



Full wwPDB EM Validation Report ⓘ

Apr 8, 2026 – 10:15 PM UTC

PDB ID : 9TG4 / pdb_00009tg4
EMDB ID : EMD-55890
Title : Structure of the YbjP lipoprotein bound to the AcrABZ-TolC efflux pump
Authors : Kaplan, E.; Harris, A.; Horne, J.; Petsolari, E.; Luisi, B.
Deposited on : 2025-11-28
Resolution : 3.17 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

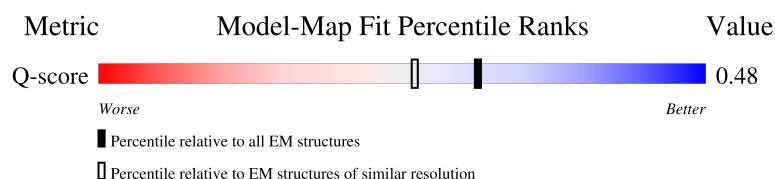
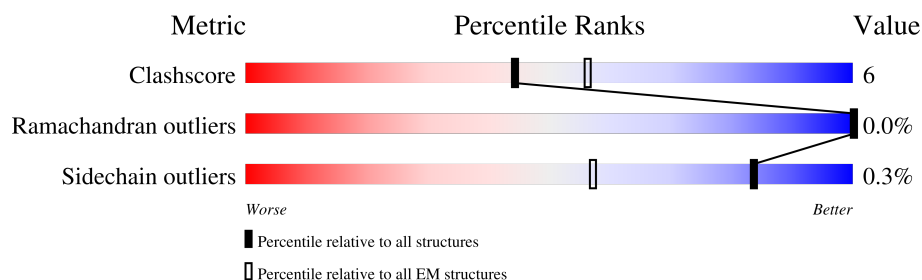
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.67 - 3.67)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	<div> <div>5%</div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	B	480	<div> <div>5%</div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	C	480	<div> <div>5%</div> <div>75%</div> <div>15%</div> <div>10%</div> </div>
2	D	397	<div> <div>6%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	397	
2	F	397	
2	G	397	
2	H	397	
2	I	397	
3	J	1049	
3	K	1049	
3	L	1049	
4	M	49	
4	N	49	
4	O	49	
5	P	160	
5	Q	160	
5	R	160	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 53653 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 Outer membrane protein TolC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3340	2059	593	683	5		
1	B	433	Total	C	N	O	S	0	0
			3340	2059	593	683	5		
1	C	433	Total	C	N	O	S	0	0
			3340	2059	593	683	5		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P02930
A	472	ASP	-	expression tag	UNP P02930
A	473	TYR	-	expression tag	UNP P02930
A	474	LYS	-	expression tag	UNP P02930
A	475	ASP	-	expression tag	UNP P02930
A	476	ASP	-	expression tag	UNP P02930
A	477	ASP	-	expression tag	UNP P02930
A	478	ASP	-	expression tag	UNP P02930
A	479	LYS	-	expression tag	UNP P02930
B	0	MET	-	initiating methionine	UNP P02930
B	472	ASP	-	expression tag	UNP P02930
B	473	TYR	-	expression tag	UNP P02930
B	474	LYS	-	expression tag	UNP P02930
B	475	ASP	-	expression tag	UNP P02930
B	476	ASP	-	expression tag	UNP P02930
B	477	ASP	-	expression tag	UNP P02930
B	478	ASP	-	expression tag	UNP P02930
B	479	LYS	-	expression tag	UNP P02930
C	0	MET	-	initiating methionine	UNP P02930
C	472	ASP	-	expression tag	UNP P02930
C	473	TYR	-	expression tag	UNP P02930
C	474	LYS	-	expression tag	UNP P02930
C	475	ASP	-	expression tag	UNP P02930
C	476	ASP	-	expression tag	UNP P02930

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASP	-	expression tag	UNP P02930
C	478	ASP	-	expression tag	UNP P02930
C	479	LYS	-	expression tag	UNP P02930

- Molecule 2 is a protein called Multidrug efflux pump subunit AcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	345	Total	C	N	O	S	0	0
			2591	1619	456	514	2		
2	E	346	Total	C	N	O	S	0	0
			2600	1624	458	516	2		
2	F	341	Total	C	N	O	S	0	0
			2564	1603	452	507	2		
2	G	346	Total	C	N	O	S	0	0
			2601	1625	459	515	2		
2	H	344	Total	C	N	O	S	0	0
			2583	1615	455	511	2		
2	I	346	Total	C	N	O	S	0	0
			2601	1625	459	515	2		

- Molecule 3 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1037	Total	C	N	O	S	0	0
			7883	5071	1304	1464	44		
3	K	1034	Total	C	N	O	S	0	0
			7855	5055	1296	1460	44		
3	L	1034	Total	C	N	O	S	0	0
			7855	5055	1296	1460	44		

- Molecule 4 is a protein called Multidrug efflux pump accessory protein AcrZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	39	Total	C	N	O	S	0	0
			294	203	41	47	3		
4	N	39	Total	C	N	O	S	0	0
			294	203	41	47	3		
4	O	39	Total	C	N	O	S	0	0
			294	203	41	47	3		

- Molecule 5 is a protein called Uncharacterized lipoprotein YbjP.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	153	Total	C	N	O	S	0	0
			1205	737	223	241	4		
5	Q	153	Total	C	N	O	S	0	0
			1205	737	223	241	4		
5	R	153	Total	C	N	O	S	0	0
			1205	737	223	241	4		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	27	MET	-	initiating methionine	UNP P75818
P	172	GLU	-	expression tag	UNP P75818
P	173	ASN	-	expression tag	UNP P75818
P	174	LEU	-	expression tag	UNP P75818
P	175	TYR	-	expression tag	UNP P75818
P	176	PHE	-	expression tag	UNP P75818
P	177	GLN	-	expression tag	UNP P75818
P	178	SER	-	expression tag	UNP P75818
P	179	LEU	-	expression tag	UNP P75818
P	180	GLU	-	expression tag	UNP P75818
P	181	HIS	-	expression tag	UNP P75818
P	182	HIS	-	expression tag	UNP P75818
P	183	HIS	-	expression tag	UNP P75818
P	184	HIS	-	expression tag	UNP P75818
P	185	HIS	-	expression tag	UNP P75818
P	186	HIS	-	expression tag	UNP P75818
Q	27	MET	-	initiating methionine	UNP P75818
Q	172	GLU	-	expression tag	UNP P75818
Q	173	ASN	-	expression tag	UNP P75818
Q	174	LEU	-	expression tag	UNP P75818
Q	175	TYR	-	expression tag	UNP P75818
Q	176	PHE	-	expression tag	UNP P75818
Q	177	GLN	-	expression tag	UNP P75818
Q	178	SER	-	expression tag	UNP P75818
Q	179	LEU	-	expression tag	UNP P75818
Q	180	GLU	-	expression tag	UNP P75818
Q	181	HIS	-	expression tag	UNP P75818
Q	182	HIS	-	expression tag	UNP P75818
Q	183	HIS	-	expression tag	UNP P75818
Q	184	HIS	-	expression tag	UNP P75818
Q	185	HIS	-	expression tag	UNP P75818
Q	186	HIS	-	expression tag	UNP P75818
R	27	MET	-	initiating methionine	UNP P75818

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	172	GLU	-	expression tag	UNP P75818
R	173	ASN	-	expression tag	UNP P75818
R	174	LEU	-	expression tag	UNP P75818
R	175	TYR	-	expression tag	UNP P75818
R	176	PHE	-	expression tag	UNP P75818
R	177	GLN	-	expression tag	UNP P75818
R	178	SER	-	expression tag	UNP P75818
R	179	LEU	-	expression tag	UNP P75818
R	180	GLU	-	expression tag	UNP P75818
R	181	HIS	-	expression tag	UNP P75818
R	182	HIS	-	expression tag	UNP P75818
R	183	HIS	-	expression tag	UNP P75818
R	184	HIS	-	expression tag	UNP P75818
R	185	HIS	-	expression tag	UNP P75818
R	186	HIS	-	expression tag	UNP P75818

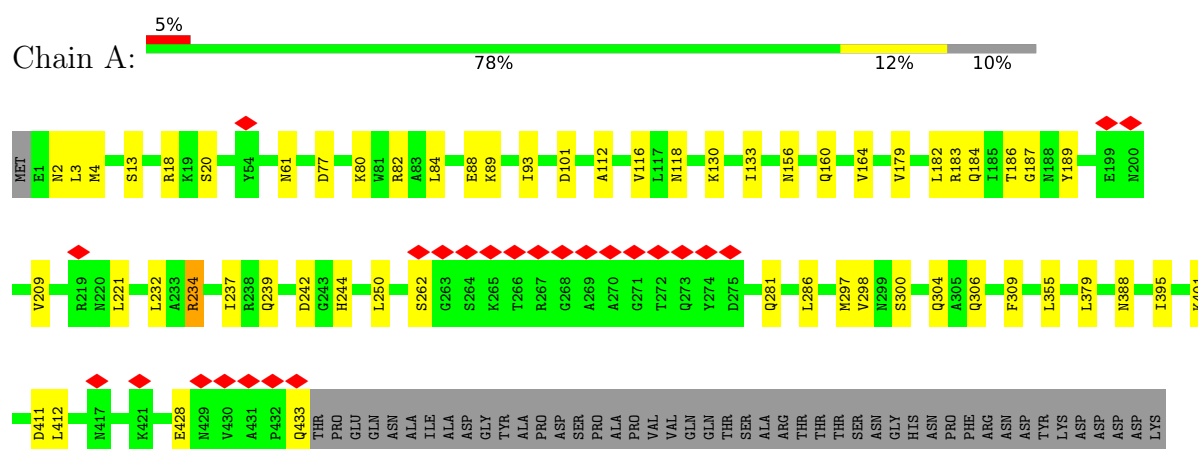
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Cl 1 1	0
6	B	1	Total Cl 1 1	0
6	C	1	Total Cl 1 1	0

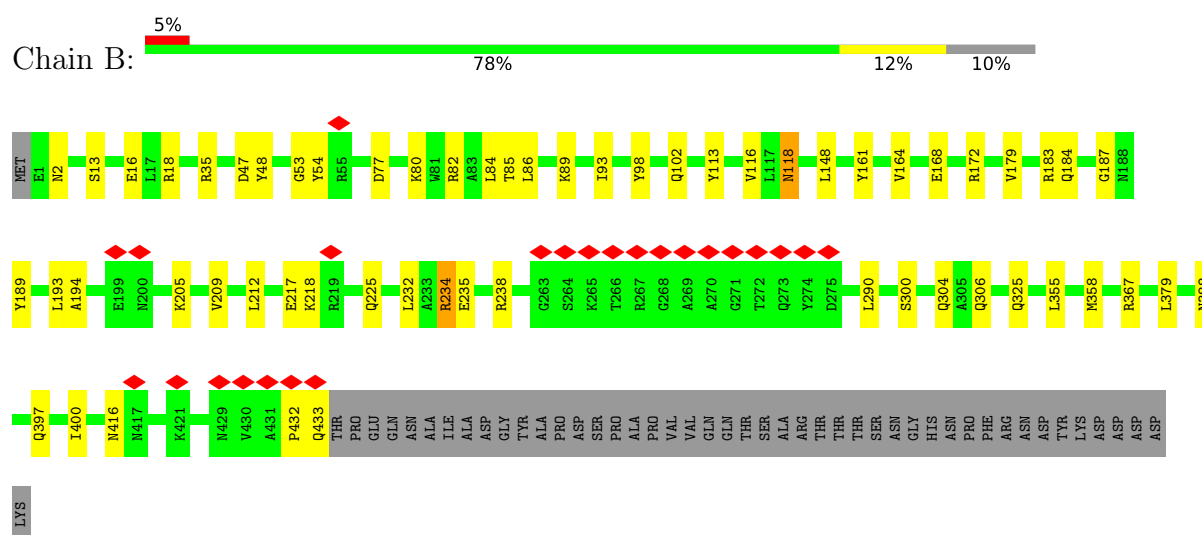
3 Residue-property plots

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

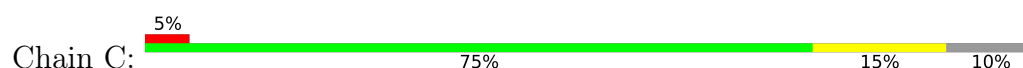
- Molecule 1: Outer membrane protein TolC

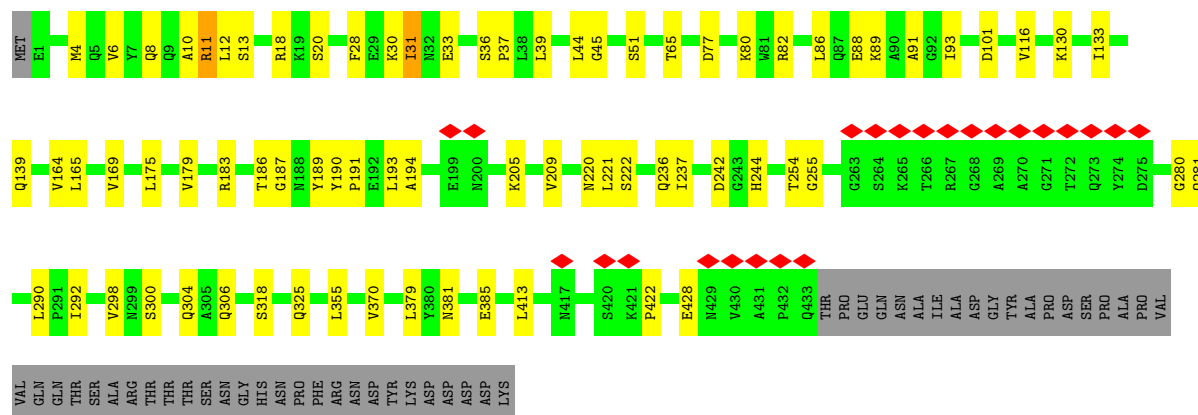


- Molecule 1: Outer membrane protein TolC

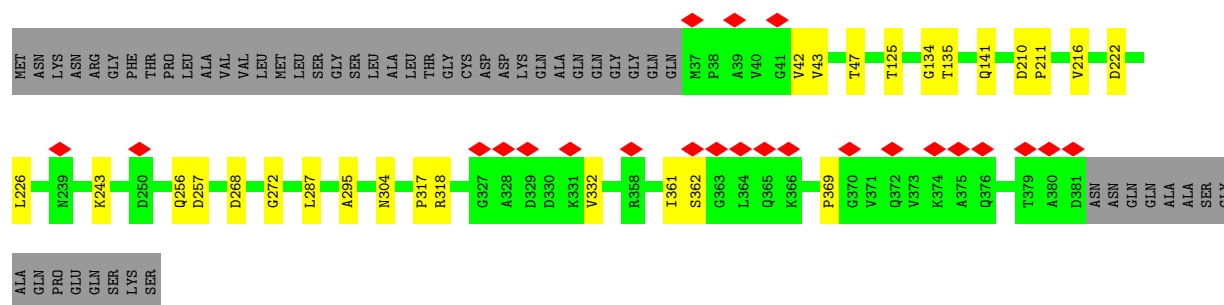
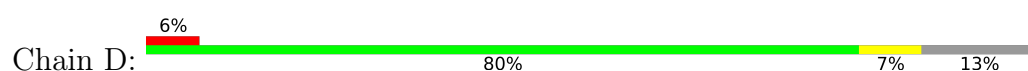


- Molecule 1: Outer membrane protein TolC

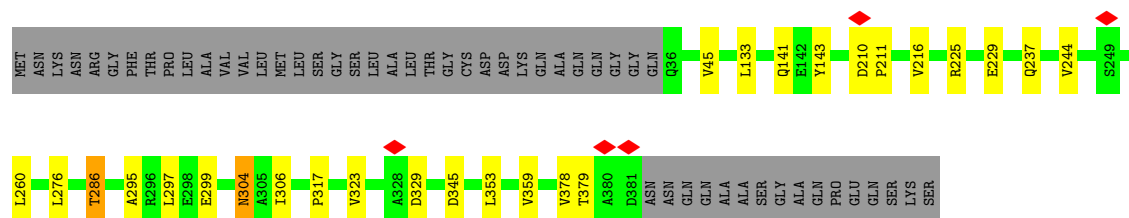
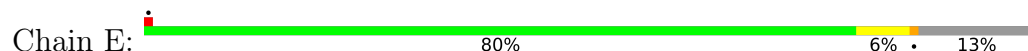




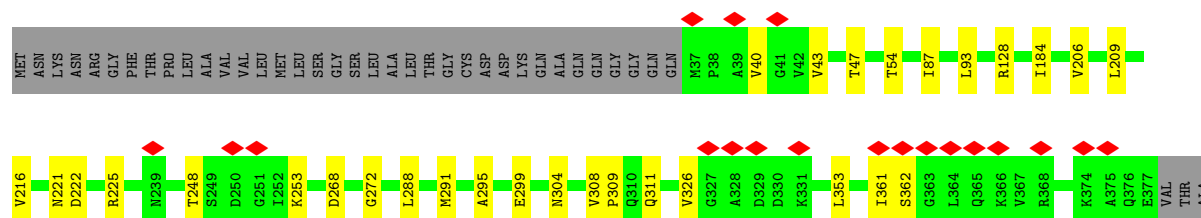
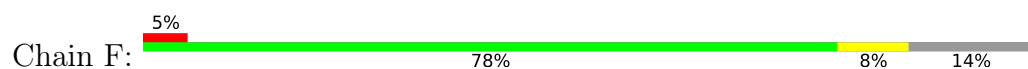
• Molecule 2: Multidrug efflux pump subunit AcrA



