Full wwPDB EM Validation Report ⓘ

Feb 18, 2023 – 03:59 pm GMT

PDB ID	:	8B0H
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	:	2J8B, 7NYD

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

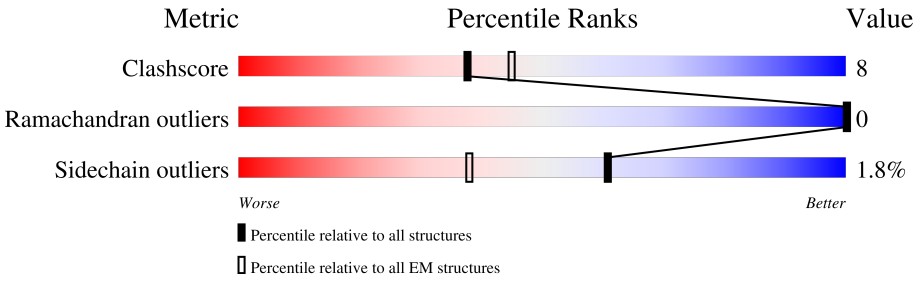
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	11%, 55%, 5%, 39%
2	D	591	71%, 14%, 14%
3	F	202	58%, 24%, 17%
4	E	584	76%, 11%, 12%
5	A	1676	57%, 16%, 26%
6	C	843	69%, 7%, 23%
7	B	934	67%, 11%, 21%
8	H	559	62%, 11%, 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	559	

2 Entry composition

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		

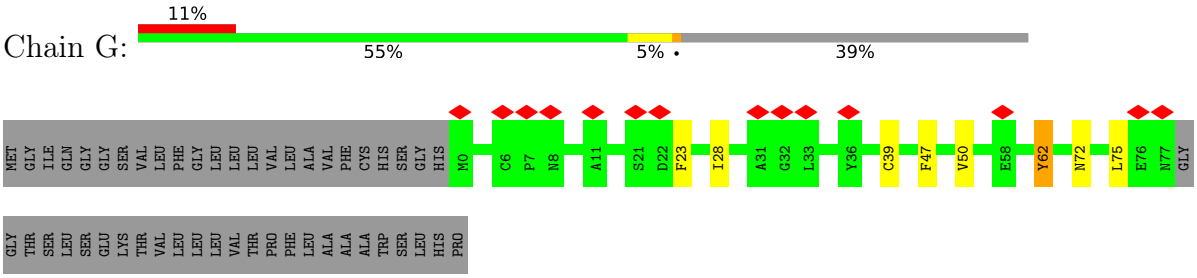
- Molecule 8 is a protein called Complement component C9.

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		

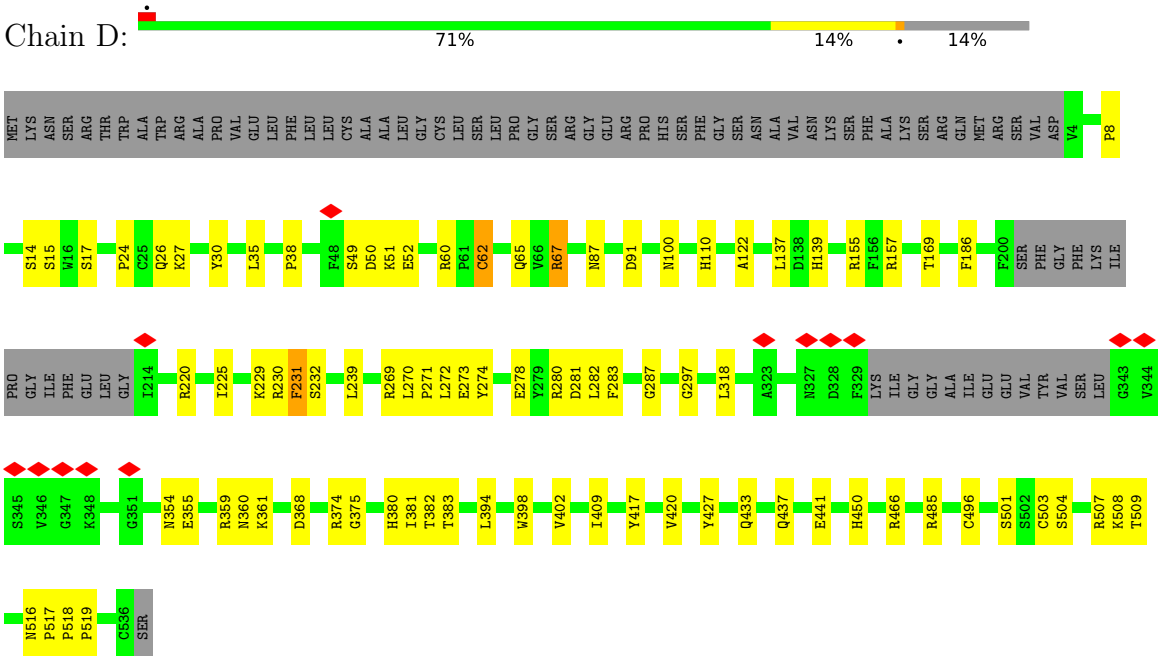
3 Residue-property plots (i)

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

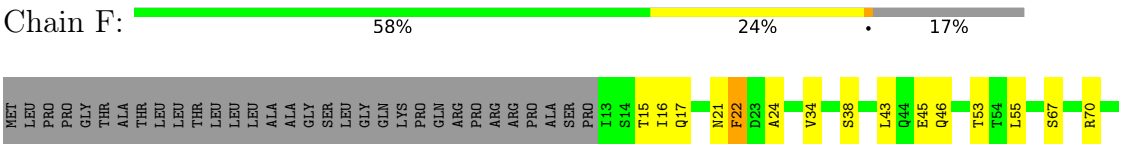
• Molecule 1: CD59 glycoprotein

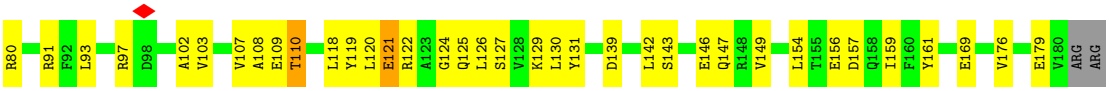


• Molecule 2: Complement component C8 beta chain



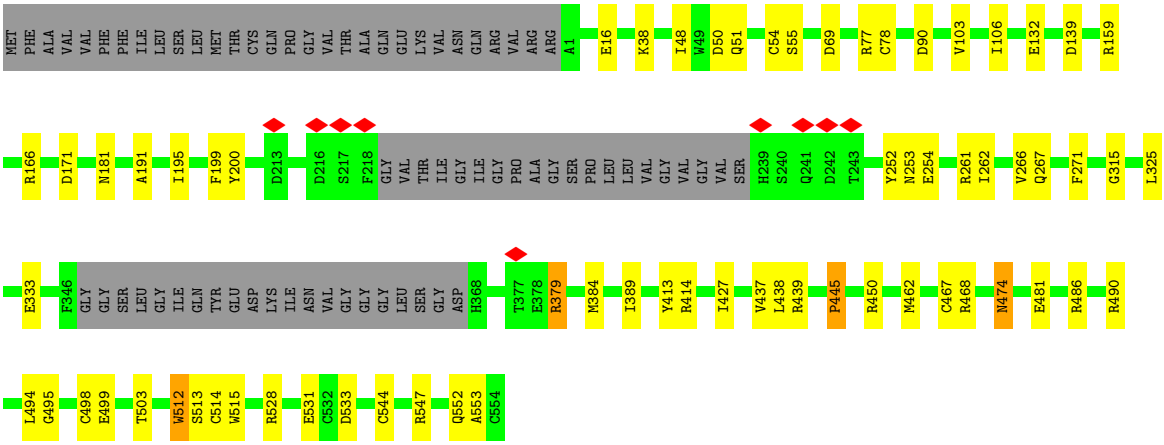
• Molecule 3: Complement component C8 gamma chain





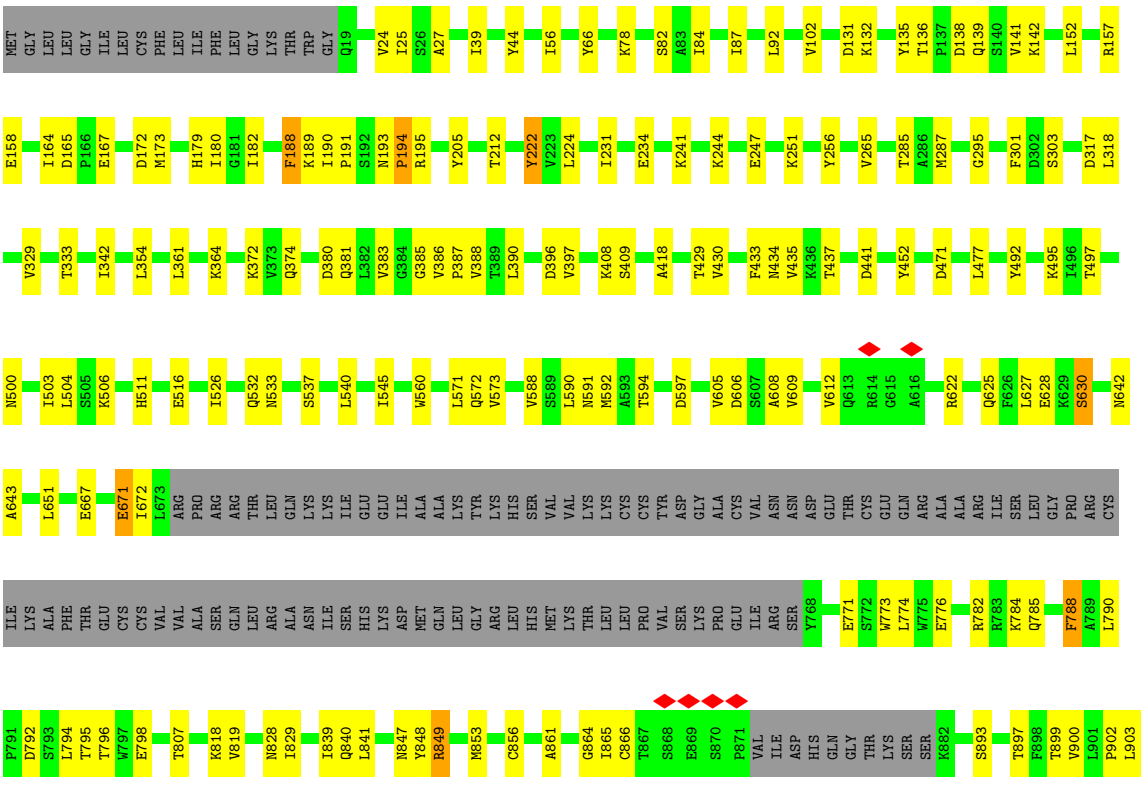
• Molecule 4: Complement component C8 alpha chain

