Full wwPDB EM Validation Report ⓘ

Jul 15, 2024 – 01:13 PM EDT

PDB ID	:	8TJO
EMDB ID	:	EMD-41306
Title	:	Crosslinked 6-deoxyerythronolide B synthase (DEBS) Module 1 in complex with antibody fragment 1B2: Crosslinked Intra-State 1
Authors	:	Cogan, D.P.; Soohoo, A.M.; Chen, M.; Brodsky, K.L.; Liu, Y.; Khosla, C.
Deposited on	:	2023-07-23
Resolution	:	3.61 Å(reported)
Based on initial model	:	7M7F

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:

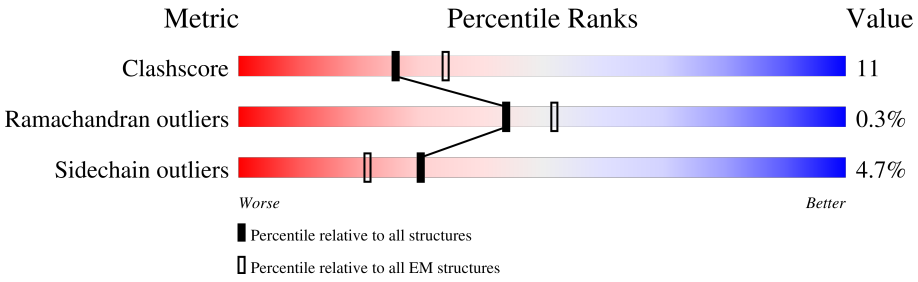
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.61 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	A	1784	12% 60% 16% • 23%
1	B	1784	• 35% 10% • 55%
2	C	249	• 52% 28% • 18%
2	E	249	57% 24% • 18%
3	D	236	59% 25% • 13%
3	F	236	61% 22% • • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22287 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1370	Total	C	N	O	P	S	0	0
			10158	6319	1865	1941	1	32		
1	B	800	Total	C	N	O	S		0	0
			5915	3690	1076	1126	23			

- Molecule 2 is a protein called Antibody Fragment 1B2, Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

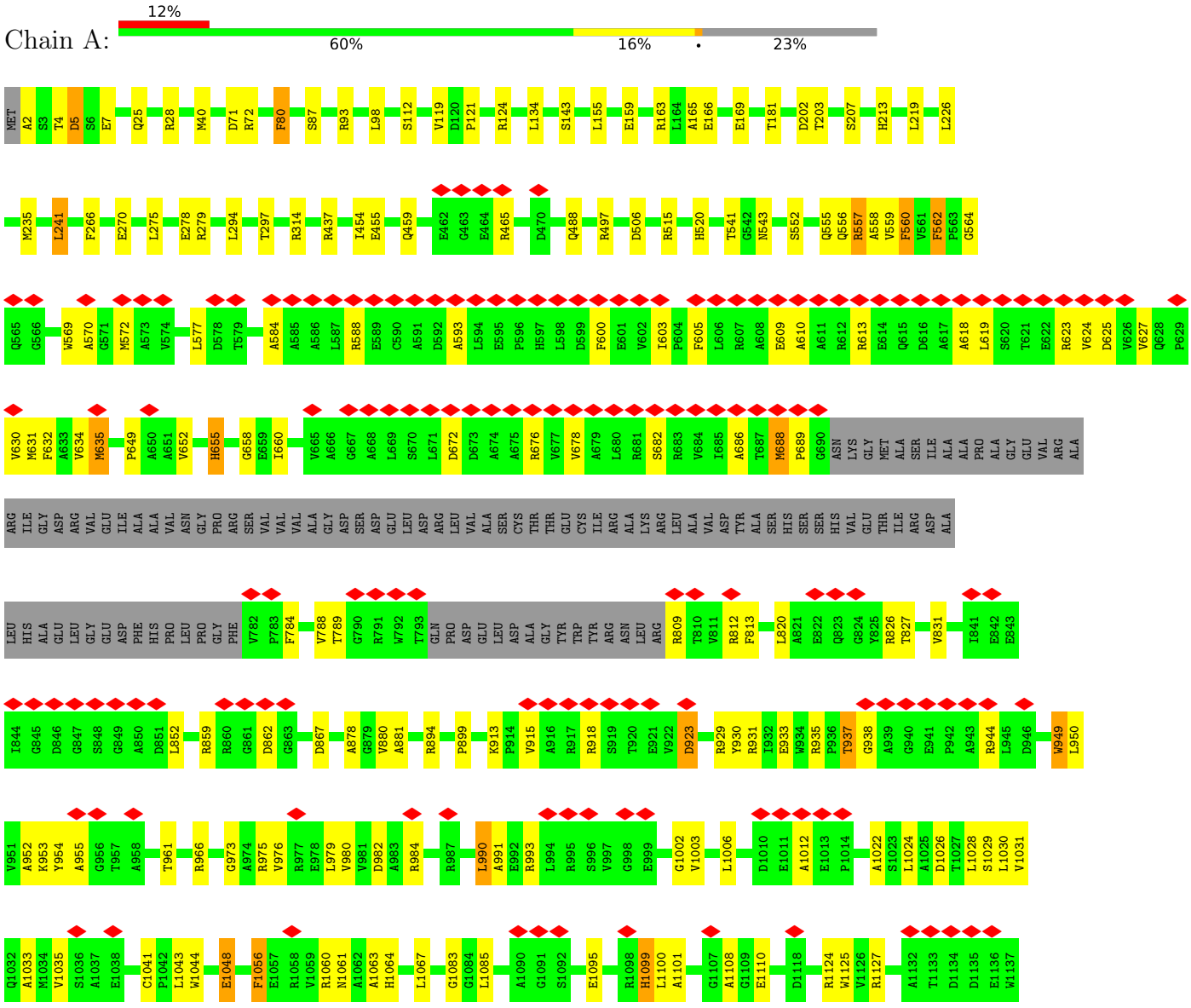
- Molecule 3 is a protein called Antibody Fragment 1B2, Light Chain.

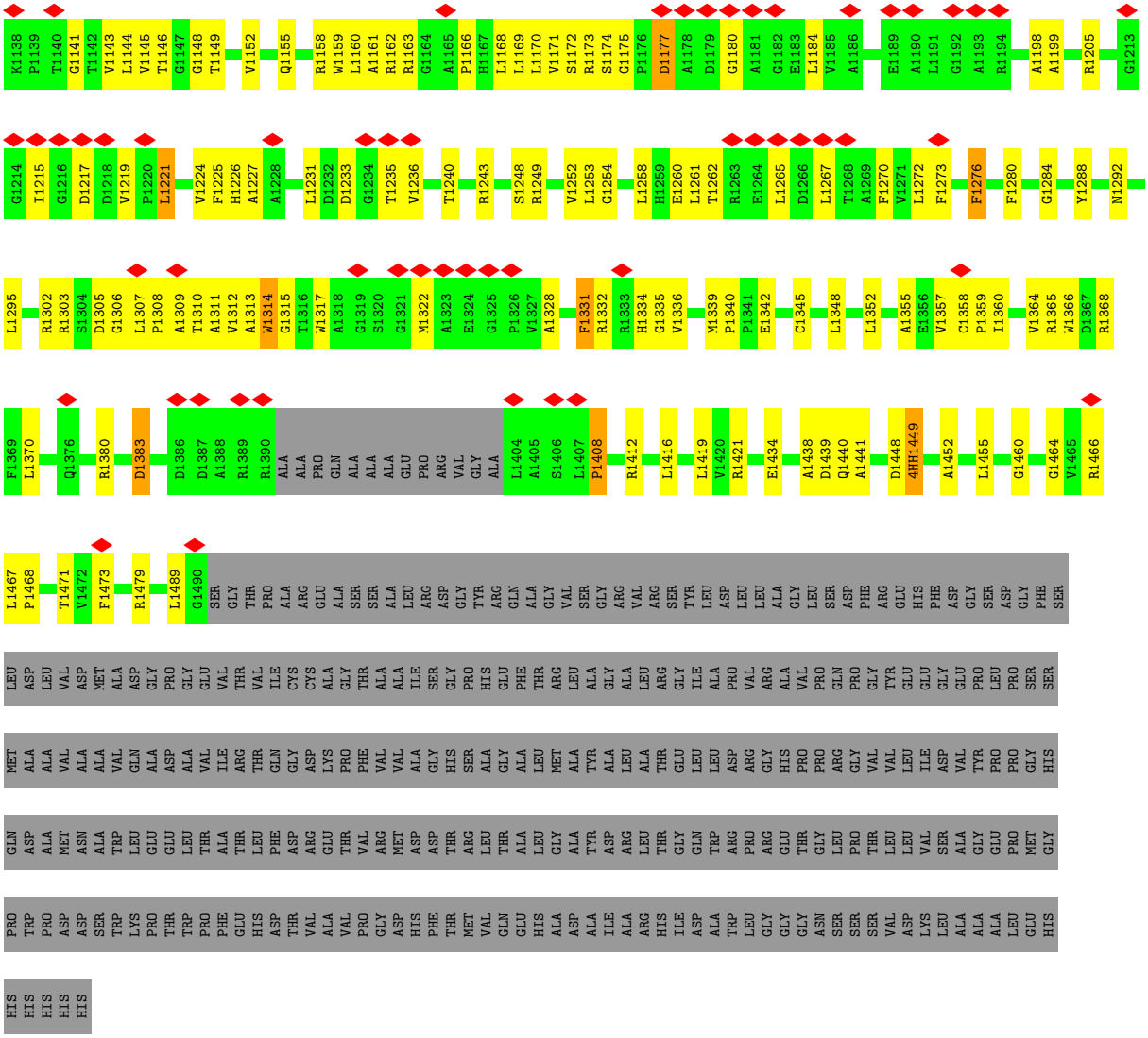
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

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.

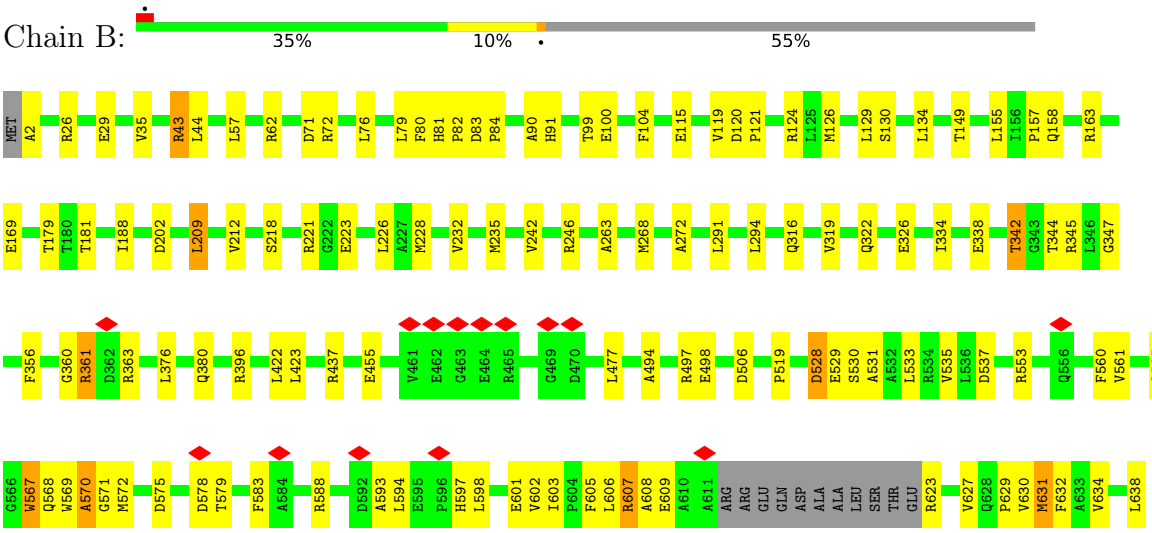
- Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6

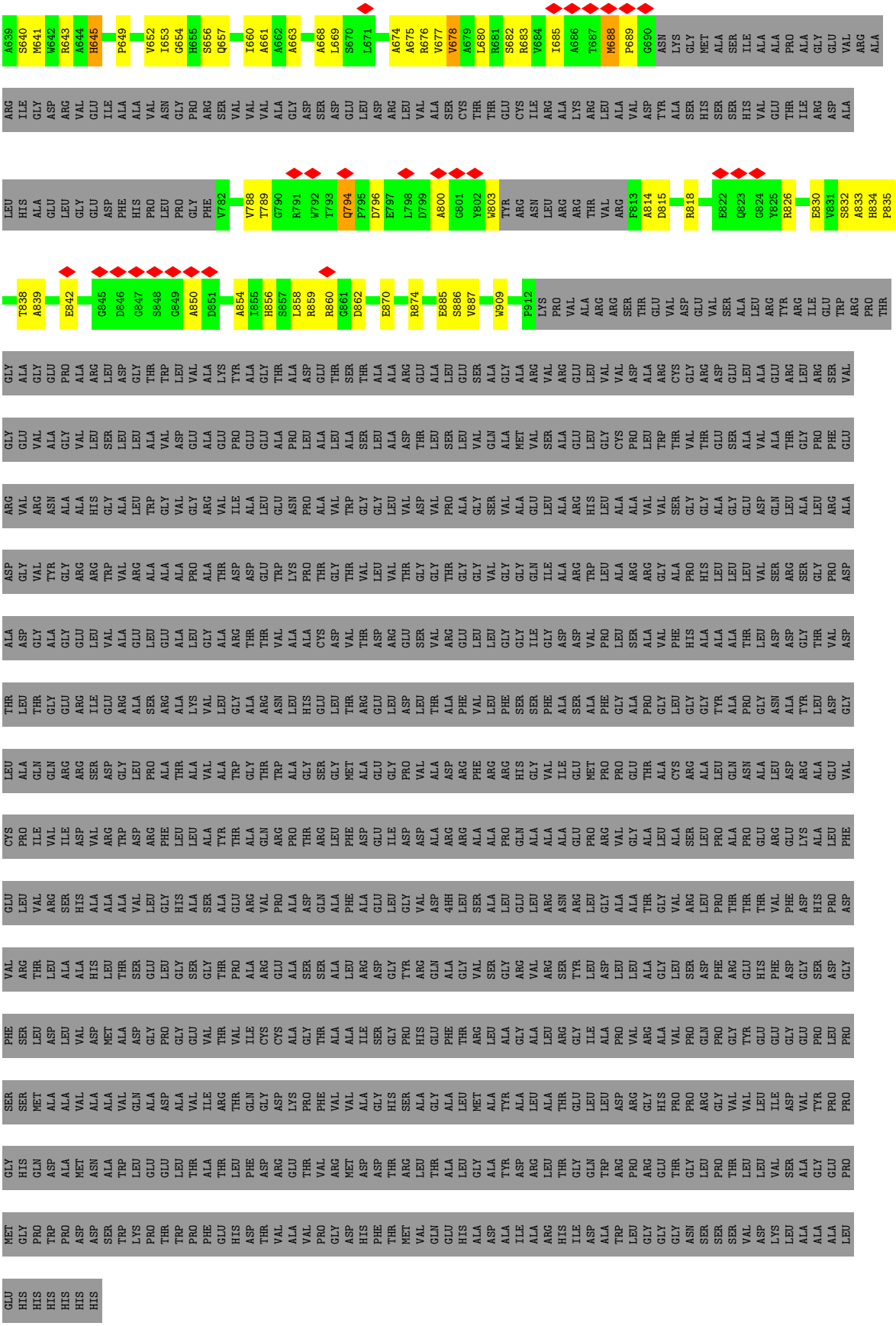




• Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6

Chain B:



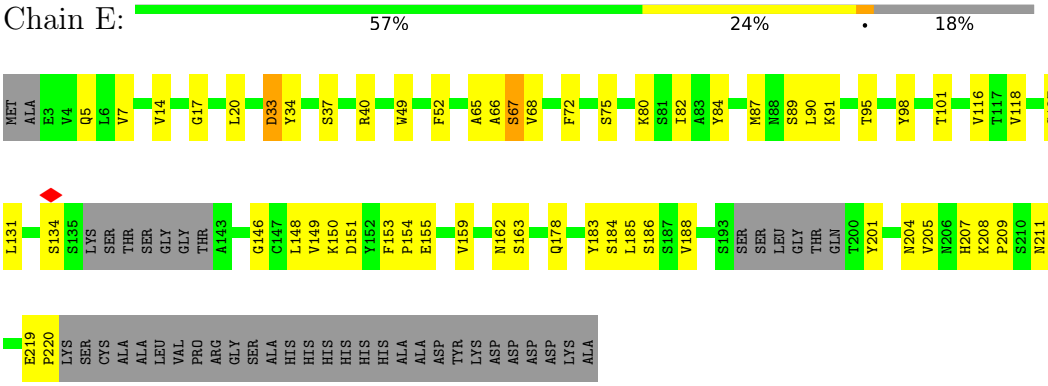

A639 S640 M641 W642 R643 A644 H645 P649 V652 I653 G654 H655 S656 Q657 I660 A661 A662 A663 A668 L669 S670 L671 A674 A675 R676 V677 V678 A679 L680 R681 S682 R683 V684 I685 A686 T687 M688 P689 G690 ASN LYS GLY MET ALA SER ILE ALA ALA PRO ALA GLY GLU VAL ARG ALA
ARG ILE GLY ASP ARG VAL GLU ILE ALA ALA VAL ASN GLY PRO ARG SER VAL VAL VAL ALA ALA GLY ASP SER ASP GLU LEU ASP ARG LEU VAL ALA SER CYS THR THR GLU CYS ILE ARG ALA LYS ARG LEU ALA VAL ASP TYR ALA SER HIS SER HIS SER HIS VAL GLU THR ILE ARG ASP ALA
LEU HIS ALA GLU LEU GLY GLU ASP PHE HIS PRO LEU PRO GLY PHE V782 V788 T789 G790 R791 W792 T793 Q794 P795 D796 E797 L798 D799 A800 G801 Y802 W803 TYR ARG ASN LEU ARG ARG THR VAL ARG F813 A814 D815 R818 E822 Q823 G824 Y825 R826 E830 V831 S832 A833 H834 P835
T838 A839 E842 G845 D846 G847 S848 G849 A850 D851 A854 I855 H856 S857 L858 R859 R860 G861 D862 E870 R874 E885 S886 V887 W909 P912 LYS PRO VAL ALA ARG ARG SER THR GLU VAL ASP GLU VAL SER ALA LEU ARG TYR ARG ILE GLU TRP ARG PRO THR
GLY ALA GLY GLU PRO ALA ARG LEU ASP GLY THR THR LEU ALA ASP GLU THR SER THR ALA ARG GLU ALA LEU GLU ALA ARG GLU LEU VAL VAL ASP ALA ARG CYS GLY ARG ASP GLU LEU ALA GLU ARG LEU ARG SER VAL
GLY GLU VAL ALA GLY VAL LEU LEU SER LEU LEU ALA VAL ASP GLU ALA GLU PRO GLU GLU ALA PRO LEU ALA LEU ALA SER LEU SER LEU GLU ALA ASP THR LEU SER LEU VAL GLN ALA MET VAL SER ALA GLU LEU GLY CYS PRO LEU TRP THR VAL THR GLU SER ALA VAL ALA THR GLY PRO PHE GLU
ARG VAL ARG ASN ALA ALA HIS GLY GLY ALA LEU TRP GLY VAL GLY ARG VAL ILE ALA LEU GLU ASN PRO ALA VAL TRP GLY GLY LEU VAL ASP VAL PRO ALA GLY SER VAL ALA GLY GLU LEU ALA ARG HIS LEU ALA ALA ALA VAL SER GLY GLY ALA GLY GLU ASP GLN LEU ALA LEU ARG ALA
ASP GLY VAL TYR GLY ARG ARG TRP VAL ARG ALA ALA ALA PRO ALA THR ASP ASP GLU TRP LYS PRO THR GLY THR VAL LEU VAL THR GLY GLY THR GLY VAL GLY GLY GLN ILE ALA ARG ARG GLY PRO ALA PRO ASP
ALA ASP GLY ALA GLU LEU VAL ALA GLU LEU GLU LEU GLU LEU GLY ALA ARG THR THR VAL ALA ALA CYS ASP VAL THR ASP ARG GLU SER VAL ARG GLU ILE GLY ASP ASP VAL PRO LEU SER ALA ARG ARG GLY PHE HIS LEU LEU LEU VAL SER ARG GLY ASP VAL THR VAL ASP
THR LEU THR GLY GLU ILE GLU ARG ALA ARG ASN LEU HIS GLU GLU LEU THR ARG GLU LEU ASP LEU THR ALA PHE VAL LEU PHE SER SER PHE ALA SER ALA PHE GLY ALA PRO GLY LEU GLY GLY TYR ALA PRO GLY GLY ASN ALA LEU ASP ASP GLY
LEU ALA GLN GLN ARG ASP GLY LEU PRO ALA THR ALA VAL ALA TRP GLY THR TRP ALA GLY GLU GLY PRO VAL ALA ASP ARG PHE ARG ARG HIS GLY VAL ILE GLU MET PRO PRO GLU THR ALA CYS ARG ALA LEU GLN ASN ALA LEU ASP ARG GLU ALA GLU VAL
CYS PRO ILE VAL ILE ASP VAL ARG TRP ASP ARG PHE LEU LEU ALA TYR THR ARG LEU PHE ASP GLU ILE ASP ASP ALA ARG ARG ALA ALA PRO GLN ALA ALA ALA GLU GLU PRO ARG VAL GLY ALA ALA LEU ALA SER LEU PRO ALA PRO GLU ARG GLU LYS ALA LEU LEU PHE
GLU LEU VAL ARG SER HIS ALA ALA ALA VAL LEU GLY HIS ALA SER ALA GLU GLU ARG VAL PRO ALA ALA GLU ALA PHE ALA ASP GLN ALA ALA GLU LEU GLY VAL ASP 4HH LEU SER ALA LEU GLU LEU ARG ASN ARG GLY LEU GLY ALA ALA THR GLY VAL ARG LEU PRO THR THR THR VAL PHE ASP HIS ASP PRO
VAL ARG THR LEU ALA ALA HIS LEU THR SER GLU LEU GLY SER GLU LEU ALA ALA ARG ASP GLY TYR ARG GLN ALA GLY VAL SER GLY ARG VAL ARG SER TYR LEU ASP LEU LEU ALA GLY LEU SER ASP PHE ARG GLU HIS PHE ASP GLY SER ASP GLY
PHE SER LEU ASP LEU VAL THR VAL ILE CYS CYS ALA GLY THR ALA ALA ILE SER GLY PRO HIS GLU PHE THR ARG LEU GLY ALA GLY ALA LEU ARG GLY ILE ALA PRO VAL ARG ALA VAL PRO HIS GLU GLY GLU PRO LEU PRO
SER SER MET ALA ALA VAL GLN ALA ASP VAL ALA VAL ALA GLY HIS SER ALA GLY ALA LEU MET ALA TYR ALA LEU ALA THR GLU GLU LEU LEU ASP ARG GLY VAL VAL LEU ILE ASP VAL TYR PRO PRO
GLY HIS GLN ASP ALA MET ASN ALA TRP LEU GLU GLU LEU THR PHE ASP ARG GLU ASP ARG THR LEU THR ALA LEU GLY ALA TYR ASP ARG LEU GLY GLN TRP ARG PRO ARG GLU THR GLY LEU LEU PRO THR LEU LEU VAL SER ALA GLY GLU PRO
MET GLY PRO TRP PRO ASP ASP SER TRP LYS PRO THR TRP PRO PHE GLU HIS ASP THR VAL ALA VAL PRO GLY ASP HIS PHE THR MET VAL GLN GLU HIS ILE ALA ARG HIS ILE ASP ALA TRP LEU GLY GLY GLY ASN SER SER SER VAL VAL ASP LYS LEU ALA ALA LEU
GLU HIS HIS HIS HIS HIS

• Molecule 2: Antibody Fragment 1B2, Heavy Chain

Chain C:

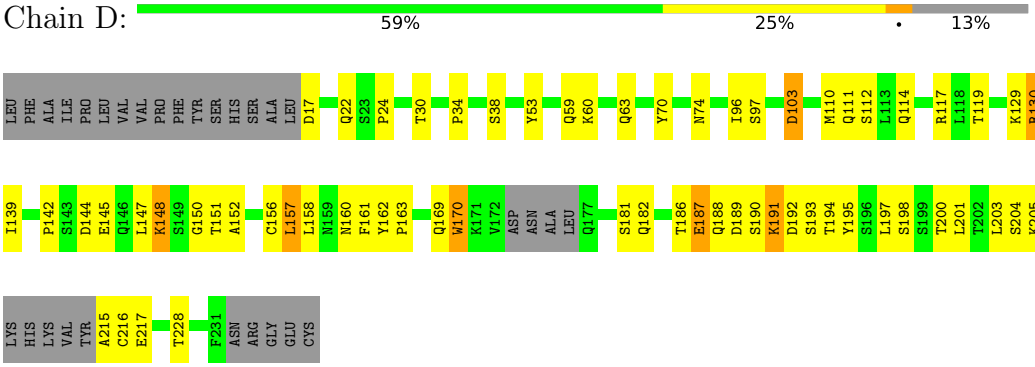
• Molecule 2: Antibody Fragment 1B2, Heavy Chain

Chain E:



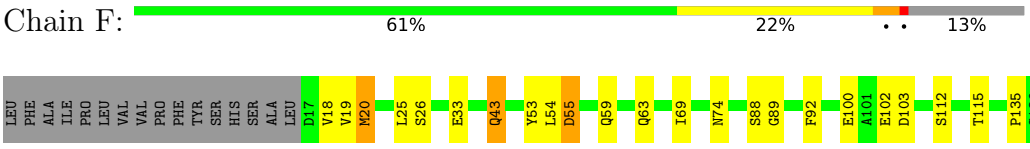
• Molecule 3: Antibody Fragment 1B2, Light Chain

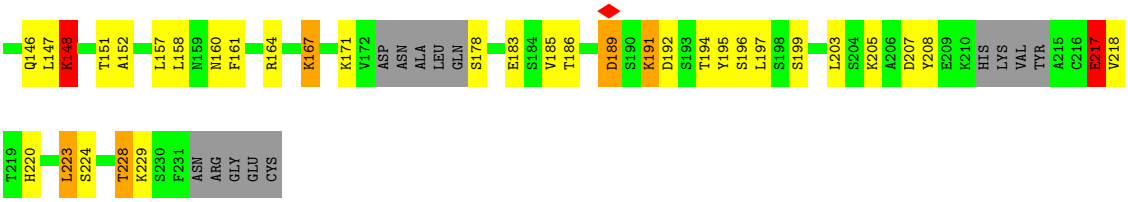
Chain D:



• Molecule 3: Antibody Fragment 1B2, Light Chain

Chain F:




Q146
L147
K148
T151
A152
L157
L158
N159
N160
F161
R164
K167
K171
V172
ASP
ASN
ALA
LEU
GLN
S178
E183
S184
V185
T186
D189
S190
K191
D192
S193
T194
Y195
S196
L197
S198
S199
L203
S204
K205
A206
D207
Y208
E209
K210
HIS
LYS
VAL
TYR
A215
C216
E217
V218
T219
H220
L223
S224
T228
K229
S230
F231
ASN
ARG
GLY
GLU
CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92037	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)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.462	Depositor
Minimum map value	-0.366	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.416	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/10326	0.55	1/14057 (0.0%)
1	B	0.25	0/6038	0.54	0/8215
2	C	0.26	0/1575	0.54	0/2141
2	E	0.28	0/1575	0.54	0/2141
3	D	0.26	0/1601	0.54	0/2175
3	F	0.35	0/1601	0.66	4/2174 (0.2%)
All	All	0.26	0/22716	0.55	5/30903 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	217	GLU	CB-CG-CD	-9.22	89.30	114.20
3	F	228	THR	CA-CB-OG1	-5.67	97.10	109.00
3	F	228	THR	N-CA-CB	-5.51	99.84	110.30
3	F	223	LEU	CA-CB-CG	5.22	127.32	115.30
1	A	1169	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10158	0	10022	212	0
1	B	5915	0	5803	114	0
2	C	1539	0	1513	49	0
2	E	1539	0	1511	48	0
3	D	1568	0	1528	48	0
3	F	1568	0	1532	44	0
All	All	22287	0	21909	497	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 11.