• Molecule 2: Multidrug efflux pump subunit AcrA



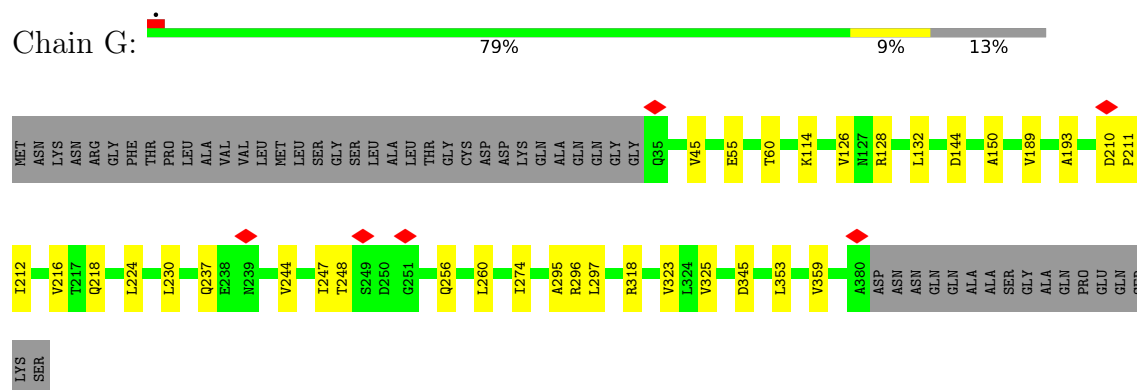
• Molecule 2: Multidrug efflux pump subunit AcrA



ASP
ASN
ASN
GLN
GLN
ALA
ALA
SER
GLY
GLN
ALA
PRO
GLU
GLN
LYS
SER

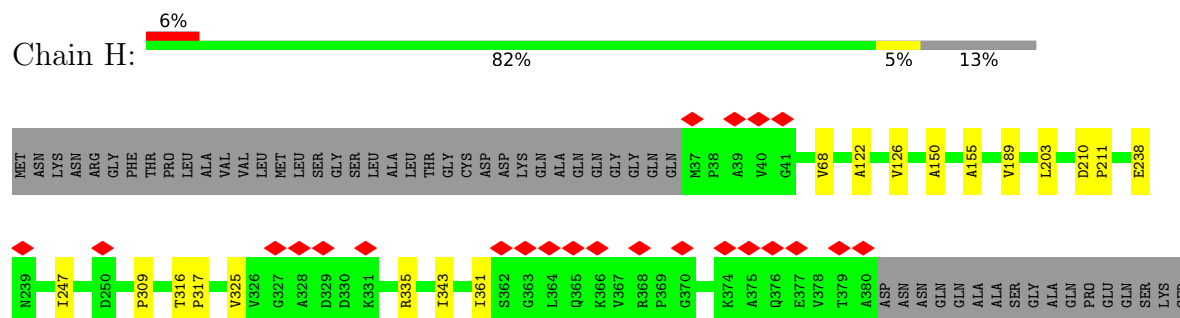
• Molecule 2: Multidrug efflux pump subunit AcrA

Chain G:



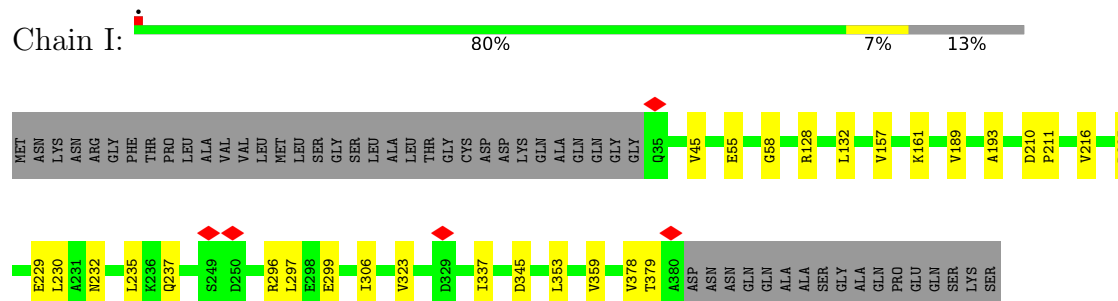
• Molecule 2: Multidrug efflux pump subunit AcrA

Chain H:



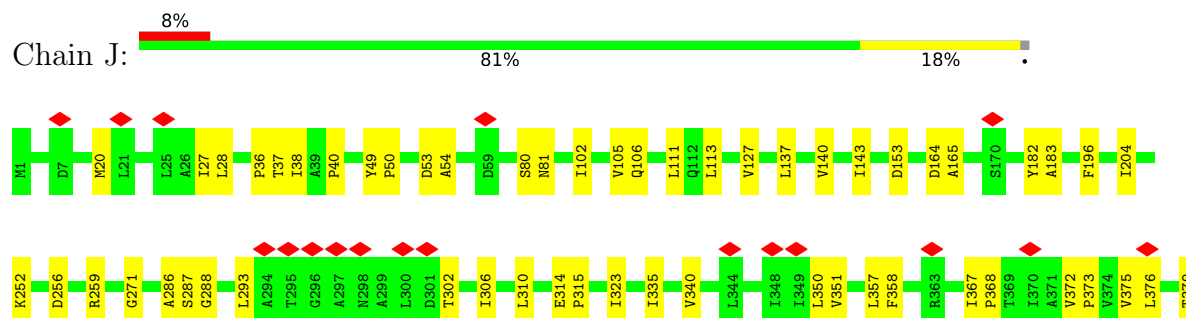
• Molecule 2: Multidrug efflux pump subunit AcrA

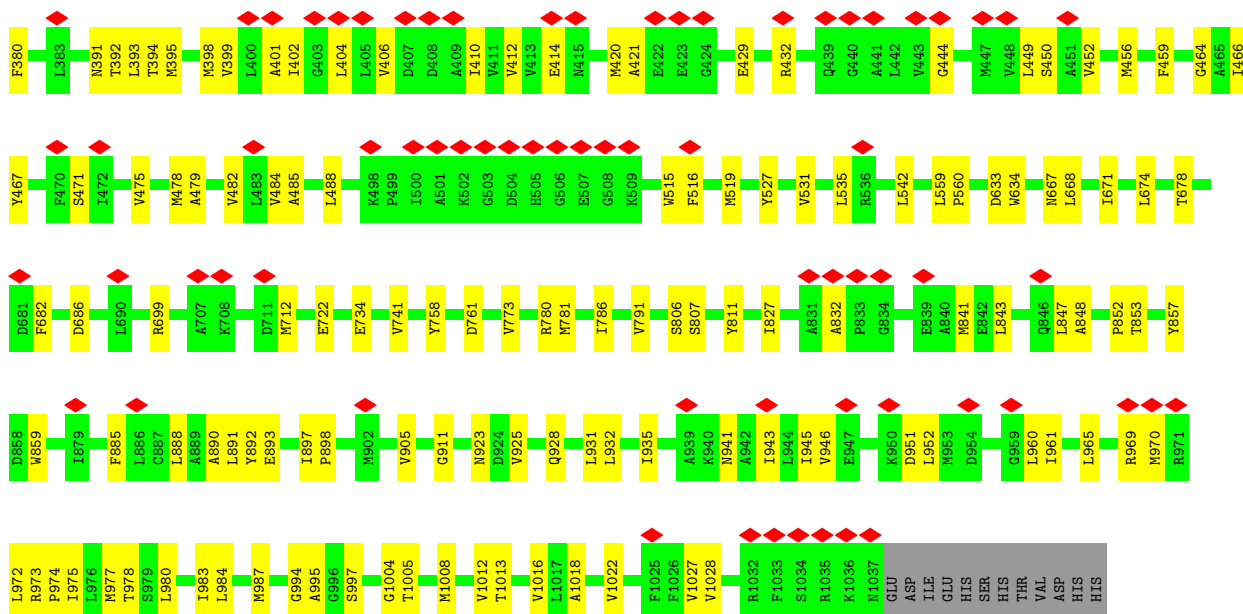
Chain I:



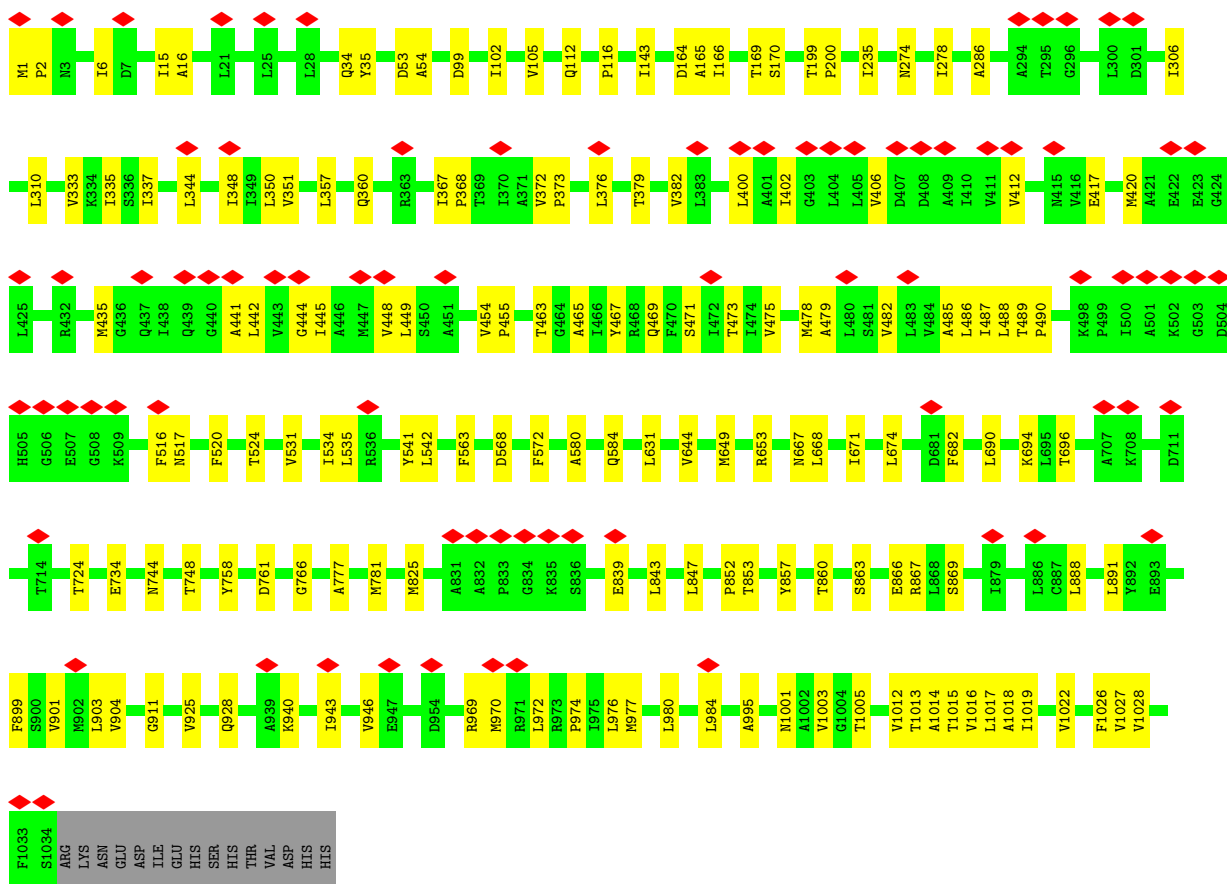
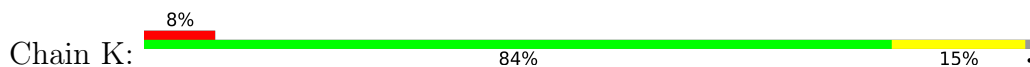
• Molecule 3: Multidrug efflux pump subunit AcrB

Chain J:

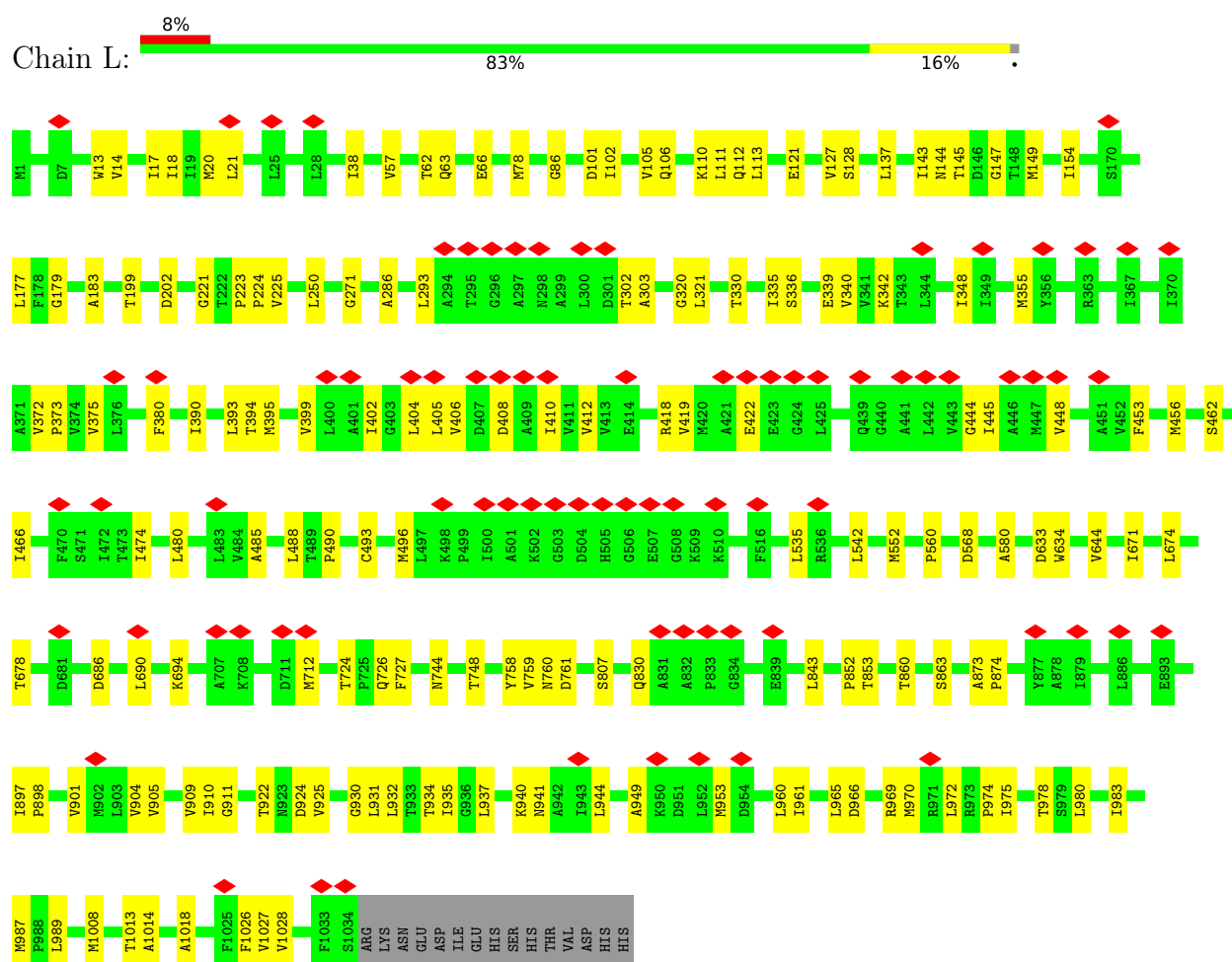




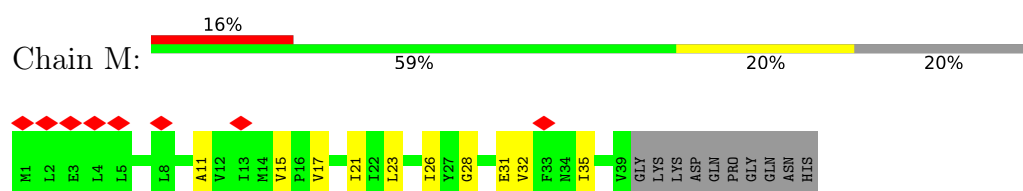
• Molecule 3: Multidrug efflux pump subunit AcrB



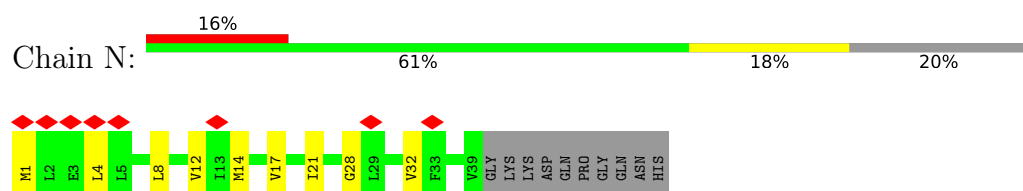
• Molecule 3: Multidrug efflux pump subunit AcrB



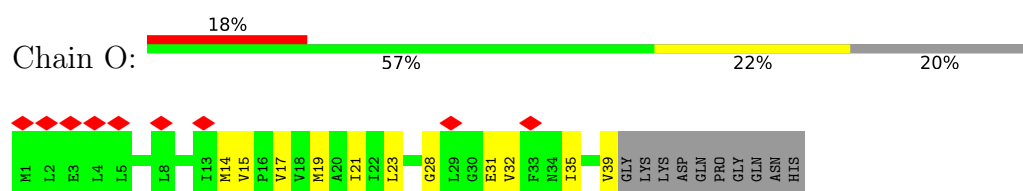
• Molecule 4: Multidrug efflux pump accessory protein AcrZ