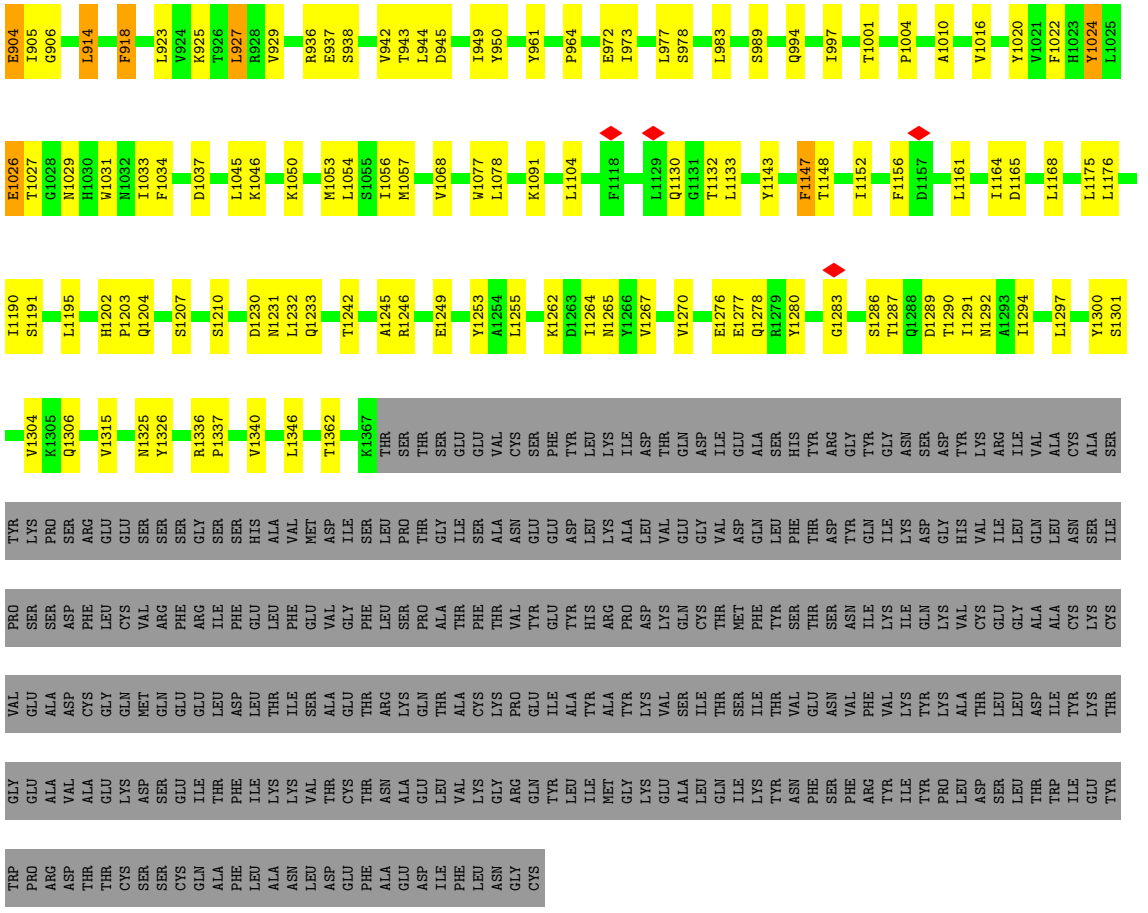
Chain E:



• Molecule 5: Complement C5

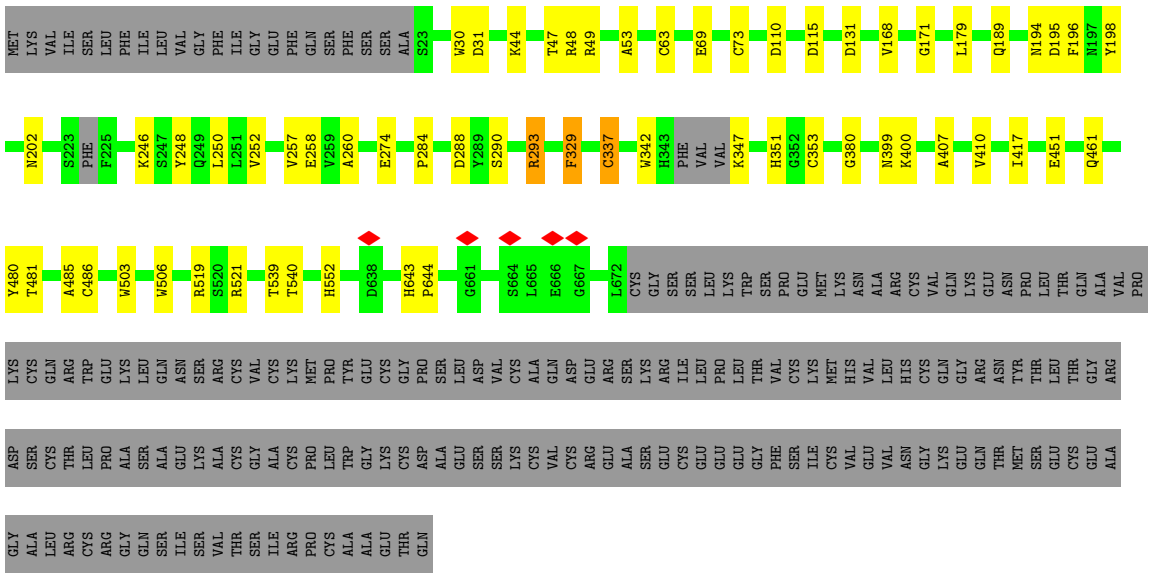
Chain A:





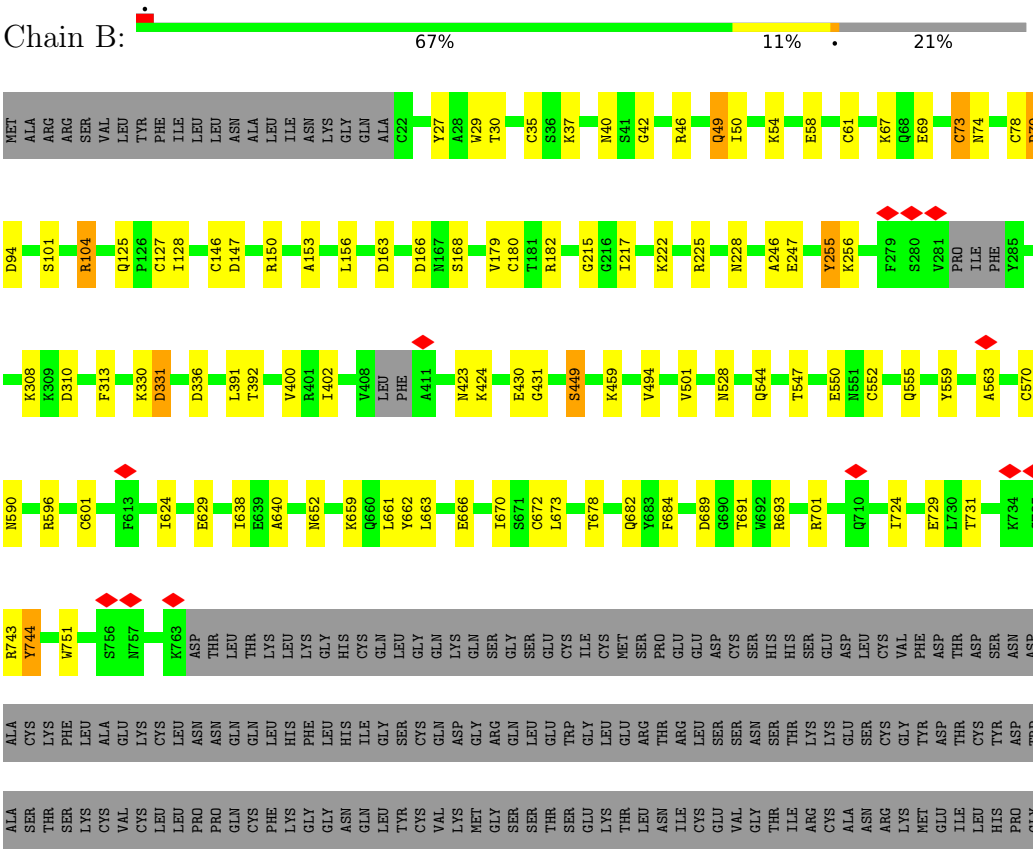
• Molecule 6: Complement component C7

Chain C:



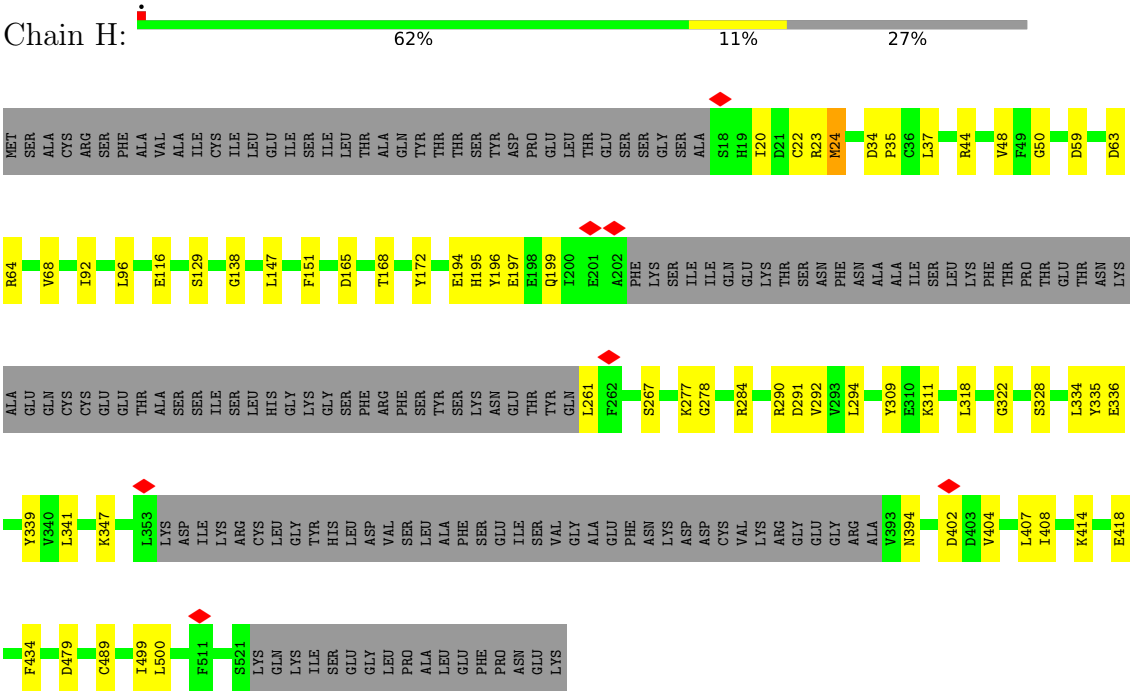
• Molecule 7: Complement component C6

Chain B:



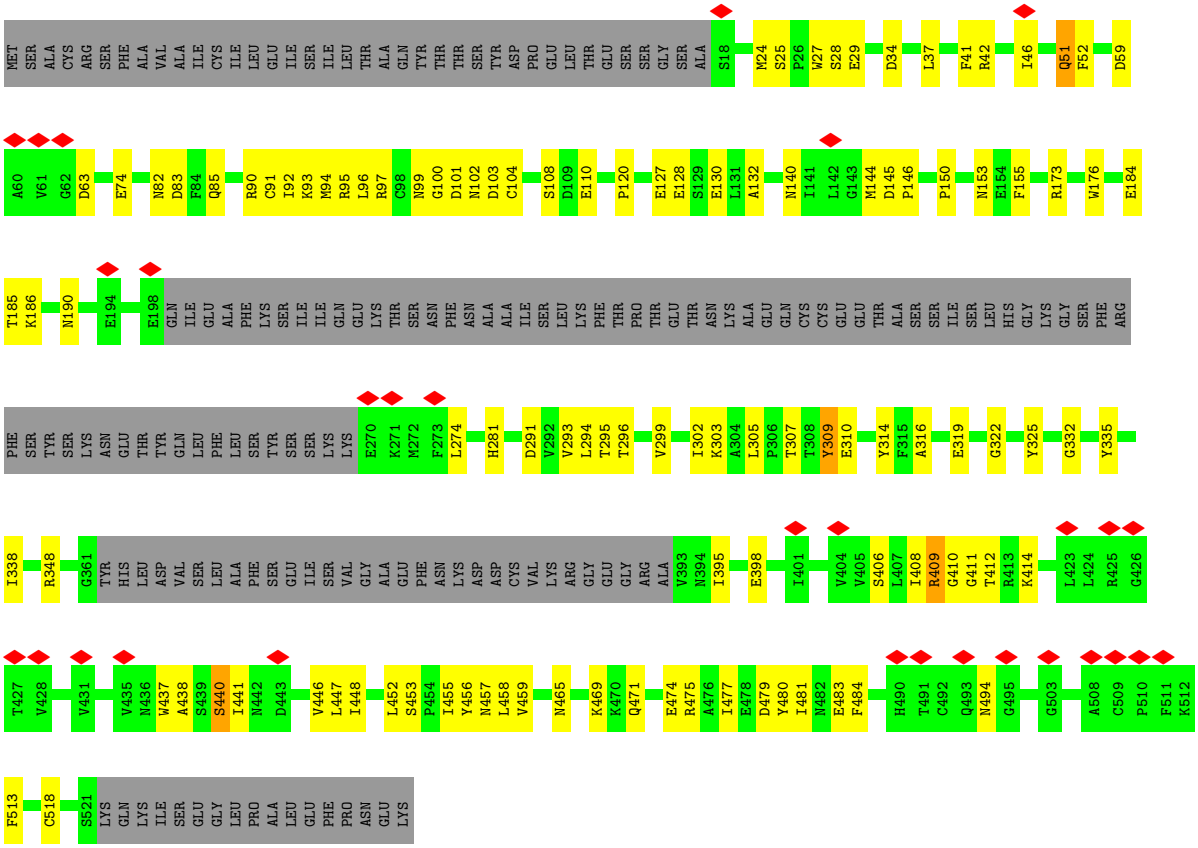
• Molecule 8: Complement component C9

Chain H:



• Molecule 8: Complement component C9

Chain I:


MET SER ALA CYS ARG SER PHE ALA VAL ALA ILE CYS ILE LEU GLU ILE SER ILE LEU THR ALA GLN TYR THR THR SER TYR ASP PRO GLU LEU THR GLU SER SER GLY SER ALA S18 M24 S25 P26 W27 S28 E29 D34 L37 F41 R42 I46 Q51 F52 D59
A60 V61 G62 D63 E74 N82 D83 F84 Q85 R90 C91 I92 K93 M94 R95 L96 R97 C98 N99 G100 D101 N102 D103 C104 S108 D109 E110 P120 E127 E128 S129 E130 L131 A132 N140 I141 L142 G143 M144 D145 P146 P150 N153 E154 F155 R173 W176 E184
T185 K186 N190 E194 E198 GLN ILE GLU ALA PHE LYS SER ILE ILE GLN GLU LYS THR SER ASN PHE ASN ALA ALA ILE SER LEU LYS PHE THR PRO THR GLU THR ASN LYS ALA GLU GLN CYS CYS GLU GLU THR ALA SER SER ILE SER LEU HIS GLY LYS GLY SER PHE ARG
PHE SER TYR SER LYS ASN GLU THR TYR GLN LEU LEU PHE LEU SER TYR SER SER LYS LYS E270 K271 M272 F273 L274 H281 D291 V292 V293 L294 T295 T296 V299 I302 K303 A304 L305 P306 T307 T308 Y309 E310 Y314 F315 A316 E319 G322 Y325 G332 Y335
I338 R348 G361 TYR HIS LEU ASP VAL SER LEU ALA PHE SER GLU ILE SER VAL GLY ALA GLU PHE ASN LYS ASP ASP CYS VAL LYS ARG GLY GLU GLY ARG ALA V393 N394 I395 E398 I401 V404 V405 S406 L407 I408 R409 G410 G411 T412 R413 K414 L423 L424 R425 G426
T427 V428 V431 V435 N436 W437 A438 S439 S440 I441 N442 D443 V446 L447 I448 L452 S453 P454 I455 Y456 N457 L458 V459 N465 K469 K470 Q471 E474 R475 A476 I477 E478 D479 Y480 I481 N482 E483 F484 H490 T491 C492 Q493 N494 G495 G503 A508 C509 P510 F511 K512
F513 C518 S521 LYS GLN LYS ILE SER GLU GLY LEU PRO ALA LEU GLU PHE PRO ASN GLU LYS