All (497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:142:PRO:HB3	3:D:147:LEU:HD13	1.49	0.94
3:D:144:ASP:OD1	3:D:145:GLU:N	2.07	0.86
1:A:1328:ALA:O	1:A:1332:ARG:HB2	1.75	0.84
1:A:1215:ILE:HG13	1:A:1217:ASP:H	1.46	0.80
3:F:135:PRO:HB3	3:F:161:PHE:HB3	1.67	0.76
1:A:1262:THR:HG22	1:A:1262:THR:O	1.86	0.75
2:E:75:SER:HB3	2:E:84:TYR:HB2	1.68	0.75
1:A:1313:ALA:HB3	1:A:1360:ILE:HG23	1.70	0.73
1:A:1262:THR:CG2	1:A:1267:LEU:HD13	2.20	0.72
1:B:569:TRP:O	1:B:571:GLY:N	2.22	0.72
2:C:128:VAL:HG12	2:C:149:VAL:HG13	1.72	0.72
1:A:991:ALA:HB2	1:A:1033:ALA:HB1	1.70	0.72
2:E:95:THR:HG22	2:E:118:VAL:H	1.56	0.71
1:A:1144:LEU:HD12	1:A:1224:VAL:HG22	1.70	0.70
1:A:1273:PHE:HA	1:A:1312:VAL:HB	1.73	0.70
1:A:560:PHE:HE1	1:A:831:VAL:HB	1.56	0.70
1:A:1252:VAL:HG23	1:A:1253:LEU:HD22	1.74	0.70
2:C:171:HIS:HB2	2:C:173:PHE:HE1	1.56	0.70
1:A:1240:THR:HG22	1:A:1243:ARG:HE	1.55	0.70
3:F:217:GLU:OE2	3:F:218:VAL:N	2.25	0.70
3:F:102:GLU:OE1	3:F:102:GLU:N	2.25	0.69
1:B:588:ARG:HH12	1:B:602:VAL:HG21	1.56	0.69
2:E:66:ALA:O	2:E:68:VAL:N	2.26	0.69
1:B:79:LEU:O	1:B:90:ALA:N	2.25	0.69
1:B:567:TRP:HE3	1:B:833:ALA:H	1.41	0.68
1:A:1099:HIS:O	1:A:1101:ALA:N	2.26	0.68
1:A:955:ALA:HA	1:A:980:VAL:HB	1.76	0.67
1:A:1180:GLY:HA2	1:A:1184:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:ALA:HB3	1:A:1358:CYS:HA	1.76	0.67
1:A:556:GLN:O	1:A:557:ARG:NH1	2.27	0.66
1:B:833:ALA:HA	1:B:858:LEU:HB2	1.76	0.66
1:B:497:ARG:HH21	1:B:533:LEU:HD13	1.60	0.66
1:B:794:GLN:HG2	1:B:796:ASP:H	1.57	0.66
2:C:77:ASP:O	2:C:81:SER:HA	1.96	0.66
2:E:129:PHE:HB3	2:E:148:LEU:O	1.96	0.66
1:A:1272:LEU:HD22	1:A:1311:ALA:HA	1.78	0.65
2:E:154:PRO:HD2	2:E:207:HIS:HE2	1.60	0.65
1:A:1162:ARG:NH1	1:A:1342:GLU:OE2	2.29	0.65
1:A:559:VAL:HG11	1:A:820:LEU:HD21	1.79	0.65
1:A:515:ARG:NH2	1:A:899:PRO:O	2.30	0.65
1:A:1235:THR:HG22	1:A:1236:VAL:HG12	1.79	0.65
1:A:72:ARG:NH2	1:A:270:GLU:OE2	2.29	0.65
1:B:578:ASP:OD1	1:B:579:THR:N	2.31	0.63
3:F:33:GLU:OE2	3:F:33:GLU:N	2.26	0.63
1:A:1227:ALA:HA	1:A:1273:PHE:HB2	1.79	0.63
2:E:89:SER:O	2:E:91:LYS:NZ	2.32	0.63
1:A:459:GLN:N	1:A:459:GLN:OE1	2.31	0.63
1:A:966:ARG:HB2	1:A:976:VAL:HG11	1.79	0.63
1:B:567:TRP:HE1	1:B:631:MET:HE2	1.63	0.63
2:E:129:PHE:CB	2:E:148:LEU:O	2.47	0.63
1:A:203:THR:H	1:A:207:SER:HB3	1.62	0.62
1:A:610:ALA:HB2	1:A:613:ARG:HH21	1.63	0.62
1:A:630:VAL:O	1:A:634:VAL:HG23	2.00	0.62
1:A:1272:LEU:H	1:A:1310:THR:HB	1.64	0.62
3:D:188:GLN:HE21	3:D:193:SER:HB2	1.63	0.62
1:A:4:THR:OG1	1:A:5:ASP:N	2.33	0.62
1:A:1152:VAL:HG13	1:A:1317:TRP:HE1	1.64	0.62
3:D:130:ARG:NH2	3:D:131:THR:OG1	2.32	0.62
1:A:929:ARG:HA	1:A:929:ARG:NH1	2.15	0.62
3:D:111:GLN:O	3:D:117:ARG:NH1	2.33	0.62
1:A:437:ARG:HG2	1:A:455:GLU:HG3	1.80	0.62
1:A:1143:VAL:HA	1:A:1221:LEU:HD13	1.80	0.62
3:F:55:ASP:OD1	3:F:55:ASP:N	2.32	0.62
1:A:923:ASP:N	1:A:923:ASP:OD1	2.32	0.61
1:B:830:GLU:OE2	1:B:830:GLU:N	2.33	0.61
3:F:18:VAL:HG13	3:F:20:MET:H	1.65	0.61
1:B:560:PHE:HD2	1:B:649:PRO:HB3	1.64	0.61
2:C:154:PRO:HD2	2:C:209:PRO:HG2	1.83	0.61
3:F:160:ASN:HA	3:F:194:THR:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:GLN:OE1	2:E:5:GLN:N	2.26	0.61
1:B:656:SER:OG	1:B:657:GLN:N	2.34	0.61
1:A:213:HIS:ND1	1:A:297:THR:OG1	2.34	0.60
2:C:133:PRO:HA	2:C:144:ALA:HB2	1.83	0.60
1:A:1172:SER:H	1:A:1198:ALA:HB3	1.64	0.60
1:A:1235:THR:HG23	1:A:1284:GLY:HA2	1.83	0.60
2:E:20:LEU:H	2:E:87:MET:HB2	1.66	0.60
1:A:953:LYS:HB2	1:A:1006:LEU:HB3	1.82	0.60
1:A:72:ARG:NH1	1:A:235:MET:O	2.35	0.60
1:A:1307:LEU:HD21	1:A:1355:ALA:HB1	1.83	0.60
3:F:183:GLU:N	3:F:183:GLU:OE2	2.34	0.60
1:A:1452:ALA:O	1:A:1455:LEU:HB3	2.02	0.60
3:F:191:LYS:H	3:F:191:LYS:HZ2	1.48	0.60
1:A:1144:LEU:HG	1:A:1221:LEU:HD11	1.82	0.60
1:A:1310:THR:HA	1:A:1357:VAL:HA	1.84	0.60
2:E:129:PHE:HZ	3:F:147:LEU:HD13	1.66	0.59
3:F:100:GLU:N	3:F:100:GLU:OE2	2.35	0.59
2:E:37:SER:HG	2:E:101:THR:HG1	1.46	0.59
1:B:263:ALA:O	1:B:345:ARG:NH2	2.35	0.59
1:A:159:GLU:OE2	1:B:163:ARG:NE	2.35	0.59
1:B:593:ALA:O	1:B:597:HIS:NE2	2.35	0.59
2:C:173:PHE:HB2	2:C:186:SER:HB3	1.85	0.58
3:D:53:TYR:HB3	3:D:112:SER:HB3	1.85	0.58
1:A:593:ALA:O	1:A:676:ARG:NH2	2.31	0.58
3:F:158:LEU:HD12	3:F:197:LEU:HD22	1.85	0.58
2:C:132:ALA:HB1	2:C:133:PRO:HD2	1.85	0.58
1:A:913:LYS:O	1:A:913:LYS:NZ	2.28	0.58
3:D:59:GLN:NE2	3:D:63:GLN:O	2.29	0.58
1:B:84:PRO:O	1:B:246:ARG:NH2	2.37	0.57
3:F:205:LYS:O	3:F:205:LYS:HD3	2.04	0.57
1:A:169:GLU:N	1:A:169:GLU:OE2	2.37	0.57
1:A:929:ARG:HA	1:A:929:ARG:HH11	1.69	0.57
1:A:953:LYS:HD3	1:A:954:TYR:HB2	1.86	0.57
1:A:1022:ALA:O	1:A:1026:ASP:HB2	2.04	0.57
1:B:885:GLU:OE2	1:B:885:GLU:N	2.24	0.57
2:C:151:ASP:HA	2:C:182:LEU:HD12	1.86	0.57
1:B:814:ALA:O	1:B:818:ARG:HG2	2.04	0.57
2:C:41:GLN:NE2	2:C:45:LYS:O	2.35	0.57
1:A:506:ASP:OD2	1:A:894:ARG:NH1	2.38	0.57
1:B:99:THR:OG1	1:B:100:GLU:OE2	2.22	0.57
2:C:204:ASN:HB3	2:C:214:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:HIS:HA	1:A:1368:ARG:HE	1.69	0.57
1:A:572:MET:SD	1:A:572:MET:N	2.78	0.57
1:A:1159:TRP:CD1	1:A:1345:CYS:HB3	2.39	0.57
1:B:361:ARG:HE	1:B:361:ARG:N	2.02	0.57
3:D:215:ALA:HB3	3:D:228:THR:HG23	1.87	0.57
2:E:207:HIS:O	2:E:211:ASN:N	2.34	0.57
1:A:181:THR:OG1	1:B:202:ASP:OD1	2.20	0.56
1:A:1366:TRP:HD1	1:A:1370:LEU:HD21	1.70	0.56
1:B:565:GLN:OE1	1:B:565:GLN:N	2.33	0.56
2:E:20:LEU:N	2:E:87:MET:HB2	2.20	0.56
3:F:59:GLN:NE2	3:F:63:GLN:O	2.38	0.56
1:A:1158:ARG:O	1:A:1161:ALA:HB3	2.04	0.56
1:A:1307:LEU:HG	1:A:1308:PRO:HD2	1.87	0.56
3:F:139:ILE:HG22	3:F:229:LYS:HE3	1.87	0.56
1:A:1024:LEU:O	1:A:1028:LEU:HG	2.05	0.56
2:C:150:LYS:NZ	2:C:151:ASP:OD1	2.31	0.56
1:A:1262:THR:O	1:A:1262:THR:CG2	2.54	0.56
1:A:202:ASP:OD2	1:B:181:THR:OG1	2.24	0.56
1:A:1031:VAL:O	1:A:1035:VAL:HG12	2.06	0.56
2:E:87:MET:HB3	2:E:90:LEU:HD21	1.88	0.56
2:C:67:SER:O	2:C:71:ARG:NH1	2.39	0.56
2:C:128:VAL:HG23	2:C:129:PHE:H	1.70	0.56
1:A:933:GLU:OE2	1:A:935:ARG:NH1	2.38	0.55
1:A:1026:ASP:O	1:A:1030:LEU:HG	2.07	0.55
1:A:1288:TYR:O	1:A:1292:ASN:ND2	2.39	0.55
1:A:1438:ALA:HB1	1:A:1479:ARG:HD3	1.87	0.55
1:B:607:ARG:HH12	1:B:609:GLU:HB2	1.72	0.55
2:E:149:VAL:N	2:E:185:LEU:O	2.26	0.55
2:E:148:LEU:HA	2:E:186:SER:HA	1.88	0.55
1:A:1145:VAL:HB	1:A:1170:LEU:HD22	1.89	0.55
2:C:86:GLN:NE2	2:C:88:ASN:OD1	2.33	0.55
1:B:26:ARG:NH1	1:B:29:GLU:OE2	2.39	0.55
1:A:1308:PRO:HD3	1:B:82:PRO:HD2	1.88	0.55
1:B:221:ARG:NH1	1:B:223:GLU:OE1	2.39	0.55
1:A:627:VAL:O	1:A:631:MET:N	2.32	0.55
1:B:356:PHE:HD1	1:B:361:ARG:HH22	1.52	0.55
1:A:71:ASP:OD1	1:A:71:ASP:N	2.34	0.55
1:A:949:TRP:CE2	1:A:1002:GLY:HA3	2.42	0.55
1:A:1160:LEU:HD12	1:A:1160:LEU:H	1.71	0.55
1:A:1440:GLN:HE21	1:B:553:ARG:HH21	1.54	0.55
3:D:203:LEU:HD12	3:D:204:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:THR:OG1	1:A:543:ASN:OD1	2.24	0.55
3:D:30:THR:HG23	3:D:129:LYS:HB3	1.89	0.55
2:E:188:VAL:HG21	3:F:157:LEU:HD11	1.88	0.55
1:B:529:GLU:N	1:B:529:GLU:OE1	2.38	0.54
1:B:169:GLU:OE1	1:B:169:GLU:N	2.29	0.54
3:D:207:ASP:N	3:D:207:ASP:OD1	2.41	0.54
1:A:2:ALA:HB3	1:A:7:GLU:HG3	1.89	0.54
1:B:627:VAL:O	1:B:631:MET:HG3	2.07	0.54
2:C:41:GLN:HB2	2:C:47:LEU:HD23	1.89	0.54
1:A:1440:GLN:HE21	1:B:553:ARG:NH2	2.06	0.54
2:E:146:GLY:HA3	2:E:188:VAL:HG12	1.88	0.54
2:E:127:SER:HB2	2:E:150:LYS:HB3	1.89	0.54
1:A:1440:GLN:OE1	1:A:1441:ALA:N	2.40	0.54
1:A:552:SER:OG	1:A:878:ALA:O	2.26	0.54
1:A:610:ALA:HA	1:A:613:ARG:HB2	1.89	0.54
1:B:334:ILE:O	1:B:363:ARG:NH1	2.31	0.54
1:A:560:PHE:HD2	1:A:649:PRO:HB3	1.71	0.53
1:A:1095:GLU:OE1	1:A:1095:GLU:N	2.42	0.53
1:A:1248:SER:O	1:A:1252:VAL:HG22	2.08	0.53
1:A:1302:ARG:NH1	1:A:1305:ASP:O	2.41	0.53
3:F:53:TYR:HB3	3:F:112:SER:HB2	1.89	0.53
1:A:937:THR:OG1	1:A:938:GLY:N	2.41	0.53