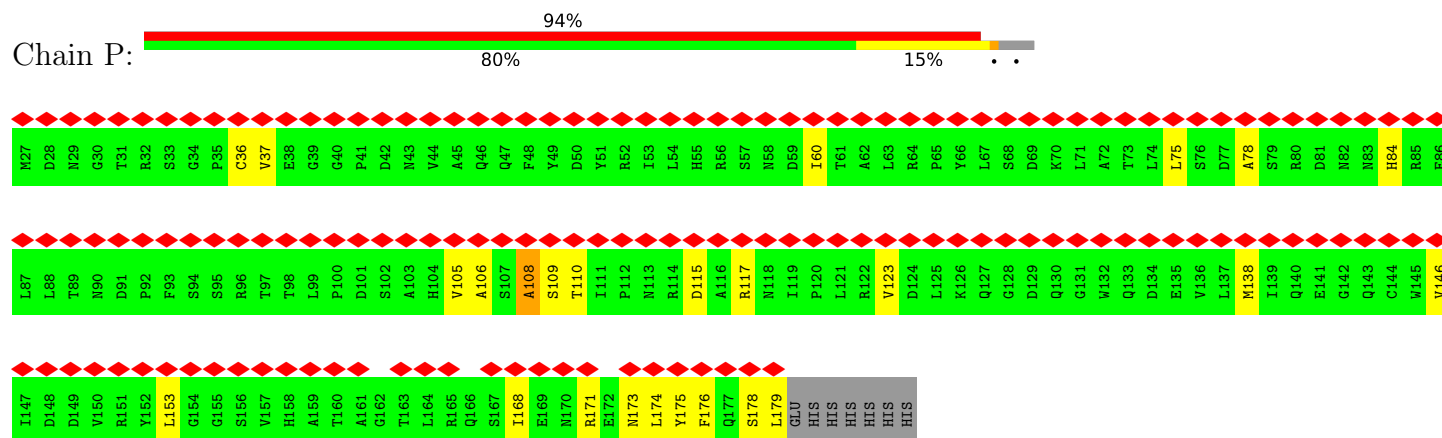
• Molecule 4: Multidrug efflux pump accessory protein AcrZ



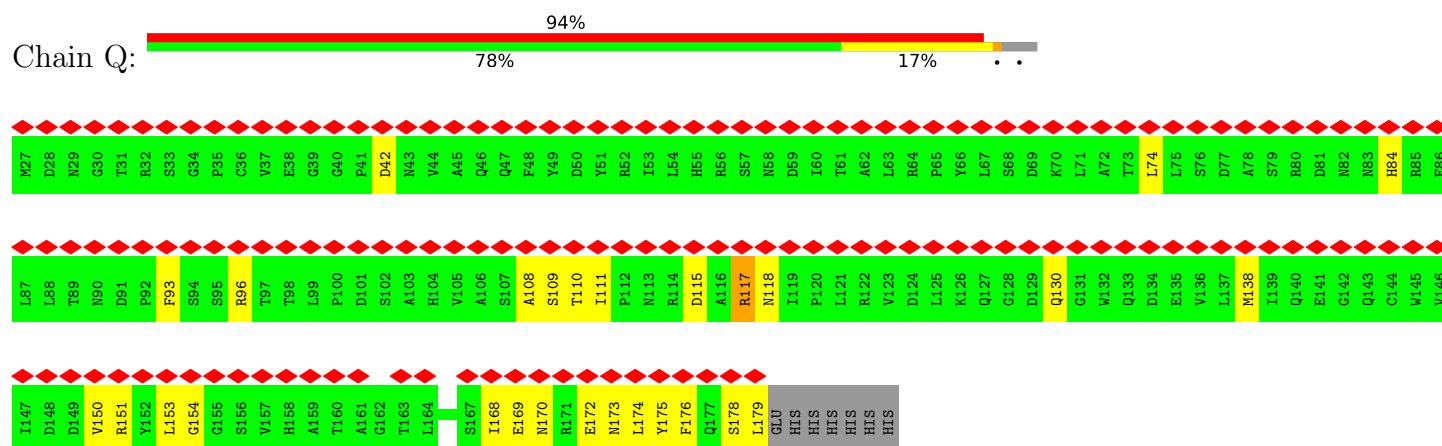
• Molecule 4: Multidrug efflux pump accessory protein AcrZ



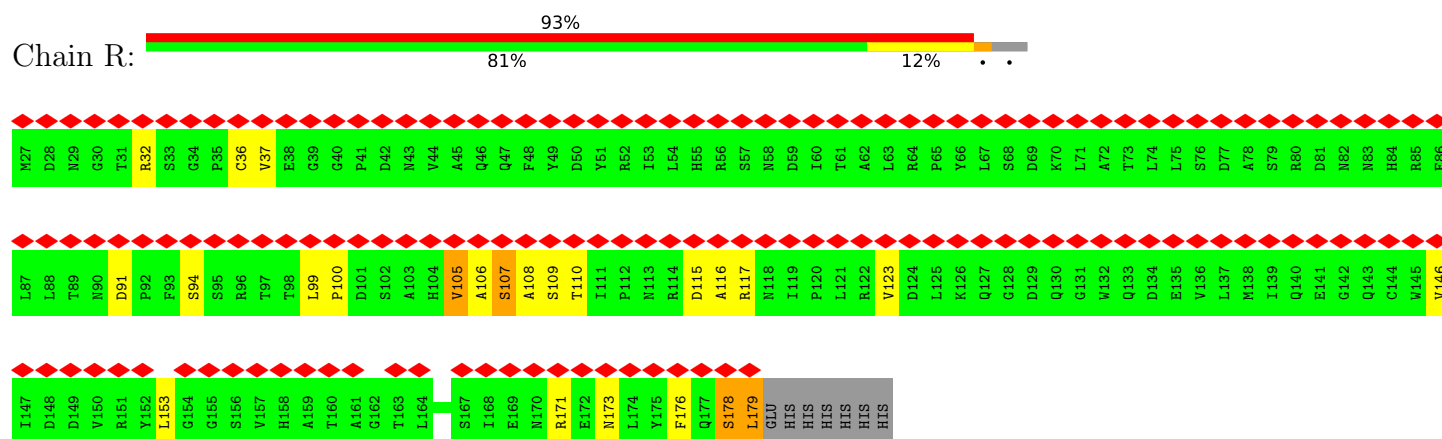
● Molecule 5: Uncharacterized lipoprotein YbjP



● Molecule 5: Uncharacterized lipoprotein YbjP



● Molecule 5: Uncharacterized lipoprotein YbjP



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97441	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.551	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	686.784, 686.784, 686.784	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.168, 1.168, 1.168	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/3382	0.31	0/4596
1	B	0.20	0/3382	0.31	0/4596
1	C	0.30	2/3382 (0.1%)	0.52	4/4596 (0.1%)
2	D	0.14	0/2624	0.31	0/3570
2	E	0.16	0/2633	0.30	0/3582
2	F	0.14	0/2597	0.31	0/3532
2	G	0.16	0/2634	0.30	0/3583
2	H	0.15	0/2616	0.30	0/3559
2	I	0.15	0/2634	0.30	0/3583
3	J	0.15	0/8033	0.35	0/10907
3	K	0.15	0/8005	0.36	2/10871 (0.0%)
3	L	0.15	0/8005	0.35	0/10871
4	M	0.15	0/298	0.31	0/403
4	N	0.16	0/298	0.28	0/403
4	O	0.16	0/298	0.33	0/403
5	P	0.33	1/1227 (0.1%)	0.44	1/1667 (0.1%)
5	Q	0.24	0/1227	0.40	1/1667 (0.1%)
5	R	0.32	0/1227	0.41	0/1667
All	All	0.18	3/54502 (0.0%)	0.35	8/74056 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	PRO	CG-CD	-9.71	1.17	1.50
1	C	191	PRO	CB-CG	-8.72	1.06	1.49
5	P	108	ALA	CA-C	-5.52	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	PRO	N-CD-CG	-19.03	74.66	103.20
1	C	191	PRO	CA-CB-CG	-15.60	74.87	104.50
1	C	191	PRO	CB-CG-CD	10.39	139.35	106.10
3	K	116	PRO	N-CD-CG	-9.32	89.22	103.20
5	P	108	ALA	N-CA-C	-8.04	96.12	109.07
1	C	191	PRO	CA-N-CD	-7.46	101.55	112.00
5	Q	117	ARG	N-CA-C	-6.50	98.72	107.88
3	K	116	PRO	CA-CB-CG	-5.37	94.30	104.50

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	3340	0	3289	42	0
1	B	3340	0	3289	54	0
1	C	3340	0	3289	60	0
2	D	2591	0	2649	15	0
2	E	2600	0	2657	22	0
2	F	2564	0	2624	21	0
2	G	2601	0	2661	21	0
2	H	2583	0	2645	15	0
2	I	2601	0	2661	20	0
3	J	7883	0	8038	146	0
3	K	7855	0	8006	107	0
3	L	7855	0	8006	129	0
4	M	294	0	330	7	0
4	N	294	0	330	5	0
4	O	294	0	330	7	0
5	P	1205	0	1150	27	0
5	Q	1205	0	1150	36	0
5	R	1205	0	1150	22	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	53653	0	54254	693	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 6.