4 Experimental information (i)

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 ($e^-/Å^2$)	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	0.28	0/641	0.52	0/867
2	D	0.28	0/4146	0.59	0/5598
3	F	0.28	0/1348	0.64	0/1829
4	E	0.35	2/4135 (0.0%)	0.64	4/5568 (0.1%)
5	A	0.31	2/10072 (0.0%)	0.58	2/13685 (0.0%)
6	C	0.31	1/5160 (0.0%)	0.58	1/6982 (0.0%)
7	B	0.28	1/5897 (0.0%)	0.58	1/7962 (0.0%)
8	H	0.29	0/3280	0.60	0/4424
8	I	0.28	0/3242	0.65	2/4371 (0.0%)
All	All	0.30	6/37921 (0.0%)	0.60	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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	514	CYS	CB-SG	-9.71	1.65	1.82
5	A	671	GLU	CD-OE2	8.30	1.34	1.25
5	A	667	GLU	CD-OE2	8.27	1.34	1.25
4	E	467	CYS	CB-SG	-8.12	1.68	1.82
6	C	337	CYS	CB-SG	-5.77	1.72	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	570	CYS	CB-SG	-5.63	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	445	PRO	CA-N-CD	-9.38	98.37	111.50
6	C	337	CYS	CA-CB-SG	9.30	130.74	114.00
4	E	514	CYS	CA-CB-SG	8.05	128.48	114.00
7	B	79	PRO	CA-N-CD	-7.47	101.04	111.50
4	E	467	CYS	CB-CA-C	-7.43	95.53	110.40
4	E	467	CYS	CA-CB-SG	6.93	126.47	114.00
8	I	146	PRO	CA-N-CD	-6.80	101.98	111.50
5	A	193	ASN	C-N-CD	-6.38	106.57	120.60
8	I	146	PRO	N-CD-CG	-5.67	94.70	103.20
5	A	194	PRO	CA-N-CD	-5.32	104.06	111.50

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	60	0
3	F	1319	1283	1282	31	0
4	E	4052	3814	3814	51	0
5	A	9849	9829	9826	232	0
6	C	5035	4727	4724	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	5776	5491	5488	73	0
8	H	3219	3091	3089	42	0
8	I	3182	3048	3045	80	0
All	All	37115	35735	35720	593	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 8.

All (593) 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:537:SER:HG	5:A:560:TRP:HE1	1.33	0.73
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
5:A:537:SER:OG	5:A:560:TRP:NE1	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:829:ILE:HD13	5:A:925:LYS:HZ1	1.66	0.59
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
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:849:ARG:HG3	5:A:853:MET:HE1	1.85	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
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
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: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
8:I:140:ASN:OD1	8:I:322:GLY:HA2	2.05	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
8:H:35:PRO:O	8:H:37:LEU:HD23	2.10	0.52
7:B:693:ARG:HG3	7:B:693:ARG:O	2.09	0.52
5:A:1278:GLN:CD	7:B:624:ILE:HG21	2.30	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
5:A:1057:MET:HE3	5:A:1057:MET:O	2.10	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:507:ARG:NH1	2:D:509:THR:HG23	2.26	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
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
8:H:339:TYR:HE1	8:H:341:LEU:HD21	1.76	0.50
8:I:291:ASP:CG	8:I:291:ASP:O	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:506:TRP:HB3	6:C:519:ARG:HD3	1.92	0.50
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:82:ASN:O	8:I:94:MET:HE1	2.11	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
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
7:B:291:GLU:OE1	7:B:402:ILE:HG22	2.12	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
5:A:241:LYS:HA	5:A:244:LYS:HZ1	1.77	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: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
8:H:116:GLU:O	8:H:116:GLU:HG2	2.13	0.48
2:D:433:GLN:O	2:D:437:GLN:HG3	2.13	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:773:TRP:CZ3	5:A:788:PHE:CE1	3.01	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
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: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
6:C:539:THR:HG23	6:C:540:THR:HG23	1.96	0.47
7:B:79:PRO:HD2	7:B:79:PRO:O	2.13	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
5:A:903:LEU:HB2	5:A:904:GLU:CD	2.35	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:333:THR:O	5:A:893:SER:OG	2.20	0.47
5:A:387:PRO:HB3	5:A:408:LYS:HZ1	1.80	0.47
6:C:115:ASP:N	6:C:115:ASP:OD1	2.47	0.47
7:B:590:ASN:CG	7:B:590:ASN:O	2.54	0.47
8:I:316:ALA:O	8:I:319:GLU:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:136:THR:HG23	5:A:222:TYR:HE1	1.80	0.46
5:A:592:MET:HE2	5:A:784:LYS:HB3	1.97	0.46
5:A:829:ILE:HG21	5:A:925:LYS:HZ1	1.79	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: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
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
7:B:659:LYS:NZ	7:B:666:GLU:OE2	2.29	0.46
8:I:332:GLY:C	8:I:448:ILE:HD11	2.35	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:1207:SER:O	5:A:1210:SER:OG	2.25	0.45
8:I:184:GLU:HG3	8:I:185:THR:N	2.31	0.45
5:A:138:ASP:OD1	5:A:138:ASP:O	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
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
2:D:239:LEU:C	2:D:239:LEU:HD23	2.37	0.45
5:A:840:GLN:NE2	5:A:899:THR:HG23	2.31	0.45
7:B:693:ARG:O	7:B:693:ARG:CG	2.64	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
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
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:1147:PHE:CD1	5:A:1147:PHE:C	2.90	0.45
5:A:1176:LEU:HD11	5:A:1202:HIS:CE1	2.52	0.45
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:165:ASP:C	5:A:165:ASP:OD1	2.55	0.44
8:I:398:GLU:CD	8:I:398:GLU:O	2.56	0.44
3:F:16:ILE:HG22	3:F:17:GLN:N	2.32	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:285:THR:O	5:A:287:MET:SD	2.76	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
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
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
6:C:329:PHE:C	6:C:329:PHE:CD2	2.92	0.43
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
5:A:56:ILE:HG22	5:A:66:TYR:HD2	1.84	0.43
5:A:138:ASP:O	5:A:138:ASP:CG	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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: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
7:B:299:PHE:C	7:B:299:PHE:CD2	2.93	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
5:A:606:ASP:O	5:A:609:VAL:HG23	2.20	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
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
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
5:A:671:GLU:C	5:A:672:ILE:HD13	2.39	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:828:ASN:O	5:A:828:ASN:CG	2.58	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:I:494:ASN:O	8:I:494:ASN:CG	2.58	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:450:HIS:ND1	2:D:496:CYS:SG	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:337:CYS:HB3	6:C:353:CYS:CA	2.20	0.41
7:B:128:ILE:O	7:B:128:ILE:HG23	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
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:96:LEU:HD23	8:I:103:ASP:HB3	2.03	0.41
2:D:273:GLU:H	2:D:273:GLU:CD	2.24	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: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
4:E:48:ILE:HG12	4:E:48:ILE:O	2.19	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
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:1077:TRP:HE1	5:A:1143:TYR:HH	1.68	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:30:TYR:CE2	2:D:271:PRO:HB3	2.56	0.41
3:F:119:TYR:C	3:F:120:LEU:HD12	2.41	0.41
3:F:126:LEU:HD23	3:F:127:SER:N	2.36	0.41
5:A:222:TYR:CD2	5:A:612:VAL:HG11	2.55	0.41
5:A:471:ASP:O	5:A:471:ASP:CG	2.58	0.41
5:A:477:LEU:HD22	5:A:477:LEU:H	1.86	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: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: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:731:THR:HG23	7:B:731:THR:O	2.21	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
3:F:176:VAL:HG13	3:F:176:VAL:O	2.22	0.40
4:E:533:ASP:OD1	4:E:533:ASP:C	2.59	0.40
5:A:188:PHE:C	5:A:188:PHE:CD1	2.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1024:TYR:C	5:A:1024:TYR:CD1	2.95	0.40
6:C:407:ALA:O	6:C:410:VAL:HG12	2.21	0.40
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
2:D:65:GLN:CD	2:D:65:GLN:H	2.25	0.40
2:D:360:ASN:OD1	2:D:360:ASN:C	2.60	0.40
4:E:494:LEU:HD23	4:E:495:GLY:N	2.37	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:305:LEU:HD22	8:I:314:TYR:CE2	2.57	0.40
8:I:309:TYR:C	8:I:309:TYR:CD1	2.95	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
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 (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	G	73/112 (65%)	71 (97%)	2 (3%)	44	71
2	D	449/517 (87%)	438 (98%)	11 (2%)	49	73
3	F	136/163 (83%)	132 (97%)	4 (3%)	42	69
4	E	438/493 (89%)	430 (98%)	8 (2%)	59	78
5	A	1101/1484 (74%)	1088 (99%)	13 (1%)	71	83
6	C	562/733 (77%)	558 (99%)	4 (1%)	84	90
7	B	646/827 (78%)	634 (98%)	12 (2%)	57	77
8	H	356/494 (72%)	347 (98%)	9 (2%)	47	72
8	I	352/494 (71%)	342 (97%)	10 (3%)	43	70
All	All	4113/5317 (77%)	4040 (98%)	73 (2%)	61	78

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	62	TYR
1	G	72	ASN
2	D	62	CYS
2	D	67	ARG
2	D	100	ASN
2	D	110	HIS
2	D	157	ARG
2	D	186	PHE
2	D	220	ARG
2	D	231	PHE
2	D	281	ASP
2	D	374	ARG
2	D	466	ARG
3	F	22	PHE
3	F	121	GLU
3	F	139	ASP
3	F	157	ASP
4	E	166	ARG
4	E	171	ASP
4	E	261	ARG
4	E	379	ARG
4	E	413	TYR
4	E	462	MET
4	E	474	ASN
4	E	490	ARG
5	A	82	SER
5	A	188	PHE
5	A	222	TYR
5	A	630	SER
5	A	788	PHE
5	A	849	ARG
5	A	904	GLU
5	A	914	LEU
5	A	918	PHE
5	A	927	LEU
5	A	950	TYR
5	A	1024	TYR
5	A	1147	PHE
6	C	44	LYS
6	C	73	CYS
6	C	293	ARG
6	C	329	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	B	49	GLN
7	B	73	CYS
7	B	94	ASP
7	B	101	SER
7	B	127	CYS
7	B	255	TYR
7	B	313	PHE
7	B	331	ASP
7	B	449	SER
7	B	601	CYS
7	B	652	ASN
7	B	744	TYR
8	H	22	CYS
8	H	24	MET
8	H	261	LEU
8	H	267	SER
8	H	311	LYS
8	H	347	LYS
8	H	394	ASN
8	H	434	PHE
8	H	489	CYS
8	I	51	GLN
8	I	95	ARG
8	I	145	ASP
8	I	309	TYR
8	I	335	TYR
8	I	406	SER
8	I	409	ARG
8	I	440	SER
8	I	457	ASN
8	I	480	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	487	ASN
2	D	521	ASN
3	F	78	GLN
4	E	82	HIS
5	A	591	ASN
5	A	613	GLN
5	A	1278	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	C	472	HIS
8	I	195	HIS
8	I	275	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