3:D:17:ASP:OD1	3:D:17:ASP:N	2.42	0.53
3:D:203:LEU:HD12	3:D:204:SER:H	1.71	0.53
1:B:528:ASP:OD1	1:B:530:SER:N	2.41	0.53
2:C:54:ARG:O	2:C:76:ARG:NH1	2.42	0.53
1:A:1448:ASP:N	1:A:1448:ASP:OD1	2.41	0.53
1:B:104:PHE:HB2	1:B:124:ARG:HD3	1.91	0.53
3:D:34:PRO:HB3	3:D:97:SER:HA	1.89	0.53
1:B:43:ARG:HG3	1:B:129:LEU:HD21	1.91	0.53
2:E:134:SER:HA	3:F:140:PHE:HE1	1.73	0.53
1:A:788:VAL:O	1:A:812:ARG:NH2	2.31	0.52
1:A:1225:PHE:HE1	1:A:1352:LEU:HD11	1.74	0.52
1:A:859:ARG:NH1	1:A:862:ASP:OD2	2.42	0.52
1:A:950:LEU:HB3	1:A:1003:VAL:HG22	1.92	0.52
2:C:207:HIS:O	2:C:213:LYS:NZ	2.43	0.52
1:B:570:ALA:HB3	1:B:572:MET:HE2	1.91	0.52
3:F:186:THR:HG22	3:F:196:SER:H	1.74	0.52
1:B:519:PRO:HB3	1:B:553:ARG:HD2	1.91	0.52
1:A:990:LEU:HA	1:A:993:ARG:HE	1.75	0.52
2:C:49:TRP:HZ2	2:C:52:PHE:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LEU:HD23	1:A:241:LEU:H	1.75	0.51
1:A:556:GLN:HG3	1:A:881:ALA:HB2	1.92	0.51
2:C:148:LEU:HA	2:C:185:LEU:O	2.11	0.51
3:D:189:ASP:HB2	3:D:194:THR:H	1.75	0.51
3:D:158:LEU:HD22	3:D:158:LEU:H	1.75	0.51
2:E:68:VAL:HB	2:E:72:PHE:CD1	2.45	0.51
3:F:137:VAL:HG11	3:F:218:VAL:HG11	1.92	0.51
1:A:1108:ALA:O	1:A:1380:ARG:NH2	2.29	0.51
1:A:1273:PHE:CE1	1:A:1348:LEU:HD11	2.45	0.51
2:C:54:ARG:NH1	2:C:63:GLU:OE2	2.42	0.51
1:A:1416:LEU:HA	1:A:1419:LEU:HD23	1.93	0.51
1:B:660:ILE:HD12	1:B:660:ILE:H	1.75	0.51
1:A:569:TRP:CG	1:A:570:ALA:N	2.79	0.51
3:F:147:LEU:HD21	3:F:152:ALA:HA	1.93	0.50
1:A:226:LEU:HD23	1:A:278:GLU:HB2	1.92	0.50
1:B:338:GLU:HA	1:B:338:GLU:OE2	2.12	0.50
1:B:361:ARG:N	1:B:361:ARG:NE	2.59	0.50
1:A:278:GLU:OE1	1:A:279:ARG:N	2.42	0.50
2:C:188:VAL:HG11	3:D:157:LEU:HD21	1.93	0.50
1:A:1024:LEU:HD13	1:A:1067:LEU:HD23	1.93	0.50
1:A:558:ALA:HB2	1:A:880:VAL:HG13	1.93	0.50
1:A:1172:SER:OG	1:A:1198:ALA:O	2.28	0.50
1:B:575:ASP:OD1	1:B:575:ASP:N	2.44	0.50
2:E:154:PRO:HD2	2:E:207:HIS:NE2	2.27	0.50
1:A:1366:TRP:O	1:A:1370:LEU:HG	2.11	0.50
1:B:630:VAL:O	1:B:634:VAL:HG13	2.11	0.50
1:B:645:HIS:CE1	1:B:887:VAL:HG12	2.47	0.50
2:C:162:ASN:HD21	2:C:166:LEU:H	1.58	0.50
1:B:119:VAL:O	1:B:124:ARG:NH2	2.44	0.50
1:B:835:PRO:HB2	1:B:838:THR:OG1	2.12	0.50
1:A:688:MET:N	1:A:689:PRO:HD2	2.27	0.50
3:D:187:GLU:OE1	3:D:188:GLN:N	2.45	0.50
2:E:151:ASP:N	2:E:151:ASP:OD1	2.45	0.50
1:A:624:VAL:HA	1:A:627:VAL:HG22	1.93	0.49
1:A:1148:GLY:N	1:A:1171:VAL:O	2.45	0.49
1:A:1249:ARG:HA	1:A:1253:LEU:HD23	1.94	0.49
2:C:14:VAL:HB	2:C:18:ARG:HD2	1.93	0.49
2:E:67:SER:OG	2:E:68:VAL:N	2.45	0.49
2:E:219:GLU:OE1	2:E:220:PRO:HD2	2.13	0.49
1:A:688:MET:N	1:A:688:MET:SD	2.81	0.49
2:C:133:PRO:HB3	2:C:143:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:GLN:HB2	3:D:217:GLU:HB2	1.95	0.49
1:A:1224:VAL:HB	1:A:1270:PHE:HA	1.94	0.49
3:D:59:GLN:NE2	3:D:60:LYS:O	2.38	0.49
2:C:158:THR:OG1	2:C:159:VAL:N	2.46	0.49
3:F:203:LEU:HD22	3:F:207:ASP:HB3	1.94	0.49
3:F:223:LEU:HD12	3:F:224:SER:H	1.78	0.49
3:D:160:ASN:HA	3:D:194:THR:HB	1.94	0.49
3:F:223:LEU:HD12	3:F:224:SER:N	2.28	0.49
1:A:1160:LEU:HA	1:A:1163:ARG:HB2	1.95	0.48
2:C:173:PHE:HE2	3:D:198:SER:HB3	1.78	0.48
1:B:130:SER:HB2	1:B:228:MET:HE1	1.94	0.48
2:C:32:GLY:HA2	2:C:56:LYS:HZ3	1.77	0.48
2:E:204:ASN:OD1	2:E:204:ASN:N	2.46	0.48
1:B:870:GLU:OE2	1:B:874:ARG:NH1	2.46	0.48
3:D:22:GLN:NE2	3:D:38:SER:HB3	2.28	0.48
1:A:219:LEU:O	1:A:279:ARG:NH1	2.43	0.48
1:A:1056:PHE:HE2	1:B:76:LEU:HD11	1.79	0.48
1:B:688:MET:SD	1:B:689:PRO:HD3	2.54	0.48
1:B:788:VAL:HG13	1:B:789:THR:HG23	1.95	0.48
3:F:185:VAL:HG22	3:F:197:LEU:HD12	1.95	0.48
1:A:1254:GLY:O	1:A:1258:LEU:HG	2.13	0.48
3:F:171:LYS:NZ	3:F:178:SER:OG	2.41	0.48
1:A:562:PHE:HB2	1:A:658:GLY:HA3	1.96	0.48
2:C:202:ILE:HG23	2:C:216:LYS:HB3	1.96	0.48
1:A:632:PHE:HD2	1:A:678:VAL:HG21	1.79	0.48
1:B:834:HIS:CD2	1:B:860:ARG:HD2	2.49	0.48
1:A:1272:LEU:N	1:A:1310:THR:HB	2.29	0.47
1:A:1273:PHE:CZ	1:A:1348:LEU:HD11	2.48	0.47
1:A:1439:ASP:OD1	1:A:1439:ASP:N	2.38	0.47
1:B:179:THR:O	1:B:179:THR:OG1	2.32	0.47
2:C:216:LYS:HD2	2:C:218:VAL:HG12	1.96	0.47
1:A:1335:GLY:O	1:A:1365:ARG:N	2.42	0.47
1:B:601:GLU:HG3	1:B:603:ILE:HG12	1.95	0.47
2:E:128:VAL:HG12	2:E:130:PRO:HD3	1.96	0.47
1:B:57:LEU:HB2	1:B:62:ARG:HH21	1.79	0.47
3:D:142:PRO:HG2	3:D:152:ALA:HA	1.97	0.47
3:D:152:ALA:HB3	3:D:203:LEU:HD23	1.95	0.47
1:A:672:ASP:OD1	1:A:676:ARG:NH1	2.47	0.47
1:B:602:VAL:HA	1:B:606:LEU:HD13	1.97	0.47
2:E:159:VAL:HG23	2:E:205:VAL:HG12	1.97	0.47
3:D:139:ILE:HB	3:D:156:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:ASP:OD1	2:E:33:ASP:N	2.47	0.47
1:A:543:ASN:OD1	1:A:543:ASN:N	2.48	0.47
1:A:577:LEU:HD23	1:A:577:LEU:H	1.78	0.47
1:A:1331:PHE:O	1:A:1336:VAL:HG12	2.14	0.47
1:A:1468:PRO:O	1:A:1471:THR:OG1	2.31	0.47
1:B:815:ASP:OD1	1:B:815:ASP:N	2.46	0.47
3:D:135:PRO:HB3	3:D:161:PHE:HB3	1.97	0.47
2:E:153:PHE:HB3	2:E:154:PRO:HD3	1.96	0.47
1:A:1421:ARG:HH21	1:A:1434:GLU:HA	1.80	0.46
1:B:209:LEU:O	1:B:212:VAL:HG22	2.14	0.46
3:F:164:ARG:HB3	3:F:195:TYR:CE2	2.50	0.46
2:C:162:ASN:HD22	2:C:165:ALA:HB3	1.79	0.46
1:A:166:GLU:N	1:A:166:GLU:OE1	2.49	0.46
1:A:1168:LEU:HD12	1:A:1168:LEU:HA	1.81	0.46
1:A:1383:ASP:OD1	1:A:1383:ASP:N	2.49	0.46
1:B:859:ARG:HB2	1:B:862:ASP:HB3	1.97	0.46
1:A:952:ALA:HB2	1:A:979:LEU:HB3	1.97	0.46
1:A:1012:ALA:HA	1:A:1060:ARG:HH21	1.79	0.46
1:A:619:LEU:H	1:A:623:ARG:HD2	1.79	0.46
1:A:859:ARG:NH1	1:A:867:ASP:HB3	2.30	0.46
1:A:1148:GLY:HA3	1:A:1172:SER:HB3	1.96	0.46
1:A:1489:LEU:H	1:A:1489:LEU:HD23	1.79	0.46
2:C:128:VAL:O	2:C:129:PHE:HD1	1.98	0.46
3:F:19:VAL:HG12	3:F:43:GLN:HB3	1.98	0.46
1:B:856:HIS:ND1	1:B:858:LEU:O	2.49	0.46
3:F:171:LYS:HD3	3:F:171:LYS:HA	1.78	0.46
1:A:600:PHE:HE2	1:A:605:PHE:HB2	1.81	0.46
1:A:1043:LEU:O	1:A:1083:GLY:N	2.48	0.46
1:A:1061:ASN:HD21	1:A:1064:HIS:CD2	2.34	0.46
1:A:1231:LEU:HD13	1:A:1322:MET:HB3	1.96	0.46
1:A:660:ILE:HD13	1:A:678:VAL:HG12	1.98	0.45
2:C:92:THR:HA	2:C:118:VAL:HG11	1.99	0.45
3:F:88:SER:OG	3:F:89:GLY:N	2.48	0.45
1:A:1272:LEU:HB3	1:A:1310:THR:O	2.16	0.45
2:C:128:VAL:O	2:C:129:PHE:CD1	2.69	0.45
1:A:1048:GLU:HB3	1:A:1060:ARG:HH12	1.81	0.45
1:A:1175:GLY:HA3	1:A:1199:ALA:HA	1.99	0.45
1:B:826:ARG:NH1	1:B:850:ALA:H	2.15	0.45
1:B:157:PRO:O	1:B:158:GLN:HG2	2.15	0.45
1:B:494:ALA:O	1:B:498:GLU:HG2	2.17	0.45
2:C:118:VAL:HG22	2:C:119:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:GLY:O	1:A:1184:LEU:HB3	2.15	0.45
1:B:423:LEU:HD12	1:B:423:LEU:HA	1.86	0.45
1:A:990:LEU:HD23	1:A:990:LEU:H	1.81	0.45
1:A:1226:HIS:HB2	1:A:1273:PHE:H	1.82	0.45
1:A:1466:ARG:HE	1:A:1467:LEU:H	1.65	0.45
1:B:568:GLN:C	1:B:570:ALA:H	2.19	0.45
3:D:170:TRP:HA	3:D:215:ALA:O	2.17	0.45
1:A:789:THR:HG22	1:A:809:ARG:HH22	1.81	0.45
1:A:1061:ASN:OD1	1:A:1063:ALA:N	2.50	0.45
1:B:834:HIS:NE2	1:B:860:ARG:HA	2.32	0.45
1:B:838:THR:HG23	1:B:854:ALA:HB3	1.99	0.45
1:A:121:PRO:HA	1:A:124:ARG:HG2	1.99	0.45
1:A:1048:GLU:HB3	1:A:1060:ARG:NH1	2.31	0.45
1:B:209:LEU:HD23	1:B:209:LEU:HA	1.84	0.45
1:B:594:LEU:HD21	1:B:629:PRO:HB2	1.98	0.45
1:B:627:VAL:O	1:B:630:VAL:HG22	2.16	0.45
1:B:839:ALA:HA	1:B:842:GLU:HB2	1.99	0.45
3:F:102:GLU:H	3:F:102:GLU:CD	2.20	0.45
1:A:557:ARG:O	1:A:557:ARG:HG2	2.17	0.45
1:A:1155:GLN:OE1	1:A:1158:ARG:NH1	2.50	0.45
1:A:1460:GLY:O	1:A:1464:GLY:N	2.37	0.45
1:A:609:GLU:O	1:A:613:ARG:N	2.49	0.45
1:A:682:SER:O	1:A:686:ALA:HB2	2.17	0.45
1:A:1314:TRP:CZ2	1:A:1348:LEU:HD13	2.52	0.45
1:A:1352:LEU:HD13	1:A:1352:LEU:HA	1.82	0.45
1:B:35:VAL:HG22	1:B:294:LEU:HB2	1.99	0.45
2:C:161:TRP:CZ2	2:C:203:CYS:HB2	2.52	0.45
3:D:200:THR:OG1	3:D:201:LEU:N	2.50	0.44
1:A:1141:GLY:H	1:A:1166:PRO:HD2	1.81	0.44
2:C:38:TRP:CD1	2:C:85:LEU:HD13	2.52	0.44
1:A:40:MET:HB3	1:A:275:LEU:HD23	1.99	0.44
1:B:268:MET:HB3	1:B:380:GLN:HE22	1.83	0.44
