	Depositor
Map size (Å)	448.74, 448.74, 448.74	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

5 Model quality

5.1 Standard geometry

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	G	0.17	0/641	0.43	0/867
2	D	0.17	0/4146	0.49	0/5598
3	F	0.19	0/1348	0.56	0/1829
4	E	0.22	0/4135	0.55	4/5568 (0.1%)
5	A	0.21	0/10072	0.55	1/13685 (0.0%)
6	C	0.20	0/5160	0.49	1/6982 (0.0%)
7	B	0.18	0/5897	0.49	1/7962 (0.0%)
8	H	0.18	0/3280	0.48	0/4424
8	I	0.19	0/3242	0.58	3/4371 (0.1%)
All	All	0.20	0/37921	0.52	10/51286 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
3	F	0	1
4	E	0	1
5	A	0	1
6	C	0	1
7	B	0	1
All	All	0	6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	445	PRO	CA-N-CD	-9.74	98.37	112.00
7	B	79	PRO	CA-N-CD	-7.83	101.04	112.00
4	E	467	CYS	CB-CA-C	-7.69	95.53	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	146	PRO	CA-N-CD	-7.16	101.98	112.00
6	C	337	CYS	CA-CB-SG	7.10	130.74	114.40
4	E	514	CYS	CA-CB-SG	6.12	128.48	114.40
5	A	194	PRO	CA-N-CD	-5.67	104.06	112.00
8	I	146	PRO	N-CD-CG	-5.67	94.70	103.20
8	I	409	ARG	CB-CG-CD	5.43	123.78	111.30
4	E	467	CYS	CA-CB-SG	5.25	126.47	114.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1026	GLU	Peptide
7	B	104	ARG	Sidechain
6	C	171	GLY	Peptide
2	D	17	SER	Peptide
4	E	512	TRP	Peptide
3	F	110	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	629	580	582	4	0
2	D	4054	3872	3870	63	0
3	F	1319	1283	1282	32	0
4	E	4052	3814	3814	59	0
5	A	9849	9829	9826	248	0
6	C	5035	4727	4724	48	0
7	B	5776	5491	5488	74	0
8	H	3219	3091	3089	47	0
8	I	3182	3048	3045	89	0
All	All	37115	35735	35720	638	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 9.