All (693) 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)
1:B:234:ARG:NH1	5:Q:109:SER:CB	2.07	1.17
1:B:234:ARG:NH1	5:Q:109:SER:HB2	1.60	1.15
1:B:234:ARG:HH11	5:Q:109:SER:CB	1.66	1.09
3:L:348:ILE:HD11	3:L:372:VAL:HG11	1.36	1.08
5:R:105:VAL:HG13	5:R:123:VAL:HG22	1.39	1.01
1:B:234:ARG:HH11	5:Q:109:SER:HB3	1.23	0.98
1:B:234:ARG:NH1	5:Q:109:SER:HB3	1.79	0.91
1:B:234:ARG:HH12	5:Q:109:SER:HB2	1.28	0.90
1:A:184:GLN:OE1	1:B:325:GLN:NE2	2.06	0.88
3:K:350:LEU:HD21	3:K:984:LEU:HG	1.56	0.87
3:K:351:VAL:HG21	3:K:406:VAL:HG21	1.57	0.87
2:F:222:ASP:OD1	2:F:225:ARG:NH2	2.10	0.83
3:J:905:VAL:HG13	3:J:935:ILE:HG23	1.60	0.83
3:K:467:TYR:OH	3:K:928:GLN:OE1	1.97	0.83
1:B:18:ARG:NH1	5:P:115:ASP:O	2.12	0.81
3:J:450:SER:OG	3:J:478:MET:SD	2.39	0.80
1:C:133:ILE:HG13	1:C:164:VAL:HG21	1.66	0.78
3:L:375:VAL:HG11	3:L:405:LEU:HD13	1.66	0.77
5:P:105:VAL:HG13	5:P:123:VAL:HG22	1.66	0.77
1:A:118:ASN:OD1	1:A:388:ASN:ND2	2.17	0.77
3:L:418:ARG:NE	3:L:970:MET:HE1	2.00	0.77
3:L:101:ASP:O	3:L:105:VAL:HG23	1.84	0.77
3:L:930:GLY:O	3:L:934:THR:HG23	1.85	0.76
3:J:53:ASP:OD1	3:J:54:ALA:N	2.19	0.76
3:L:121:GLU:N	3:L:121:GLU:OE1	2.17	0.76
1:C:65:THR:O	1:C:65:THR:HG22	1.86	0.76
3:L:580:ALA:HB1	3:L:724:THR:HG22	1.68	0.75
1:C:20:SER:OG	1:C:101:ASP:OD2	2.03	0.75
1:B:205:LYS:HG3	5:Q:179:LEU:HG	1.69	0.75
4:O:19:MET:SD	4:O:23:LEU:HD23	2.27	0.75
4:N:28:GLY:O	4:N:32:VAL:HG23	1.87	0.74
2:D:243:LYS:NZ	2:D:257:ASP:OD1	2.17	0.74
3:J:994:GLY:O	3:J:997:SER:OG	2.05	0.74
2:D:134:GLY:O	2:D:135:THR:OG1	2.03	0.74
5:Q:178:SER:C	5:Q:179:LEU:HD22	2.14	0.73
2:G:244:VAL:HG22	2:G:297:LEU:HD23	1.68	0.73
5:Q:138:MET:HE3	5:Q:138:MET:HA	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:105:VAL:HG22	5:P:123:VAL:HG13	1.72	0.72
1:B:118:ASN:OD1	1:B:388:ASN:ND2	2.23	0.71
5:P:138:MET:HE3	5:P:138:MET:HA	1.72	0.71
1:A:209:VAL:HG12	5:R:173:ASN:HD22	1.56	0.71
2:G:55:GLU:OE1	2:G:296:ARG:NH1	2.25	0.70
2:E:237:GLN:NE2	2:E:299:GLU:O	2.23	0.70
3:K:1018:ALA:O	3:K:1022:VAL:HG23	1.91	0.70
3:J:414:GLU:OE2	3:J:973:ARG:NH2	2.24	0.70
3:J:391:ASN:O	3:J:394:THR:OG1	2.09	0.70
1:C:189:TYR:CE2	5:R:171:ARG:HG3	2.27	0.69
5:P:153:LEU:HD23	5:P:153:LEU:O	1.93	0.69
5:P:178:SER:O	5:P:179:LEU:HD13	1.93	0.68
3:L:375:VAL:HG23	3:L:480:LEU:HB3	1.75	0.68
5:Q:178:SER:O	5:Q:179:LEU:HD22	1.94	0.67
1:C:12:LEU:HD21	5:R:117:ARG:NH1	2.10	0.67
1:C:183:ARG:O	1:C:187:GLY:N	2.28	0.67
3:J:542:LEU:HD11	3:J:1028:VAL:HG11	1.74	0.67
3:J:897:ILE:HD11	3:J:946:VAL:HG11	1.77	0.67
3:L:412:VAL:HG21	3:L:485:ALA:HB1	1.76	0.67
3:J:699:ARG:NH2	3:J:722:GLU:OE2	2.28	0.67
4:O:28:GLY:O	4:O:32:VAL:HG12	1.95	0.67
1:C:31:ILE:HD11	1:C:88:GLU:HA	1.77	0.66
1:B:433:GLN:C	5:P:178:SER:HB3	2.20	0.66
5:Q:153:LEU:O	5:Q:153:LEU:HD23	1.94	0.66
1:C:428:GLU:N	1:C:428:GLU:OE1	2.29	0.66
3:L:535:LEU:CD2	3:L:1027:VAL:HG21	2.26	0.66
2:I:45:VAL:HG21	2:I:353:LEU:HD23	1.76	0.66
1:C:165:LEU:O	1:C:169:VAL:HG23	1.96	0.65
3:K:980:LEU:HD22	4:O:19:MET:HE2	1.78	0.65
5:Q:168:ILE:HD12	5:Q:169:GLU:N	2.10	0.65
1:A:18:ARG:NH1	5:Q:115:ASP:O	2.30	0.65
3:J:80:SER:O	3:J:81:ASN:ND2	2.30	0.65
3:K:568:ASP:OD2	3:K:644:VAL:HG23	1.97	0.64
3:K:445:ILE:HD12	3:K:940:LYS:HZ2	1.62	0.64
5:P:178:SER:C	5:P:179:LEU:HD22	2.22	0.64
1:A:133:ILE:HD13	1:A:164:VAL:HG21	1.79	0.64
3:L:418:ARG:NH1	3:L:422:GLU:OE1	2.31	0.64
1:A:237:ILE:HD11	1:A:309:PHE:CB	2.27	0.64
2:E:244:VAL:HG22	2:E:297:LEU:HD22	1.79	0.64
3:J:412:VAL:HG21	3:J:485:ALA:HB1	1.79	0.64
3:L:924:ASP:OD1	3:L:925:VAL:N	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:951:ASP:OD1	3:J:952:LEU:N	2.31	0.63
3:J:535:LEU:CD1	3:J:1027:VAL:HG11	2.28	0.63
2:E:45:VAL:HG21	2:E:353:LEU:HD23	1.81	0.63
2:I:230:LEU:HD11	2:I:237:GLN:HG3	1.81	0.63
3:K:758:TYR:OH	3:K:761:ASP:OD1	2.11	0.63
4:O:35:ILE:O	4:O:39:VAL:HG23	1.98	0.63
2:H:247:ILE:HD12	2:H:247:ILE:O	1.99	0.62
3:K:360:GLN:OE1	3:K:517:ASN:ND2	2.31	0.62
3:L:987:MET:HE2	4:N:14:MET:HE2	1.80	0.62
3:J:140:VAL:HG11	3:J:310:LEU:HD21	1.81	0.62
3:J:449:LEU:HD22	3:J:478:MET:HE3	1.82	0.62
1:A:77:ASP:OD2	1:A:80:LYS:NZ	2.33	0.62
3:J:393:LEU:HD23	3:J:393:LEU:H	1.64	0.62
3:J:164:ASP:OD1	3:J:165:ALA:N	2.33	0.62
3:J:395:MET:SD	3:J:395:MET:N	2.73	0.62
3:L:375:VAL:HG13	3:L:405:LEU:HD22	1.82	0.62
3:L:568:ASP:OD1	3:L:644:VAL:HG23	1.99	0.62
3:J:932:LEU:HA	3:J:935:ILE:HD12	1.82	0.62
5:R:178:SER:O	5:R:178:SER:OG	2.17	0.61
3:K:1:MET:SD	3:K:1:MET:N	2.73	0.61
1:B:212:LEU:HD13	1:B:400:ILE:HD11	1.82	0.61
1:A:433:GLN:O	5:Q:178:SER:N	2.34	0.61
1:C:12:LEU:HD21	5:R:117:ARG:CZ	2.31	0.61
3:J:531:VAL:O	3:J:535:LEU:HD23	2.01	0.61
3:J:38:ILE:HD11	3:J:671:ILE:HD13	1.83	0.60
3:J:843:LEU:O	3:J:847:LEU:HD12	2.01	0.60
2:I:225:ARG:NH1	2:I:229:GLU:OE2	2.34	0.60
2:F:311:GLN:OE1	2:F:361:ILE:HG22	2.01	0.60
2:G:218:GLN:O	2:G:274:ILE:N	2.32	0.60
2:H:343:ILE:HD12	2:H:343:ILE:O	2.01	0.60
3:J:893:GLU:N	3:J:893:GLU:OE1	2.34	0.60
3:K:449:LEU:HB2	3:K:478:MET:HE1	1.83	0.60
4:M:11:ALA:O	4:M:15:VAL:HG23	2.01	0.60
2:H:309:PRO:HG2	2:H:361:ILE:HD13	1.84	0.60
3:J:358:PHE:CD2	3:J:977:MET:HE2	2.37	0.60
1:A:428:GLU:N	1:A:428:GLU:OE1	2.35	0.59
1:B:54:TYR:N	1:C:280:GLY:O	2.34	0.59
3:J:350:LEU:HD11	3:J:984:LEU:HG	1.82	0.59
1:B:47:ASP:OD1	1:B:48:TYR:N	2.35	0.59
3:K:1014:ALA:O	3:K:1018:ALA:HB3	2.03	0.59
3:K:667:ASN:OD1	3:K:668:LEU:N	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1012:VAL:O	3:K:1016:VAL:HG22	2.03	0.59
3:L:303:ALA:CB	3:L:330:THR:HG21	2.33	0.58
3:K:463:THR:HG21	3:K:869:SER:HB2	1.86	0.58
3:J:1018:ALA:O	3:J:1022:VAL:HG23	2.03	0.58
3:L:355:MET:SD	3:L:410:ILE:HD13	2.44	0.58
1:B:183:ARG:O	1:B:187:GLY:N	2.34	0.58
3:J:897:ILE:HD11	3:J:946:VAL:CG1	2.33	0.58
3:K:946:VAL:HG13	3:K:1026:PHE:HE2	1.68	0.58
1:C:209:VAL:HG12	5:P:173:ASN:HD22	1.69	0.58
5:R:173:ASN:HA	5:R:176:PHE:HB2	1.84	0.58
3:K:463:THR:HG22	3:K:563:PHE:CE1	2.38	0.58
2:H:343:ILE:HD12	2:H:343:ILE:C	2.29	0.58
3:J:960:LEU:CD2	3:J:1027:VAL:HG12	2.34	0.58
5:Q:169:GLU:OE1	5:Q:174:LEU:HD21	2.03	0.58
3:K:843:LEU:O	3:K:847:LEU:HD13	2.03	0.57
3:K:53:ASP:OD1	3:K:54:ALA:N	2.37	0.57
3:L:453:PHE:CE2	3:L:474:ILE:HG21	2.40	0.57
1:C:44:LEU:HD23	1:C:45:GLY:N	2.18	0.57
3:J:380:PHE:CD1	3:J:398:MET:HE1	2.39	0.57
3:J:970:MET:SD	3:J:970:MET:N	2.77	0.57
3:K:531:VAL:O	3:K:534:ILE:HG22	2.04	0.57
3:L:20:MET:HE3	3:L:21:LEU:N	2.19	0.57
3:K:901:VAL:O	3:K:904:VAL:HG12	2.04	0.57
2:E:133:LEU:HD11	2:E:143:TYR:CD2	2.40	0.57
2:H:122:ALA:O	2:H:126:VAL:HG23	2.05	0.57
2:I:323:VAL:CG1	2:I:359:VAL:HG13	2.35	0.57
3:J:741:VAL:HG11	3:J:791:VAL:HG21	1.87	0.57
3:L:375:VAL:HG23	3:L:480:LEU:CB	2.34	0.56
1:A:300:SER:O	1:A:304:GLN:HG2	2.05	0.56
1:C:116:VAL:HG11	1:C:193:LEU:HD12	1.87	0.56
5:Q:117:ARG:O	5:Q:118:ASN:C	2.47	0.56
2:H:126:VAL:HG21	2:H:150:ALA:HB2	1.87	0.56
3:L:348:ILE:HD11	3:L:372:VAL:CG1	2.23	0.56
3:K:969:ARG:NE	3:K:970:MET:HE3	2.20	0.56
3:J:897:ILE:HG23	3:J:898:PRO:HD3	1.86	0.56
3:J:945:ILE:HD11	3:J:975:ILE:HD11	1.88	0.56
3:J:974:PRO:O	3:J:978:THR:HG22	2.06	0.56
3:L:395:MET:N	3:L:395:MET:HE2	2.21	0.56
5:R:105:VAL:HG12	5:R:106:ALA:H	1.71	0.56
1:A:20:SER:OG	1:A:101:ASP:OD2	2.12	0.56
1:A:112:ALA:O	1:A:116:VAL:HG23	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:VAL:HG11	1:C:189:TYR:CE1	2.41	0.56
3:L:860:THR:O	3:L:863:SER:OG	2.14	0.56
1:C:300:SER:O	1:C:304:GLN:HG3	2.05	0.56
3:J:781:MET:HE2	3:L:225:VAL:HG12	1.88	0.56
3:J:984:LEU:HD12	3:J:984:LEU:O	2.05	0.56
1:C:33:GLU:C	1:C:33:GLU:OE1	2.49	0.56
3:L:488:LEU:HD13	3:L:488:LEU:C	2.31	0.55
3:L:102:ILE:O	3:L:106:GLN:HG3	2.05	0.55
1:B:53:GLY:N	1:C:281:GLN:OE1	2.39	0.55
3:L:372:VAL:HG13	3:L:405:LEU:CD2	2.37	0.55
3:J:712:MET:SD	3:J:843:LEU:HD22	2.47	0.55
3:J:980:LEU:HD12	3:J:980:LEU:O	2.07	0.55
1:A:232:LEU:HD23	1:A:232:LEU:O	2.06	0.55
2:F:291:MET:HE1	2:G:224:LEU:HD11	1.88	0.55
3:L:335:ILE:C	3:L:335:ILE:HD12	2.31	0.55
3:L:980:LEU:HD13	3:L:980:LEU:C	2.31	0.55
1:C:4:MET:HE1	1:C:8:GLN:HE21	1.71	0.55
2:G:210:ASP:HB3	2:G:211:PRO:HD3	1.89	0.55
3:J:667:ASN:O	3:J:678:THR:HG23	2.07	0.55
3:L:375:VAL:HG11	3:L:405:LEU:CD1	2.37	0.55
3:J:969:ARG:NE	3:J:970:MET:SD	2.80	0.55
3:K:400:LEU:HD21	3:K:1003:VAL:HG11	1.88	0.55
2:F:43:VAL:HB	2:F:361:ILE:HD11	1.89	0.54
2:I:58:GLY:HA3	2:I:216:VAL:HG12	1.90	0.54
1:B:2:ASN:OD1	1:B:416:ASN:ND2	2.40	0.54
3:K:417:GLU:O	3:K:420:MET:HE3	2.06	0.54
3:L:744:ASN:O	3:L:748:THR:HG23	2.08	0.54
3:L:932:LEU:HA	3:L:935:ILE:HG22	1.89	0.54
5:R:153:LEU:HD23	5:R:153:LEU:O	2.07	0.54
3:L:412:VAL:HG21	3:L:485:ALA:CB	2.37	0.54
1:A:133:ILE:CD1	1:A:164:VAL:HG21	2.38	0.54
2:F:216:VAL:HG11	2:F:295:ALA:HB3	1.90	0.54
2:D:210:ASP:HB3	2:D:211:PRO:HD3	1.90	0.54
3:J:27:ILE:HD11	3:J:380:PHE:CG	2.43	0.54
1:B:358:MET:HE3	1:B:367:ARG:HG2	1.88	0.54
3:K:445:ILE:HD12	3:K:940:LYS:NZ	2.22	0.54
3:K:379:THR:HA	3:K:382:VAL:HG12	1.89	0.54
3:L:335:ILE:HD12	3:L:336:SER:N	2.23	0.54
3:K:164:ASP:OD1	3:K:165:ALA:N	2.41	0.54
3:J:102:ILE:O	3:J:106:GLN:HG3	2.08	0.53
3:J:758:TYR:OH	3:J:761:ASP:OD1	2.15	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:535:LEU:CD2	3:L:1027:VAL:HG11	2.39	0.53
3:J:984:LEU:CD2	4:M:15:VAL:HG22	2.38	0.53
3:L:759:VAL:HG23	3:L:760:ASN:N	2.24	0.53
2:E:378:VAL:O	2:E:379:THR:HG22	2.09	0.53
3:J:961:ILE:O	3:J:965:LEU:HD13	2.08	0.53
1:C:130:LYS:HA	1:C:164:VAL:HG11	1.90	0.53
2:F:288:LEU:H	2:F:291:MET:HE3	1.74	0.53
3:L:372:VAL:HB	3:L:373:PRO:HD3	1.90	0.53
3:J:40:PRO:HD2	3:J:674:LEU:HD21	1.90	0.53
3:J:444:GLY:HA3	3:J:891:LEU:HD21	1.91	0.53
3:J:535:LEU:HD11	3:J:1027:VAL:HG11	1.89	0.53
5:Q:172:GLU:HB3	5:Q:176:PHE:CE2	2.44	0.53
3:J:153:ASP:OD1	3:J:182:TYR:OH	2.27	0.53
5:P:105:VAL:HG22	5:P:123:VAL:CG1	2.38	0.53
3:J:699:ARG:HG3	3:J:827:ILE:HD11	1.90	0.53
3:L:712:MET:SD	3:L:843:LEU:HD11	2.49	0.53
2:H:68:VAL:HG23	2:H:68:VAL:O	2.10	0.52
4:O:17:VAL:O	4:O:21:ILE:HG13	2.09	0.52
3:J:204:ILE:HG12	3:J:773:VAL:HG21	1.92	0.52
3:J:399:VAL:O	3:J:402:ILE:HG22	2.09	0.52
3:L:144:ASN:OD1	3:L:147:GLY:N	2.43	0.52
3:L:444:GLY:O	3:L:448:VAL:HG22	2.08	0.52
4:M:17:VAL:O	4:M:21:ILE:HG13	2.09	0.52
1:A:237:ILE:HD11	1:A:309:PHE:HB2	1.92	0.52
3:J:293:LEU:CD2	3:J:302:THR:HG21	2.39	0.52
5:R:36:CYS:SG	5:R:37:VAL:N	2.82	0.52
3:L:490:PRO:HA	3:L:493:CYS:SG	2.50	0.52
5:R:178:SER:O	5:R:179:LEU:HD22	2.10	0.52
2:I:210:ASP:HB3	2:I:211:PRO:HD3	1.91	0.52
3:J:335:ILE:HG21	3:J:995:ALA:HB3	1.91	0.52
2:F:268:ASP:O	2:F:272:GLY:N	2.42	0.52
1:B:179:VAL:HG11	1:B:189:TYR:CE2	2.45	0.51
3:L:535:LEU:HD23	3:L:1027:VAL:HG21	1.91	0.51
3:L:758:TYR:OH	3:L:761:ASP:OD2	2.13	0.51
3:L:974:PRO:O	3:L:978:THR:HG22	2.11	0.51
1:C:237:ILE:HD11	1:C:306:GLN:HA	1.91	0.51
3:J:931:LEU:HD23	3:J:935:ILE:HD11	1.91	0.51
1:C:8:GLN:OE1	1:C:11:ARG:NH2	2.43	0.51
3:L:38:ILE:HG22	3:L:462:SER:OG	2.11	0.51
1:C:244:HIS:ND1	1:C:298:VAL:HG11	2.25	0.51
3:J:395:MET:O	3:J:399:VAL:HG12	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:890:ALA:HB2	3:L:14:VAL:HG11	1.92	0.51
3:K:35:TYR:CE1	3:K:671:ILE:HG22	2.46	0.51
3:K:690:LEU:HD11	3:K:694:LYS:HB3	1.91	0.51
3:K:972:LEU:HD13	3:K:972:LEU:C	2.36	0.51
5:Q:175:TYR:HD1	5:Q:175:TYR:O	1.92	0.51
1:B:16:GLU:OE1	1:C:318:SER:OG	2.14	0.51
2:I:237:GLN:NE2	2:I:299:GLU:O	2.38	0.51
4:N:1:MET:HA	4:N:4:LEU:HD13	1.93	0.51
1:C:65:THR:O	1:C:65:THR:CG2	2.56	0.51
3:K:376:LEU:O	3:K:379:THR:HG22	2.11	0.50