1:B:652:VAL:HG12	1:B:654:GLY:H	1.81	0.44
2:C:147:CYS:HB2	2:C:187:SER:HB3	1.99	0.44
3:D:145:GLU:O	3:D:148:LYS:HB3	2.16	0.44
3:D:197:LEU:HD12	3:D:198:SER:N	2.32	0.44
2:E:129:PHE:CD1	3:F:146:GLN:HB2	2.52	0.44
1:A:25:GLN:OE1	1:A:28:ARG:NH1	2.51	0.44
1:B:638:LEU:O	1:B:641:MET:HG3	2.18	0.44
3:D:190:SER:OG	3:D:191:LYS:N	2.50	0.44
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:THR:HG23	1:B:347:GLY:H	1.83	0.44
3:F:69:ILE:HG23	3:F:74:ASN:H	1.82	0.44
1:A:915:VAL:O	1:A:918:ARG:NE	2.51	0.44
2:E:49:TRP:CZ3	2:E:65:ALA:HB2	2.53	0.44
1:B:800:ALA:HA	1:B:803:TRP:CD1	2.52	0.44
2:C:31:PHE:O	2:C:56:LYS:NZ	2.51	0.44
1:A:119:VAL:O	1:A:124:ARG:NH2	2.50	0.44
2:C:64:TYR:HE1	2:C:74:ILE:HG13	1.83	0.44
2:C:162:ASN:ND2	2:C:165:ALA:HB3	2.33	0.44
1:A:1205:ARG:HH22	1:A:1260:GLU:HG2	1.83	0.43
1:B:291:LEU:HD22	1:B:396:ARG:HH22	1.82	0.43
1:A:1026:ASP:O	1:A:1029:SER:OG	2.28	0.43
1:A:1043:LEU:HD12	1:A:1044:TRP:N	2.33	0.43
3:D:169:GLN:O	3:D:216:CYS:HA	2.18	0.43
3:D:186:THR:OG1	3:D:187:GLU:N	2.51	0.43
1:A:294:LEU:HD23	1:A:454:ILE:HG22	1.99	0.43
1:A:1149:THR:OG1	1:A:1180:GLY:N	2.51	0.43
1:B:44:LEU:HD12	1:B:376:LEU:HD13	2.00	0.43
1:B:598:LEU:HD23	1:B:598:LEU:HA	1.87	0.43
2:C:173:PHE:CD1	2:C:173:PHE:N	2.85	0.43
2:E:155:GLU:HA	2:E:155:GLU:OE2	2.19	0.43
1:A:588:ARG:NH2	1:A:603:ILE:HG12	2.34	0.43
1:A:930:TYR:HB3	1:A:1125:TRP:HE1	1.84	0.43
1:B:72:ARG:NH1	1:B:235:MET:O	2.50	0.43
1:A:555:GLN:HB3	1:A:557:ARG:CZ	2.49	0.43
1:B:561:VAL:HG12	1:B:653:ILE:HG22	2.01	0.43
2:E:213:LYS:H	2:E:213:LYS:HG3	1.64	0.43
1:B:663:ALA:HB1	1:B:668:ALA:HB3	2.00	0.43
2:E:14:VAL:HG23	2:E:118:VAL:HG22	1.99	0.43
2:E:49:TRP:HZ2	2:E:52:PHE:HD1	1.67	0.43
1:A:975:ARG:NH1	1:A:976:VAL:O	2.44	0.43
1:A:1331:PHE:HA	1:A:1334:HIS:CE1	2.54	0.43
1:B:360:GLY:HA3	1:B:361:ARG:HH21	1.83	0.43
2:C:131:LEU:HB2	3:D:145:GLU:OE2	2.18	0.43
2:E:207:HIS:HD2	2:E:209:PRO:HD2	1.83	0.43
3:F:146:GLN:HA	3:F:148:LYS:HE2	1.99	0.43
1:B:675:ALA:O	1:B:678:VAL:HG12	2.19	0.43
1:B:680:LEU:HA	1:B:683:ARG:NE	2.34	0.43
2:E:163:SER:HA	2:E:204:ASN:HD21	1.84	0.43
3:F:158:LEU:HD21	3:F:218:VAL:HG21	2.01	0.43
3:F:167:LYS:HE3	3:F:167:LYS:HB3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:150:GLY:HA3	3:D:205:LYS:HG3	2.01	0.43
3:F:220:HIS:HB3	3:F:223:LEU:HD23	2.00	0.43
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.75	0.42
1:B:567:TRP:CE3	1:B:832:SER:HA	2.53	0.42
2:C:200:THR:O	2:C:217:LYS:NZ	2.46	0.42
2:C:207:HIS:CD2	2:C:209:PRO:HD2	2.54	0.42
2:E:208:LYS:HD2	2:E:208:LYS:HA	1.85	0.42
1:A:165:ALA:HA	1:B:242:VAL:HG11	2.00	0.42
1:B:2:ALA:HB3	3:F:115:THR:HG21	2.00	0.42
1:B:676:ARG:O	1:B:680:LEU:HG	2.18	0.42
1:B:682:SER:HA	1:B:685:ILE:HG22	2.01	0.42
1:A:944:ARG:HD2	1:A:973:GLY:HA3	2.01	0.42
1:A:1339:MET:HA	1:A:1340:PRO:HD3	1.91	0.42
1:B:218:SER:HB2	1:B:223:GLU:HG2	2.01	0.42
3:D:162:TYR:HB3	3:D:163:PRO:HD3	2.02	0.42
1:B:531:ALA:O	1:B:535:VAL:HG13	2.18	0.42
1:A:859:ARG:HD2	1:A:862:ASP:HB3	2.01	0.42
1:B:583:PHE:CZ	1:B:641:MET:HG2	2.54	0.42
1:A:1174:SER:HB3	1:A:1177:ASP:HB3	2.02	0.42
1:A:1226:HIS:HB3	1:A:1295:LEU:HD13	2.02	0.42
3:F:103:ASP:OD1	3:F:103:ASP:N	2.53	0.42
1:A:826:ARG:HH21	1:A:852:LEU:HD22	1.85	0.42
1:A:930:TYR:CZ	1:A:1366:TRP:HH2	2.37	0.42
1:A:1270:PHE:CG	1:A:1302:ARG:HG2	2.55	0.42
1:A:1306:GLY:C	1:B:82:PRO:HG2	2.40	0.42
1:A:618:ALA:HA	1:A:623:ARG:HD2	2.02	0.42
1:A:1146:THR:HA	1:A:1171:VAL:HG22	2.01	0.42
1:A:1265:LEU:HA	1:A:1265:LEU:HD23	1.79	0.42
1:B:342:THR:HG23	1:B:344:THR:HG22	2.02	0.42
2:E:80:LYS:HB2	2:E:82:ILE:HG12	2.00	0.42
1:A:564:GLY:HA3	1:A:655:HIS:ND1	2.34	0.42
1:A:631:MET:O	1:A:635:MET:SD	2.78	0.42
1:B:570:ALA:HB3	1:B:572:MET:CE	2.50	0.42
3:F:54:LEU:HD22	3:F:92:PHE:CG	2.55	0.42
1:A:1408:PRO:HD2	1:A:1412:ARG:HB3	2.01	0.41
1:B:437:ARG:HG3	1:B:455:GLU:HG3	2.02	0.41
3:D:103:ASP:OD1	3:D:103:ASP:N	2.52	0.41
3:D:188:GLN:HG3	3:D:195:TYR:CE2	2.55	0.41
1:A:1358:CYS:N	1:A:1359:PRO:HD3	2.34	0.41
1:B:856:HIS:CE1	1:B:859:ARG:HG2	2.55	0.41
2:C:176:VAL:HG12	2:C:184:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:37:SER:OG	2:E:101:THR:OG1	2.27	0.41
2:E:178:GLN:HE22	2:E:184:SER:HB3	1.85	0.41
2:E:183:TYR:N	2:E:183:TYR:CD1	2.88	0.41
3:F:148:LYS:HE2	3:F:148:LYS:HB2	1.87	0.41
1:A:169:GLU:CD	1:A:169:GLU:H	2.24	0.41
1:A:1334:HIS:O	1:A:1334:HIS:ND1	2.51	0.41
1:B:669:LEU:HD21	1:B:676:ARG:NH2	2.35	0.41
2:C:143:ALA:HB2	2:C:190:THR:H	1.85	0.41
3:D:197:LEU:HD12	3:D:198:SER:H	1.85	0.41
1:A:588:ARG:HA	1:A:588:ARG:NE	2.35	0.41
2:C:77:ASP:O	2:C:81:SER:CA	2.66	0.41
3:F:189:ASP:OD2	3:F:192:ASP:HB3	2.21	0.41
1:B:623:ARG:O	1:B:627:VAL:HG22	2.20	0.41
1:A:1225:PHE:HB3	1:A:1273:PHE:CE2	2.56	0.41
3:D:181:SER:OG	3:D:182:GLN:N	2.54	0.41
1:B:322:GLN:HG2	1:B:326:GLU:OE1	2.21	0.41
3:D:22:GLN:NE2	3:D:38:SER:O	2.43	0.41
1:A:961:THR:OG1	1:A:1006:LEU:HD21	2.21	0.41
1:A:1217:ASP:O	1:A:1219:VAL:N	2.50	0.41
1:A:1276:PHE:HB3	1:A:1315:GLY:HA2	2.02	0.41
1:B:149:THR:HG23	1:B:226:LEU:HB3	2.02	0.41
1:B:232:VAL:HG23	1:B:272:ALA:HB2	2.03	0.41
1:B:316:GLN:O	1:B:319:VAL:HG12	2.21	0.41
3:D:147:LEU:HD23	3:D:151:THR:HG23	2.02	0.41
3:D:189:ASP:HB3	3:D:192:ASP:HB3	2.03	0.41
2:E:17:GLY:HA2	2:E:89:SER:HA	2.02	0.41
2:E:207:HIS:CD2	2:E:209:PRO:HD2	2.56	0.41
3:F:25:LEU:HB3	3:F:26:SER:H	1.76	0.41
1:A:80:PHE:HB2	1:A:93:ARG:HH22	1.85	0.41
1:B:632:PHE:HE1	1:B:661:ALA:HA	1.85	0.41
2:C:48:GLU:HA	3:D:119:THR:HA	2.03	0.41
2:E:40:ARG:HB2	2:E:98:TYR:CE1	2.56	0.41
1:A:931:ARG:HG3	1:A:1358:CYS:HB3	2.03	0.40
1:A:1249:ARG:O	1:A:1253:LEU:HD23	2.22	0.40
2:C:75:SER:OG	2:C:84:TYR:HB2	2.21	0.40
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.84	0.40
1:A:266:PHE:HZ	1:A:1449:4HH:HT2	1.86	0.40
1:A:584:ALA:O	1:A:588:ARG:HG2	2.22	0.40
1:A:625:ASP:N	1:A:625:ASP:OD1	2.53	0.40
1:A:852:LEU:H	1:A:852:LEU:HD23	1.86	0.40
1:A:930:TYR:OH	1:A:1127:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:ALA:O	1:A:1357:VAL:HA	2.21	0.40
1:B:81:HIS:O	1:B:83:ASP:N	2.54	0.40
1:B:640:SER:HA	1:B:643:ARG:HG2	2.02	0.40
3:F:191:LYS:HE3	3:F:191:LYS:HB3	1.95	0.40
1:A:1261:LEU:HD23	1:A:1261:LEU:HA	1.93	0.40
1:A:1449:4HH:HL3	1:A:1449:4HH:HO2	1.79	0.40
1:A:1466:ARG:HE	1:A:1467:LEU:N	2.19	0.40
3:D:96:ILE:HG22	3:D:97:SER:H	1.87	0.40
1:A:560:PHE:HB3	1:A:652:VAL:HG12	2.03	0.40
1:A:1303:ARG:HG2	1:A:1308:PRO:HA	2.04	0.40
1:B:79:LEU:HA	1:B:79:LEU:HD23	1.85	0.40
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.20	0.40
1:B:126:MET:HB3	1:B:188:ILE:HD11	2.03	0.40
3:D:188:GLN:NE2	3:D:193:SER:HB2	2.31	0.40
1:B:674:ALA:O	1:B:677:VAL:HG12	2.22	0.40
3:D:70:TYR:O	3:D:74:ASN:HB2	2.21	0.40
2:E:150:LYS:HD3	2:E:150:LYS:HA	1.87	0.40
2:E:162:ASN:HD22	2:E:201:TYR:HB3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1361/1784 (76%)	1258 (92%)	101 (7%)	2 (0%)	51 83
1	B	792/1784 (44%)	744 (94%)	46 (6%)	2 (0%)	41 74
2	C	199/249 (80%)	162 (81%)	37 (19%)	0	100 100
2	E	199/249 (80%)	178 (89%)	17 (8%)	4 (2%)	7 41
3	D	200/236 (85%)	173 (86%)	27 (14%)	0	100 100
3	F	200/236 (85%)	164 (82%)	35 (18%)	1 (0%)	29 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2951/4538 (65%)	2679 (91%)	263 (9%)	9 (0%)	44 74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1100	LEU
1	B	570	ALA
2	E	67	SER
2	E	116	VAL
1	A	1233	ASP
2	E	128	VAL
1	B	608	ALA
2	E	7	VAL
3	F	148	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1007/1324 (76%)	961 (95%)	46 (5%)	27 61
1	B	591/1324 (45%)	567 (96%)	24 (4%)	30 64
2	C	170/203 (84%)	158 (93%)	12 (7%)	14 47
2	E	170/203 (84%)	165 (97%)	5 (3%)	42 71
3	D	182/208 (88%)	172 (94%)	10 (6%)	21 56
3	F	182/208 (88%)	170 (93%)	12 (7%)	16 50
All	All	2302/3470 (66%)	2193 (95%)	109 (5%)	30 60