All (638) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:394:LEU:HD21	4:E:414:ARG:NH1	1.36	1.37
2:D:394:LEU:CD2	4:E:414:ARG:NH1	2.09	1.14
6:C:337:CYS:HB3	6:C:353:CYS:HA	1.49	0.95
8:I:309:TYR:OH	8:I:479:ASP:OD2	1.85	0.94
2:D:394:LEU:CD2	4:E:414:ARG:HH12	1.78	0.93
5:A:961:TYR:OH	5:A:972:GLU:OE2	1.86	0.92
2:D:394:LEU:HD21	4:E:414:ARG:HH12	1.10	0.86
2:D:394:LEU:HD21	4:E:414:ARG:HH11	1.41	0.84
3:F:45:GLU:OE1	3:F:46:GLN:N	2.12	0.82
8:H:24:MET:SD	8:H:24:MET:N	2.53	0.81
5:A:591:ASN:ND2	5:A:785:GLN:OE1	2.14	0.80
5:A:333:THR:HG23	5:A:893:SER:OG	1.82	0.80
3:F:97:ARG:NH1	3:F:179:GLU:O	2.16	0.78
5:A:372:LYS:NZ	5:A:471:ASP:OD1	2.16	0.77
5:A:1289:ASP:OD2	5:A:1290:THR:N	2.17	0.77
5:A:172:ASP:OD1	5:A:173:MET:N	2.18	0.77
5:A:1278:GLN:NE2	7:B:624:ILE:HG21	2.00	0.76
8:I:302:ILE:O	8:I:469:LYS:NZ	2.13	0.75
4:E:132:GLU:OE1	8:H:284:ARG:NH2	2.20	0.75
6:C:257:VAL:HG22	6:C:417:ILE:HD11	1.69	0.74
5:A:782:ARG:O	5:A:782:ARG:NH1	2.22	0.73
5:A:1001:THR:O	5:A:1001:THR:HG22	1.89	0.73
8:I:74:GLU:OE1	8:I:74:GLU:N	2.22	0.72
5:A:158:GLU:N	5:A:158:GLU:OE1	2.22	0.72
8:I:104:CYS:SG	8:I:108:SER:OG	2.47	0.72
7:B:182:ARG:NH2	7:B:228:ASN:OD1	2.22	0.72
2:D:272:LEU:HD21	2:D:427:TYR:HB3	1.71	0.71
5:A:841:LEU:HD13	5:A:900:VAL:HG22	1.72	0.71
5:A:1278:GLN:NE2	7:B:624:ILE:CG2	2.54	0.71
6:C:258:GLU:OE1	7:B:449:SER:OG	2.08	0.71
4:E:547:ARG:HB2	4:E:547:ARG:NH1	2.07	0.69
4:E:77:ARG:NH1	4:E:90:ASP:O	2.26	0.69
6:C:49:ARG:NH1	6:C:451:GLU:OE2	2.26	0.69
8:H:63:ASP:OD2	8:H:64:ARG:N	2.26	0.69
5:A:152:LEU:HD11	5:A:627:LEU:CD2	2.23	0.69
6:C:461:GLN:N	6:C:461:GLN:OE1	2.25	0.67
5:A:78:LYS:NZ	5:A:516:GLU:OE1	2.27	0.67
5:A:849:ARG:HG3	5:A:853:MET:HE1	1.76	0.67
5:A:1340:VAL:HG12	5:A:1340:VAL:O	1.93	0.67
8:I:456:TYR:O	8:I:459:VAL:HG12	1.94	0.67
8:H:34:ASP:CB	8:H:37:LEU:HD21	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:594:THR:O	5:A:782:ARG:NH1	2.29	0.65
4:E:445:PRO:HD2	4:E:445:PRO:O	1.95	0.65
8:H:404:VAL:O	8:I:190:ASN:ND2	2.24	0.65
8:I:348:ARG:O	8:I:348:ARG:HD3	1.97	0.65
2:D:274:TYR:OH	2:D:441:GLU:OE2	2.07	0.65
5:A:152:LEU:HD11	5:A:627:LEU:HD22	1.79	0.65
5:A:537:SER:OG	5:A:560:TRP:NE1	2.30	0.65
5:A:190:ILE:HG22	5:A:194:PRO:HG3	1.78	0.64
8:I:411:GLY:HA2	8:I:441:ILE:HD13	1.79	0.64
8:H:151:PHE:CD2	8:H:287:MET:HE2	2.32	0.64
7:B:670:ILE:HD11	7:B:684:PHE:CE1	2.33	0.63
5:A:918:PHE:CG	5:A:918:PHE:O	2.52	0.63
8:I:132:ALA:O	8:I:153:ASN:ND2	2.31	0.63
6:C:196:PHE:CE2	7:B:459:LYS:HE3	2.34	0.63
5:A:222:TYR:HE2	5:A:612:VAL:HG21	1.64	0.63
5:A:905:ILE:HG22	5:A:906:GLY:N	2.15	0.62
8:I:99:ASN:OD1	8:I:100:GLY:N	2.32	0.62
4:E:16:GLU:OE1	4:E:16:GLU:N	2.24	0.62
8:H:194:GLU:HB3	8:H:196:TYR:HE1	1.63	0.62
8:H:414:LYS:O	8:H:418:GLU:HG3	2.00	0.62
8:I:102:ASN:N	8:I:110:GLU:OE2	2.33	0.62
8:I:408:ILE:O	8:I:409:ARG:CZ	2.48	0.62
5:A:905:ILE:HA	5:A:929:VAL:HG12	1.82	0.61
2:D:272:LEU:HD21	2:D:427:TYR:CB	2.29	0.61
2:D:87:ASN:ND2	2:D:91:ASP:OD2	2.33	0.61
5:A:1148:THR:O	5:A:1152:ILE:HG13	2.01	0.61
5:A:1230:ASP:OD1	5:A:1233:GLN:NE2	2.34	0.61
5:A:792:ASP:OD1	5:A:792:ASP:O	2.18	0.61
8:I:51:GLN:HG2	8:I:52:PHE:CE2	2.36	0.61
7:B:423:ASN:OD1	7:B:424:LYS:N	2.34	0.60
8:I:128:GLU:OE2	8:I:128:GLU:N	2.33	0.60
2:D:417:TYR:O	2:D:420:VAL:HG22	2.01	0.60
8:I:307:THR:OG1	8:I:465:ASN:OD1	2.19	0.60
7:B:35:CYS:SG	7:B:74:ASN:ND2	2.75	0.60
4:E:103:VAL:O	4:E:106:ILE:HG23	2.02	0.60
5:A:256:TYR:OH	5:A:848:TYR:OH	2.12	0.60
5:A:1203:PRO:HG3	7:B:673:LEU:HD23	1.84	0.60
3:F:121:GLU:OE2	3:F:124:GLY:N	2.35	0.59
4:E:50:ASP:OD1	4:E:51:GLN:N	2.35	0.59
5:A:1277:GLU:O	5:A:1277:GLU:HG3	2.02	0.59
3:F:156:GLU:OE1	3:F:159:ILE:HD12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1024:TYR:CD2	5:A:1294:ILE:HD11	2.37	0.59
8:H:37:LEU:HD23	8:H:37:LEU:H	1.67	0.59
7:B:629:GLU:N	7:B:629:GLU:OE2	2.35	0.59
5:A:241:LYS:HD2	5:A:241:LYS:N	2.19	0.58
5:A:1133:LEU:HD12	5:A:1133:LEU:H	1.69	0.58
8:H:165:ASP:O	8:H:165:ASP:OD2	2.22	0.58
8:H:144:MET:HE1	8:H:452:LEU:HD11	1.85	0.58
5:A:573:VAL:HG22	5:A:590:LEU:HD21	1.84	0.57
5:A:606:ASP:OD2	5:A:608:ALA:HB3	2.04	0.57
5:A:179:HIS:O	5:A:180:ILE:HD13	2.04	0.57
5:A:903:LEU:HB2	5:A:904:GLU:OE1	2.04	0.57
4:E:462:MET:HE2	4:E:462:MET:HA	1.87	0.57
7:B:555:GLN:OE1	7:B:559:TYR:CD1	2.58	0.56
2:D:507:ARG:HG2	2:D:507:ARG:HH11	1.70	0.56
2:D:297:GLY:HA3	2:D:409:ILE:HD13	1.87	0.56
5:A:1278:GLN:CD	7:B:624:ILE:HG21	2.30	0.56
5:A:383:VAL:HG11	5:A:386:VAL:HG23	1.87	0.56
2:D:155:ARG:NH2	6:C:131:ASP:OD2	2.39	0.56
5:A:1175:LEU:HD22	5:A:1195:LEU:HD21	1.87	0.56
8:I:459:VAL:HG13	8:I:459:VAL:O	2.06	0.56
8:I:42:ARG:NH1	8:I:63:ASP:OD2	2.39	0.56
8:I:395:ILE:HG23	8:I:398:GLU:HG3	1.88	0.55
5:A:964:PRO:HD3	5:A:973:ILE:HD11	1.88	0.55
5:A:829:ILE:HD13	5:A:925:LYS:HZ1	1.71	0.55
8:I:140:ASN:OD1	8:I:322:GLY:HA2	2.05	0.55
8:I:291:ASP:CG	8:I:291:ASP:O	2.50	0.55
5:A:1175:LEU:HD21	5:A:1191:SER:HB2	1.89	0.55
6:C:481:THR:O	6:C:481:THR:HG22	2.07	0.55
5:A:1276:GLU:HB3	5:A:1278:GLN:HG3	1.87	0.55
5:A:131:ASP:OD2	5:A:142:LYS:HG3	2.07	0.54
5:A:596:MET:HE3	5:A:596:MET:HA	1.89	0.54
7:B:40:ASN:ND2	7:B:78:CYS:SG	2.80	0.54
2:D:50:ASP:OD2	2:D:280:ARG:NH2	2.41	0.54
2:D:381:ILE:CG2	4:E:191:ALA:HB2	2.38	0.54
8:I:410:GLY:HA3	8:I:446:VAL:HG12	1.90	0.54
2:D:229:LYS:O	2:D:230:ARG:HD3	2.08	0.54
5:A:918:PHE:O	5:A:918:PHE:CD1	2.61	0.54
7:B:50:ILE:HD12	7:B:67:LYS:HD3	1.88	0.54
8:H:278:GLY:HA3	8:H:335:TYR:CE2	2.42	0.54
5:A:936:ARG:HD3	5:A:937:GLU:N	2.23	0.54
7:B:330:LYS:O	7:B:331:ASP:OD1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:294:LEU:HD21	8:I:458:LEU:HB3	1.90	0.54
5:A:592:MET:N	5:A:592:MET:SD	2.80	0.54
8:I:94:MET:SD	8:I:97:ARG:NH2	2.75	0.54
3:F:55:LEU:HD11	3:F:131:TYR:CE1	2.43	0.53
7:B:67:LYS:HD2	7:B:67:LYS:O	2.09	0.53
2:D:225:ILE:HD13	2:D:318:LEU:HD22	1.91	0.53
2:D:14:SER:OG	2:D:15:SER:O	2.22	0.53
3:F:53:THR:HG22	3:F:70:ARG:HG3	1.91	0.53
5:A:224:LEU:H	5:A:224:LEU:HD22	1.74	0.53
5:A:1016:VAL:HG12	5:A:1291:ILE:HD11	1.90	0.53
7:B:494:VAL:HG23	7:B:494:VAL:O	2.09	0.53
8:I:99:ASN:ND2	8:I:103:ASP:OD2	2.35	0.52
6:C:198:TYR:CD2	6:C:248:TYR:OH	2.62	0.52
5:A:24:VAL:HG23	5:A:545:ILE:HD11	1.91	0.52
5:A:361:LEU:HD12	5:A:361:LEU:N	2.25	0.52
5:A:977:LEU:HD12	5:A:978:SER:N	2.23	0.52
8:I:140:ASN:ND2	8:I:144:MET:O	2.43	0.52
7:B:222:LYS:HE2	7:B:225:ARG:HA	1.91	0.52
7:B:659:LYS:NZ	7:B:666:GLU:OE2	2.29	0.52
7:B:528:ASN:ND2	7:B:552:CYS:O	2.33	0.52
5:A:27:ALA:HB2	5:A:39:ILE:HD12	1.89	0.52
5:A:1231:ASN:OD1	5:A:1246:ARG:NH2	2.43	0.52
4:E:77:ARG:NH2	4:E:139:ASP:OD2	2.42	0.52
5:A:189:LYS:O	5:A:1336:ARG:NH2	2.42	0.52
5:A:1104:LEU:HD22	5:A:1152:ILE:HG23	1.92	0.52
5:A:1207:SER:O	5:A:1210:SER:OG	2.25	0.52
8:H:35:PRO:O	8:H:37:LEU:HD23	2.10	0.52
5:A:829:ILE:HG21	5:A:925:LYS:HZ1	1.74	0.52
5:A:903:LEU:HB2	5:A:904:GLU:CD	2.35	0.52
7:B:693:ARG:HG3	7:B:693:ARG:O	2.09	0.52
7:B:150:ARG:NH1	7:B:336:ASP:OD1	2.42	0.52
2:D:503:CYS:SG	2:D:504:SER:N	2.83	0.51
3:F:129:LYS:HE2	3:F:131:TYR:OH	2.09	0.51
8:I:474:GLU:OE1	8:I:475:ARG:N	2.44	0.51
3:F:149:VAL:HG13	3:F:154:LEU:HB2	1.92	0.51
8:I:293:VAL:O	8:I:293:VAL:HG23	2.11	0.51
5:A:364:LYS:HD3	5:A:364:LYS:N	2.25	0.51
5:A:949:ILE:HD11	5:A:1306:GLN:HB3	1.90	0.51
3:F:142:LEU:O	3:F:146:GLU:HG3	2.10	0.51
6:C:196:PHE:CE1	6:C:252:VAL:HG22	2.45	0.51
7:B:29:TRP:HB3	7:B:46:ARG:CZ	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:507:ARG:NH1	2:D:509:THR:HG23	2.26	0.51
5:A:1057:MET:HE3	5:A:1057:MET:O	2.11	0.51
2:D:394:LEU:HD22	4:E:414:ARG:NH1	2.19	0.51
5:A:1020:TYR:CD2	5:A:1291:ILE:HD12	2.44	0.51
6:C:552:HIS:CG	7:B:125:GLN:OE1	2.64	0.51
4:E:547:ARG:HB2	4:E:547:ARG:HH11	1.74	0.51
5:A:212:THR:O	5:A:212:THR:HG23	2.11	0.51
7:B:391:LEU:HD23	7:B:392:THR:N	2.26	0.51
7:B:54:LYS:O	7:B:58:GLU:HG3	2.11	0.51
3:F:55:LEU:N	3:F:55:LEU:HD12	2.26	0.51
5:A:388:VAL:O	5:A:408:LYS:HD2	2.12	0.50
5:A:841:LEU:HD12	5:A:841:LEU:N	2.26	0.50
5:A:1133:LEU:HD11	5:A:1242:THR:OG1	2.11	0.50
6:C:189:GLN:CG	6:C:260:ALA:HB2	2.41	0.50
8:I:332:GLY:C	8:I:448:ILE:HD11	2.35	0.50
3:F:34:VAL:HB	3:F:130:LEU:HD22	1.91	0.50
5:A:828:ASN:OD1	5:A:828:ASN:O	2.29	0.50
5:A:942:VAL:HG22	5:A:943:THR:N	2.27	0.50
6:C:637:MET:HE1	6:C:666:GLU:CD	2.36	0.50
7:B:590:ASN:CG	7:B:590:ASN:O	2.54	0.50
8:H:339:TYR:HE1	8:H:341:LEU:HD21	1.76	0.50
5:A:849:ARG:HA	5:A:849:ARG:NH1	2.26	0.50
8:I:130:GLU:OE1	8:I:130:GLU:N	2.44	0.50
2:D:49:SER:OG	4:E:439:ARG:NH1	2.44	0.50
5:A:222:TYR:CE2	5:A:612:VAL:HG21	2.46	0.50
5:A:1325:ASN:OD1	5:A:1326:TYR:N	2.45	0.50
8:H:44:ARG:NH2	8:H:59:ASP:OD1	2.44	0.50
2:D:297:GLY:CA	2:D:409:ILE:HD13	2.41	0.50
4:E:159:ARG:HG3	4:E:159:ARG:HH11	1.77	0.50
6:C:481:THR:HG22	6:C:486:CYS:HB3	1.93	0.50
8:I:411:GLY:CA	8:I:441:ILE:HD13	2.42	0.50
2:D:375:GLY:O	2:D:381:ILE:HD11	2.11	0.50
7:B:30:THR:HG23	7:B:49:GLN:OE1	2.11	0.50
2:D:368:ASP:OD2	2:D:485:ARG:NH2	2.45	0.50
2:D:382:THR:HG22	4:E:266:VAL:HG21	1.94	0.50
5:A:989:SER:O	5:A:989:SER:OG	2.20	0.50
7:B:673:LEU:HD12	7:B:673:LEU:H	1.77	0.50
8:I:437:TRP:CE2	8:I:441:ILE:HD11	2.47	0.50
5:A:380:ASP:O	5:A:381:GLN:NE2	2.44	0.50
5:A:771:GLU:OE2	5:A:771:GLU:HA	2.12	0.50
6:C:506:TRP:HB3	6:C:519:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:LEU:C	2:D:239:LEU:HD23	2.37	0.49
4:E:199:PHE:O	4:E:200:TYR:HD2	1.94	0.49
5:A:190:ILE:CG2	5:A:194:PRO:HG3	2.41	0.49
5:A:231:ILE:HG22	5:A:342:ILE:HD11	1.94	0.49
5:A:1190:ILE:HD13	5:A:1253:TYR:CE2	2.47	0.49
2:D:517:PRO:N	2:D:518:PRO:CD	2.76	0.49
6:C:399:ASN:OD1	6:C:400:LYS:N	2.45	0.49
5:A:905:ILE:CG2	5:A:906:GLY:N	2.76	0.49
5:A:1156:PHE:HE2	5:A:1164:ILE:HG22	1.78	0.49
8:I:150:PRO:O	8:I:295:THR:HG23	2.13	0.49
1:G:62:TYR:HB3	1:G:75:LEU:HD21	1.94	0.49
5:A:231:ILE:CG2	5:A:342:ILE:HD11	2.43	0.49
5:A:408:LYS:NZ	5:A:409:SER:O	2.45	0.49
5:A:847:ASN:OD1	5:A:849:ARG:N	2.45	0.49