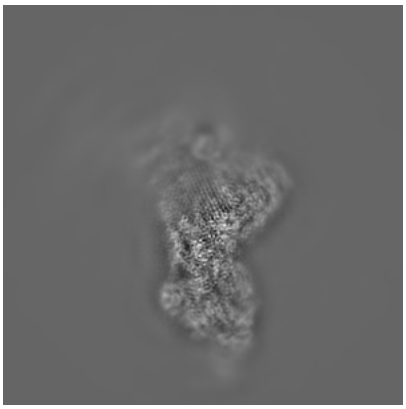
6 Map visualisation

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.

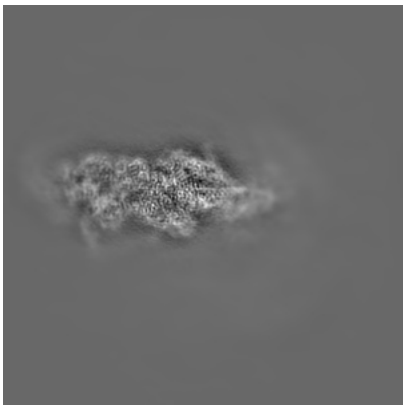
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

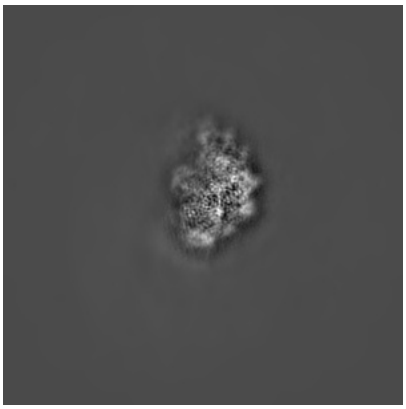
6.1.1 Primary map



X

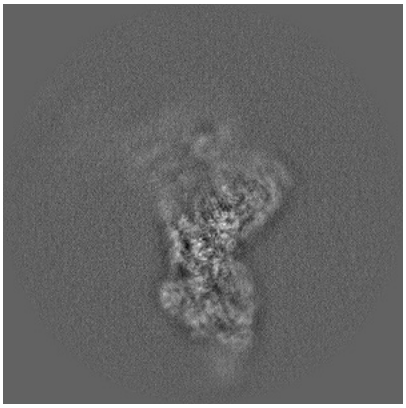


Y

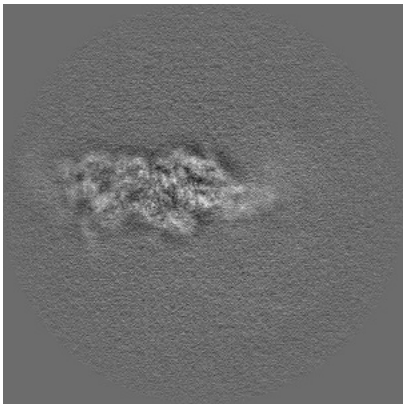


Z

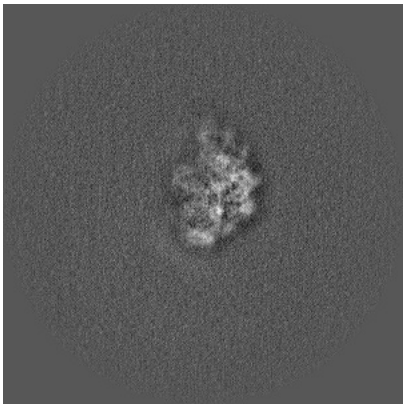
6.1.2 Raw map



X



Y

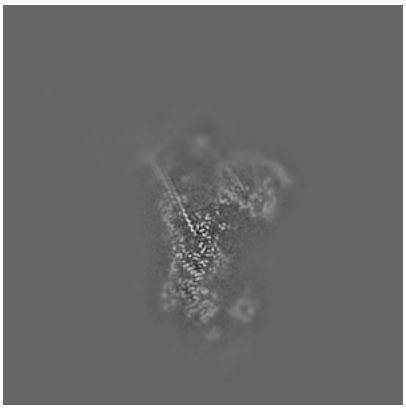


Z

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

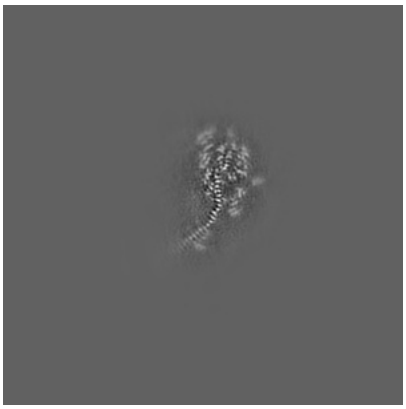
6.2 Central slices (i)

6.2.1 Primary map



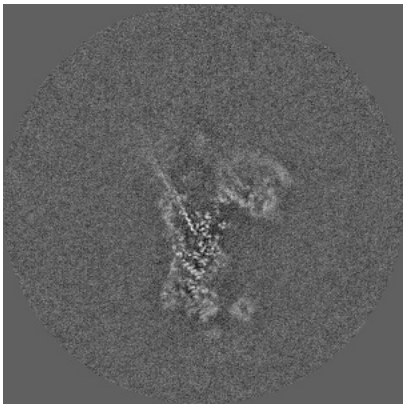
X Index: 270

Y Index: 270

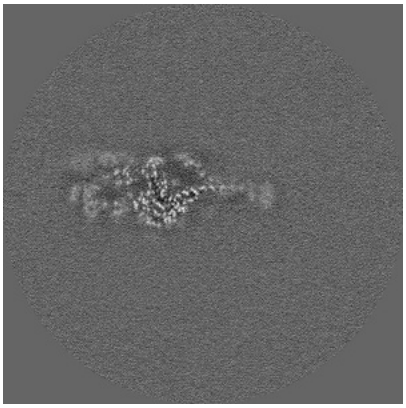


Z Index: 270

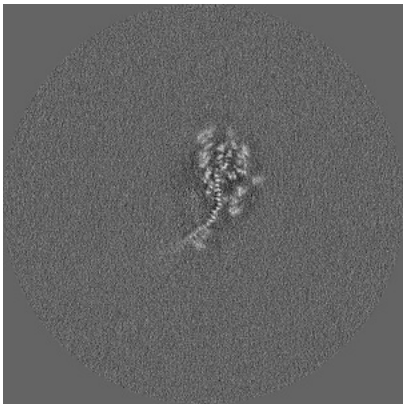
6.2.2 Raw map



X Index: 270



Y Index: 270

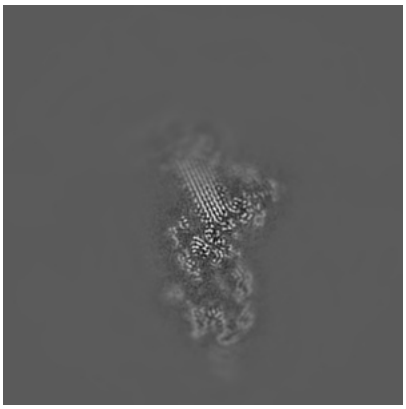


Z Index: 270

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

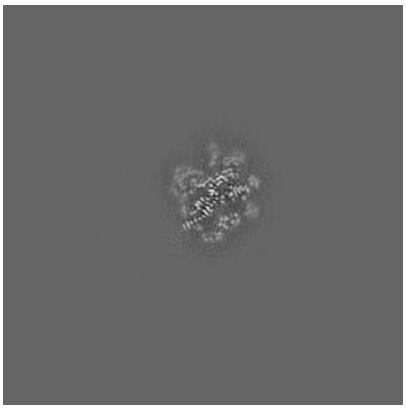
6.3 Largest variance slices (i)