3:K:454:VAL:HG22	3:K:455:PRO:HD3	1.93	0.50
1:A:304:GLN:OE1	1:C:30:LYS:HG3	2.11	0.50
5:P:60:ILE:HD12	5:P:75:LEU:HD13	1.91	0.50
5:Q:96:ARG:NH2	5:Q:130:GLN:OE1	2.44	0.50
1:B:116:VAL:HG11	1:B:193:LEU:HD12	1.93	0.50
3:K:306:ILE:O	3:K:310:LEU:HD23	2.12	0.50
3:L:57:VAL:HG21	3:L:86:GLY:HA2	1.94	0.50
5:P:36:CYS:SG	5:P:37:VAL:N	2.84	0.50
3:K:463:THR:HG22	3:K:563:PHE:HE1	1.77	0.50
1:B:189:TYR:CE1	5:P:171:ARG:HG3	2.47	0.50
2:H:210:ASP:HB3	2:H:211:PRO:HD3	1.93	0.50
2:D:361:ILE:O	2:D:362:SER:OG	2.28	0.49
2:E:286:THR:O	2:E:286:THR:OG1	2.29	0.49
3:J:287:SER:OG	3:J:288:GLY:N	2.45	0.49
3:J:394:THR:OG1	3:J:395:MET:SD	2.70	0.49
3:J:973:ARG:C	3:J:977:MET:HE3	2.37	0.49
3:K:367:ILE:HB	3:K:368:PRO:HD3	1.94	0.49
3:K:534:ILE:HG13	3:K:541:TYR:CE2	2.47	0.49
1:C:82:ARG:NE	1:C:242:ASP:OD2	2.40	0.49
3:J:420:MET:SD	3:J:421:ALA:N	2.85	0.49
3:K:969:ARG:HE	3:K:970:MET:HE3	1.77	0.49
5:Q:84:HIS:NE2	5:Q:168:ILE:O	2.46	0.49
2:D:361:ILE:HD12	2:D:362:SER:HB3	1.94	0.49
3:J:686:ASP:OD1	3:J:686:ASP:C	2.56	0.49
3:K:572:PHE:HE2	3:K:631:LEU:HD21	1.77	0.49
3:L:340:VAL:HG13	3:L:399:VAL:CG2	2.43	0.49
3:L:686:ASP:OD1	3:L:686:ASP:C	2.56	0.49
2:G:128:ARG:O	2:G:132:LEU:HD23	2.12	0.49
3:L:393:LEU:CD1	3:L:466:ILE:HG23	2.42	0.49
2:H:316:THR:HG23	2:H:317:PRO:HD2	1.95	0.49
3:J:28:LEU:C	3:J:28:LEU:HD23	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:542:LEU:HD11	3:L:1028:VAL:HG21	1.94	0.49
3:L:901:VAL:O	3:L:904:VAL:HG12	2.13	0.49
2:G:323:VAL:CG1	2:G:359:VAL:HG13	2.43	0.49
3:K:143:ILE:HG22	3:K:286:ALA:HB2	1.95	0.49
3:K:235:ILE:HD11	3:L:726:GLN:OE1	2.13	0.49
3:J:402:ILE:HD12	3:J:406:VAL:HG23	1.95	0.49
1:A:179:VAL:HG11	1:A:189:TYR:CE2	2.47	0.49
5:P:109:SER:O	5:P:110:THR:C	2.56	0.49
3:K:839:GLU:O	3:K:843:LEU:HD22	2.13	0.48
3:K:984:LEU:HD11	4:O:15:VAL:HG22	1.93	0.48
1:B:93:ILE:HG23	1:B:225:GLN:HG3	1.95	0.48
3:J:456:MET:HE2	3:J:471:SER:HB3	1.95	0.48
3:L:408:ASP:O	3:L:412:VAL:HG23	2.13	0.48
2:H:189:VAL:HG21	2:H:203:LEU:HD22	1.94	0.48
3:J:306:ILE:O	3:J:310:LEU:HD13	2.13	0.48
3:J:449:LEU:HD23	3:J:449:LEU:O	2.14	0.48
3:J:983:ILE:HG23	3:J:1008:MET:SD	2.53	0.48
3:K:972:LEU:HD22	3:K:976:LEU:HD23	1.95	0.48
3:L:199:THR:OG1	3:L:202:ASP:OD2	2.26	0.48
1:C:6:VAL:HG22	1:C:190:TYR:CE2	2.49	0.48
3:J:105:VAL:HG11	3:K:105:VAL:HG11	1.95	0.48
2:G:345:ASP:OD1	2:G:345:ASP:N	2.43	0.48
1:C:220:ASN:OD1	1:C:222:SER:N	2.46	0.48
3:K:671:ILE:HD11	3:K:674:LEU:HD12	1.96	0.48
2:E:210:ASP:HB3	2:E:211:PRO:HD3	1.94	0.48
3:L:183:ALA:N	3:L:271:GLY:O	2.45	0.48
5:P:174:LEU:N	5:P:174:LEU:HD23	2.28	0.48
2:F:326:VAL:HG12	2:F:326:VAL:O	2.12	0.48
3:L:911:GLY:CA	3:L:1013:THR:HG21	2.44	0.48
4:O:31:GLU:O	4:O:35:ILE:HG13	2.14	0.48
1:C:89:LYS:O	1:C:93:ILE:HG13	2.14	0.47
2:F:288:LEU:HD13	2:G:274:ILE:HD11	1.96	0.47
3:J:380:PHE:CE1	3:J:398:MET:HE1	2.49	0.47
3:L:111:LEU:HD21	3:L:127:VAL:CG1	2.44	0.47
3:L:113:LEU:C	3:L:113:LEU:HD23	2.39	0.47
2:D:256:GLN:NE2	2:D:287:LEU:HD12	2.30	0.47
3:L:408:ASP:OD1	3:L:940:LYS:NZ	2.44	0.47
4:M:28:GLY:O	4:M:32:VAL:HG12	2.15	0.47
5:Q:74:LEU:HB3	5:Q:168:ILE:HD13	1.97	0.47
5:R:178:SER:O	5:R:179:LEU:HB2	2.13	0.47
2:G:189:VAL:HG13	2:G:193:ALA:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:310:LEU:HD23	3:J:323:ILE:HG21	1.96	0.47
3:J:535:LEU:HD12	3:J:1027:VAL:HG11	1.95	0.47
3:L:759:VAL:HG23	3:L:760:ASN:H	1.78	0.47
5:Q:172:GLU:OE1	5:Q:172:GLU:HA	2.14	0.47
5:R:115:ASP:O	5:R:116:ALA:HB2	2.13	0.47
2:I:337:ILE:HG21	2:I:353:LEU:HD13	1.97	0.47
3:L:496:MET:O	3:L:496:MET:SD	2.72	0.47
5:Q:138:MET:HE3	5:Q:138:MET:CA	2.43	0.47
1:B:432:PRO:HD2	5:P:175:TYR:O	2.15	0.47
2:D:216:VAL:HG11	2:D:295:ALA:HB3	1.96	0.47
2:E:260:LEU:HD11	2:E:276:LEU:HB3	1.96	0.47
2:H:247:ILE:HD12	2:H:247:ILE:C	2.40	0.47
3:K:888:LEU:HD21	3:K:943:ILE:HD11	1.96	0.47
3:L:941:ASN:HB3	3:L:975:ILE:HD11	1.96	0.47
2:D:222:ASP:O	2:D:226:LEU:HD23	2.15	0.47
2:E:45:VAL:HG13	2:E:306:ILE:HG23	1.95	0.47
3:J:559:LEU:HD12	3:J:560:PRO:HD2	1.96	0.47
3:J:984:LEU:HD21	4:M:15:VAL:HG22	1.96	0.47
3:K:690:LEU:HD13	3:K:690:LEU:O	2.15	0.47
3:K:839:GLU:O	3:K:843:LEU:CD2	2.63	0.47
3:L:13:TRP:O	3:L:17:ILE:HG12	2.15	0.47
3:L:535:LEU:HD22	3:L:1027:VAL:HG11	1.97	0.47
1:B:397:GLN:O	1:B:400:ILE:HG22	2.15	0.47
2:I:337:ILE:HG21	2:I:353:LEU:CD1	2.44	0.47
3:J:351:VAL:HG13	3:J:410:ILE:HD11	1.97	0.47
3:L:66:GLU:HG3	3:L:78:MET:HE3	1.97	0.47
3:J:36:PRO:O	3:J:38:ILE:HG23	2.15	0.47
3:J:806:SER:OG	3:J:807:SER:N	2.48	0.47
3:J:941:ASN:O	3:J:945:ILE:HD12	2.15	0.47
3:K:15:ILE:HG21	3:K:487:ILE:HG21	1.97	0.47
1:A:306:GLN:NE2	5:R:110:THR:O	2.45	0.47
2:D:42:VAL:HG12	2:D:43:VAL:N	2.30	0.47
2:D:125:THR:HG22	2:E:141:GLN:HE22	1.79	0.47
2:D:141:GLN:OE1	2:I:128:ARG:NH1	2.48	0.47
2:F:209:LEU:H	2:F:209:LEU:HD23	1.80	0.47
3:J:102:ILE:HA	3:J:105:VAL:HG22	1.95	0.47
3:J:515:TRP:O	3:J:519:MET:HG2	2.14	0.47
1:B:209:VAL:CG1	5:Q:173:ASN:HB2	2.45	0.46
3:L:393:LEU:HD11	3:L:466:ILE:HG23	1.96	0.46
1:C:179:VAL:HG11	1:C:189:TYR:HE1	1.80	0.46
2:G:126:VAL:HG21	2:G:150:ALA:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:667:ASN:OD1	3:J:668:LEU:N	2.46	0.46
3:K:420:MET:SD	3:K:420:MET:C	2.97	0.46
3:K:442:LEU:HD12	3:K:445:ILE:HD11	1.96	0.46
3:K:631:LEU:HD11	3:K:644:VAL:HG22	1.97	0.46
3:L:911:GLY:HA2	3:L:1013:THR:HG21	1.98	0.46
1:C:77:ASP:OD2	1:C:80:LYS:NZ	2.48	0.46
3:J:113:LEU:HD13	3:L:128:SER:HA	1.97	0.46
3:J:488:LEU:HD13	3:J:488:LEU:C	2.41	0.46
3:K:199:THR:HG23	3:K:200:PRO:HD2	1.97	0.46
3:K:766:GLY:O	3:L:63:GLN:NE2	2.48	0.46
3:L:355:MET:HA	3:L:355:MET:HE2	1.96	0.46
3:L:961:ILE:O	3:L:965:LEU:HD23	2.15	0.46
5:P:108:ALA:O	5:P:109:SER:C	2.56	0.46
1:B:82:ARG:O	1:B:86:LEU:HD13	2.15	0.46
2:D:268:ASP:O	2:D:272:GLY:N	2.44	0.46
3:J:467:TYR:OH	3:J:928:GLN:OE1	2.33	0.46
3:J:1004:GLY:O	3:J:1005:THR:C	2.59	0.46
3:K:169:THR:HG22	3:K:170:SER:N	2.31	0.46
1:A:183:ARG:O	1:A:187:GLY:N	2.45	0.46
1:A:244:HIS:CG	1:A:298:VAL:HG11	2.50	0.46
1:B:18:ARG:HG2	1:B:18:ARG:HH11	1.81	0.46
2:F:308:VAL:HG13	2:F:309:PRO:HD2	1.97	0.46
2:I:189:VAL:HG13	2:I:193:ALA:HB3	1.97	0.46
2:I:378:VAL:HG13	2:I:379:THR:N	2.31	0.46
3:K:980:LEU:HD12	3:K:984:LEU:HD22	1.96	0.46
3:L:853:THR:O	3:L:853:THR:HG23	2.16	0.46
3:K:860:THR:O	3:K:863:SER:OG	2.31	0.46
3:K:1016:VAL:HG23	3:K:1017:LEU:H	1.80	0.46
3:L:456:MET:HE2	3:L:932:LEU:HD13	1.97	0.46
5:P:173:ASN:HA	5:P:176:PHE:HB2	1.96	0.46
1:B:218:LYS:NZ	5:Q:154:GLY:O	2.44	0.46
3:J:945:ILE:HD11	3:J:975:ILE:CD1	2.46	0.46
3:L:404:LEU:HD13	3:L:937:LEU:HD21	1.98	0.46
3:L:966:ASP:OD1	3:L:969:ARG:NH2	2.48	0.46
5:Q:110:THR:O	5:Q:111:ILE:C	2.58	0.46
1:B:13:SER:OG	5:P:117:ARG:NH1	2.49	0.46
1:B:35:ARG:HG3	1:B:84:LEU:HD13	1.97	0.46
2:E:329:ASP:C	2:E:329:ASP:OD2	2.58	0.46
3:K:696:THR:OG1	3:K:825:MET:HE1	2.15	0.46
3:K:866:GLU:OE1	3:K:866:GLU:C	2.59	0.46
3:K:1001:ASN:O	3:K:1005:THR:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:THR:O	1:B:89:LYS:HG2	2.16	0.46
3:L:552:MET:HB2	3:L:910:ILE:HD13	1.98	0.46
1:C:12:LEU:C	1:C:12:LEU:HD23	2.41	0.46
2:F:40:VAL:HG23	2:F:362:SER:O	2.16	0.46
5:R:109:SER:O	5:R:110:THR:C	2.59	0.46
1:A:130:LYS:HA	1:A:164:VAL:HG11	1.98	0.45
3:J:380:PHE:CG	3:J:398:MET:HE1	2.51	0.45
3:J:892:TYR:CE2	3:J:943:ILE:HD11	2.51	0.45
1:C:39:LEU:N	1:C:39:LEU:HD23	2.31	0.45
1:C:44:LEU:HD23	1:C:44:LEU:C	2.41	0.45
3:J:449:LEU:O	3:J:452:VAL:HG22	2.16	0.45
3:L:983:ILE:HG23	3:L:1008:MET:SD	2.56	0.45
1:B:77:ASP:OD1	1:B:80:LYS:NZ	2.47	0.45
1:B:148:LEU:CD1	2:I:132:LEU:HD11	2.46	0.45
3:J:841:MET:HE1	3:J:859:TRP:CD2	2.52	0.45
3:K:16:ALA:HB2	3:K:488:LEU:HD22	1.98	0.45
3:L:372:VAL:HG13	3:L:405:LEU:HD21	1.99	0.45
3:K:1015:THR:O	3:K:1019:ILE:HG23	2.16	0.45
1:A:250:LEU:HD12	1:A:286:LEU:HD21	1.99	0.45
3:J:897:ILE:CG2	3:J:898:PRO:HD3	2.47	0.45
3:K:911:GLY:CA	3:K:1013:THR:HG21	2.46	0.45
3:K:980:LEU:O	3:K:984:LEU:HD22	2.17	0.45
1:B:306:GLN:NE2	5:Q:110:THR:O	2.50	0.45
1:C:116:VAL:CG1	1:C:193:LEU:HD12	2.46	0.45
3:J:372:VAL:N	3:J:373:PRO:HD2	2.32	0.45
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.81	0.45
1:B:168:GLU:OE2	1:B:172:ARG:NH2	2.50	0.45
3:J:340:VAL:HG11	3:J:395:MET:HB3	1.99	0.45
1:A:82:ARG:NE	1:A:242:ASP:OD2	2.50	0.45
1:A:433:GLN:C	5:Q:179:LEU:HD23	2.41	0.45
1:C:254:THR:HG23	1:C:255:GLY:N	2.31	0.45
2:E:323:VAL:HG13	2:E:359:VAL:HG13	1.98	0.45
3:J:314:GLU:OE1	3:J:314:GLU:C	2.60	0.45
3:K:535:LEU:HD22	3:K:1027:VAL:HG23	1.99	0.45
3:L:712:MET:HB3	3:L:843:LEU:HD11	1.99	0.45
1:C:139:GLN:OE1	1:C:370:VAL:HG21	2.17	0.45
3:J:137:LEU:HD22	3:J:293:LEU:HD21	1.98	0.45
3:K:442:LEU:HD23	3:K:486:LEU:HD21	1.99	0.45
1:A:401:LYS:HG2	1:A:411:ASP:OD2	2.17	0.45
1:B:212:LEU:CD1	1:B:400:ILE:HD11	2.45	0.45
1:B:290:LEU:HD23	1:B:290:LEU:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:690:LEU:HD13	3:K:690:LEU:C	2.42	0.45
3:L:406:VAL:O	3:L:410:ILE:HG22	2.17	0.45
3:L:905:VAL:HG22	3:L:935:ILE:HG13	1.99	0.45
2:F:184:ILE:HD12	2:F:206:VAL:HG22	1.98	0.44
3:L:340:VAL:HG11	3:L:395:MET:HB3	1.99	0.44
2:H:325:VAL:HG11	2:H:335:ARG:NH1	2.32	0.44
2:I:230:LEU:CD2	2:I:235:LEU:HD22	2.47	0.44
3:J:471:SER:O	3:J:475:VAL:HG23	2.17	0.44
3:L:671:ILE:O	3:L:671:ILE:HG13	2.17	0.44
5:Q:170:ASN:O	5:Q:174:LEU:HB2	2.18	0.44
1:C:36:SER:OG	1:C:37:PRO:HD3	2.16	0.44
3:J:183:ALA:N	3:J:271:GLY:O	2.51	0.44
3:J:633:ASP:OD1	3:J:634:TRP:N	2.50	0.44
3:J:931:LEU:O	3:J:935:ILE:HG13	2.18	0.44
1:A:234:ARG:CZ	5:R:107:SER:O	2.65	0.44
3:K:542:LEU:HD11	3:K:1028:VAL:HG11	1.99	0.44
3:L:62:THR:O	3:L:66:GLU:HB2	2.16	0.44
3:J:393:LEU:H	3:J:393:LEU:CD2	2.31	0.44
3:K:344:LEU:CD1	3:K:402:ILE:HD11	2.47	0.44
1:B:433:GLN:O	5:P:178:SER:N	2.47	0.44
2:D:332:VAL:HG23	2:D:369:PRO:HA	1.99	0.44
2:F:47:THR:HG23	2:F:304:ASN:HA	2.00	0.44
3:L:177:LEU:HD23	3:L:179:GLY:N	2.32	0.44
3:L:372:VAL:HG22	3:L:405:LEU:HG	1.99	0.44
3:L:399:VAL:HG11	3:L:989:LEU:HD11	1.98	0.44
5:Q:170:ASN:O	5:Q:174:LEU:HD13	2.17	0.44
1:B:209:VAL:HG13	5:Q:173:ASN:HB2	1.98	0.44
1:B:235:GLU:OE1	1:B:238:ARG:NH1	2.51	0.44
1:C:12:LEU:CD2	5:R:117:ARG:CZ	2.96	0.44
3:J:143:ILE:HG22	3:J:286:ALA:HB2	2.00	0.44
3:J:259:ARG:HD3	3:K:734:GLU:OE1	2.18	0.44
3:J:843:LEU:O	3:J:843:LEU:HD12	2.18	0.44
3:J:961:ILE:HD12	3:J:961:ILE:N	2.33	0.44
2:F:54:THR:OG1	2:F:299:GLU:OE2	2.28	0.44
2:F:209:LEU:HD23	2:F:209:LEU:N	2.33	0.44
2:F:308:VAL:HG21	2:F:353:LEU:HD12	2.00	0.44
3:J:105:VAL:HG11	3:K:105:VAL:CG1	2.48	0.44
3:K:333:VAL:HG12	3:K:337:ILE:HD12	1.99	0.44
3:K:866:GLU:OE1	3:K:867:ARG:N	2.51	0.44
1:C:18:ARG:HG2	1:C:18:ARG:HH11	1.83	0.44
1:C:381:ASN:O	1:C:385:GLU:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:55:GLU:OE2	2:I:296:ARG:NH2	2.51	0.44
3:J:459:PHE:HB3	3:J:464:GLY:HA2	1.99	0.44
3:J:888:LEU:HD11	3:J:943:ILE:HD13	2.00	0.44
3:L:106:GLN:O	3:L:110:LYS:HG2	2.17	0.44
3:L:144:ASN:HB2	3:L:154:ILE:HD11	1.98	0.44
1:A:239:GLN:C	1:A:239:GLN:OE1	2.61	0.43
1:C:413:LEU:HD23	1:C:413:LEU:C	2.43	0.43
2:F:248:THR:HG22	2:F:253:LYS:HA	2.01	0.43
3:K:441:ALA:HA	3:K:891:LEU:HD11	2.00	0.43
3:J:848:ALA:HB1	3:J:857:TYR:CD2	2.54	0.43
3:J:892:TYR:CG	3:J:897:ILE:HD13	2.53	0.43
3:L:1026:PHE:HD1	3:L:1026:PHE:O	2.01	0.43
1:A:182:LEU:O	1:A:186:THR:OG1	2.35	0.43
2:I:232:ASN:C	2:I:232:ASN:OD1	2.60	0.43
3:K:99:ASP:OD1	3:K:102:ILE:HD11	2.18	0.43
3:K:357:LEU:HD11	3:K:516:PHE:CZ	2.53	0.43
3:K:520:PHE:O	3:K:524:THR:HG22	2.18	0.43