5:A:1147:PHE:CD1	5:A:1147:PHE:C	2.90	0.49
8:H:151:PHE:CE1	8:H:292:VAL:HG21	2.48	0.49
5:A:25:ILE:HD12	5:A:25:ILE:N	2.28	0.49
5:A:165:ASP:C	5:A:165:ASP:OD1	2.55	0.49
7:B:291:GLU:OE1	7:B:402:ILE:HG22	2.12	0.49
8:I:398:GLU:CD	8:I:398:GLU:O	2.56	0.49
8:I:477:ILE:O	8:I:481:ILE:HG13	2.12	0.49
2:D:380:HIS:HA	2:D:383:THR:HG22	1.93	0.49
5:A:927:LEU:CD2	5:A:929:VAL:HG23	2.43	0.49
6:C:196:PHE:CD2	6:C:198:TYR:CE1	3.01	0.49
8:I:51:GLN:HG3	8:I:52:PHE:N	2.28	0.49
5:A:167:GLU:OE1	5:A:167:GLU:HA	2.13	0.49
7:B:153:ALA:HB3	7:B:156:LEU:HD12	1.93	0.49
8:H:20:ILE:HG23	8:H:23:ARG:CZ	2.43	0.49
5:A:866:CYS:HB2	5:A:903:LEU:HD11	1.95	0.49
5:A:84:ILE:N	5:A:84:ILE:HD12	2.29	0.48
5:A:241:LYS:HA	5:A:244:LYS:HZ1	1.78	0.48
5:A:497:THR:HG22	5:A:516:GLU:OE2	2.12	0.48
5:A:642:ASN:OD1	5:A:643:ALA:N	2.43	0.48
8:H:195:HIS:NE2	8:H:197:GLU:OE2	2.46	0.48
8:I:274:LEU:O	8:I:338:ILE:HG23	2.13	0.48
8:I:412:THR:HG22	8:I:414:LYS:HD2	1.94	0.48
5:A:1176:LEU:HD11	5:A:1204:GLN:HB2	1.95	0.48
5:A:131:ASP:OD1	5:A:132:LYS:HG3	2.13	0.48
2:D:24:PRO:HB3	2:D:60:ARG:HB2	1.93	0.48
2:D:433:GLN:O	2:D:437:GLN:HG3	2.13	0.48
6:C:329:PHE:C	6:C:329:PHE:CD2	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:670:ILE:HD12	7:B:682:GLN:O	2.13	0.48
8:I:41:PHE:CD1	8:I:310:GLU:HG3	2.49	0.48
5:A:773:TRP:CZ3	5:A:788:PHE:CE1	3.01	0.48
5:A:138:ASP:CG	5:A:138:ASP:O	2.57	0.48
8:I:101:ASP:OD1	8:I:120:PRO:HD2	2.14	0.48
2:D:516:ASN:O	2:D:519:PRO:HD2	2.14	0.48
5:A:794:LEU:HD23	5:A:819:VAL:HG12	1.96	0.48
7:B:46:ARG:HD2	7:B:46:ARG:O	2.14	0.48
8:I:155:PHE:CD1	8:I:293:VAL:HG11	2.49	0.48
2:D:49:SER:OG	4:E:439:ARG:CZ	2.62	0.48
2:D:501:SER:OG	2:D:507:ARG:NH2	2.47	0.48
5:A:195:ARG:HA	5:A:195:ARG:NE	2.29	0.48
7:B:156:LEU:HD22	7:B:163:ASP:OD2	2.14	0.47
2:D:503:CYS:O	2:D:504:SER:OG	2.28	0.47
4:E:253:ASN:OD1	4:E:254:GLU:N	2.47	0.47
7:B:689:ASP:OD2	7:B:691:THR:HG23	2.14	0.47
2:D:8:PRO:O	4:E:547:ARG:NH2	2.48	0.47
6:C:30:TRP:CE2	6:C:63:CYS:HB3	2.49	0.47
5:A:56:ILE:HG23	5:A:102:VAL:HG11	1.95	0.47
5:A:1001:THR:O	5:A:1001:THR:CG2	2.61	0.47
5:A:1020:TYR:HD2	5:A:1291:ILE:HD12	1.79	0.47
7:B:299:PHE:C	7:B:299:PHE:CD2	2.93	0.47
7:B:430:GLU:OE1	7:B:431:GLY:N	2.48	0.47
4:E:54:CYS:SG	4:E:55:SER:N	2.88	0.47
5:A:287:MET:HE3	5:A:287:MET:HA	1.97	0.47
6:C:539:THR:HG23	6:C:540:THR:HG23	1.96	0.47
8:I:24:MET:HG2	8:I:25:SER:H	1.80	0.47
4:E:531:GLU:N	4:E:531:GLU:OE1	2.48	0.47
5:A:807:THR:HG22	5:A:807:THR:O	2.15	0.47
7:B:661:LEU:HD23	7:B:662:TYR:N	2.29	0.47
8:H:334:LEU:HD23	8:H:335:TYR:N	2.29	0.47
8:I:471:GLN:O	8:I:475:ARG:HG3	2.15	0.47
4:E:69:ASP:HB2	4:E:78:CYS:SG	2.54	0.47
4:E:139:ASP:O	4:E:181:ASN:ND2	2.47	0.47
4:E:512:TRP:CE2	4:E:544:CYS:SG	3.08	0.47
5:A:504:LEU:HD21	5:A:651:LEU:HD21	1.97	0.47
7:B:146:CYS:N	7:B:150:ARG:O	2.46	0.47
8:H:138:GLY:O	8:H:147:LEU:N	2.47	0.47
8:I:414:LYS:HD2	8:I:414:LYS:H	1.80	0.47
4:E:437:VAL:HG13	4:E:438:LEU:HD23	1.97	0.47
5:A:1053:MET:HE3	5:A:1053:MET:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:333:THR:O	5:A:893:SER:OG	2.20	0.47
6:C:115:ASP:OD1	6:C:115:ASP:N	2.47	0.47
8:H:116:GLU:O	8:H:116:GLU:HG2	2.13	0.47
8:I:316:ALA:O	8:I:319:GLU:HG3	2.14	0.47
2:D:67:ARG:H	2:D:67:ARG:HD3	1.80	0.47
3:F:107:VAL:HA	3:F:118:LEU:HD13	1.96	0.47
7:B:79:PRO:HD2	7:B:79:PRO:O	2.13	0.47
5:A:136:THR:HG23	5:A:222:TYR:HE1	1.80	0.46
5:A:671:GLU:C	5:A:672:ILE:HD13	2.39	0.46
8:I:27:TRP:CD1	8:I:27:TRP:N	2.83	0.46
8:I:28:SER:OG	8:I:29:GLU:OE2	2.32	0.46
8:I:90:ARG:O	8:I:92:ILE:HG23	2.15	0.46
3:F:21:ASN:O	3:F:21:ASN:OD1	2.33	0.46
5:A:571:LEU:HD12	5:A:572:GLN:N	2.30	0.46
5:A:828:ASN:O	5:A:828:ASN:CG	2.58	0.46
8:I:494:ASN:CG	8:I:494:ASN:O	2.58	0.46
5:A:234:GLU:OE1	5:A:247:GLU:HB2	2.15	0.46
8:I:186:LYS:HB3	8:I:281:HIS:HB3	1.96	0.46
5:A:87:ILE:CG2	5:A:92:LEU:HD11	2.46	0.46
5:A:902:PRO:HB3	5:A:929:VAL:HG21	1.96	0.46
7:B:166:ASP:OD1	7:B:168:SER:HB2	2.14	0.46
7:B:550:GLU:HA	7:B:550:GLU:OE1	2.15	0.46
6:C:503:TRP:CE3	6:C:521:ARG:HD3	2.50	0.46
7:B:86:ASP:OD1	7:B:86:ASP:N	2.45	0.46
2:D:273:GLU:CD	2:D:273:GLU:H	2.24	0.46
4:E:384:MET:HG3	8:H:196:TYR:CE2	2.51	0.46
5:A:285:THR:N	5:A:287:MET:SD	2.89	0.46
5:A:1020:TYR:CD2	5:A:1291:ILE:HG23	2.50	0.46
6:C:168:VAL:CG1	6:C:179:LEU:HD11	2.46	0.46
1:G:47:PHE:HA	1:G:50:VAL:HG22	1.98	0.46
2:D:354:ASN:OD1	2:D:355:GLU:N	2.48	0.46
4:E:333:GLU:N	4:E:333:GLU:OE2	2.49	0.46
5:A:1132:THR:HG22	5:A:1133:LEU:N	2.31	0.46
7:B:128:ILE:O	7:B:128:ILE:CG2	2.63	0.46
8:H:284:ARG:NH2	8:H:328:SER:OG	2.49	0.46
8:I:34:ASP:OD2	8:I:37:LEU:HD13	2.15	0.46
8:I:303:LYS:HE2	8:I:303:LYS:HA	1.98	0.46
2:D:122:ALA:HB2	2:D:139:HIS:CG	2.51	0.46
3:F:107:VAL:O	3:F:107:VAL:HG13	2.16	0.46
5:A:157:ARG:HB2	5:A:205:TYR:CE1	2.50	0.46
5:A:1161:LEU:O	5:A:1165:ASP:OD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1336:ARG:HG2	5:A:1337:PRO:O	2.16	0.46
6:C:461:GLN:OE1	6:C:485:ALA:HB1	2.16	0.46
8:I:483:GLU:HG3	8:I:484:PHE:CD2	2.51	0.46
5:A:1277:GLU:O	5:A:1280:TYR:HA	2.15	0.46
4:E:503:THR:HG21	8:H:196:TYR:OH	2.16	0.45
5:A:224:LEU:HD21	5:A:771:GLU:OE1	2.16	0.45
5:A:597:ASP:OD1	5:A:782:ARG:N	2.49	0.45
5:A:1255:LEU:HD13	5:A:1270:VAL:HG12	1.98	0.45
2:D:360:ASN:OD1	2:D:361:LYS:N	2.49	0.45
3:F:119:TYR:C	3:F:120:LEU:HD12	2.41	0.45
5:A:471:ASP:CG	5:A:471:ASP:O	2.58	0.45
8:I:184:GLU:HG3	8:I:185:THR:N	2.31	0.45
4:E:284:MET:HE1	4:E:434:ILE:HD11	1.99	0.45
5:A:138:ASP:O	5:A:138:ASP:OD1	2.34	0.45
2:D:283:PHE:O	2:D:287:GLY:N	2.46	0.45
4:E:547:ARG:HH11	4:E:547:ARG:CB	2.30	0.45
5:A:188:PHE:CD1	5:A:188:PHE:C	2.93	0.45
6:C:189:GLN:HG2	6:C:260:ALA:CB	2.47	0.45
8:I:294:LEU:HD12	8:I:294:LEU:N	2.31	0.45
5:A:798:GLU:OE2	5:A:798:GLU:N	2.50	0.45
5:A:1283:GLY:HA3	5:A:1289:ASP:OD1	2.16	0.45
8:I:513:PHE:CD1	8:I:518:CYS:HB3	2.51	0.45
4:E:533:ASP:OD1	4:E:533:ASP:C	2.59	0.45
5:A:840:GLN:NE2	5:A:899:THR:HG23	2.31	0.45
8:H:92:ILE:HD12	8:H:96:LEU:HB2	1.97	0.45
8:I:127:GLU:O	8:I:173:ARG:N	2.42	0.45
5:A:605:VAL:O	5:A:798:GLU:OE2	2.35	0.45
5:A:774:LEU:HD12	5:A:776:GLU:OE1	2.17	0.45
5:A:1276:GLU:CB	5:A:1278:GLN:HG3	2.47	0.45
7:B:693:ARG:O	7:B:693:ARG:CG	2.64	0.45
2:D:65:GLN:CD	2:D:65:GLN:H	2.25	0.45
5:A:994:GLN:NE2	5:A:997:ILE:HD11	2.31	0.45
5:A:1068:VAL:HG13	5:A:1078:LEU:HD22	1.98	0.45
7:B:50:ILE:CD1	7:B:67:LYS:HD3	2.47	0.45
8:I:24:MET:SD	8:I:59:ASP:OD2	2.75	0.45
8:I:309:TYR:CD1	8:I:309:TYR:C	2.95	0.45
6:C:47:THR:HG21	6:C:290:SER:OG	2.17	0.45
7:B:501:VAL:HB	7:B:624:ILE:HG13	1.99	0.45
2:D:51:LYS:HD2	2:D:278:GLU:OE1	2.16	0.45
2:D:398:TRP:O	2:D:402:VAL:HG23	2.17	0.45
5:A:1176:LEU:HD11	5:A:1202:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1232:LEU:HD23	5:A:1232:LEU:O	2.17	0.45
3:F:15:THR:HG22	3:F:91:ARG:NH2	2.32	0.44
4:E:267:GLN:HG2	4:E:427:ILE:HD11	1.99	0.44
5:A:1024:TYR:CD1	5:A:1024:TYR:C	2.95	0.44
2:D:186:PHE:CD1	2:D:186:PHE:C	2.94	0.44
5:A:354:LEU:HD12	5:A:374:GLN:O	2.18	0.44
5:A:841:LEU:HD12	5:A:841:LEU:H	1.81	0.44
5:A:1020:TYR:CE2	5:A:1291:ILE:HG23	2.52	0.44
6:C:48:ARG:NE	6:C:69:GLU:OE2	2.42	0.44
3:F:67:SER:OG	3:F:80:ARG:HG2	2.18	0.44
5:A:1245:ALA:HA	5:A:1283:GLY:HA2	2.00	0.44
8:I:93:LYS:HB3	8:I:96:LEU:HD13	1.99	0.44
5:A:622:ARG:HG2	5:A:625:GLN:HB2	1.99	0.44
5:A:1340:VAL:O	5:A:1340:VAL:CG1	2.63	0.44
4:E:379:ARG:NH1	8:H:199:GLN:HG2	2.32	0.44
5:A:383:VAL:HG12	5:A:385:GLY:H	1.82	0.44
5:A:840:GLN:OE1	5:A:897:THR:HB	2.17	0.44
5:A:1045:LEU:HD23	5:A:1046:LYS:N	2.32	0.44
6:C:196:PHE:CD1	6:C:252:VAL:HG22	2.52	0.44
4:E:98:ASP:OD1	4:E:98:ASP:C	2.61	0.44
5:A:285:THR:O	5:A:287:MET:SD	2.76	0.44
5:A:433:PHE:C	5:A:434:ASN:HD22	2.25	0.44
6:C:202:ASN:HB3	6:C:246:LYS:HE2	2.00	0.44
7:B:215:GLY:O	7:B:217:ILE:HD12	2.17	0.44
5:A:44:TYR:OH	5:A:500:ASN:OD1	2.30	0.44
5:A:526:ILE:HD12	5:A:540:LEU:HD21	1.99	0.44
5:A:1013:MET:N	5:A:1013:MET:HE2	2.33	0.44
6:C:284:PRO:HG3	6:C:288:ASP:HB3	1.99	0.44
7:B:73:CYS:SG	7:B:74:ASN:N	2.91	0.44
8:I:324:HIS:C	8:I:455:ILE:HD11	2.43	0.44
2:D:360:ASN:OD1	2:D:360:ASN:C	2.60	0.43
3:F:17:GLN:N	3:F:17:GLN:CD	2.74	0.43
3:F:93:LEU:HD22	3:F:102:ALA:HB1	1.99	0.43
5:A:1050:LYS:O	5:A:1054:LEU:HD13	2.18	0.43
2:D:52:GLU:OE2	2:D:52:GLU:HA	2.18	0.43
2:D:359:ARG:HG3	2:D:359:ARG:HH11	1.83	0.43
5:A:251:LYS:HA	5:A:295:GLY:O	2.18	0.43
6:C:250:LEU:HD21	6:C:252:VAL:HG23	2.00	0.43
7:B:563:ALA:HB1	7:B:596:ARG:HH21	1.82	0.43
5:A:390:LEU:HD12	5:A:434:ASN:O	2.19	0.43
6:C:189:GLN:HG2	6:C:260:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:96:LEU:N	8:I:96:LEU:HD12	2.33	0.43
4:E:439:ARG:CZ	4:E:450:ARG:NH1	2.81	0.43
5:A:532:GLN:OE1	5:A:532:GLN:O	2.35	0.43
5:A:537:SER:HB2	5:A:628:GLU:OE2	2.18	0.43
5:A:1130:GLN:OE1	5:A:1130:GLN:HA	2.18	0.43
7:B:291:GLU:OE2	7:B:400:VAL:HG23	2.19	0.43
8:H:44:ARG:NH1	8:H:59:ASP:OD1	2.52	0.43
8:I:452:LEU:HD22	8:I:452:LEU:H	1.82	0.43
3:F:16:ILE:HG22	3:F:17:GLN:N	2.32	0.43
5:A:56:ILE:HG22	5:A:66:TYR:HD2	1.84	0.43
5:A:503:ILE:HD12	5:A:511:HIS:HB2	1.99	0.43
5:A:506:LYS:HB3	5:A:630:SER:OG	2.19	0.43
2:D:62:CYS:O	2:D:65:GLN:NE2	2.51	0.43
2:D:122:ALA:HB1	2:D:137:LEU:O	2.19	0.43
3:F:103:VAL:HG22	3:F:122:ARG:HE	1.84	0.43
5:A:983:LEU:N	5:A:983:LEU:HD22	2.34	0.43
5:A:1026:GLU:OE1	5:A:1091:LYS:HE3	2.18	0.43
7:B:255:TYR:HD1	7:B:256:LYS:N	2.16	0.43
7:B:729:GLU:HA	7:B:743:ARG:HE	1.84	0.43
4:E:474:ASN:OD1	4:E:498:CYS:O	2.36	0.43
5:A:788:PHE:CD1	5:A:788:PHE:C	2.97	0.43
8:H:44:ARG:HG2	8:H:44:ARG:HH11	1.84	0.43
8:H:165:ASP:OD1	8:H:168:THR:HB	2.19	0.43
8:I:176:TRP:CH2	8:I:291:ASP:OD1	2.71	0.43
8:I:346:MET:HE1	8:I:347:LYS:HE2	2.00	0.43
2:D:231:PHE:CD2	2:D:232:SER:N	2.87	0.43
3:F:22:PHE:CZ	3:F:24:ALA:HB2	2.54	0.43
5:A:927:LEU:HD21	5:A:929:VAL:HG23	2.00	0.43
5:A:1245:ALA:O	5:A:1249:GLU:OE1	2.37	0.43
8:H:339:TYR:HE1	8:H:341:LEU:CD2	2.31	0.43
8:H:404:VAL:O	8:I:190:ASN:HA	2.19	0.43