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	80	PHE
1	A	87	SER

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Mol	Chain	Res	Type
1	A	98	LEU
1	A	112	SER
1	A	143	SER
1	A	163	ARG
1	A	241	LEU
1	A	314	ARG
1	A	465	ARG
1	A	488	GLN
1	A	497	ARG
1	A	520	HIS
1	A	557	ARG
1	A	560	PHE
1	A	562	PHE
1	A	635	MET
1	A	655	HIS
1	A	688	MET
1	A	784	PHE
1	A	813	PHE
1	A	827	THR
1	A	923	ASP
1	A	937	THR
1	A	949	TRP
1	A	982	ASP
1	A	984	ARG
1	A	990	LEU
1	A	1041	CYS
1	A	1048	GLU
1	A	1056	PHE
1	A	1085	LEU
1	A	1099	HIS
1	A	1110	GLU
1	A	1124	ARG
1	A	1173	ARG
1	A	1177	ASP
1	A	1221	LEU
1	A	1276	PHE
1	A	1280	PHE
1	A	1314	TRP
1	A	1331	PHE
1	A	1364	VAL
1	A	1383	ASP
1	A	1408	PRO

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Mol	Chain	Res	Type
1	A	1473	PHE
1	B	43	ARG
1	B	71	ASP
1	B	80	PHE
1	B	91	HIS
1	B	115	GLU
1	B	155	LEU
1	B	209	LEU
1	B	342	THR
1	B	361	ARG
1	B	422	LEU
1	B	477	LEU
1	B	506	ASP
1	B	528	ASP
1	B	537	ASP
1	B	567	TRP
1	B	605	PHE
1	B	607	ARG
1	B	631	MET
1	B	645	HIS
1	B	678	VAL
1	B	688	MET
1	B	794	GLN
1	B	886	SER
1	B	909	TRP
2	C	34	TYR
2	C	40	ARG
2	C	52	PHE
2	C	87	MET
2	C	100	CYS
2	C	127	SER
2	C	128	VAL
2	C	148	LEU
2	C	151	ASP
2	C	152	TYR
2	C	184	SER
2	C	185	LEU
3	D	24	PRO
3	D	103	ASP
3	D	110	MET
3	D	114	GLN
3	D	130	ARG

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Mol	Chain	Res	Type
3	D	148	LYS
3	D	157	LEU
3	D	170	TRP
3	D	187	GLU
3	D	191	LYS
2	E	33	ASP
2	E	34	TYR
2	E	129	PHE
2	E	131	LEU
2	E	215	ASP
3	F	20	MET
3	F	43	GLN
3	F	55	ASP
3	F	148	LYS
3	F	151	THR
3	F	167	LYS
3	F	189	ASP
3	F	191	LYS
3	F	199	SER
3	F	208	TYR
3	F	217	GLU
3	F	228	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1064	HIS
1	B	657	GLN
2	C	162	ASN
3	D	188	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	4HH	A	1449	1	21,26,27	1.22	1 (4%)	27,35,37	0.97	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4HH	A	1449	1	-	18/32/35/37	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1449	4HH	CL3-NN	2.46	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1449	4HH	OG-CB-CA	2.59	110.67	108.14
1	A	1449	4HH	O1P-P-O2P	2.12	122.74	112.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1449	4HH	N-CA-CB-OG
1	A	1449	4HH	CB-OG-P-O1P
1	A	1449	4HH	O3P-CJ-CK-CM
1	A	1449	4HH	CM-CL3-NN-CO
1	A	1449	4HH	NN-CO-CP-CQ
1	A	1449	4HH	ON-CL3-NN-CO
1	A	1449	4HH	CJ-O3P-P-OG
1	A	1449	4HH	O3P-CJ-CK-CL1
1	A	1449	4HH	O3P-CJ-CK-CL2
1	A	1449	4HH	NR-CS-CT-SU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	1449	4HH	CJ-O3P-P-O2P
1	A	1449	4HH	ON-CL3-CM-OM
1	A	1449	4HH	NN-CL3-CM-OM
1	A	1449	4HH	CL2-CK-CM-CL3
1	A	1449	4HH	CL2-CK-CM-OM
1	A	1449	4HH	CK-CJ-O3P-P
1	A	1449	4HH	CB-OG-P-O2P
1	A	1449	4HH	CJ-CK-CM-CL3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1449	4HH	2	0

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.

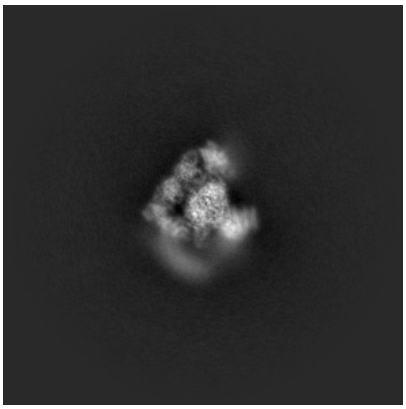
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41306. These allow visual inspection of the internal detail of the map and identification of artifacts.

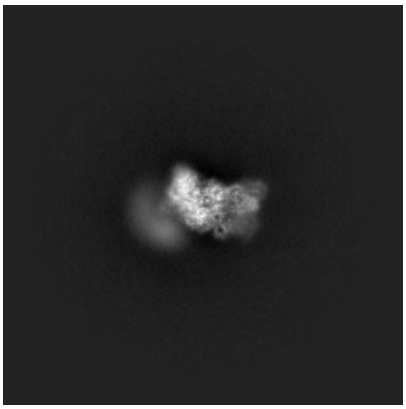
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

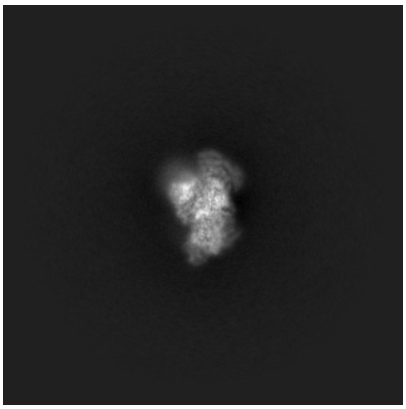
6.1.1 Primary map



X

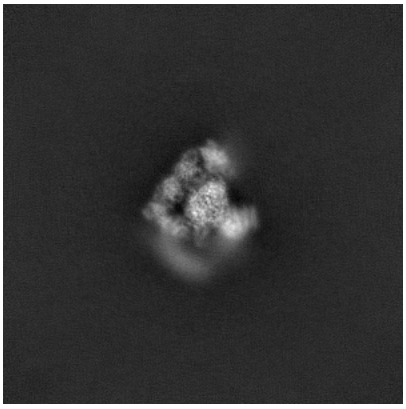


Y

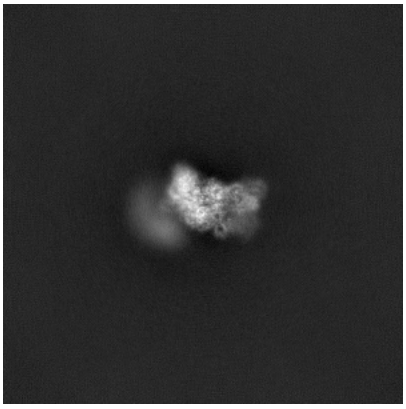


Z

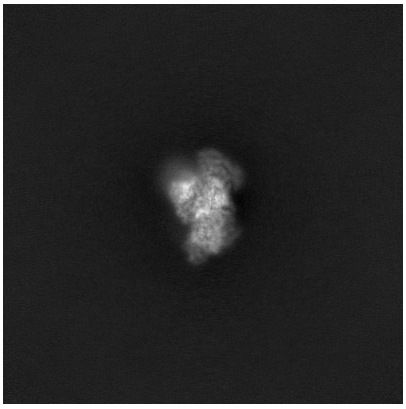
6.1.2 Raw map



X



Y

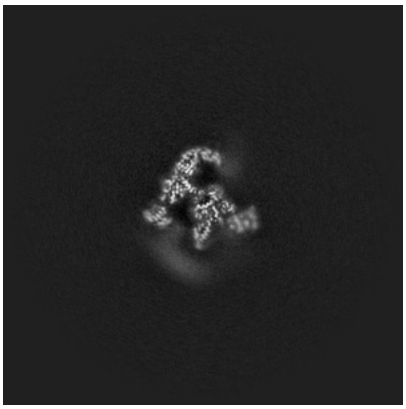


Z

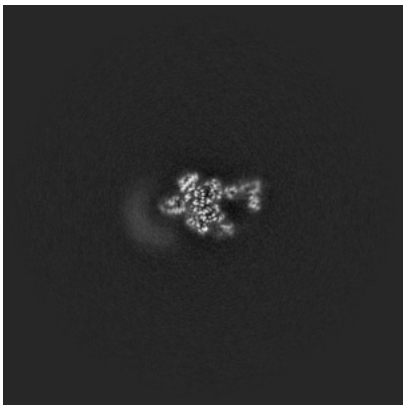
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

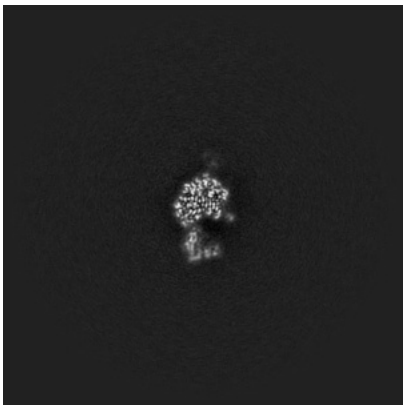
6.2.1 Primary map



X Index: 256

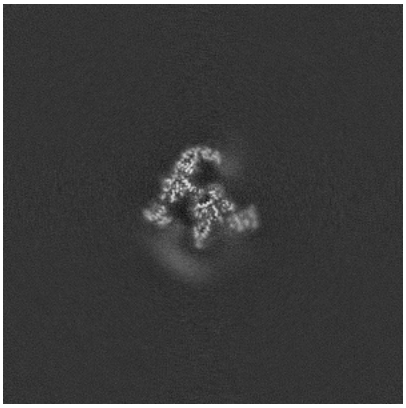


Y Index: 256

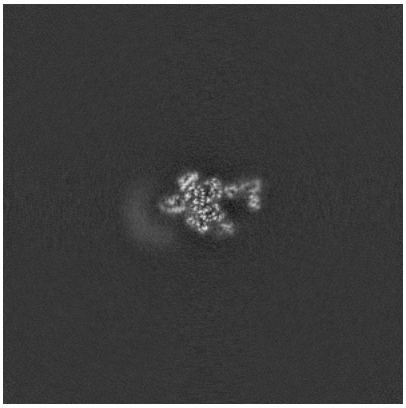


Z Index: 256

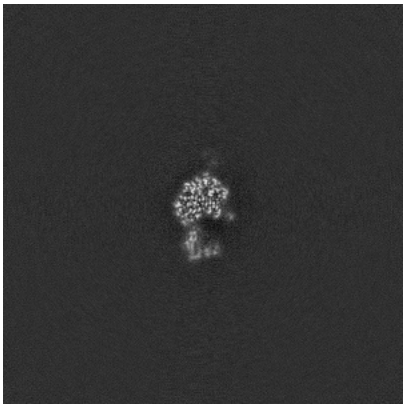
6.2.2 Raw map



X Index: 256



Y Index: 256

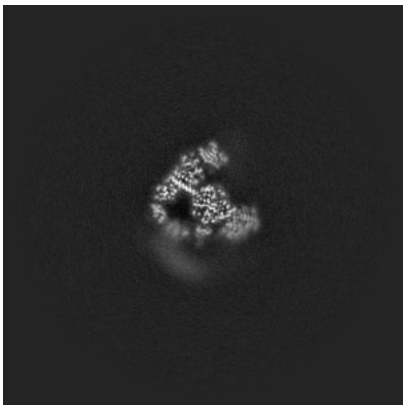


Z Index: 256

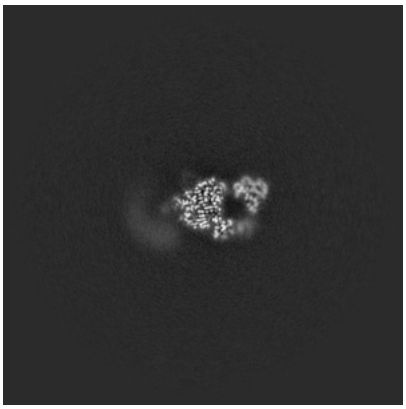
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

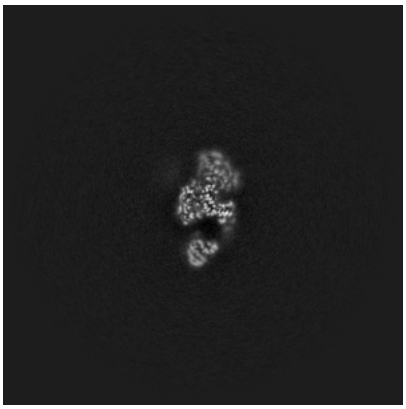
6.3.1 Primary map



X Index: 264

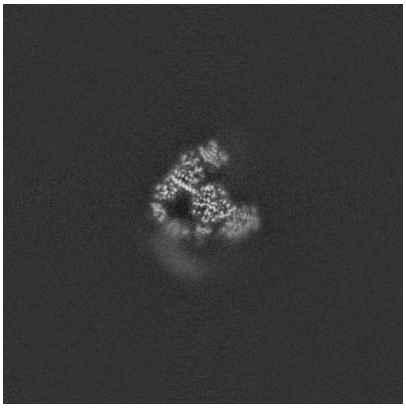


Y Index: 264

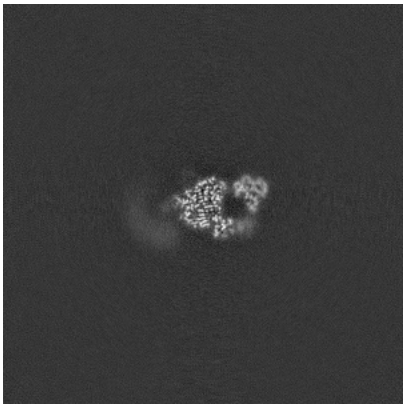


Z Index: 244

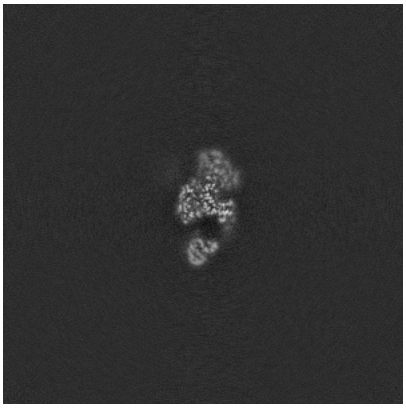
6.3.2 Raw map



X Index: 264



Y Index: 264

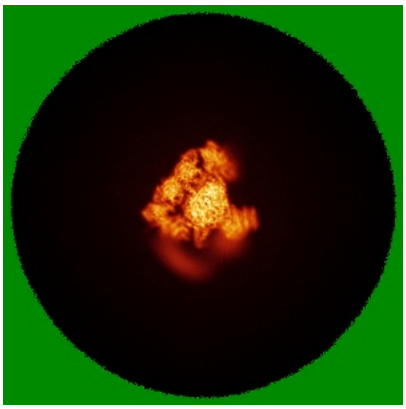


Z Index: 244

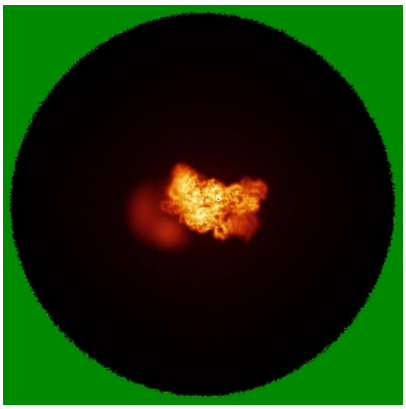
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