3:L:445:ILE:HD11	3:L:944:LEU:HD21	1.99	0.43
3:L:1014:ALA:O	3:L:1018:ALA:HB3	2.18	0.43
4:M:23:LEU:O	4:M:26:ILE:HG13	2.18	0.43
1:B:148:LEU:HD12	2:I:132:LEU:HD11	1.99	0.43
1:B:232:LEU:C	1:B:232:LEU:HD23	2.43	0.43
2:E:353:LEU:HD21	2:E:359:VAL:CG2	2.49	0.43
2:G:260:LEU:HD13	2:G:297:LEU:HD21	2.00	0.43
3:J:20:MET:SD	3:J:20:MET:C	3.02	0.43
3:K:412:VAL:HG21	3:K:485:ALA:HB1	2.00	0.43
3:L:339:GLU:HA	3:L:342:LYS:HG2	2.01	0.43
1:A:355:LEU:HD23	1:A:379:LEU:HD22	1.99	0.43
2:I:45:VAL:HG13	2:I:306:ILE:HG23	2.00	0.43
3:J:358:PHE:HD2	3:J:977:MET:HE2	1.84	0.43
3:K:335:ILE:HG21	3:K:995:ALA:HB3	2.00	0.43
1:A:281:GLN:OE1	1:C:51:SER:OG	2.34	0.43
1:C:190:TYR:N	1:C:190:TYR:CD1	2.87	0.43
2:F:221:ASN:OD1	2:F:222:ASP:N	2.52	0.43
3:J:923:ASN:OD1	3:J:923:ASN:C	2.61	0.43
5:R:91:ASP:OD2	5:R:94:SER:OG	2.34	0.43
2:D:47:THR:HG23	2:D:304:ASN:HA	2.01	0.43
2:E:323:VAL:CG1	2:E:359:VAL:HG13	2.48	0.43
3:J:402:ILE:CD1	3:J:406:VAL:HG23	2.49	0.43
3:J:449:LEU:HD22	3:J:478:MET:CE	2.46	0.43
3:K:563:PHE:O	3:K:925:VAL:HG13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HA	1:A:237:ILE:HD12	2.01	0.43
3:J:314:GLU:N	3:J:315:PRO:CD	2.82	0.43
3:L:860:THR:N	3:L:863:SER:OG	2.52	0.43
5:R:32:ARG:CZ	5:R:146:VAL:HG11	2.48	0.43
2:G:318:ARG:NH1	2:G:318:ARG:HB2	2.34	0.43
3:J:734:GLU:HG2	3:L:250:LEU:HD21	2.01	0.43
3:K:34:GLN:HA	3:K:333:VAL:HG22	2.00	0.43
3:K:580:ALA:HB1	3:K:724:THR:HG22	2.01	0.43
3:K:899:PHE:O	3:K:903:LEU:HD13	2.19	0.43
3:L:560:PRO:O	3:L:922:THR:HG22	2.19	0.43
3:L:674:LEU:O	3:L:674:LEU:HD23	2.19	0.43
1:A:395:ILE:HD13	1:A:395:ILE:HA	1.92	0.43
2:H:68:VAL:O	2:H:68:VAL:CG2	2.67	0.43
3:J:987:MET:HE2	3:J:1008:MET:HE1	2.01	0.43
3:K:112:GLN:HG3	3:L:112:GLN:HG3	2.00	0.43
1:A:89:LYS:O	1:A:93:ILE:HG13	2.19	0.42
3:J:712:MET:HA	3:J:832:ALA:HB3	2.01	0.42
3:L:953:MET:HE1	3:L:960:LEU:HA	2.01	0.42
5:P:138:MET:HE3	5:P:138:MET:CA	2.44	0.42
1:B:232:LEU:HD23	1:B:232:LEU:O	2.19	0.42
2:F:128:ARG:NH2	2:G:144:ASP:OD2	2.51	0.42
2:G:325:VAL:HG12	2:G:359:VAL:HG22	2.01	0.42
3:K:454:VAL:N	3:K:455:PRO:CD	2.82	0.42
5:Q:109:SER:O	5:Q:109:SER:OG	2.32	0.42
1:A:297:MET:HB2	1:C:36:SER:OG	2.19	0.42
1:B:82:ARG:HE	1:B:238:ARG:HB3	1.84	0.42
2:E:304:ASN:O	2:E:304:ASN:ND2	2.37	0.42
2:I:157:VAL:HG12	2:I:161:LYS:HD2	2.00	0.42
3:J:196:PHE:O	3:J:252:LYS:NZ	2.42	0.42
3:J:379:THR:HG23	3:J:398:MET:HE2	2.00	0.42
3:J:429:GLU:OE1	3:J:432:ARG:NH1	2.46	0.42
3:L:394:THR:C	3:L:395:MET:HE2	2.44	0.42
1:C:86:LEU:HD21	1:C:236:GLN:HG2	2.01	0.42
3:J:527:TYR:O	3:J:531:VAL:HG23	2.19	0.42
3:K:479:ALA:O	3:K:482:VAL:HG22	2.19	0.42
3:L:149:MET:HE1	3:L:321:LEU:HD12	2.02	0.42
3:L:375:VAL:HG13	3:L:405:LEU:CD2	2.47	0.42
3:L:678:THR:OG1	3:L:830:GLN:OE1	2.32	0.42
3:L:690:LEU:HG	3:L:694:LYS:HB2	2.01	0.42
5:R:99:LEU:HD23	5:R:100:PRO:O	2.19	0.42
1:A:61:ASN:O	1:A:262:SER:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD23	1:A:88:GLU:OE2	2.20	0.42
1:B:355:LEU:HD23	1:B:379:LEU:HD22	2.01	0.42
3:J:515:TRP:CD1	3:J:515:TRP:C	2.98	0.42
2:F:87:ILE:HD12	2:F:93:LEU:HD21	2.01	0.42
2:G:60:THR:HG21	2:G:212:ILE:HD13	2.02	0.42
3:L:14:VAL:O	3:L:18:ILE:HG12	2.20	0.42
5:Q:93:PHE:HD1	5:Q:150:VAL:HG21	1.85	0.42
1:C:10:ALA:HB2	1:C:186:THR:HG22	2.02	0.42
2:E:317:PRO:HA	3:J:811:TYR:HB2	2.01	0.42
2:G:247:ILE:O	2:G:248:THR:HG22	2.19	0.42
3:J:375:VAL:HG22	3:J:484:VAL:HG21	2.01	0.42
3:J:911:GLY:HA2	3:J:1013:THR:HG21	2.00	0.42
3:L:418:ARG:NH2	3:L:419:VAL:HG22	2.35	0.42
4:N:17:VAL:O	4:N:21:ILE:HG13	2.20	0.42
1:A:13:SER:O	1:A:13:SER:OG	2.32	0.42
1:B:161:TYR:O	1:B:164:VAL:HG12	2.20	0.42
2:E:225:ARG:O	2:E:229:GLU:HG2	2.20	0.42
2:G:216:VAL:HG11	2:G:295:ALA:HB3	2.01	0.42
3:J:111:LEU:HD21	3:J:127:VAL:CG1	2.50	0.42
3:J:466:ILE:HG21	3:J:925:VAL:HG11	2.01	0.42
3:J:972:LEU:C	3:J:972:LEU:HD13	2.45	0.42
3:K:744:ASN:O	3:K:748:THR:HG23	2.20	0.42
3:L:949:ALA:HB3	3:L:1026:PHE:CE2	2.55	0.42
1:A:156:ASN:O	1:A:160:GLN:HG3	2.20	0.42
2:E:379:THR:HG23	2:E:379:THR:O	2.19	0.42
3:J:399:VAL:O	3:J:399:VAL:HG22	2.19	0.42
3:J:1012:VAL:O	3:J:1016:VAL:HG22	2.20	0.42
3:K:2:PRO:O	3:K:6:ILE:HG12	2.20	0.42
3:K:402:ILE:O	3:K:406:VAL:HG12	2.19	0.42
3:L:535:LEU:HD21	3:L:1027:VAL:HG11	2.02	0.42
5:Q:108:ALA:HB1	5:Q:111:ILE:HD11	2.02	0.42
3:J:367:ILE:HB	3:J:368:PRO:CD	2.50	0.42
3:L:145:THR:N	3:L:320:GLY:O	2.46	0.42
3:L:727:PHE:CZ	3:L:807:SER:HB3	2.55	0.42
1:C:175:LEU:O	1:C:175:LEU:HD23	2.20	0.41
3:J:49:TYR:O	3:J:50:PRO:C	2.62	0.41
3:K:274:ASN:OD1	3:K:274:ASN:C	2.62	0.41
1:B:86:LEU:HD12	1:B:235:GLU:HG3	2.02	0.41
1:C:290:LEU:CD2	1:C:292:ILE:HD13	2.50	0.41
3:K:444:GLY:O	3:K:448:VAL:HG23	2.20	0.41
3:K:469:GLN:O	3:K:473:THR:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:852:PRO:O	3:L:853:THR:C	2.63	0.41
3:L:1026:PHE:C	3:L:1026:PHE:CD1	2.97	0.41
1:B:217:GLU:OE2	5:Q:151:ARG:HB3	2.19	0.41
1:B:300:SER:O	1:B:304:GLN:HG3	2.19	0.41
1:C:28:PHE:O	1:C:31:ILE:HB	2.21	0.41
2:E:345:ASP:OD2	2:E:345:ASP:N	2.53	0.41
2:G:230:LEU:HD11	2:G:237:GLN:HG3	2.02	0.41
3:K:372:VAL:HB	3:K:373:PRO:HD3	2.01	0.41
1:A:221:LEU:HD22	1:A:221:LEU:N	2.35	0.41
3:K:278:ILE:HD12	3:K:584:GLN:CD	2.46	0.41
3:L:633:ASP:OD1	3:L:634:TRP:N	2.54	0.41
5:P:78:ALA:HB2	5:P:168:ILE:HG23	2.02	0.41
5:P:179:LEU:HD22	5:P:179:LEU:N	2.35	0.41
3:J:852:PRO:O	3:J:853:THR:C	2.64	0.41
3:K:166:ILE:HD11	3:K:310:LEU:HD22	2.03	0.41
3:L:293:LEU:HD23	3:L:302:THR:HG21	2.02	0.41
1:C:194:ALA:HA	1:C:422:PRO:HA	2.02	0.41
2:G:45:VAL:HG21	2:G:353:LEU:HD23	2.03	0.41
3:J:479:ALA:O	3:J:482:VAL:HG22	2.20	0.41
3:K:2:PRO:HG3	3:K:435:MET:HG2	2.02	0.41
3:K:471:SER:O	3:K:475:VAL:HG23	2.19	0.41
3:L:137:LEU:HD22	3:L:293:LEU:HD21	2.02	0.41
3:L:873:ALA:N	3:L:874:PRO:HD2	2.35	0.41
3:L:909:VAL:HG22	3:L:931:LEU:HD11	2.02	0.41
4:N:8:LEU:O	4:N:12:VAL:HG23	2.20	0.41
2:G:114:LYS:HB2	2:H:155:ALA:HB3	2.01	0.41
3:J:357:LEU:HD11	3:J:516:PHE:CZ	2.56	0.41
3:L:143:ILE:HG22	3:L:286:ALA:HB2	2.03	0.41
3:L:293:LEU:CD2	3:L:302:THR:HG21	2.50	0.41
5:Q:42:ASP:N	5:Q:42:ASP:OD1	2.53	0.41
1:A:2:ASN:OD1	1:A:4:MET:N	2.50	0.41
3:K:489:THR:OG1	3:K:490:PRO:HD3	2.21	0.41
3:K:682:PHE:CZ	3:K:857:TYR:HB2	2.56	0.41
3:L:20:MET:SD	3:L:20:MET:C	3.04	0.41
1:C:355:LEU:HD23	1:C:379:LEU:HD22	2.03	0.41
2:I:345:ASP:OD1	2:I:345:ASP:O	2.39	0.41
3:J:376:LEU:O	3:J:379:THR:HG22	2.21	0.41
3:J:897:ILE:CD1	3:J:946:VAL:HG11	2.48	0.41
3:K:465:ALA:O	3:K:469:GLN:HG3	2.21	0.41
3:L:1026:PHE:HD1	3:L:1026:PHE:C	2.29	0.41
5:R:108:ALA:O	5:R:109:SER:C	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LYS:HG3	5:P:179:LEU:HG	2.03	0.41
1:C:221:LEU:N	1:C:221:LEU:HD22	2.36	0.41
2:E:378:VAL:C	2:E:379:THR:HG22	2.46	0.41
3:J:780:ARG:NH1	3:L:221:GLY:O	2.51	0.41
3:J:911:GLY:HA3	3:J:1013:THR:OG1	2.21	0.41
3:K:777:ALA:O	3:K:781:MET:HG2	2.21	0.41
3:K:852:PRO:O	3:K:853:THR:C	2.64	0.41
5:P:138:MET:HE1	5:P:146:VAL:C	2.46	0.41
1:A:3:LEU:HD21	1:A:412:LEU:HD22	2.02	0.40
1:B:184:GLN:OE1	1:C:325:GLN:OE1	2.38	0.40
3:J:392:THR:HG23	3:J:393:LEU:N	2.35	0.40
3:J:885:PHE:CD1	3:J:885:PHE:C	2.99	0.40
3:K:348:ILE:HG12	3:K:372:VAL:HG11	2.02	0.40
5:P:105:VAL:O	5:P:106:ALA:C	2.63	0.40
5:R:178:SER:O	5:R:179:LEU:CB	2.69	0.40
1:B:113:TYR:OH	1:B:194:ALA:O	2.18	0.40
1:C:18:ARG:HG2	1:C:18:ARG:NH1	2.36	0.40
2:H:238:GLU:CD	2:H:238:GLU:C	2.90	0.40
3:K:649:MET:HE2	3:K:649:MET:HB3	2.00	0.40
2:D:317:PRO:O	2:D:318:ARG:CB	2.69	0.40
2:E:216:VAL:HG11	2:E:295:ALA:HB3	2.03	0.40
3:J:980:LEU:HD12	3:J:980:LEU:C	2.46	0.40
3:K:649:MET:HE3	3:K:653:ARG:HH22	1.87	0.40
3:L:399:VAL:O	3:L:402:ILE:HG22	2.21	0.40
3:L:897:ILE:N	3:L:898:PRO:CD	2.84	0.40
4:M:31:GLU:O	4:M:35:ILE:HG13	2.21	0.40
5:P:84:HIS:NE2	5:P:168:ILE:O	2.55	0.40
1:B:98:TYR:O	1:B:102:GLN:HG3	2.21	0.40
1:B:234:ARG:O	1:B:235:GLU:C	2.61	0.40
1:C:12:LEU:HD23	1:C:13:SER:HB2	2.02	0.40
3:L:223:PRO:HA	3:L:224:PRO:HD3	1.96	0.40
3:L:340:VAL:HG13	3:L:399:VAL:HG23	2.02	0.40
1:C:28:PHE:CE1	1:C:91:ALA:HB1	2.57	0.40
1:C:33:GLU:O	1:C:37:PRO:HD3	2.22	0.40
2:E:378:VAL:O	2:E:379:THR:CG2	2.70	0.40
3:J:37:THR:O	3:J:37:THR:HG22	2.21	0.40
3:J:401:ALA:O	3:J:404:LEU:N	2.54	0.40
3:J:682:PHE:CE1	3:J:857:TYR:HB2	2.56	0.40
3:K:974:PRO:HA	3:K:977:MET:HG2	2.04	0.40
3:L:380:PHE:CE1	3:L:390:ILE:HD11	2.57	0.40
3:L:972:LEU:HD23	3:L:972:LEU:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	431/480 (90%)	429 (100%)	2 (0%)	0	100	100
1	B	431/480 (90%)	428 (99%)	3 (1%)	0	100	100
1	C	431/480 (90%)	421 (98%)	10 (2%)	0	100	100
2	D	343/397 (86%)	334 (97%)	9 (3%)	0	100	100
2	E	344/397 (87%)	332 (96%)	12 (4%)	0	100	100
2	F	339/397 (85%)	327 (96%)	12 (4%)	0	100	100
2	G	344/397 (87%)	335 (97%)	9 (3%)	0	100	100
2	H	342/397 (86%)	335 (98%)	7 (2%)	0	100	100
2	I	344/397 (87%)	335 (97%)	9 (3%)	0	100	100
3	J	1035/1049 (99%)	1011 (98%)	24 (2%)	0	100	100
3	K	1032/1049 (98%)	1006 (98%)	26 (2%)	0	100	100
3	L	1032/1049 (98%)	1005 (97%)	27 (3%)	0	100	100
4	M	37/49 (76%)	37 (100%)	0	0	100	100
4	N	37/49 (76%)	37 (100%)	0	0	100	100
4	O	37/49 (76%)	37 (100%)	0	0	100	100
5	P	151/160 (94%)	141 (93%)	10 (7%)	0	100	100
5	Q	151/160 (94%)	143 (95%)	8 (5%)	0	100	100
5	R	151/160 (94%)	140 (93%)	10 (7%)	1 (1%)	18	50
All	All	7012/7596 (92%)	6833 (97%)	178 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	R	178	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/402 (90%)	361 (100%)	1 (0%)	86	86
1	B	362/402 (90%)	360 (99%)	2 (1%)	78	82
1	C	362/402 (90%)	360 (99%)	2 (1%)	78	82
2	D	278/318 (87%)	278 (100%)	0	100	100
2	E	279/318 (88%)	277 (99%)	2 (1%)	76	81
2	F	275/318 (86%)	275 (100%)	0	100	100
2	G	279/318 (88%)	278 (100%)	1 (0%)	84	85
2	H	277/318 (87%)	277 (100%)	0	100	100
2	I	279/318 (88%)	278 (100%)	1 (0%)	84	85
3	J	843/855 (99%)	841 (100%)	2 (0%)	87	88
3	K	840/855 (98%)	840 (100%)	0	100	100
3	L	840/855 (98%)	840 (100%)	0	100	100
4	M	33/41 (80%)	33 (100%)	0	100	100
4	N	33/41 (80%)	33 (100%)	0	100	100
4	O	33/41 (80%)	32 (97%)	1 (3%)	36	63
5	P	133/140 (95%)	133 (100%)	0	100	100
5	Q	133/140 (95%)	133 (100%)	0	100	100
5	R	133/140 (95%)	130 (98%)	3 (2%)	44	68
All	All	5774/6222 (93%)	5759 (100%)	15 (0%)	84	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ARG
1	B	118	ASN
1	B	234	ARG
1	C	11	ARG
1	C	31	ILE
2	E	286	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	304	ASN
2	G	256	GLN
2	I	297	LEU
3	J	256	ASP
3	J	786	ILE
4	O	14	MET
5	R	105	VAL
5	R	107	SER
5	R	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	197	ASN
1	A	200	ASN
1	A	304	GLN
1	A	388	ASN
1	A	399	ASN
1	B	58	ASN
1	B	87	GLN
1	B	155	GLN
1	B	236	GLN
1	B	306	GLN
1	B	325	GLN
1	B	384	GLN
1	B	410	GLN
1	C	118	ASN
1	C	145	ASN
1	C	188	ASN
1	C	282	ASN
1	C	410	GLN
2	D	95	GLN
2	D	136	GLN
2	D	152	GLN
2	D	170	ASN
2	E	36	GLN
2	E	120	ASN
2	E	207	GLN
2	E	365	GLN
2	F	71	GLN
2	G	120	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	151	GLN
2	G	311	GLN
2	H	80	ASN
2	H	95	GLN
2	H	218	GLN
2	H	221	ASN
2	H	304	ASN
2	H	365	GLN
2	I	120	ASN
2	I	145	GLN
2	I	188	ASN
3	J	68	ASN
3	J	213	GLN
3	J	517	ASN
3	J	596	HIS
3	J	605	ASN
3	J	700	ASN
3	K	70	ASN
3	K	284	GLN
3	K	577	GLN
3	K	604	ASN
3	K	733	GLN
3	K	737	GLN
3	K	830	GLN
3	L	70	ASN
3	L	151	GLN
3	L	255	GLN
3	L	588	GLN
3	L	797	GLN
5	P	82	ASN
5	P	113	ASN
5	Q	177	GLN
5	R	84	HIS
5	R	173	ASN
5	R	177	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