3:F:109:GLU:OE2	3:F:110:THR:N	2.52	0.43
5:A:841:LEU:H	5:A:841:LEU:CD1	2.32	0.43
5:A:905:ILE:HA	5:A:929:VAL:CG1	2.48	0.43
7:B:578:ASP:OD1	7:B:578:ASP:C	2.62	0.43
8:H:277:LYS:HE3	8:H:336:GLU:OE1	2.19	0.43
1:G:28:ILE:CG2	1:G:62:TYR:HD1	2.32	0.43
2:D:26:GLN:O	2:D:27:LYS:HG3	2.19	0.43
2:D:35:LEU:HD21	2:D:38:PRO:N	2.33	0.43
5:A:773:TRP:HZ3	5:A:788:PHE:CE1	2.36	0.43
7:B:46:ARG:NH2	7:B:69:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:83:ASP:OD2	8:I:91:CYS:HB3	2.19	0.43
8:I:446:VAL:HG22	8:I:447:LEU:N	2.33	0.43
5:A:387:PRO:HB3	5:A:408:LYS:HZ1	1.84	0.42
5:A:396:ASP:OD1	5:A:397:VAL:N	2.46	0.42
5:A:1024:TYR:O	5:A:1027:THR:HG23	2.19	0.42
5:A:1176:LEU:C	5:A:1176:LEU:HD23	2.44	0.42
7:B:662:TYR:HA	7:B:666:GLU:OE1	2.18	0.42
7:B:672:CYS:SG	7:B:678:THR:N	2.92	0.42
8:H:407:LEU:HD12	8:H:408:ILE:N	2.34	0.42
2:D:169:THR:HG21	6:C:380:GLY:O	2.19	0.42
5:A:136:THR:N	5:A:139:GLN:OE1	2.52	0.42
5:A:852:GLY:C	5:A:853:MET:SD	3.02	0.42
5:A:986:GLU:CD	5:A:986:GLU:H	2.27	0.42
5:A:1026:GLU:HA	5:A:1031:TRP:CZ3	2.54	0.42
5:A:1267:VAL:HG11	5:A:1300:TYR:HD2	1.83	0.42
8:H:309:TYR:OH	8:H:479:ASP:OD2	2.30	0.42
4:E:38:LYS:HG2	4:E:468:ARG:O	2.19	0.42
4:E:325:LEU:HD13	4:E:389:ILE:HD11	2.00	0.42
5:A:152:LEU:HD11	5:A:627:LEU:HD21	2.00	0.42
5:A:1301:SER:O	5:A:1304:VAL:HG12	2.19	0.42
6:C:196:PHE:HD2	6:C:198:TYR:CE1	2.37	0.42
6:C:342:TRP:CH2	6:C:347:LYS:N	2.87	0.42
8:I:296:THR:HA	8:I:299:VAL:HG22	2.01	0.42
8:I:298:PHE:CD1	8:I:298:PHE:C	2.97	0.42
3:F:38:SER:OG	3:F:127:SER:OG	2.32	0.42
6:C:503:TRP:CE3	6:C:521:ARG:CD	3.02	0.42
5:A:135:TYR:CE2	5:A:141:VAL:HG22	2.54	0.42
5:A:179:HIS:C	5:A:180:ILE:HD13	2.44	0.42
5:A:1164:ILE:O	5:A:1168:LEU:HG	2.19	0.42
5:A:1315:VAL:HG22	5:A:1346:LEU:HD11	2.01	0.42
7:B:494:VAL:O	7:B:494:VAL:CG2	2.66	0.42
8:I:289:ASN:C	8:I:290:ARG:HD3	2.43	0.42
5:A:131:ASP:OD1	5:A:131:ASP:C	2.62	0.42
5:A:606:ASP:O	5:A:609:VAL:HG23	2.20	0.42
5:A:1325:ASN:OD1	5:A:1325:ASN:C	2.62	0.42
7:B:37:LYS:HG2	7:B:42:GLY:CA	2.50	0.42
3:F:38:SER:OG	3:F:127:SER:CB	2.68	0.42
4:E:481:GLU:OE2	4:E:486:ARG:NE	2.53	0.42
5:A:27:ALA:CB	5:A:39:ILE:CD1	2.98	0.42
5:A:1029:ASN:O	5:A:1033:ILE:N	2.50	0.42
5:A:1264:ILE:HG23	5:A:1265:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:24:MET:HG3	8:I:46:ILE:HD13	2.01	0.42
3:F:125:GLN:OE1	3:F:125:GLN:HA	2.19	0.42
4:E:515:TRP:CD1	4:E:528:ARG:HH21	2.37	0.42
6:C:110:ASP:OD1	6:C:274:GLU:HB2	2.19	0.42
6:C:410:VAL:O	6:C:410:VAL:HG22	2.19	0.42
7:B:27:TYR:CE2	7:B:61:CYS:SG	3.12	0.42
2:D:507:ARG:HG2	2:D:508:LYS:N	2.35	0.42
3:F:43:LEU:N	3:F:43:LEU:HD22	2.34	0.42
3:F:161:TYR:N	3:F:161:TYR:CD1	2.88	0.42
4:E:499:GLU:OE1	4:E:499:GLU:N	2.48	0.42
5:A:191:PRO:O	5:A:194:PRO:HD2	2.19	0.42
5:A:429:THR:HG22	5:A:430:VAL:HG13	2.02	0.42
7:B:246:ALA:O	7:B:247:GLU:HG2	2.20	0.42
8:I:155:PHE:HD1	8:I:293:VAL:HG21	1.83	0.42
5:A:592:MET:HE2	5:A:784:LYS:HB3	2.02	0.42
5:A:936:ARG:HD3	5:A:937:GLU:H	1.84	0.42
8:H:48:VAL:HG12	8:H:50:GLY:H	1.85	0.42
8:H:129:SER:HB2	8:H:172:TYR:CG	2.55	0.42
8:H:502:ASP:OD2	8:H:502:ASP:C	2.62	0.42
2:D:409:ILE:N	2:D:409:ILE:HD12	2.35	0.41
2:D:420:VAL:HG23	2:D:420:VAL:O	2.20	0.41
5:A:861:ALA:HB1	5:A:865:ILE:HG22	2.02	0.41
7:B:179:VAL:HG13	7:B:180:CYS:N	2.35	0.41
7:B:670:ILE:HD11	7:B:684:PHE:CZ	2.55	0.41
2:D:35:LEU:C	2:D:35:LEU:HD23	2.45	0.41
2:D:450:HIS:ND1	2:D:496:CYS:SG	2.89	0.41
5:A:191:PRO:HB2	5:A:194:PRO:HD3	2.02	0.41
7:B:663:LEU:HD12	7:B:663:LEU:H	1.84	0.41
8:H:318:LEU:O	8:H:322:GLY:N	2.51	0.41
8:I:322:GLY:O	8:I:455:ILE:HG13	2.20	0.41
4:E:325:LEU:HD12	4:E:389:ILE:HG12	2.02	0.41
4:E:388:ASP:C	4:E:388:ASP:OD1	2.62	0.41
5:A:317:ASP:OD1	5:A:318:LEU:N	2.53	0.41
5:A:386:VAL:CG1	5:A:437:THR:HG23	2.50	0.41
5:A:1004:PRO:O	5:A:1010:ALA:HB1	2.20	0.41
5:A:1133:LEU:HD22	5:A:1246:ARG:HH11	1.85	0.41
5:A:1287:THR:O	5:A:1291:ILE:CG1	2.68	0.41
6:C:320:ASP:OD2	6:C:320:ASP:C	2.63	0.41
6:C:337:CYS:HB3	6:C:353:CYS:CA	2.20	0.41
7:B:701:ARG:HD2	7:B:724:ILE:HD11	2.02	0.41
8:H:294:LEU:N	8:H:294:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:ALA:HB2	3:F:119:TYR:CD1	2.56	0.41
3:F:169:GLU:N	3:F:169:GLU:OE2	2.53	0.41
5:A:533:ASN:OD1	5:A:533:ASN:N	2.53	0.41
5:A:597:ASP:HA	5:A:782:ARG:H	1.84	0.41
8:H:500:LEU:HG	8:H:500:LEU:O	2.20	0.41
8:I:82:ASN:O	8:I:94:MET:HE1	2.21	0.41
8:I:96:LEU:HD23	8:I:103:ASP:HB3	2.03	0.41
4:E:195:ILE:HG23	4:E:262:ILE:HG12	2.02	0.41
4:E:515:TRP:HB3	4:E:528:ARG:HE	1.86	0.41
5:A:164:ILE:N	5:A:164:ILE:HD12	2.35	0.41
5:A:191:PRO:O	5:A:194:PRO:CD	2.69	0.41
5:A:591:ASN:CG	5:A:785:GLN:OE1	2.63	0.41
5:A:1034:PHE:CE2	5:A:1037:ASP:HB2	2.56	0.41
7:B:87:PHE:HA	7:B:104:ARG:HB3	2.01	0.41
8:I:285:PHE:CD1	8:I:285:PHE:C	2.98	0.41
4:E:48:ILE:HG12	4:E:48:ILE:O	2.19	0.41
4:E:99:ASP:OD1	4:E:99:ASP:C	2.63	0.41
5:A:24:VAL:C	5:A:25:ILE:HD12	2.46	0.41
5:A:180:ILE:HG22	5:A:182:ILE:CD1	2.51	0.41
5:A:829:ILE:HG21	5:A:925:LYS:NZ	2.36	0.41
5:A:839:ILE:HG23	5:A:841:LEU:CD1	2.50	0.41
5:A:1188:LEU:C	5:A:1188:LEU:HD23	2.46	0.41
8:I:85:GLN:O	8:I:85:GLN:CG	2.69	0.41
5:A:241:LYS:CE	5:A:441:ASP:HB2	2.50	0.41
5:A:390:LEU:HD13	5:A:435:VAL:HG22	2.02	0.41
5:A:1336:ARG:HG3	5:A:1337:PRO:HD2	2.01	0.41
6:C:189:GLN:HG3	6:C:260:ALA:HB2	2.02	0.41
6:C:351:HIS:NE2	6:C:353:CYS:SG	2.94	0.41
8:H:68:VAL:O	8:H:68:VAL:HG13	2.20	0.41
8:H:263:LEU:HD12	8:H:263:LEU:C	2.45	0.41
1:G:23:PHE:CG	1:G:39:CYS:HB3	2.56	0.41
2:D:270:LEU:HD11	2:D:282:LEU:HD22	2.01	0.41
5:A:492:TYR:HB3	5:A:495:LYS:HG3	2.02	0.41
5:A:903:LEU:CB	5:A:904:GLU:OE1	2.69	0.41
5:A:923:LEU:HD23	5:A:923:LEU:O	2.21	0.41
7:B:638:ILE:HG23	7:B:640:ALA:H	1.85	0.41
8:I:343:LYS:O	8:I:346:MET:HE3	2.21	0.41
8:I:474:GLU:CD	8:I:474:GLU:C	2.88	0.41
2:D:30:TYR:CE2	2:D:271:PRO:HB3	2.56	0.41
3:F:126:LEU:HD23	3:F:127:SER:N	2.36	0.41
4:E:253:ASN:OD1	4:E:253:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:222:TYR:CD2	5:A:612:VAL:HG11	2.55	0.41
5:A:477:LEU:HD22	5:A:477:LEU:H	1.86	0.41
5:A:829:ILE:HD13	5:A:925:LYS:NZ	2.35	0.41
5:A:944:LEU:HD23	5:A:945:ASP:N	2.36	0.41
5:A:1053:MET:HA	5:A:1056:ILE:HG22	2.02	0.41
5:A:1114:ASP:OD1	5:A:1114:ASP:C	2.63	0.41
5:A:1286:SER:O	5:A:1290:THR:HG22	2.21	0.41
5:A:1286:SER:O	5:A:1289:ASP:OD2	2.38	0.41
5:A:1290:THR:HG23	5:A:1291:ILE:N	2.36	0.41
6:C:293:ARG:NH2	6:C:451:GLU:OE1	2.46	0.41
7:B:308:LYS:HE2	7:B:310:ASP:OD2	2.21	0.41
7:B:744:TYR:CE2	7:B:751:TRP:O	2.74	0.41
8:I:85:GLN:O	8:I:85:GLN:HG3	2.20	0.41
3:F:143:SER:O	3:F:147:GLN:HG2	2.21	0.41
5:A:87:ILE:HG22	5:A:92:LEU:HD11	2.01	0.41
5:A:388:VAL:HG11	5:A:418:ALA:CB	2.51	0.41
5:A:938:SER:O	5:A:1362:THR:HG23	2.21	0.41
8:H:191:PHE:CD1	8:H:191:PHE:C	2.98	0.41
8:H:499:ILE:O	8:H:499:ILE:CG2	2.68	0.41
8:I:103:ASP:HB3	8:I:155:PHE:CE2	2.56	0.41
8:I:325:TYR:CE1	8:I:453:SER:HB2	2.56	0.41
8:I:438:ALA:HA	8:I:441:ILE:HG12	2.01	0.41
2:D:269:ARG:HH11	2:D:269:ARG:HB3	1.85	0.40
5:A:165:ASP:OD1	5:A:167:GLU:N	2.54	0.40
5:A:265:VAL:HG22	5:A:329:VAL:HG12	2.02	0.40
5:A:796:THR:HG22	5:A:818:LYS:HG2	2.03	0.40
5:A:1253:TYR:CE1	5:A:1292:ASN:OD1	2.74	0.40
5:A:1297:LEU:HD23	5:A:1297:LEU:O	2.21	0.40
7:B:128:ILE:O	7:B:128:ILE:HG23	2.20	0.40
7:B:731:THR:HG23	7:B:731:THR:O	2.21	0.40
8:I:195:HIS:C	8:I:196:TYR:CD1	2.99	0.40
4:E:512:TRP:HB3	4:E:513:SER:O	2.22	0.40
5:A:949:ILE:O	5:A:1262:LYS:HE3	2.21	0.40
7:B:578:ASP:OD1	7:B:580:THR:N	2.53	0.40
8:H:341:LEU:HD13	8:H:402:ASP:HA	2.02	0.40
5:A:301:PHE:CE1	5:A:303:SER:HA	2.57	0.40
5:A:433:PHE:CZ	5:A:452:TYR:HB2	2.56	0.40
5:A:588:VAL:HG13	5:A:790:LEU:HD13	2.02	0.40
5:A:856:CYS:O	5:A:914:LEU:HG	2.21	0.40
5:A:1339:GLU:H	5:A:1339:GLU:CD	2.29	0.40
6:C:407:ALA:O	6:C:410:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:643:HIS:HB2	6:C:644:PRO:HD3	2.02	0.40
7:B:544:GLN:O	7:B:547:THR:HG22	2.21	0.40
8:H:290:ARG:HG3	8:H:291:ASP:OD2	2.21	0.40
4:E:252:TYR:CD2	4:E:333:GLU:OE2	2.75	0.40
4:E:271:PHE:CZ	4:E:315:GLY:HA3	2.56	0.40
4:E:552:GLN:HG2	4:E:553:ALA:N	2.37	0.40
5:A:471:ASP:O	5:A:471:ASP:OD2	2.39	0.40
5:A:606:ASP:OD1	5:A:795:THR:HG21	2.21	0.40
5:A:864:GLY:HA2	5:A:904:GLU:OE2	2.21	0.40
5:A:1022:PHE:CZ	5:A:1091:LYS:HD3	2.57	0.40
6:C:31:ASP:OD1	6:C:53:ALA:HB2	2.22	0.40
6:C:194:ASN:O	6:C:195:ASP:OD1	2.39	0.40
6:C:480:TYR:N	6:C:480:TYR:CD1	2.85	0.40
8:I:291:ASP:O	8:I:291:ASP:OD2	2.40	0.40
8:I:412:THR:HB	8:I:440:SER:HB2	2.03	0.40
4:E:494:LEU:HD23	4:E:495:GLY:N	2.37	0.40
4:E:514:CYS:C	4:E:530:ARG:HG3	2.46	0.40
5:A:241:LYS:HD2	5:A:241:LYS:H	1.84	0.40
7:B:147:ASP:O	7:B:147:ASP:OD2	2.40	0.40
8:H:92:ILE:HD12	8:H:96:LEU:CB	2.51	0.40
8:I:96:LEU:HD23	8:I:155:PHE:HE2	1.87	0.40
8:I:140:ASN:ND2	8:I:144:MET:C	2.79	0.40
8:I:305:LEU:HD22	8:I:314:TYR:CE2	2.57	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	G	76/128 (59%)	73 (96%)	3 (4%)	0	100	100
2	D	501/591 (85%)	476 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	166/202 (82%)	160 (96%)	6 (4%)	0	100	100
4	E	507/584 (87%)	489 (96%)	18 (4%)	0	100	100
5	A	1239/1676 (74%)	1159 (94%)	80 (6%)	0	100	100
6	C	640/843 (76%)	615 (96%)	25 (4%)	0	100	100
7	B	731/934 (78%)	701 (96%)	30 (4%)	0	100	100
8	H	401/559 (72%)	373 (93%)	28 (7%)	0	100	100
8	I	396/559 (71%)	372 (94%)	24 (6%)	0	100	100
All	All	4657/6076 (77%)	4418 (95%)	239 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	G	73/112 (65%)	71 (97%)	2 (3%)	39	63
2	D	449/517 (87%)	448 (100%)	1 (0%)	87	88
3	F	136/163 (83%)	136 (100%)	0	100	100
4	E	438/493 (89%)	437 (100%)	1 (0%)	87	88
5	A	1101/1484 (74%)	1093 (99%)	8 (1%)	76	80
6	C	562/733 (77%)	562 (100%)	0	100	100
7	B	646/827 (78%)	639 (99%)	7 (1%)	65	76
8	H	356/494 (72%)	355 (100%)	1 (0%)	86	86
8	I	352/494 (71%)	350 (99%)	2 (1%)	78	81
All	All	4113/5317 (77%)	4091 (100%)	22 (0%)	78	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	62	TYR