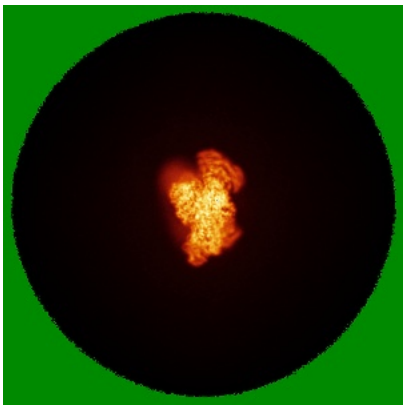
6.4.1 Primary map



X

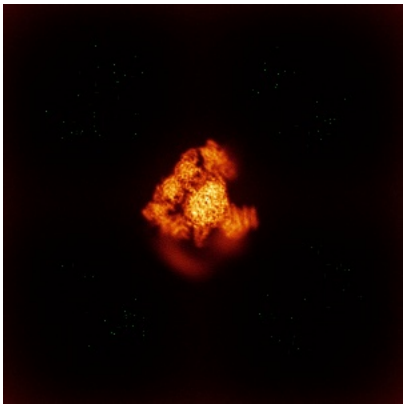


Y

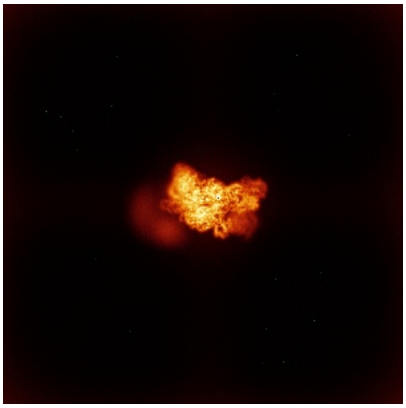


Z

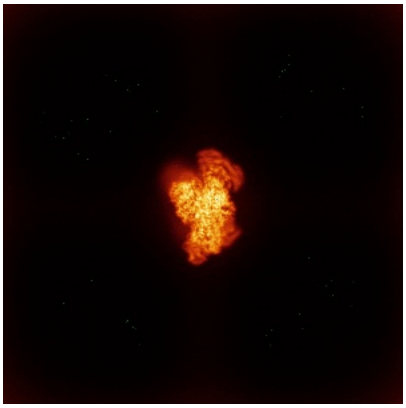
6.4.2 Raw map



X



Y

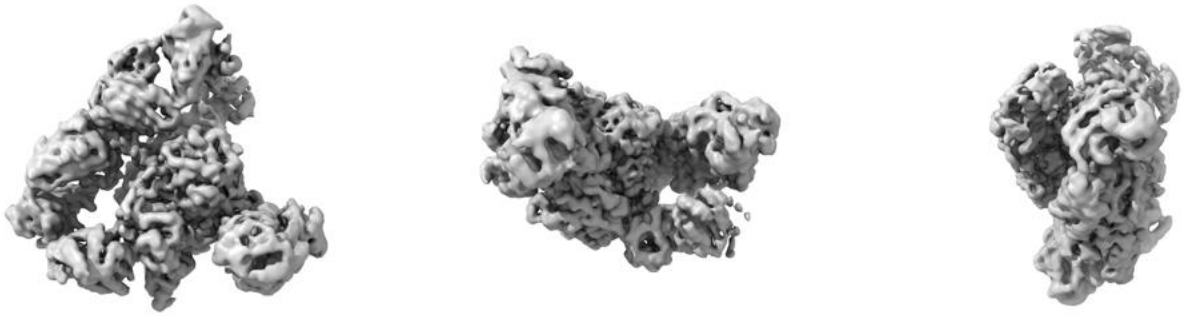


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.416. 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

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.

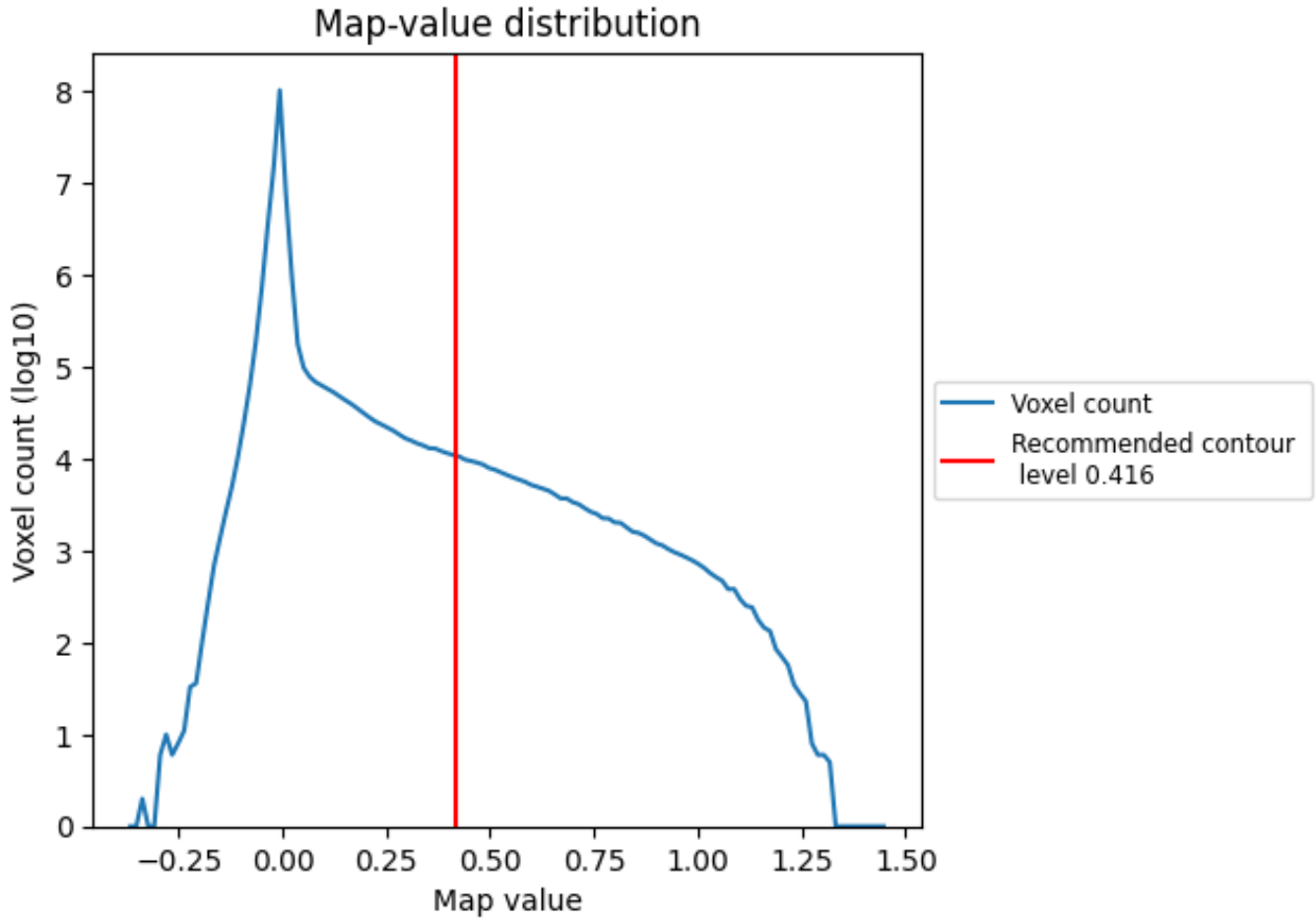
6.6 Mask visualisation (i)

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

7 Map analysis

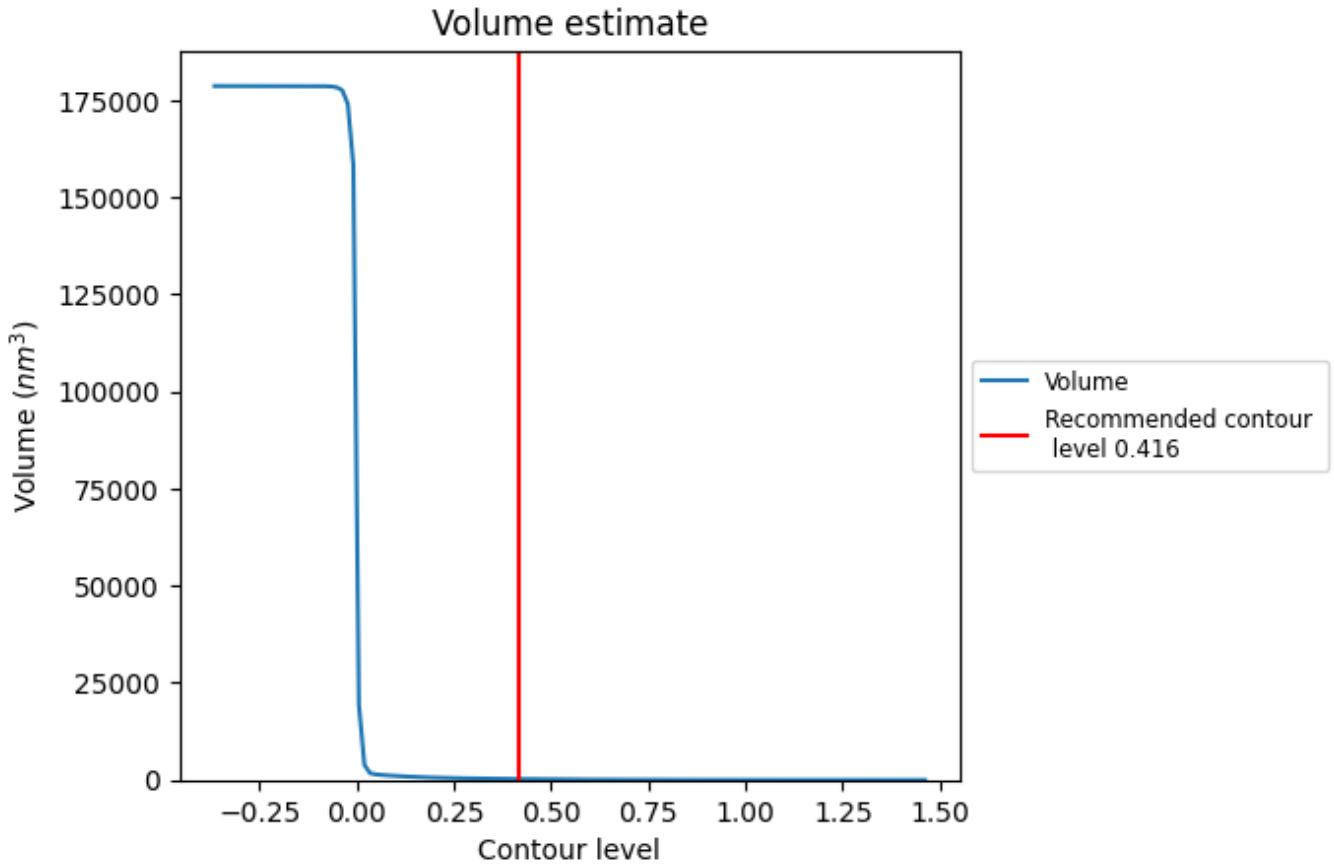
This section contains the results of statistical analysis of the map.

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.

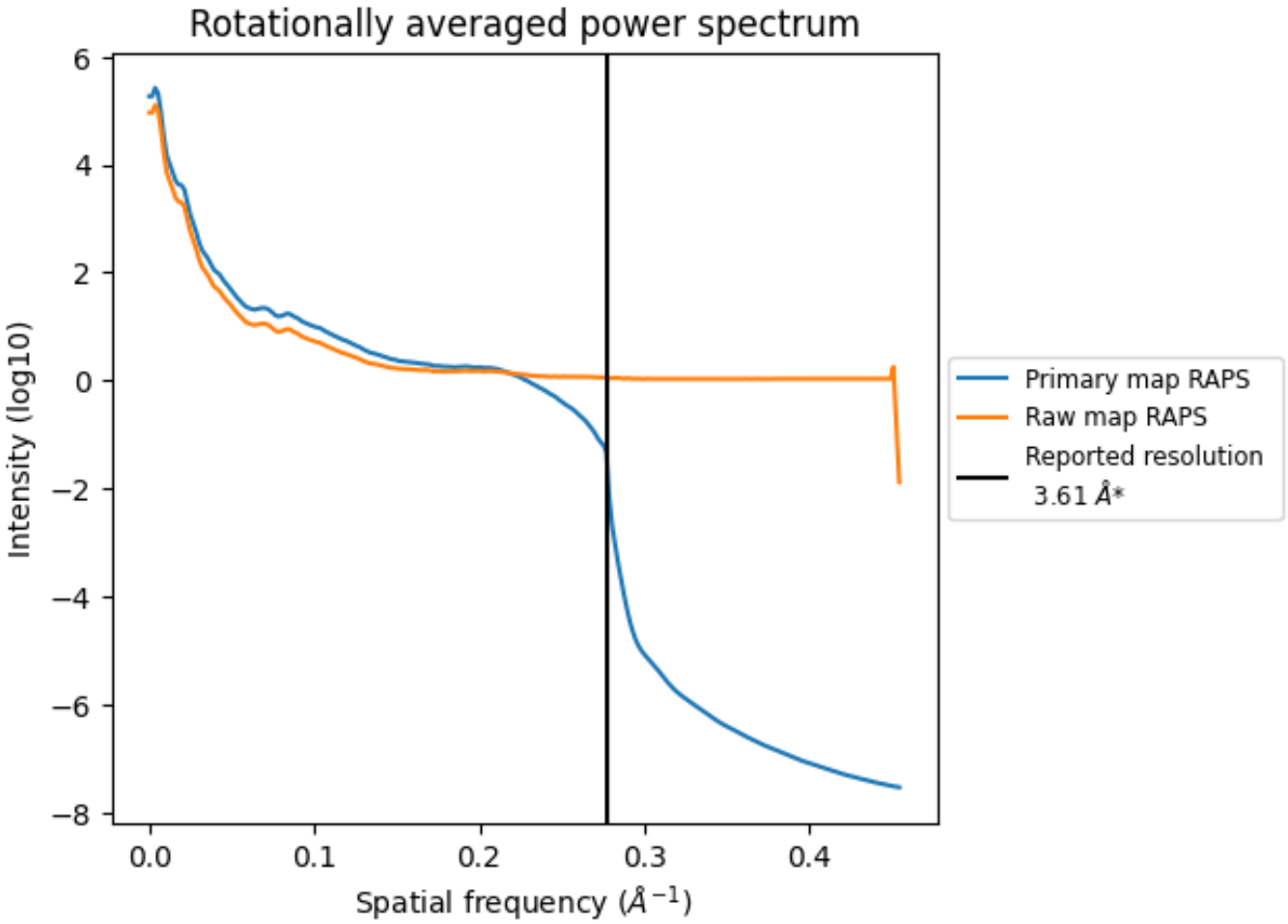
7.2 Volume estimate



The volume at the recommended contour level is 236 nm^3; this corresponds to an approximate mass of 213 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)