6.3.1 Primary map



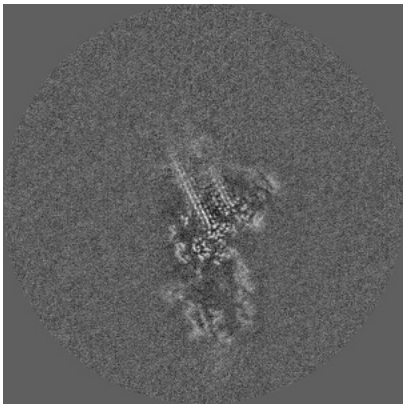
X Index: 291

Y Index: 266

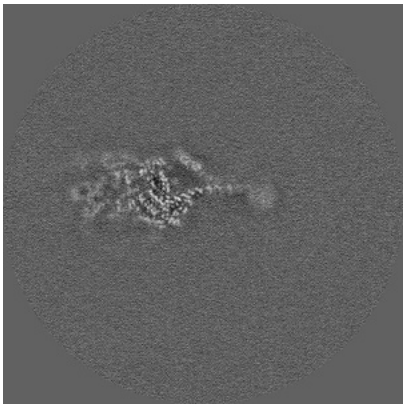


Z Index: 238

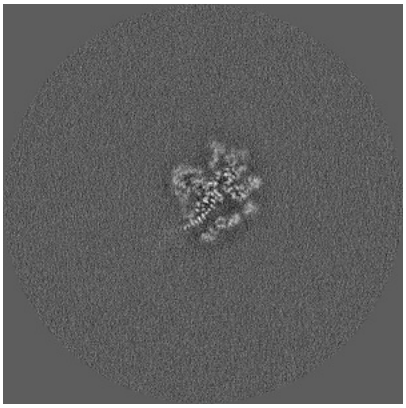
6.3.2 Raw map



X Index: 287



Y Index: 266



Z Index: 241

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

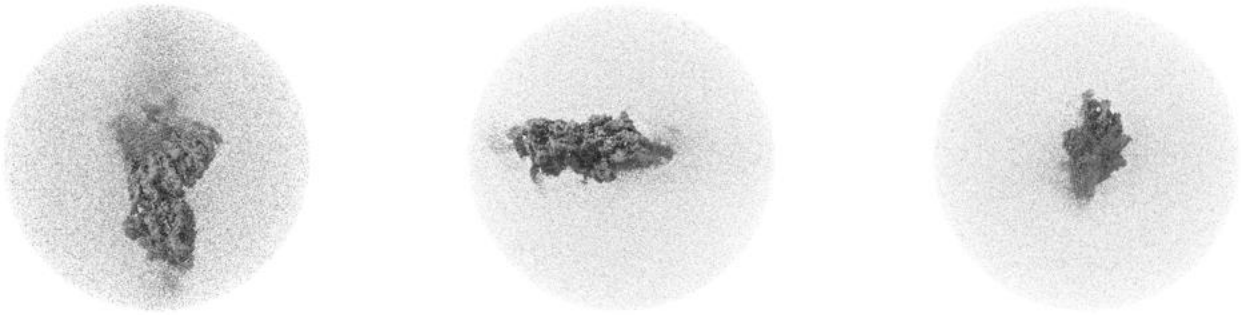
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00481. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

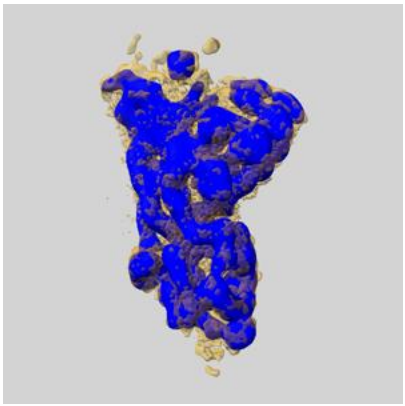
6.5 Mask visualisation (i)

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

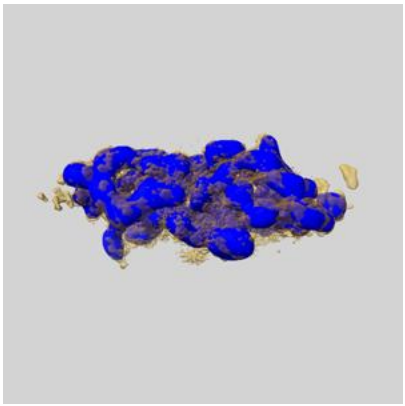
A mask typically either:

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

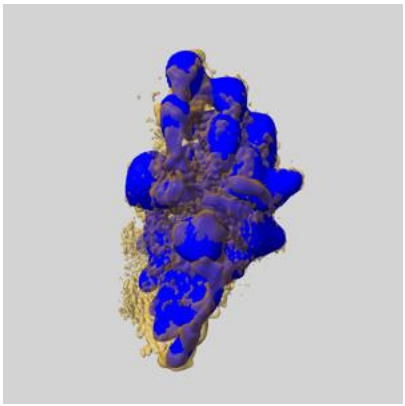
6.5.1 emd_15781_msk_1.map (i)