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Mol	Chain	Res	Type
1	G	72	ASN
2	D	281	ASP
4	E	166	ARG
5	A	361	LEU
5	A	841	LEU
5	A	865	ILE
5	A	904	GLU
5	A	927	LEU
5	A	1024	TYR
5	A	1068	VAL
5	A	1274	LEU
7	B	94	ASP
7	B	101	SER
7	B	377	LEU
7	B	402	ILE
7	B	449	SER
7	B	552	CYS
7	B	759	LEU
8	H	394	ASN
8	I	96	LEU
8	I	457	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	2	GLN
1	G	18	ASN
1	G	72	ASN
2	D	26	GLN
2	D	37	GLN
2	D	59	ASN
2	D	168	GLN
2	D	265	GLN
2	D	487	ASN
2	D	521	ASN
3	F	21	ASN
3	F	78	GLN
4	E	286	GLN
4	E	534	ASN
5	A	72	HIS
5	A	319	ASN
5	A	391	ASN

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Mol	Chain	Res	Type
5	A	423	ASN
5	A	572	GLN
5	A	591	ASN
5	A	647	HIS
5	A	1029	ASN
5	A	1110	ASN
5	A	1121	ASN
5	A	1125	GLN
5	A	1278	GLN
5	A	1366	HIS
6	C	194	ASN
6	C	255	ASN
6	C	326	GLN
6	C	330	ASN
6	C	472	HIS
6	C	625	HIS
7	B	63	GLN
7	B	191	GLN
7	B	195	ASN
7	B	301	GLN
7	B	429	HIS
7	B	479	ASN
7	B	555	GLN
7	B	694	GLN
7	B	719	GLN
8	H	99	ASN
8	H	450	GLN
8	I	102	ASN
8	I	195	HIS
8	I	275	HIS
8	I	289	ASN
8	I	394	ASN
8	I	399	ASN
8	I	467	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