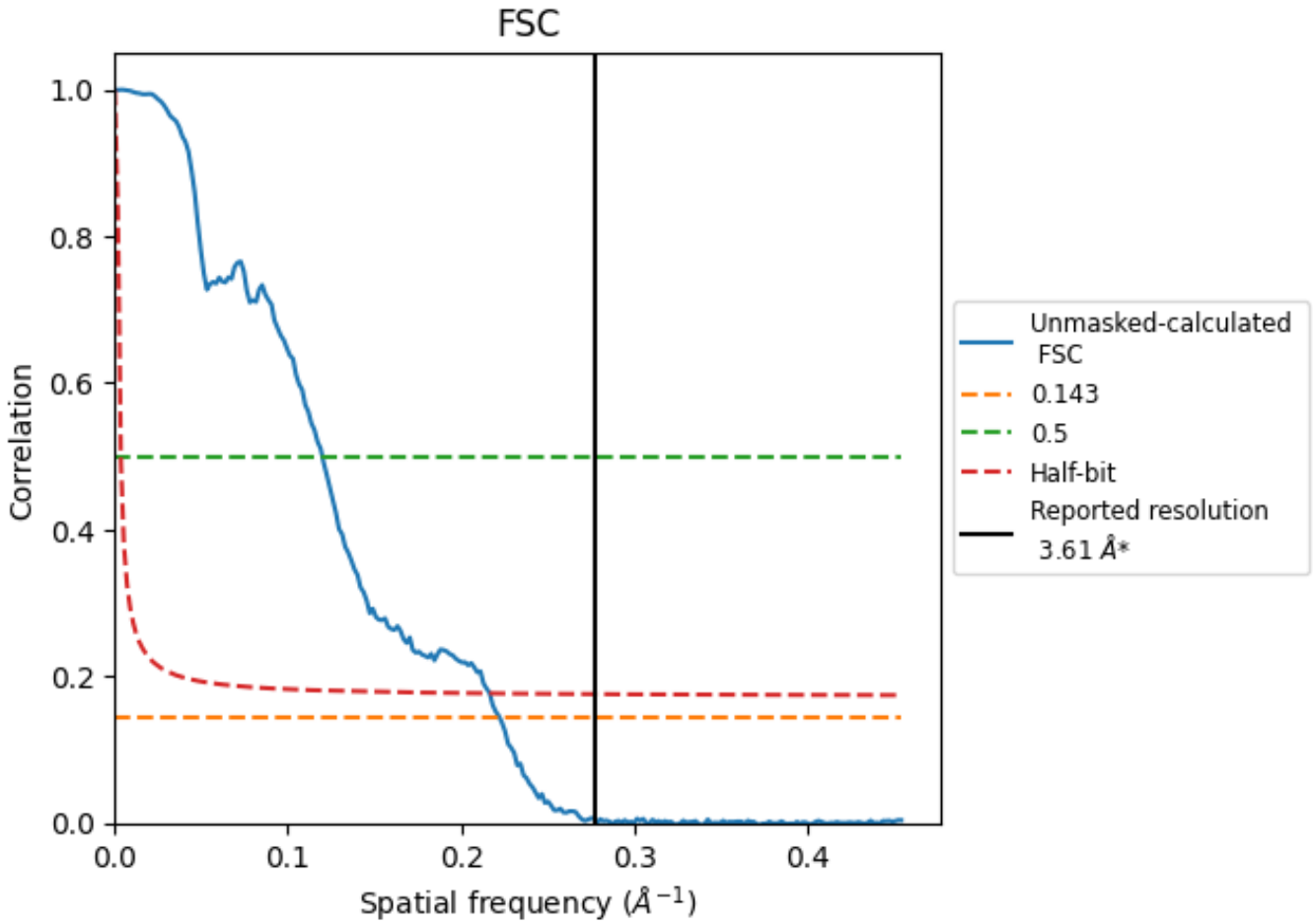


*Reported resolution corresponds to spatial frequency of 0.277 Å^{-1}

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 0.277 Å^{-1}

8.2 Resolution estimates (i)

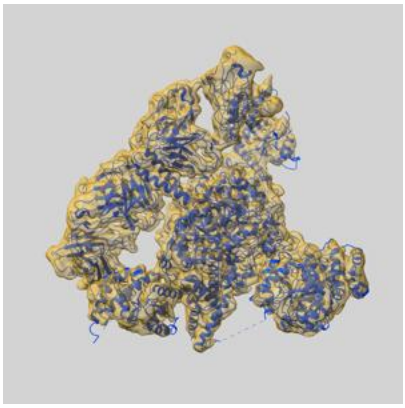
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	8.34	4.61

*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 4.49 differs from the reported value 3.61 by more than 10 %

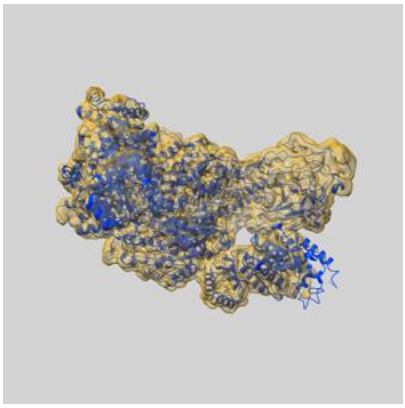
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41306 and PDB model 8TJO. Per-residue inclusion information can be found in section 3 on page 4.

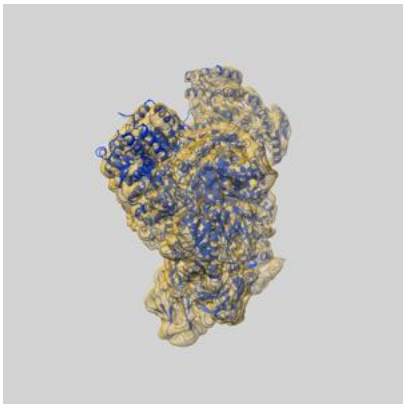
9.1 Map-model overlay



X



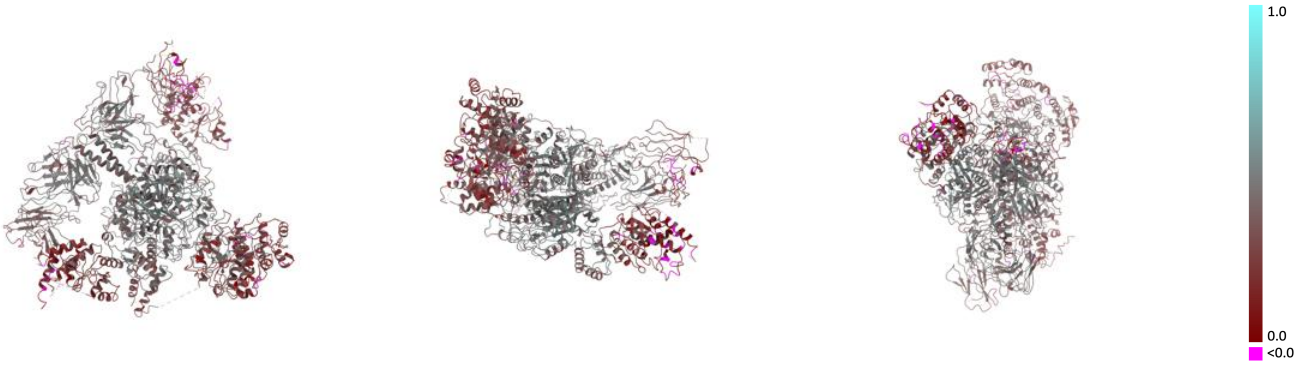
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.416 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.

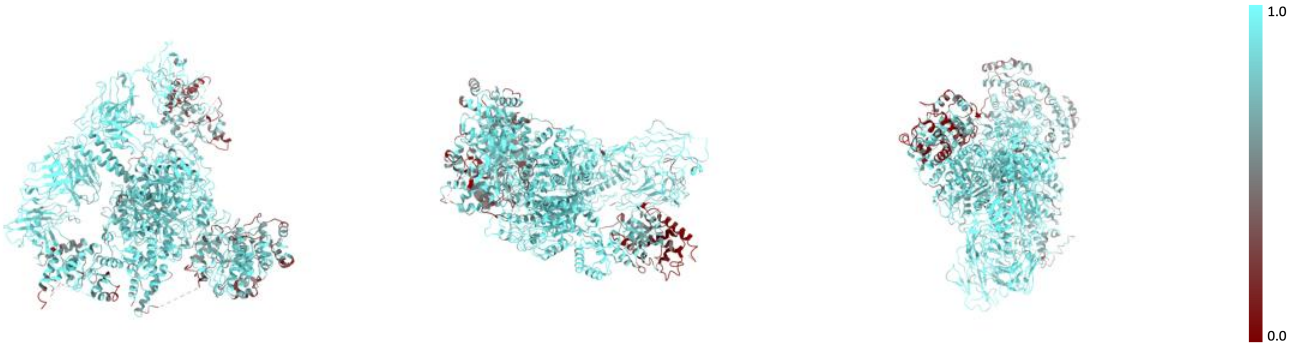
9.2 Q-score mapped to coordinate model (i)



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.

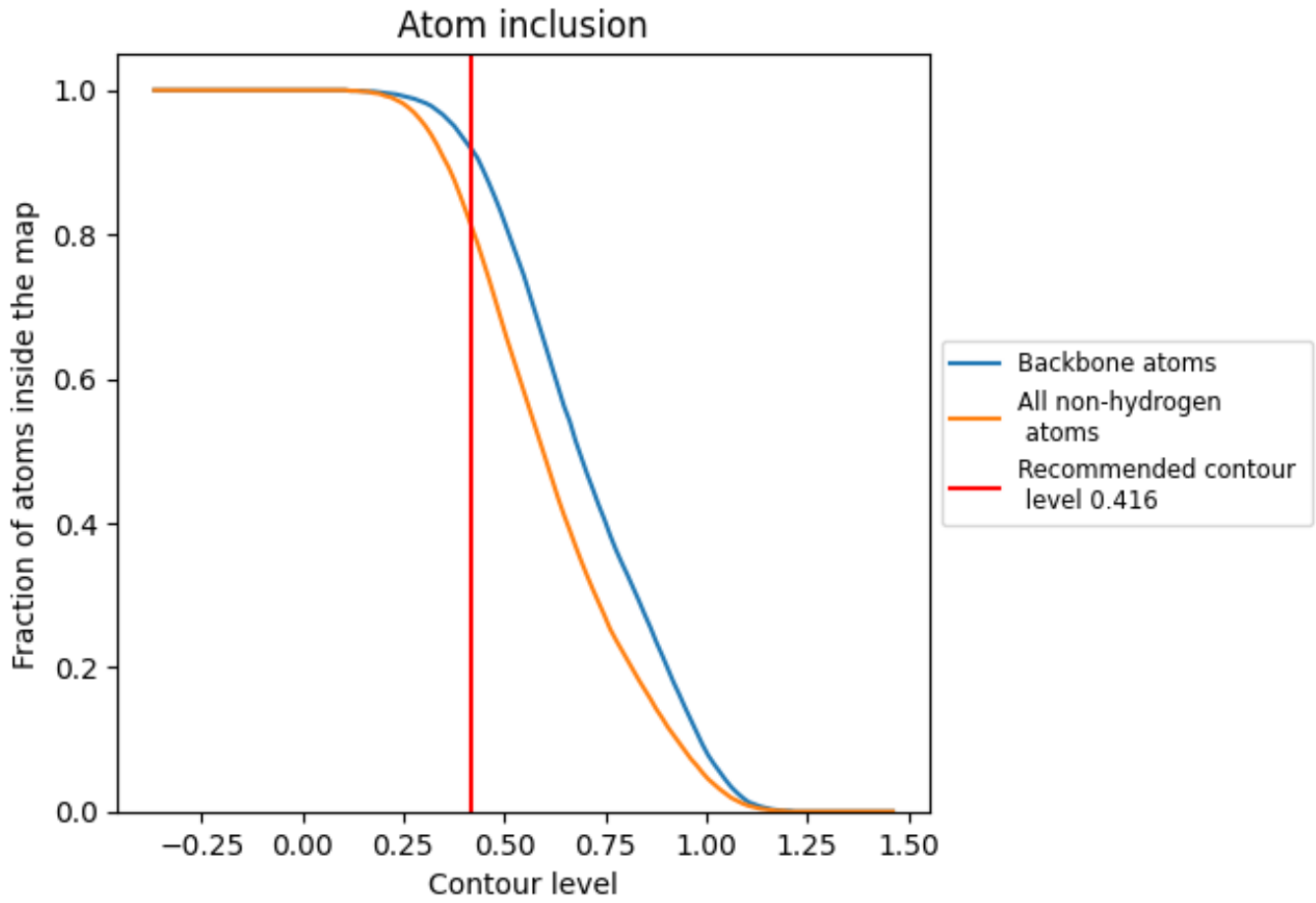
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.416).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.416) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.3650
A	0.7420	0.3380
B	0.8510	0.3880
C	0.8860	0.3530
D	0.8980	0.3800
E	0.9080	0.4020
F	0.9180	0.4090