X



Y

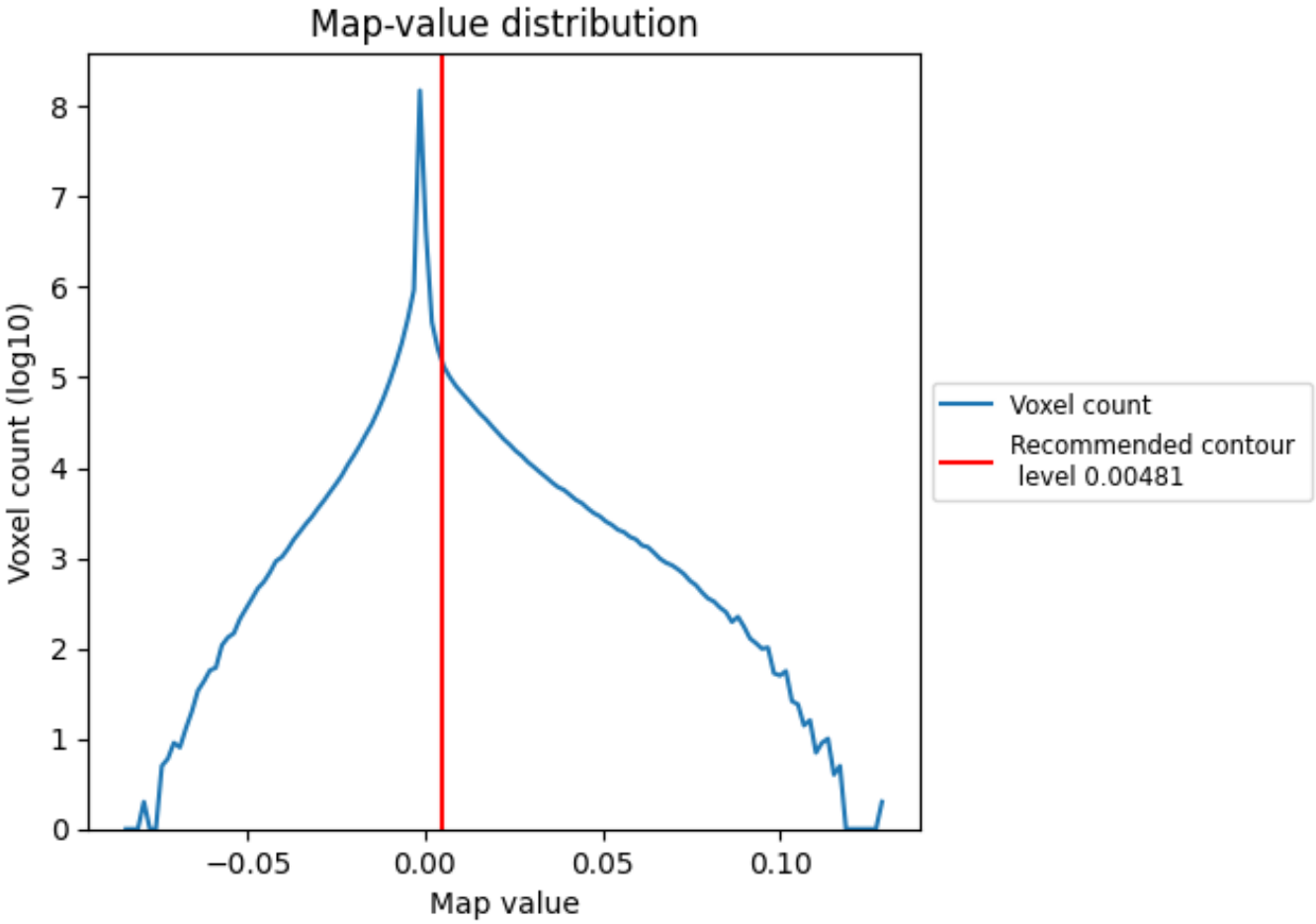


Z

7 Map analysis

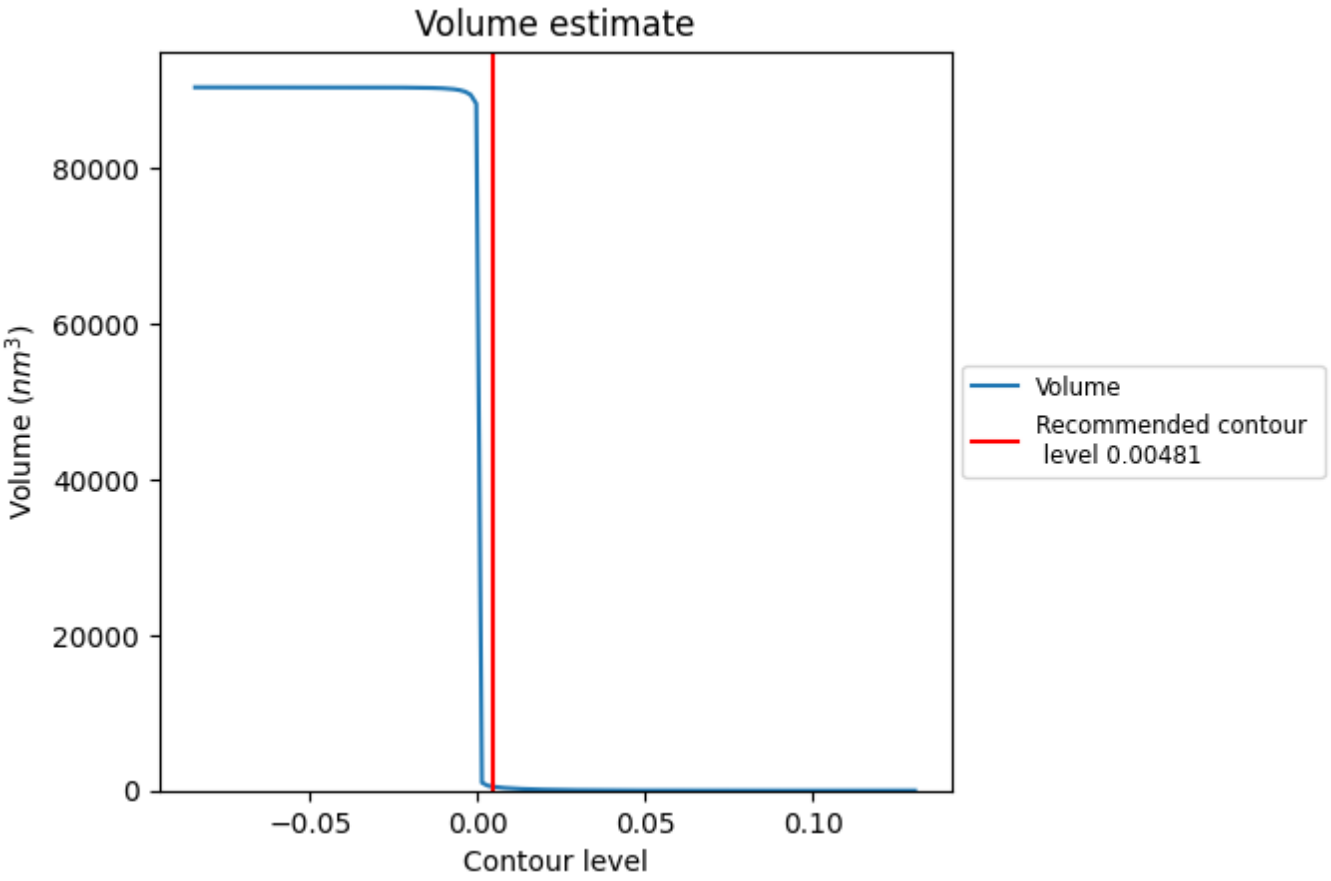
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

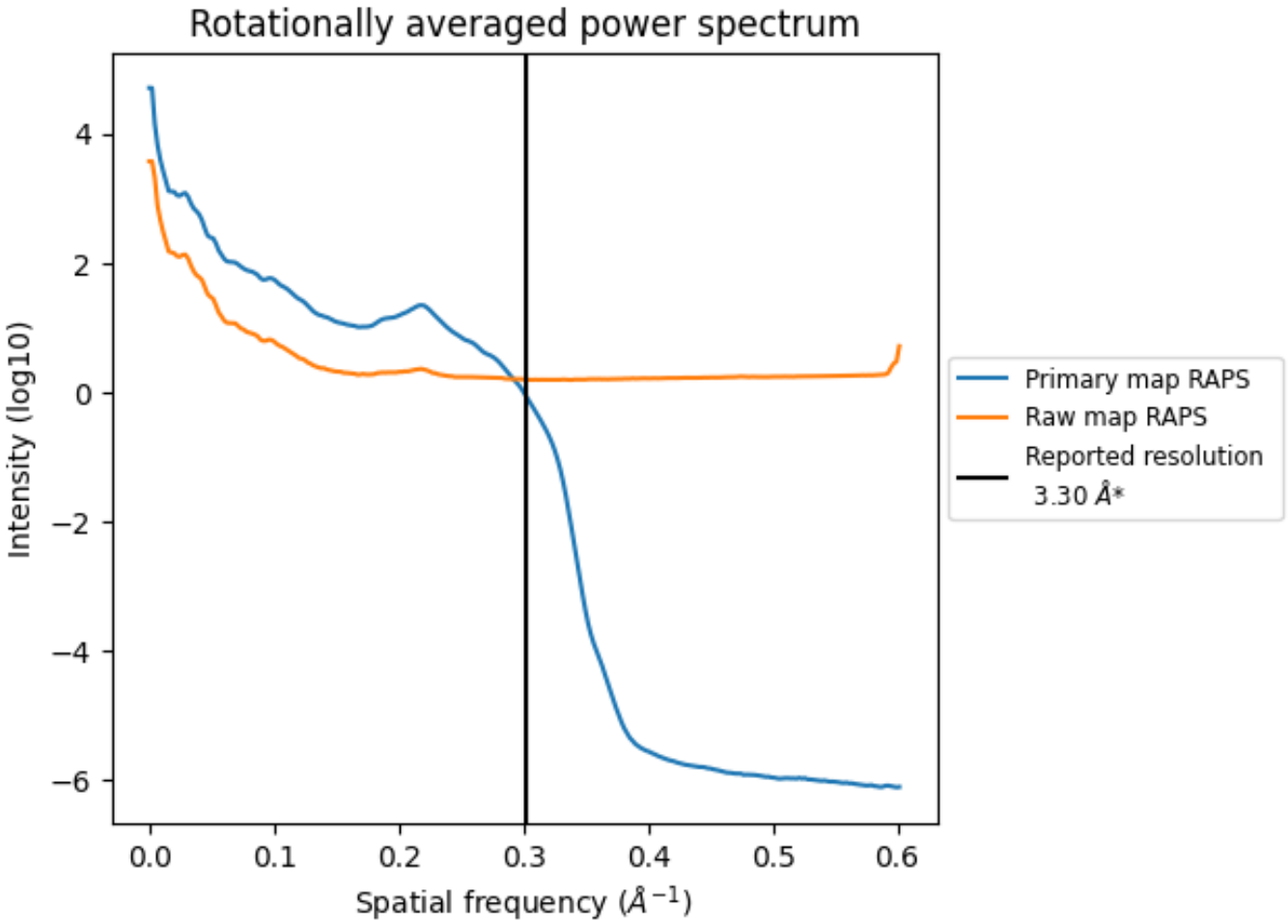
7.2 Volume estimate



The volume at the recommended contour level is 481 nm^3; 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 (i)

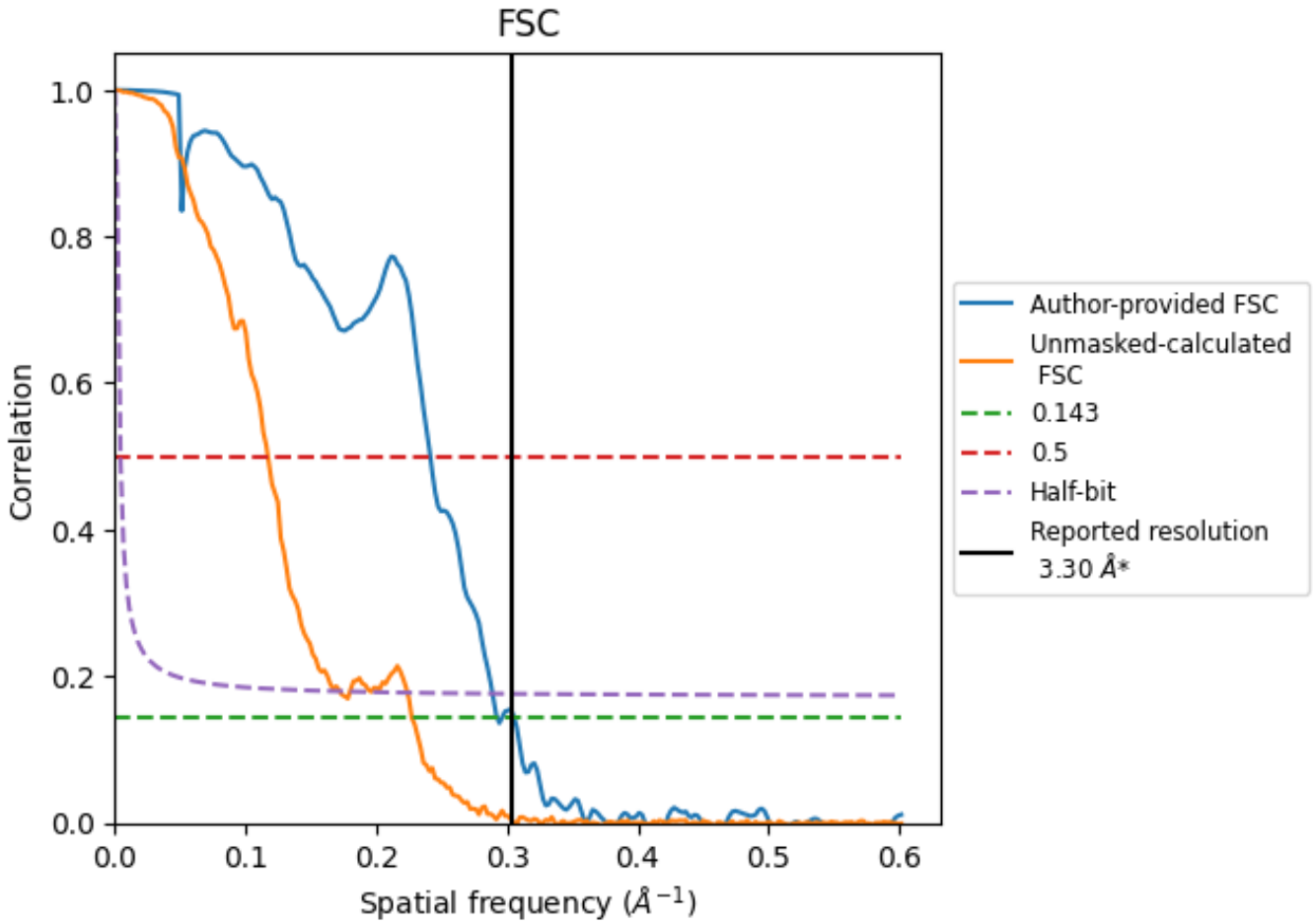


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

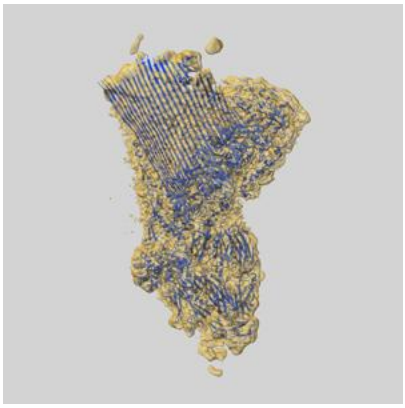
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.42	4.14	3.46
Unmasked-calculated*	4.40	8.54	5.81