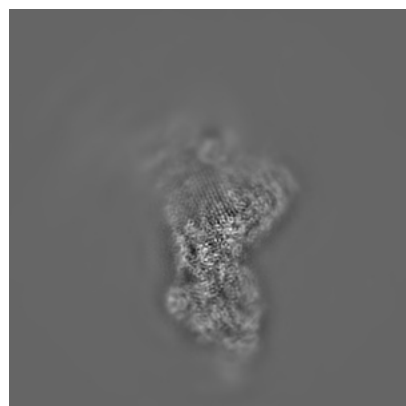
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15781. These allow visual inspection of the internal detail of the map and identification of artifacts.

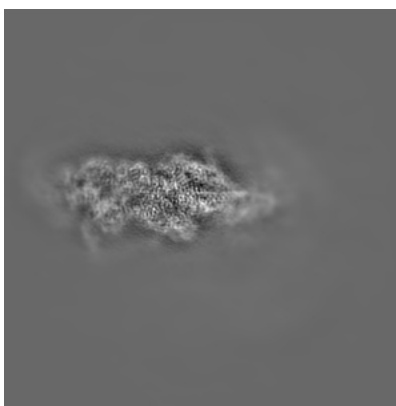
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

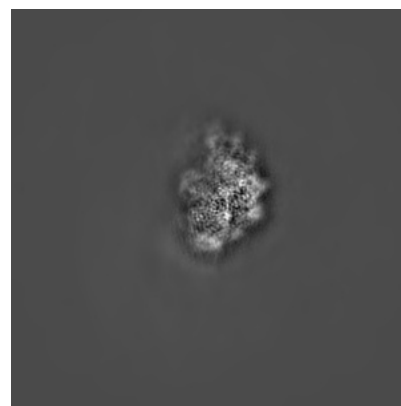
6.1.1 Primary map



X

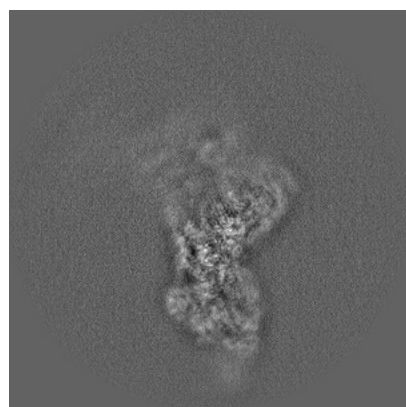


Y

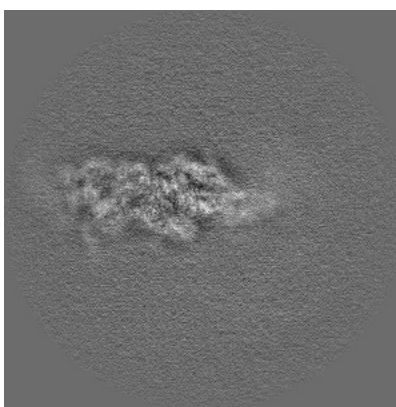


Z

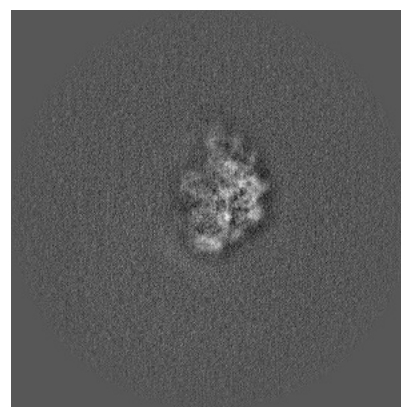
6.1.2 Raw map



X



Y

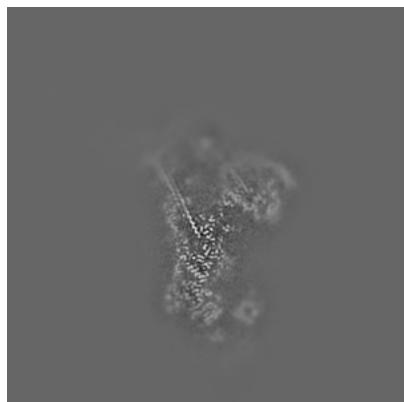


Z

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

6.2 Central slices [i](#)

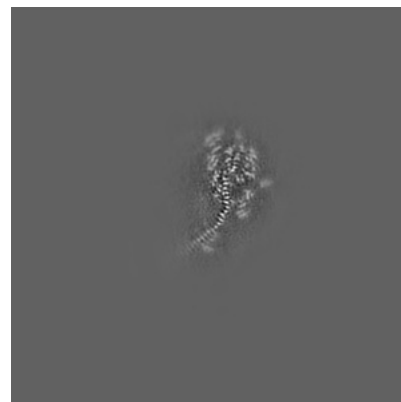
6.2.1 Primary map



X Index: 270

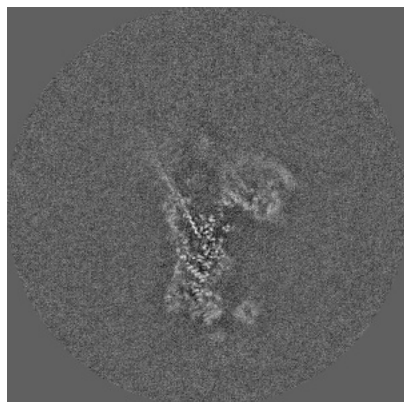


Y Index: 270

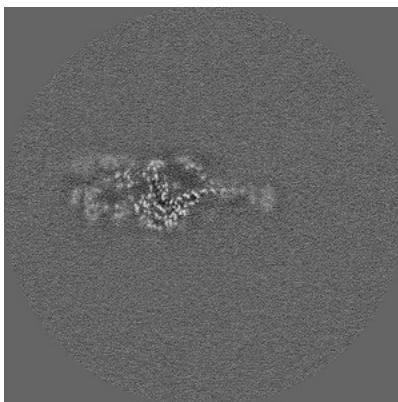


Z Index: 270

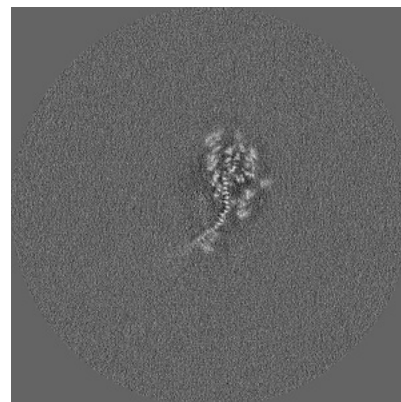
6.2.2 Raw map



X Index: 270



Y Index: 270

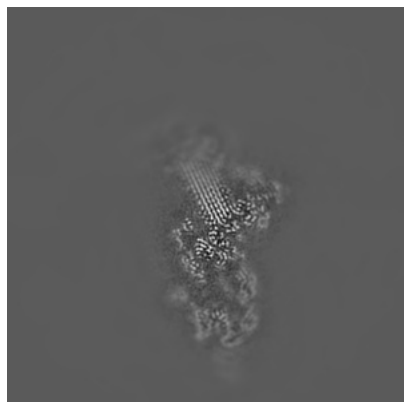


Z Index: 270

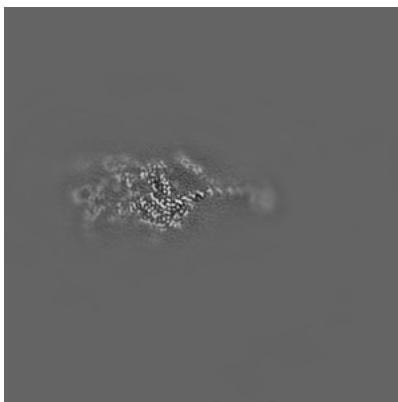
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

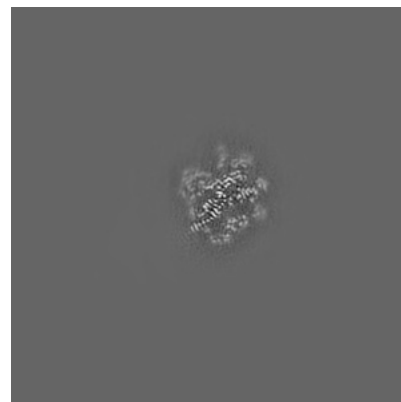
6.3.1 Primary map



X Index: 291

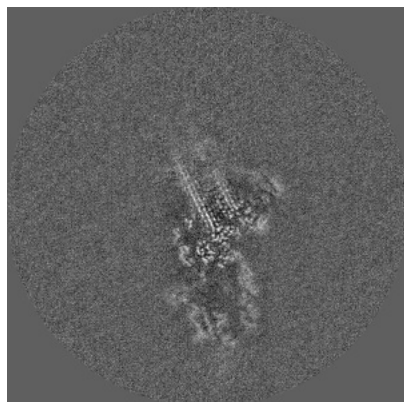


Y Index: 266

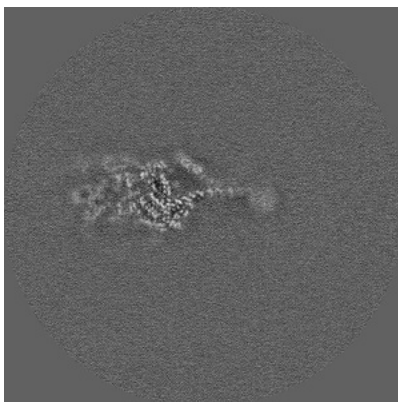


Z Index: 238

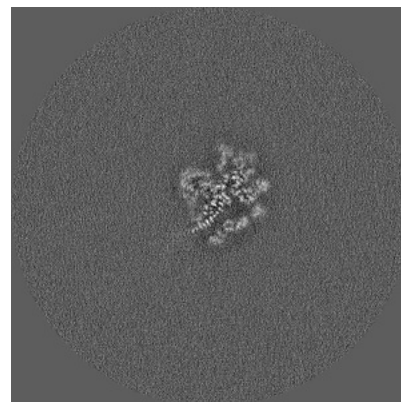
6.3.2 Raw map



X Index: 287



Y Index: 266

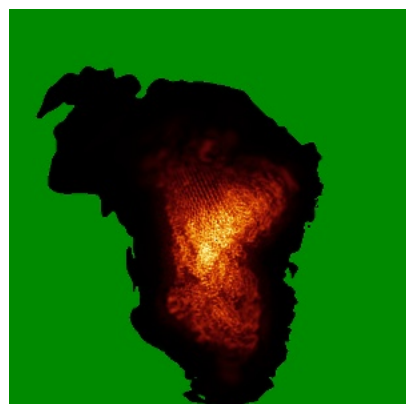


Z Index: 241

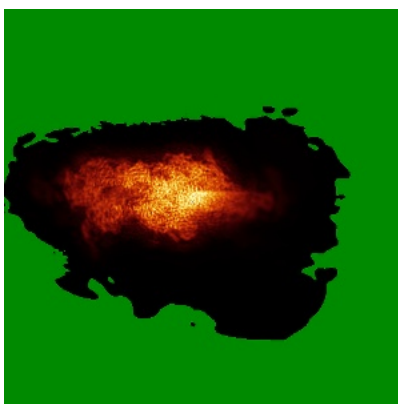
The images above show the largest variance slices of the map in three orthogonal directions.

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

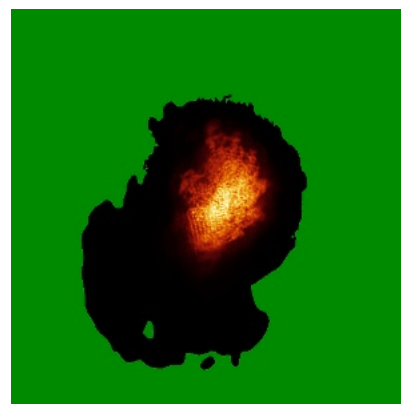
6.4.1 Primary map



X

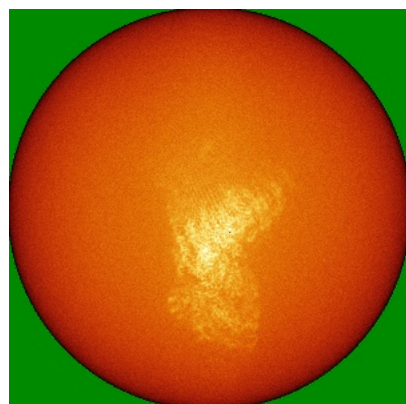


Y

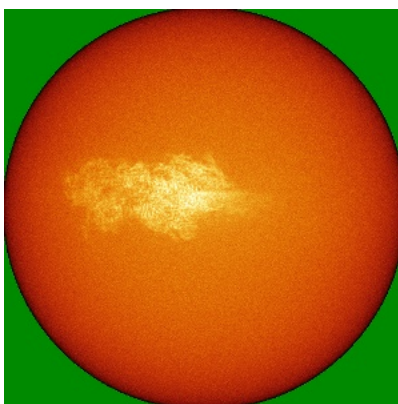


Z

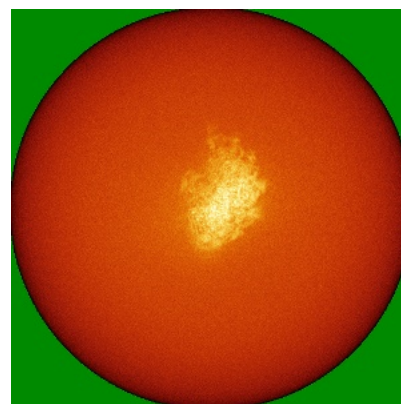
6.4.2 Raw map



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.

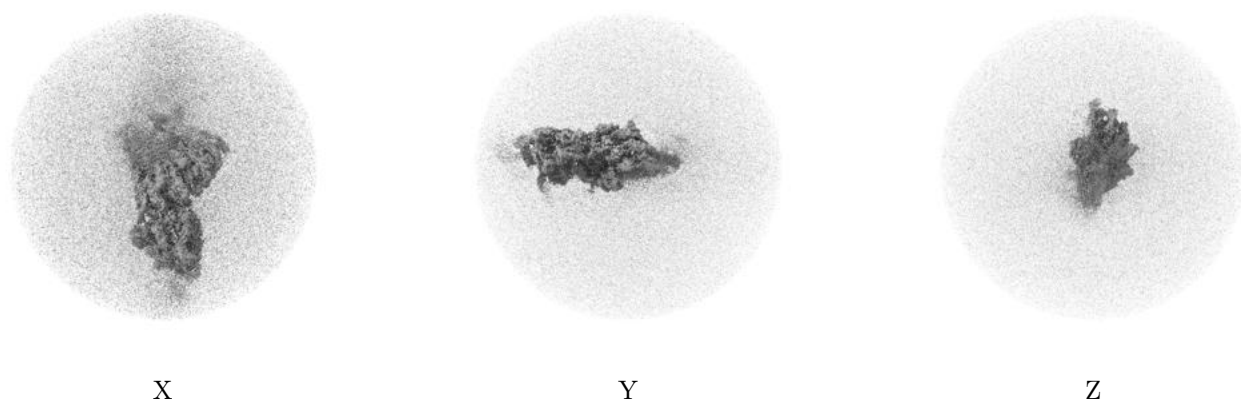
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00481. 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.