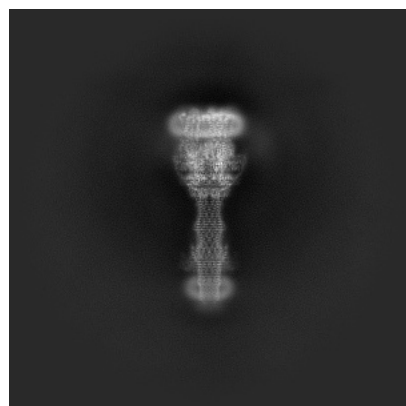
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55890. These allow visual inspection of the internal detail of the map and identification of artifacts.

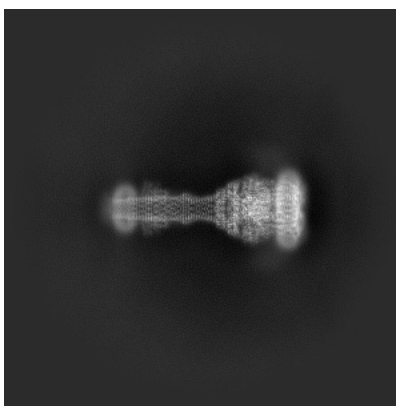
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

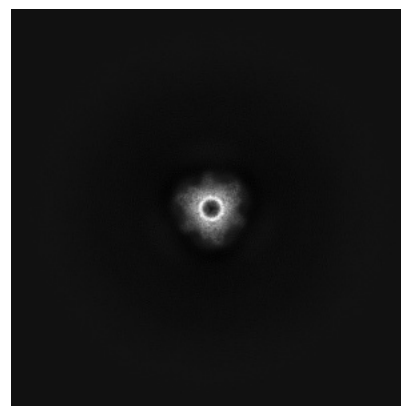
6.1.1 Primary map



X

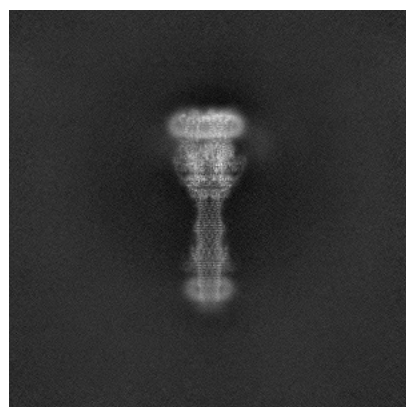


Y

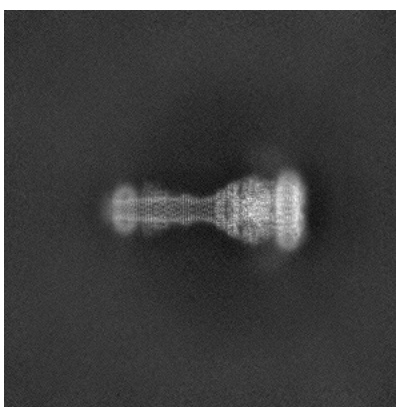


Z

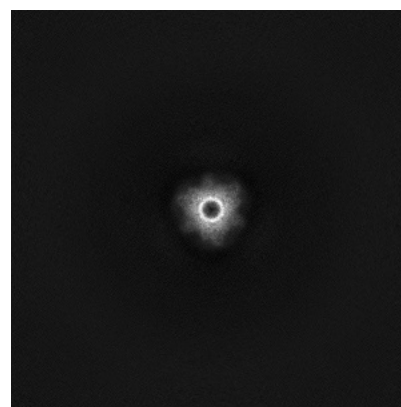
6.1.2 Raw map



X



Y

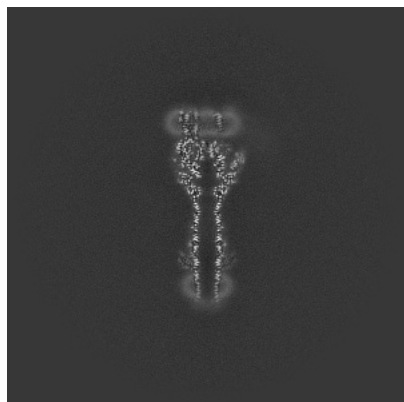


Z

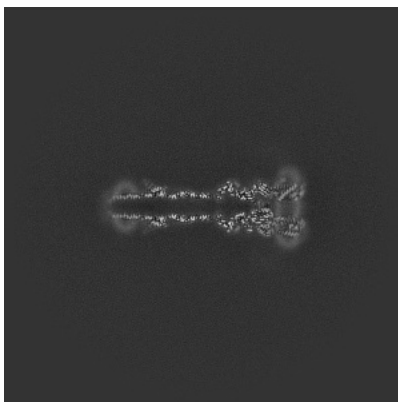
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

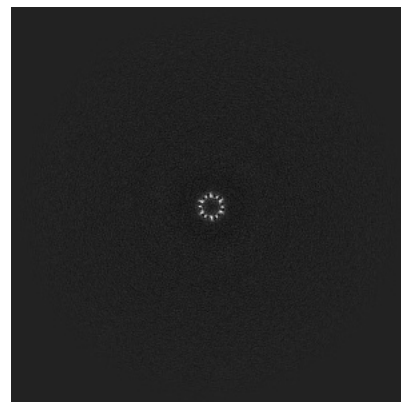
6.2.1 Primary map



X Index: 294

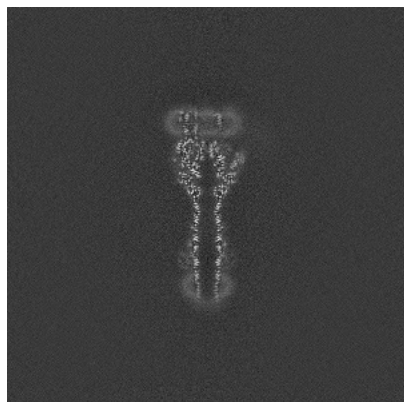


Y Index: 294

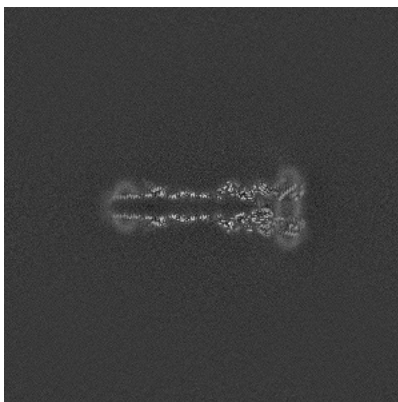


Z Index: 294

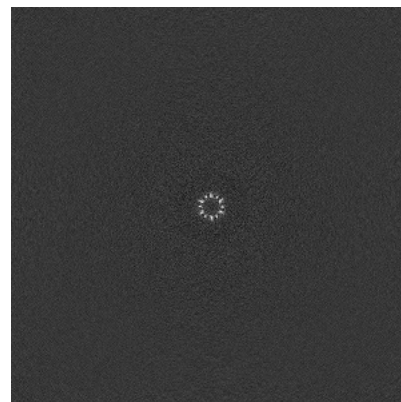
6.2.2 Raw map



X Index: 294



Y Index: 294

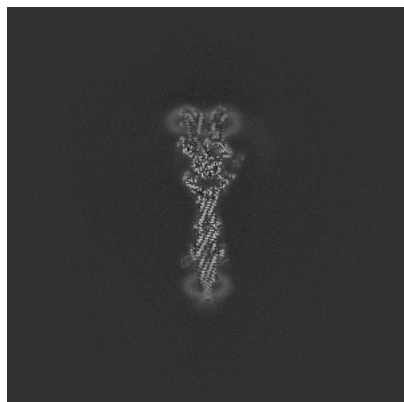


Z Index: 294

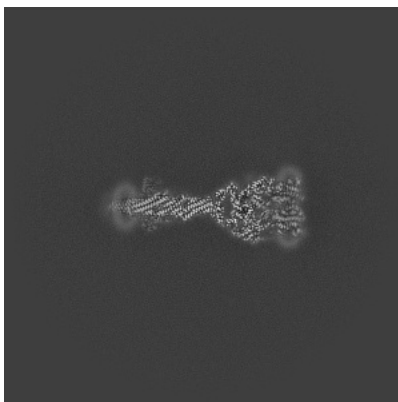
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

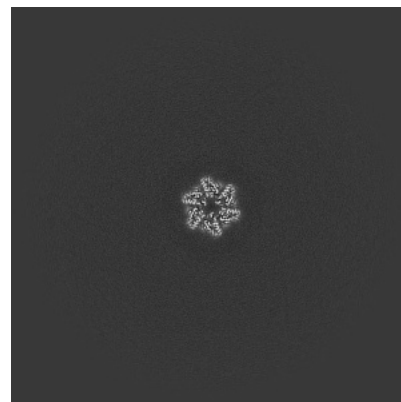
6.3.1 Primary map



X Index: 280

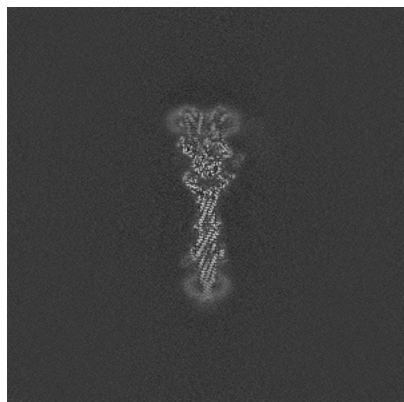


Y Index: 309

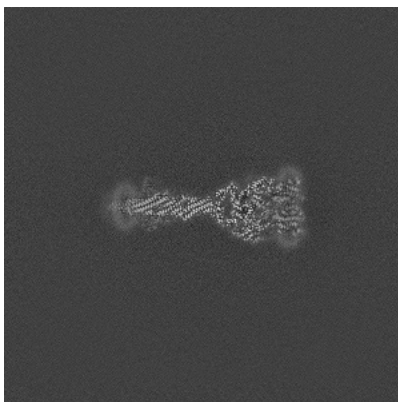


Z Index: 339

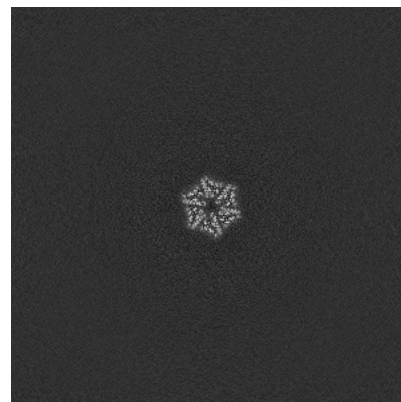
6.3.2 Raw map



X Index: 280



Y Index: 309

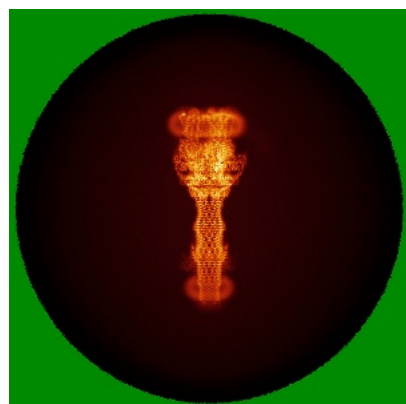


Z Index: 338

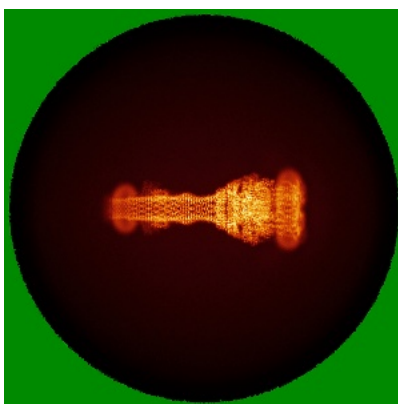
The images above show the largest variance slices of the map in three orthogonal directions.

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

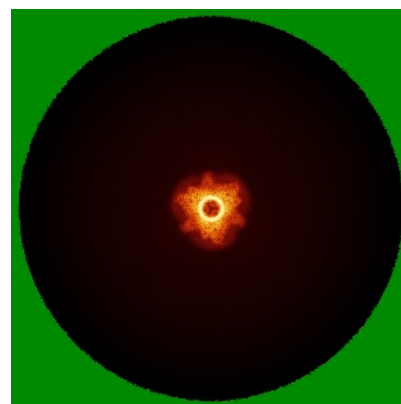
6.4.1 Primary map



X

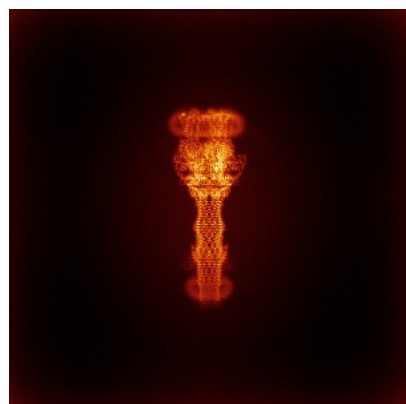


Y

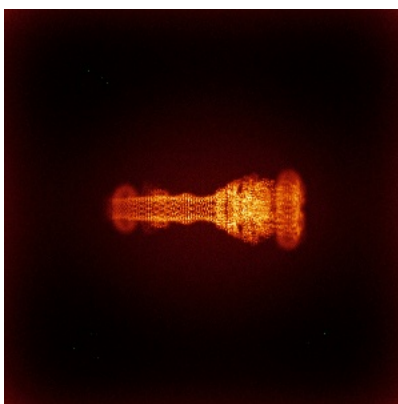


Z

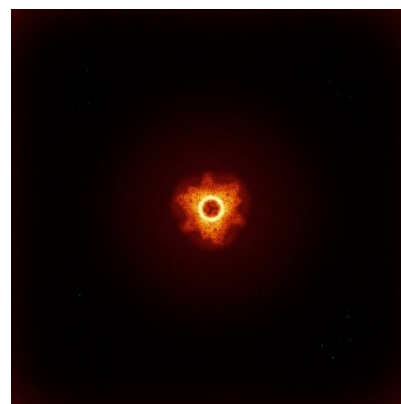
6.4.2 Raw map



X



Y

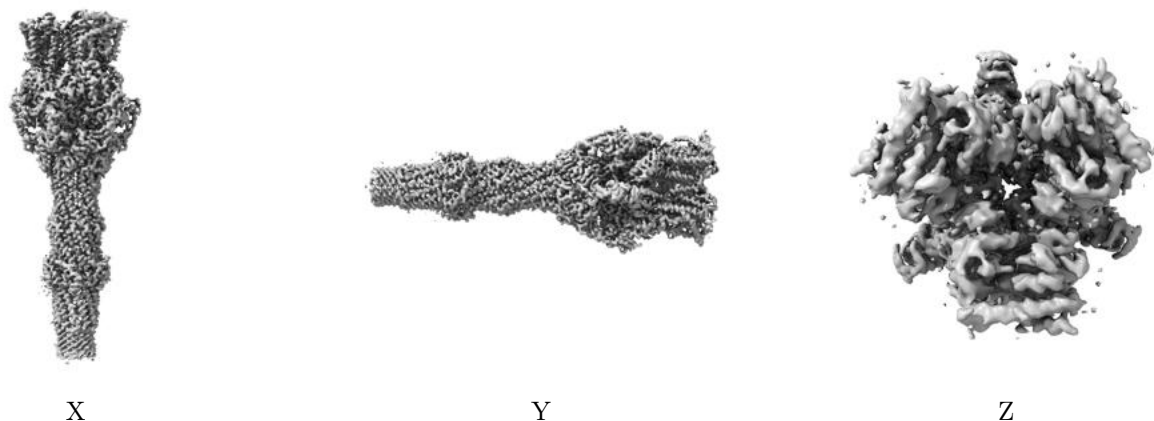


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

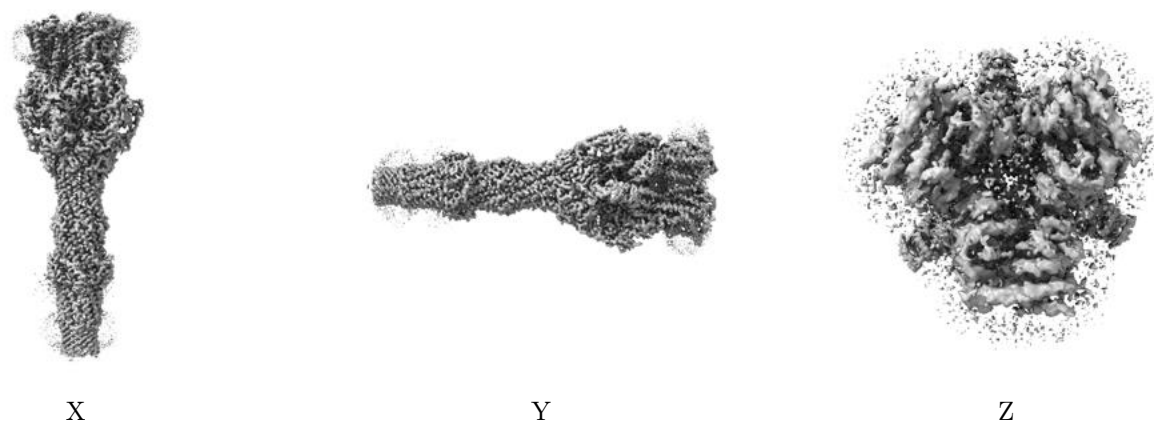
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

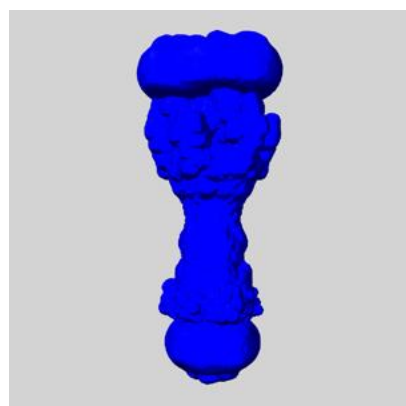
6.6 Mask visualisation [i](#)

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

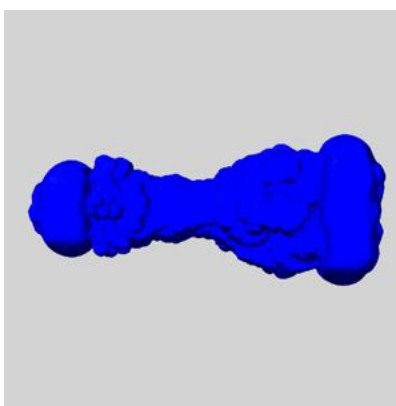
A mask typically either:

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

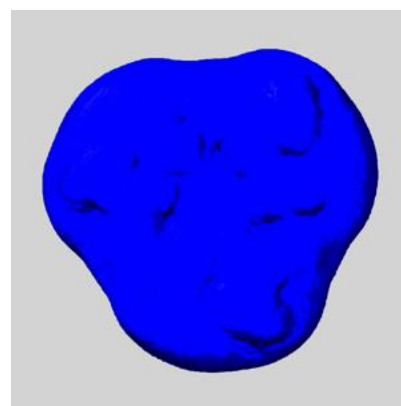
6.6.1 emd_55890_msk_1.map [i](#)