*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 %

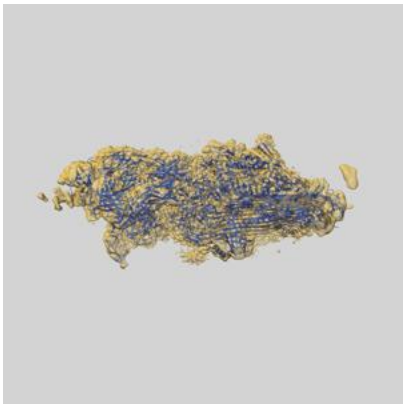
9 Map-model fit

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.

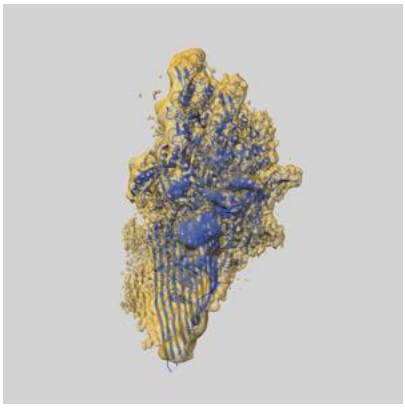
9.1 Map-model overlay



X



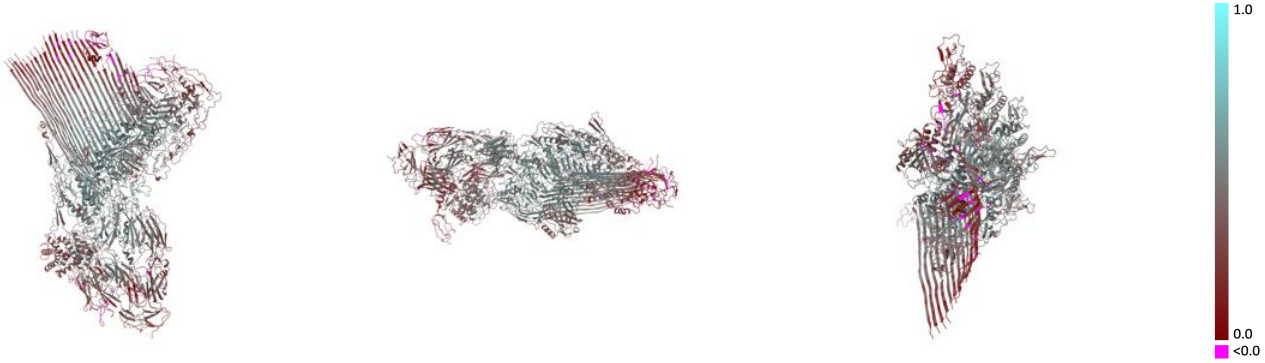
Y



Z

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.

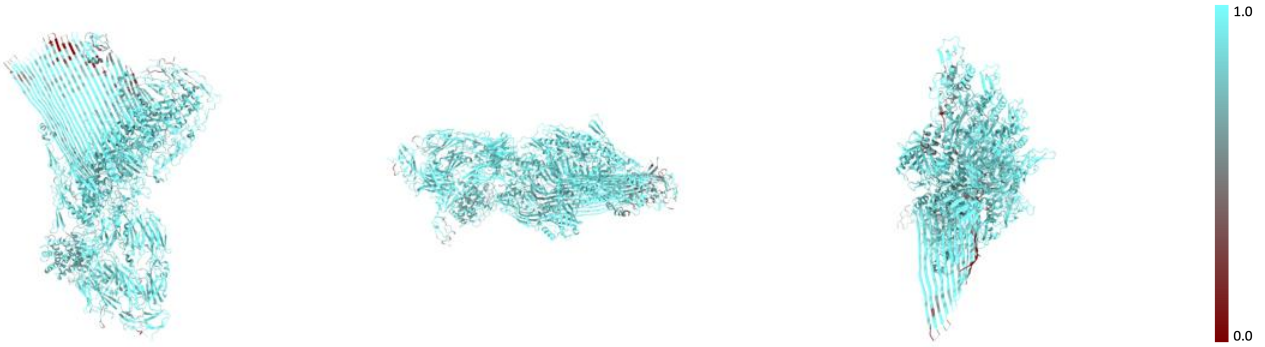
9.2 Q-score mapped to coordinate model



X Y Z

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.

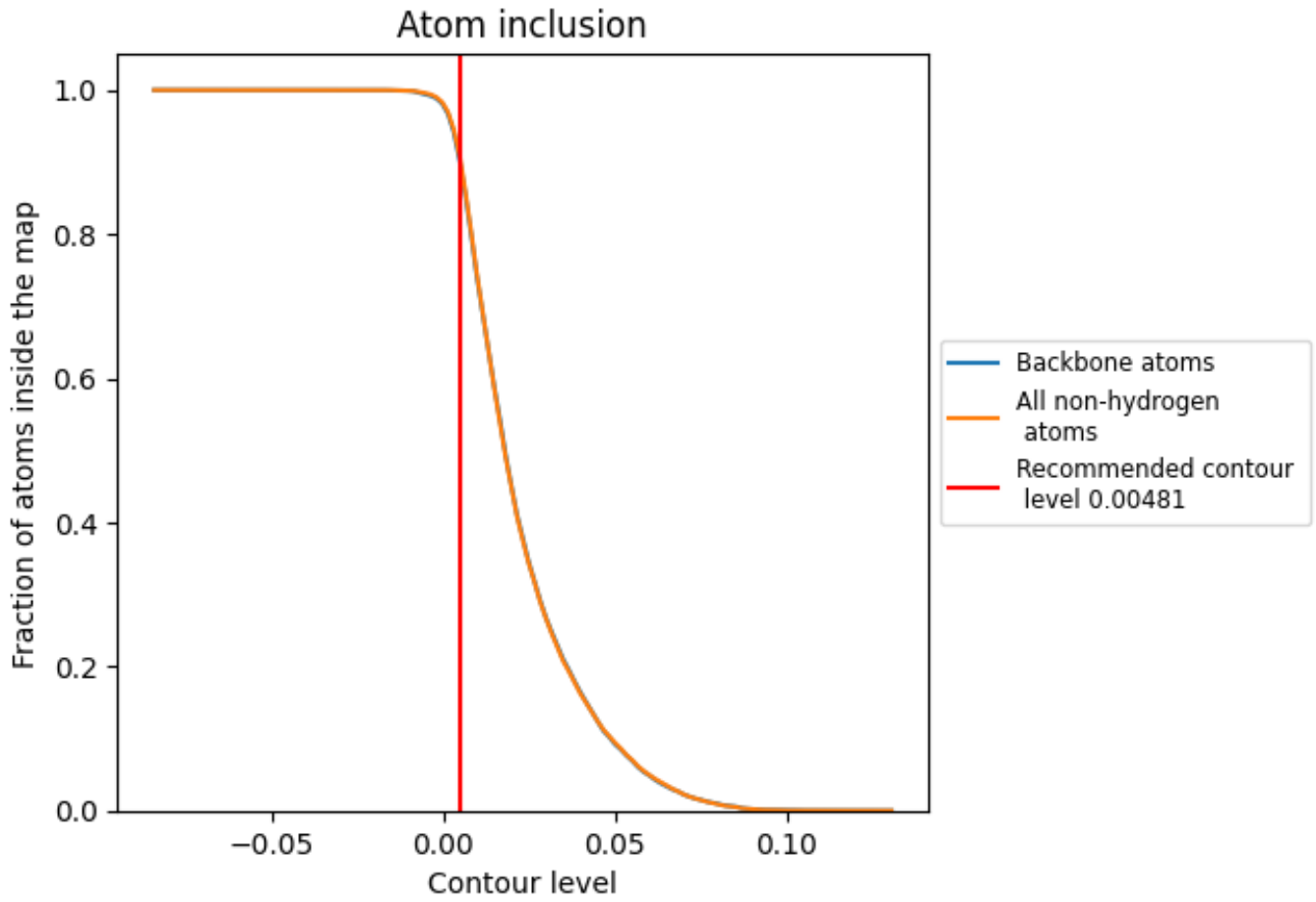
9.3 Atom inclusion mapped to coordinate model



X Y Z

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	0.9063	0.4050
A	0.9050	0.3660
B	0.9195	0.4250
C	0.9392	0.4610
D	0.9402	0.4790
E	0.9188	0.4570
F	0.9311	0.3970
G	0.7242	0.1150
H	0.9023	0.4160
I	0.8220	0.2910