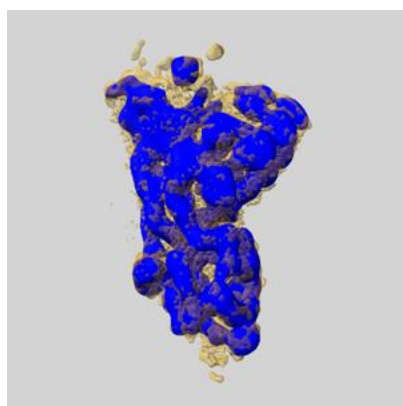
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

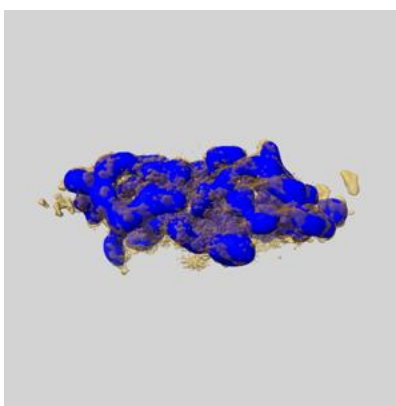
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

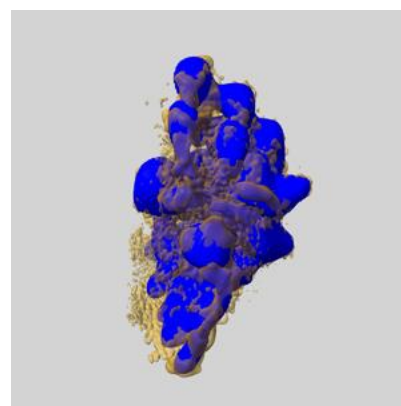
6.6.1 emd_15781_msk_1.map [i](#)



X



Y

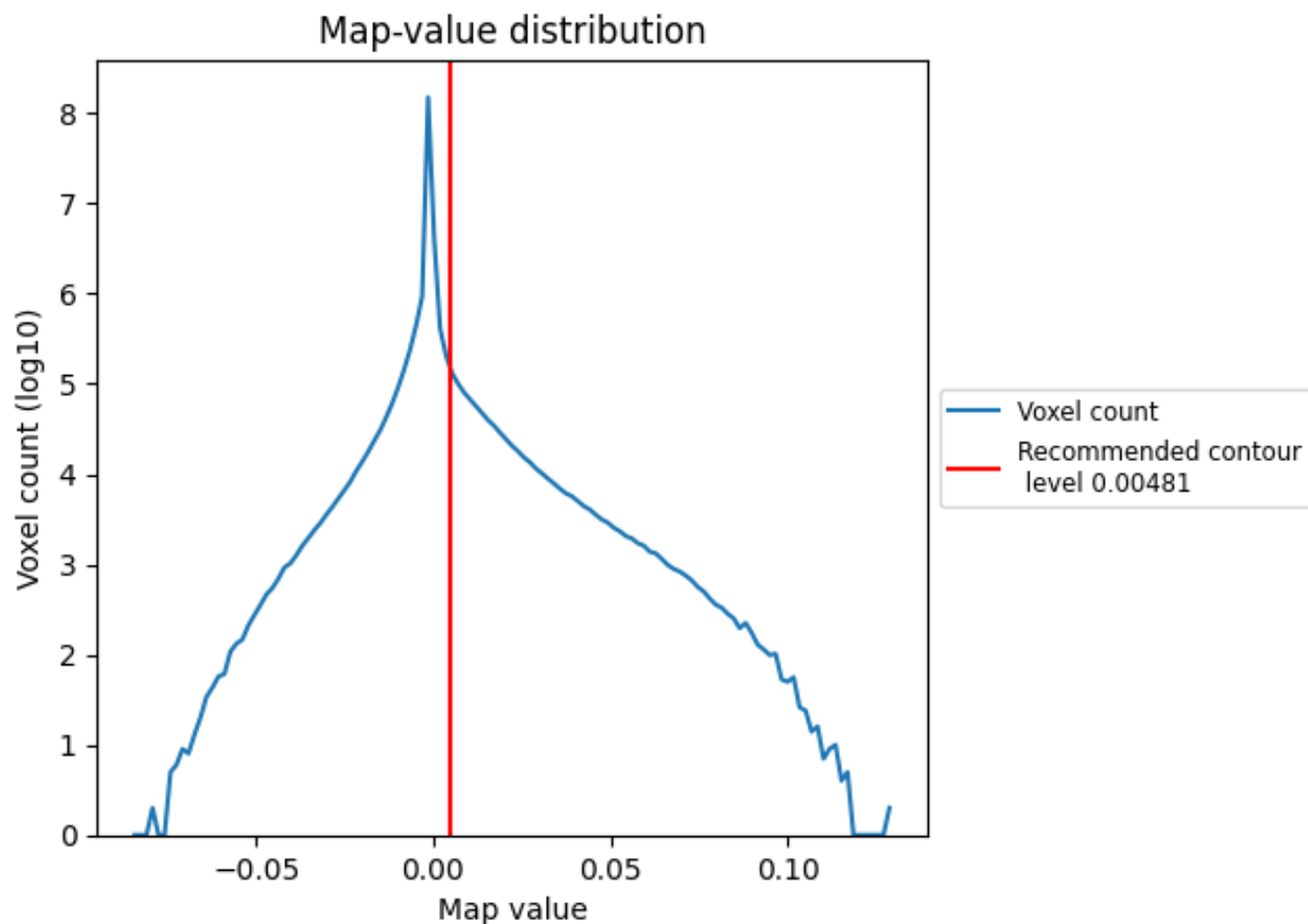


Z

7 Map analysis [i](#)

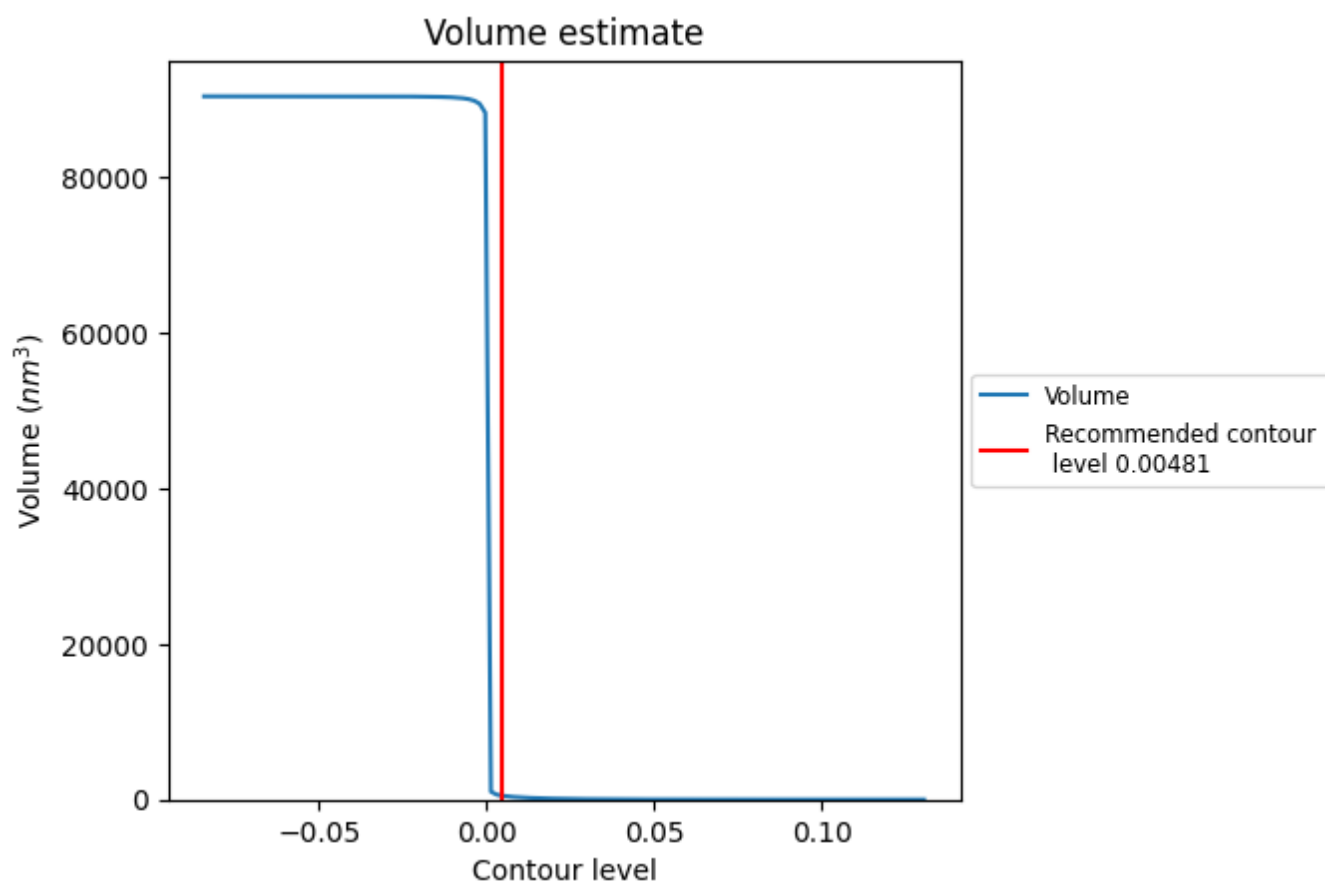
This section contains the results of statistical analysis of the map.

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.

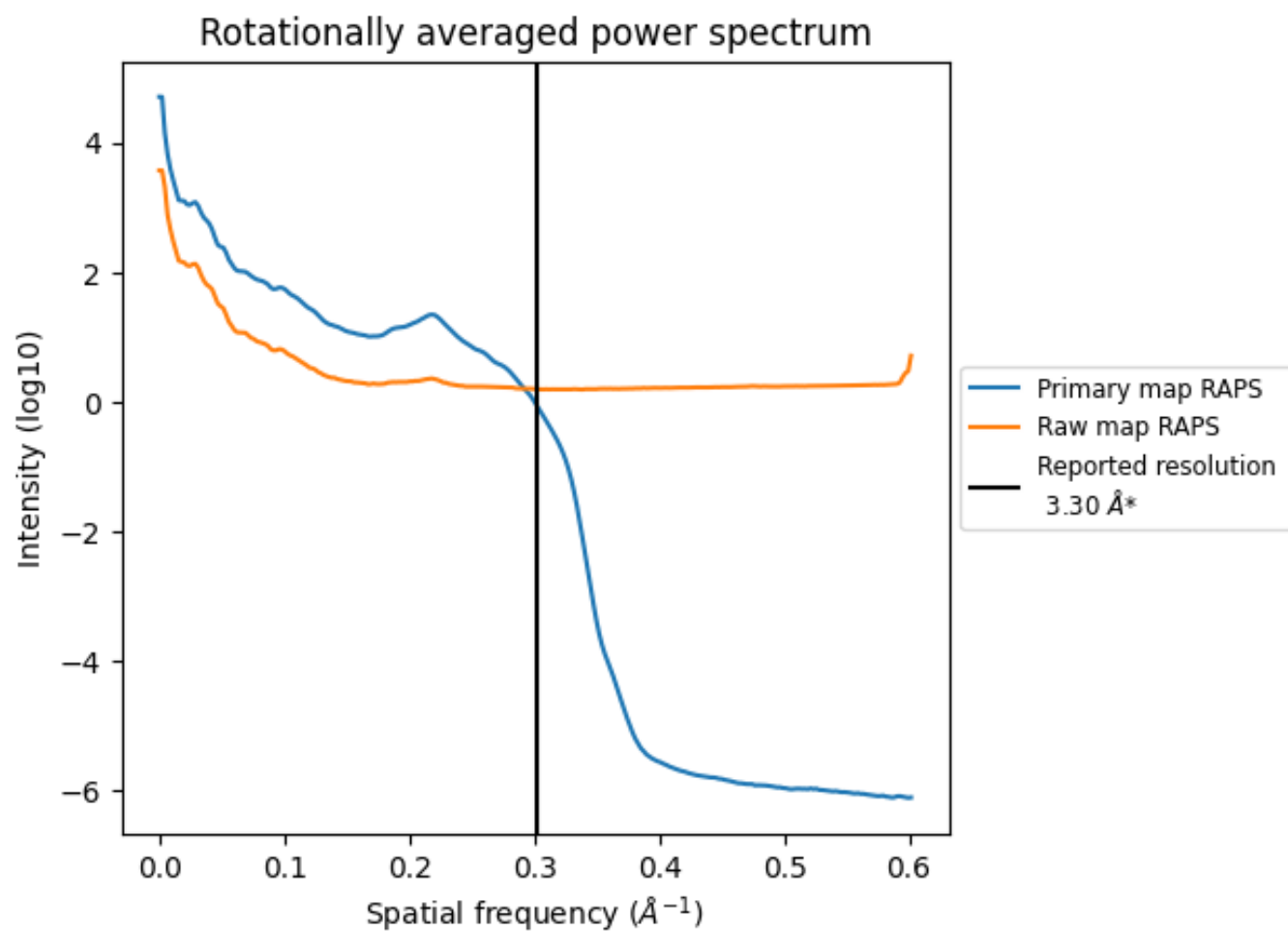
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 481 nm³; this corresponds to an approximate mass of 434 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 ⓘ

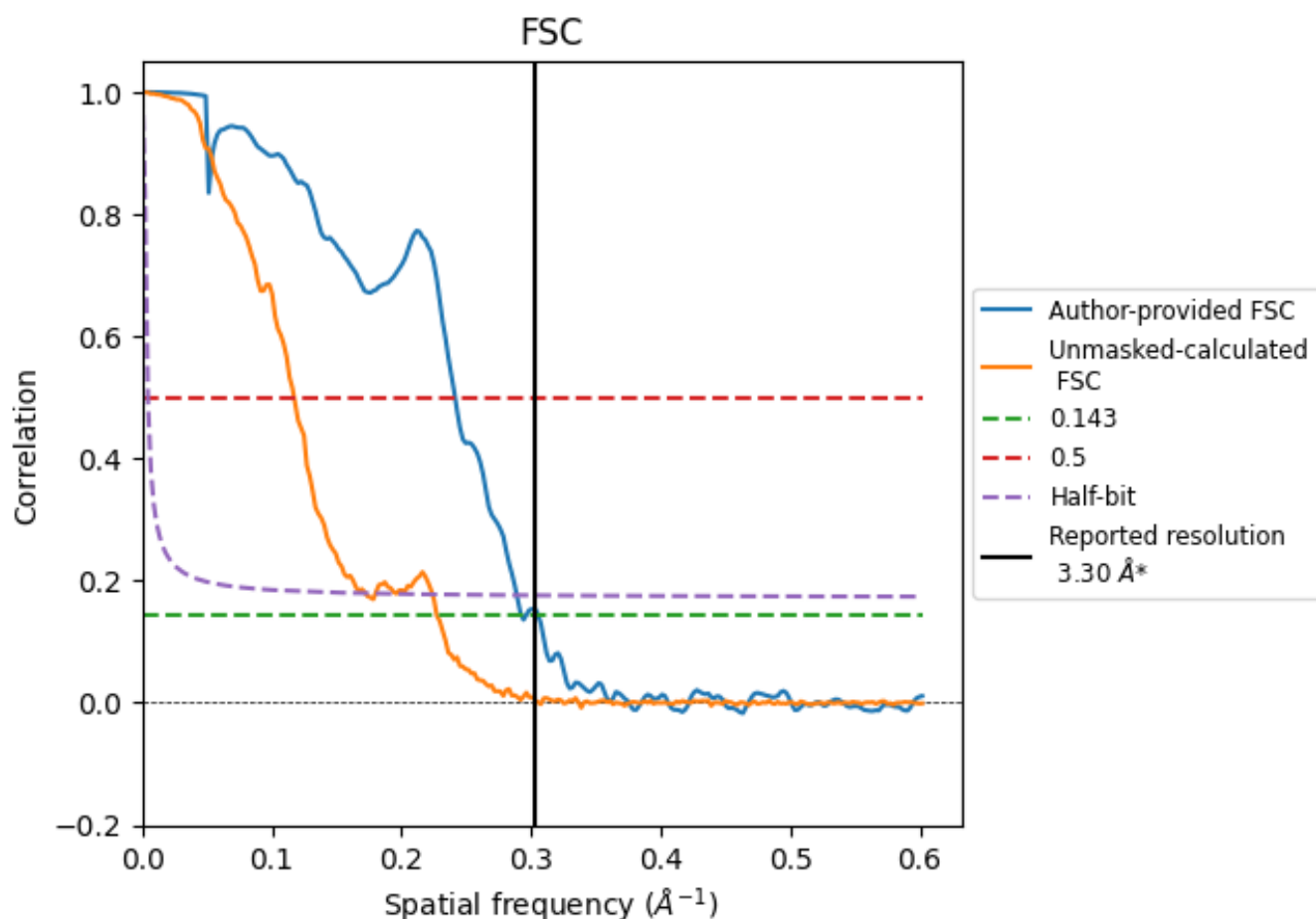


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

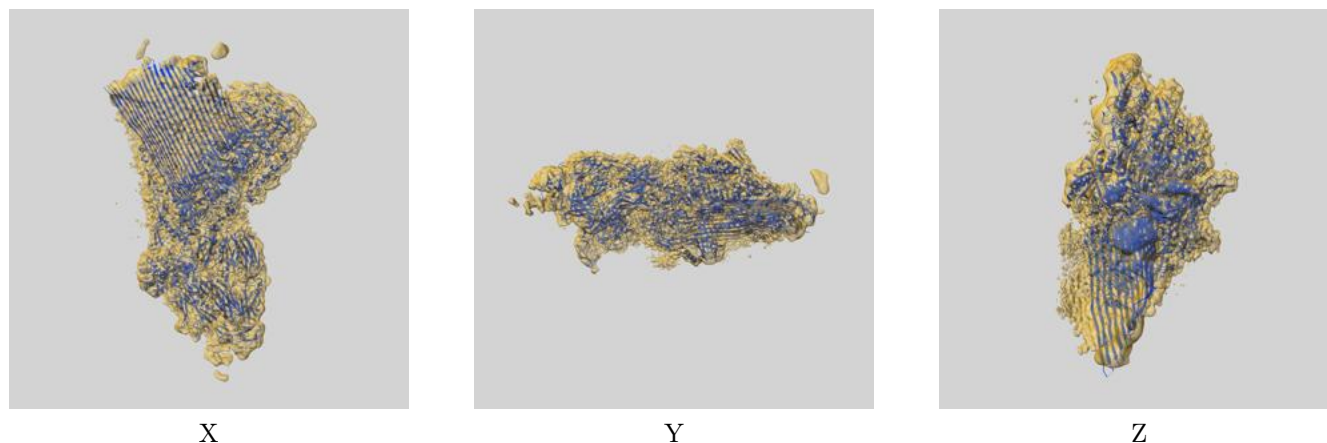
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.42	4.14	3.46
Unmasked-calculated*	4.40	8.54	5.81

*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 4.40 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

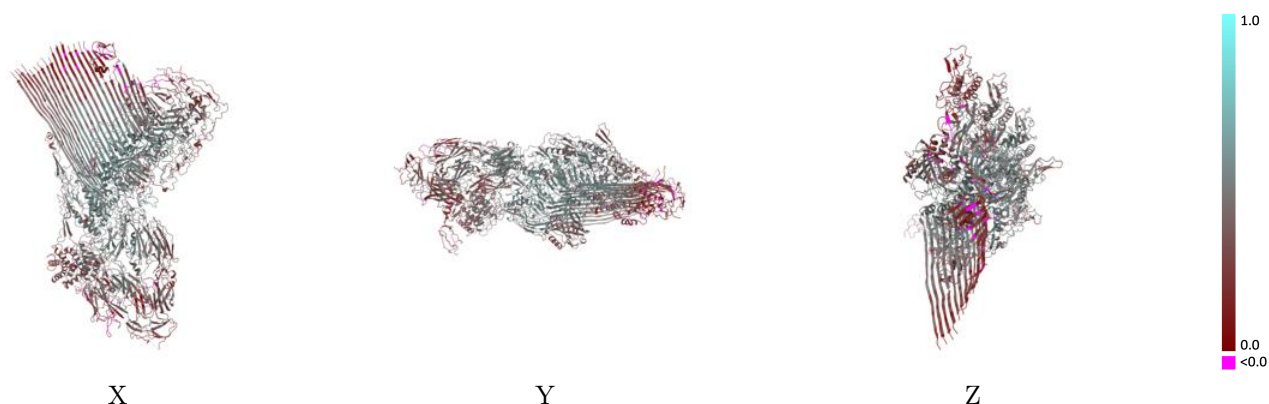
This section contains information regarding the fit between EMDB map EMD-15781 and PDB model 8B0H. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



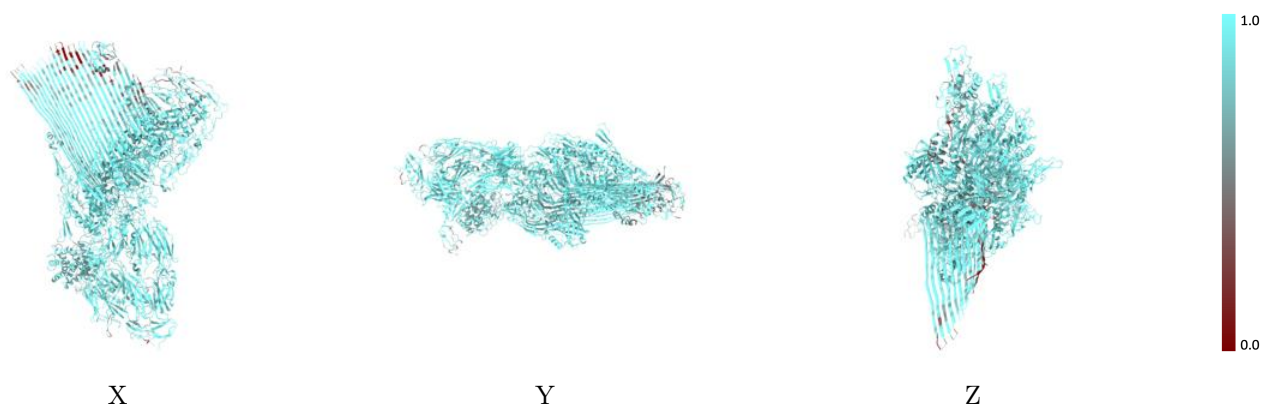
The images above show the 3D surface view of the map at the recommended contour level 0.00481 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



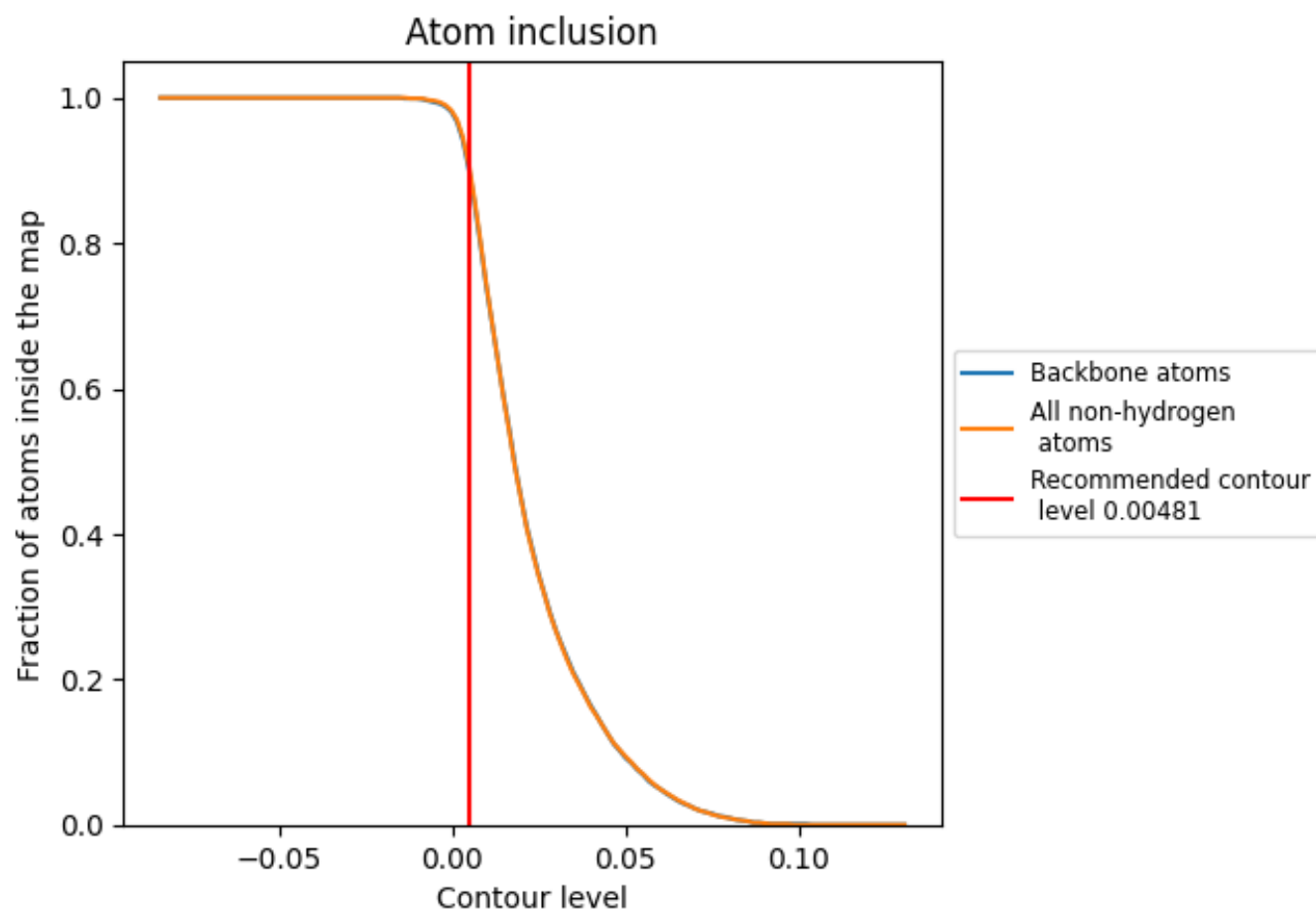
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00481).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.00481) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.4050
A	0.9050	0.3660
B	0.9190	0.4250
C	0.9390	0.4610
D	0.9400	0.4790
E	0.9190	0.4570
F	0.9310	0.3970
G	0.7240	0.1150
H	0.9020	0.4160
I	0.8220	0.2910

1.0

0.0

<0.0