X



Y

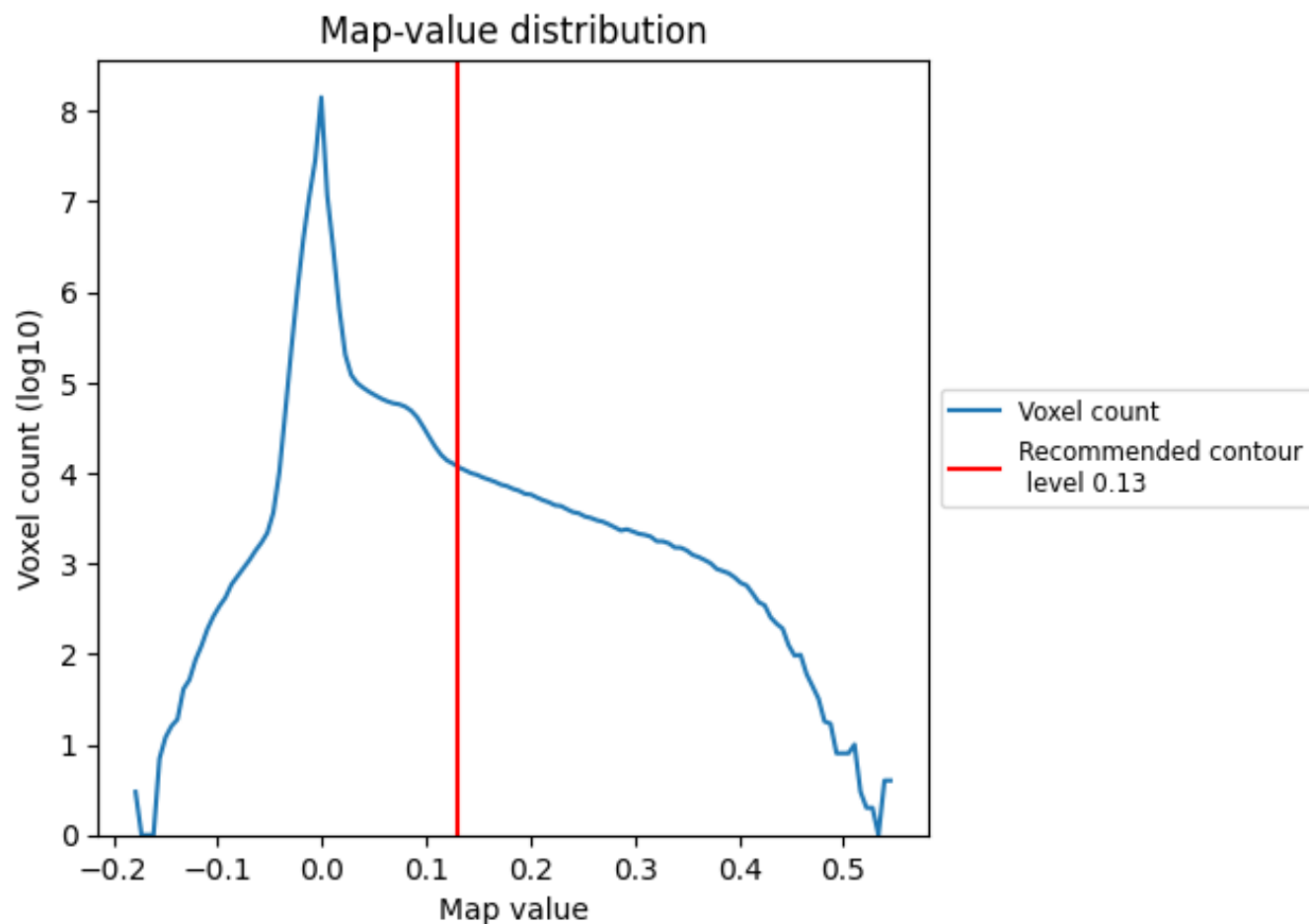


Z

7 Map analysis [i](#)

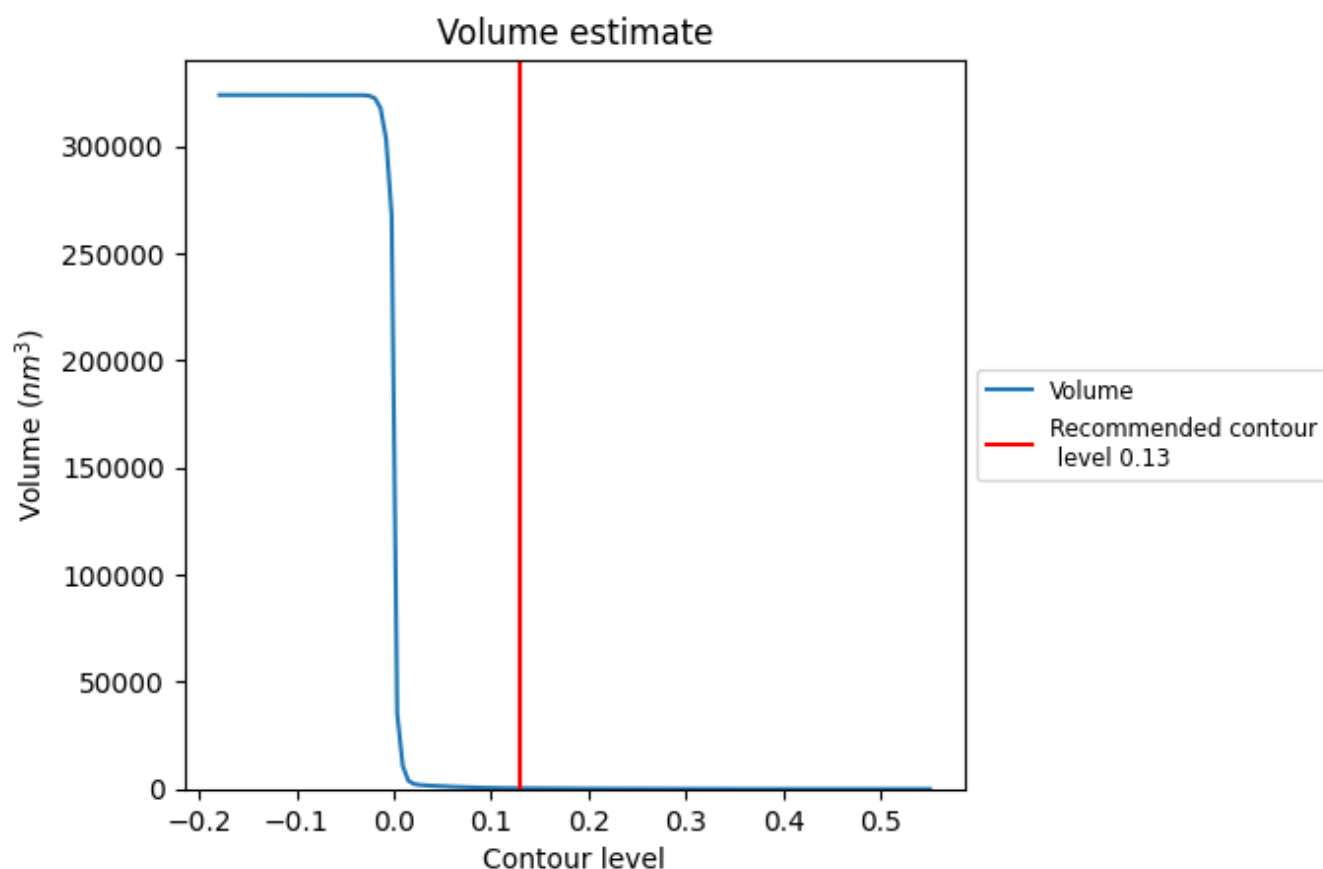
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

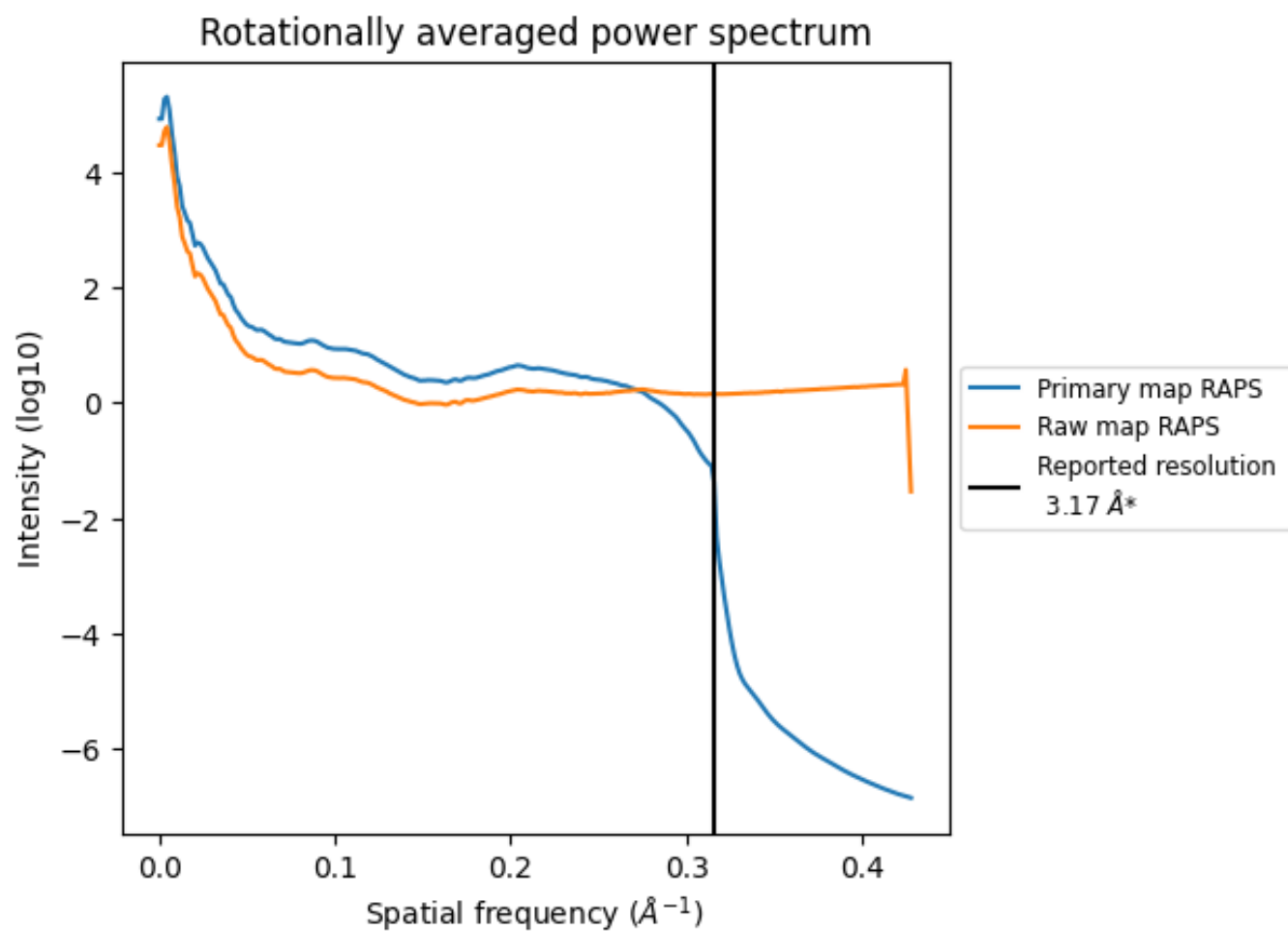
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm³; this corresponds to an approximate mass of 282 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](#)

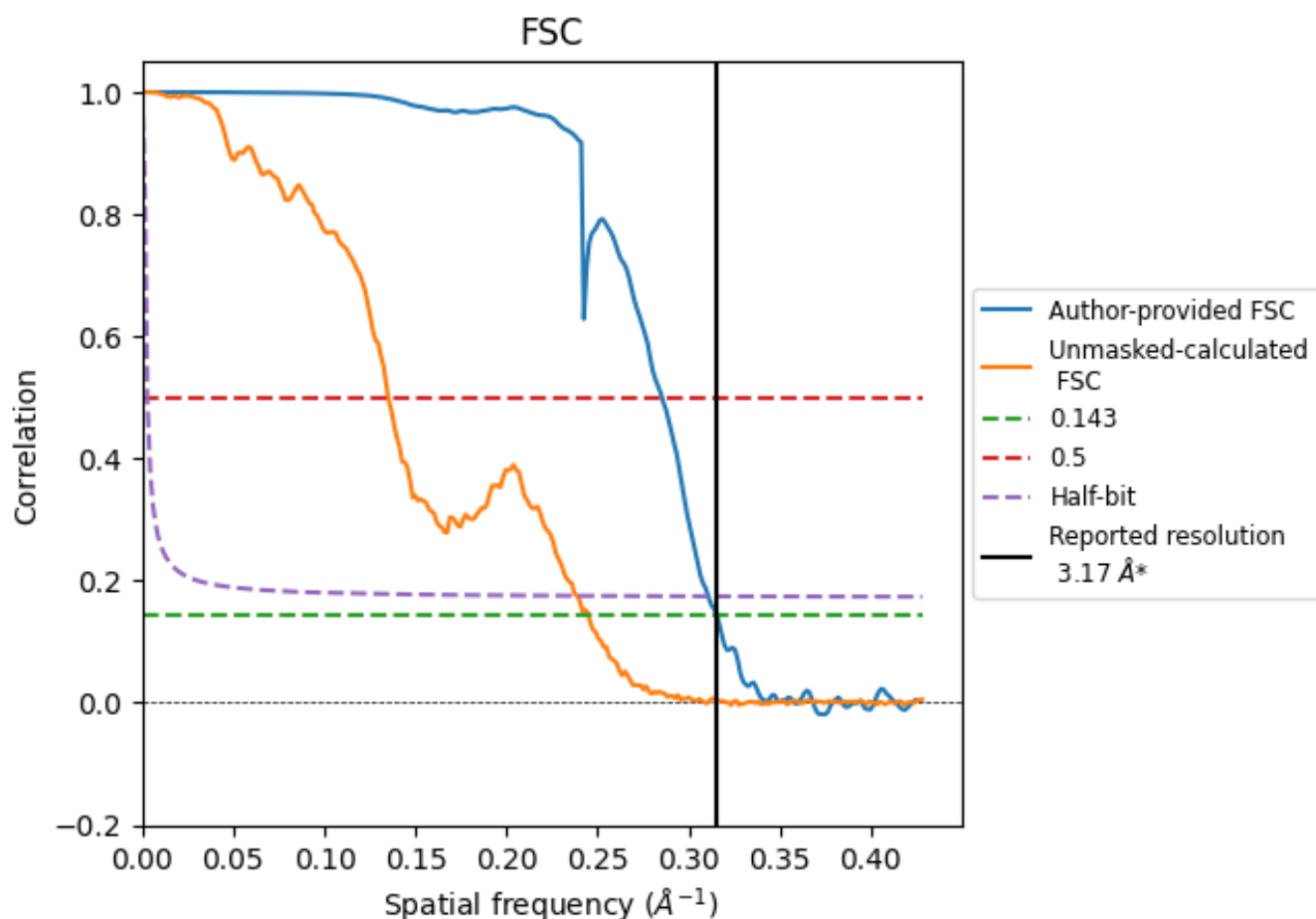


*Reported resolution corresponds to spatial frequency of 0.315 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.315 \AA^{-1}

8.2 Resolution estimates [i](#)

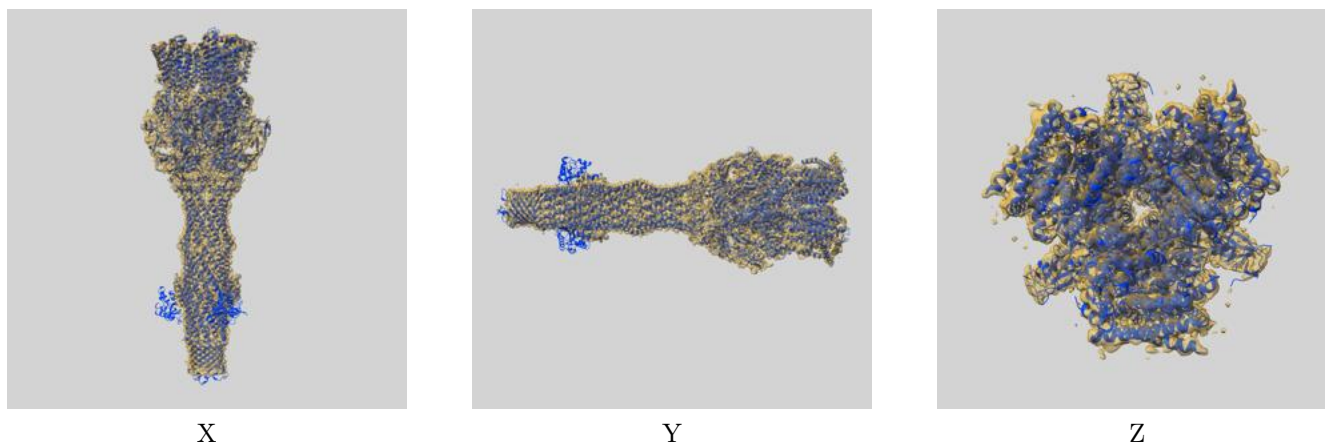
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.51	3.22
Unmasked-calculated*	4.08	7.40	4.19

*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 4.08 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

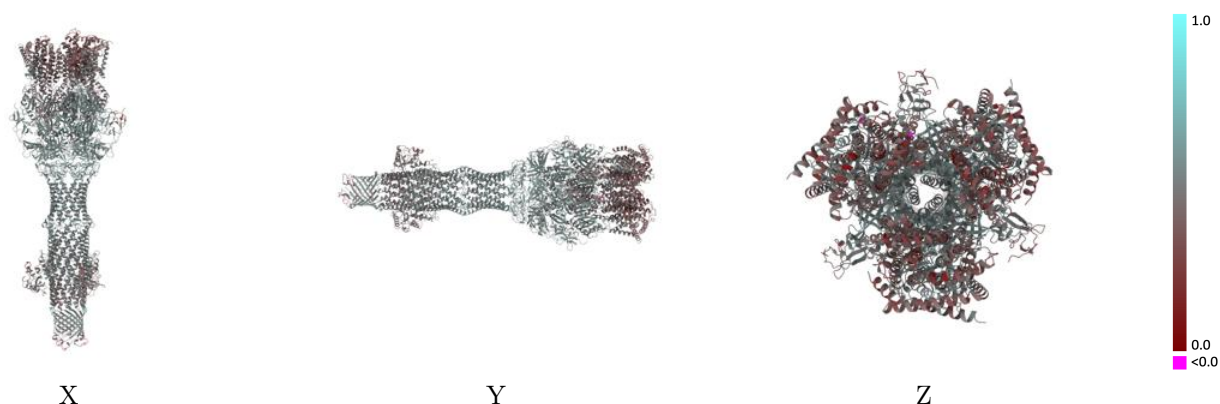
This section contains information regarding the fit between EMDB map EMD-55890 and PDB model 9TG4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



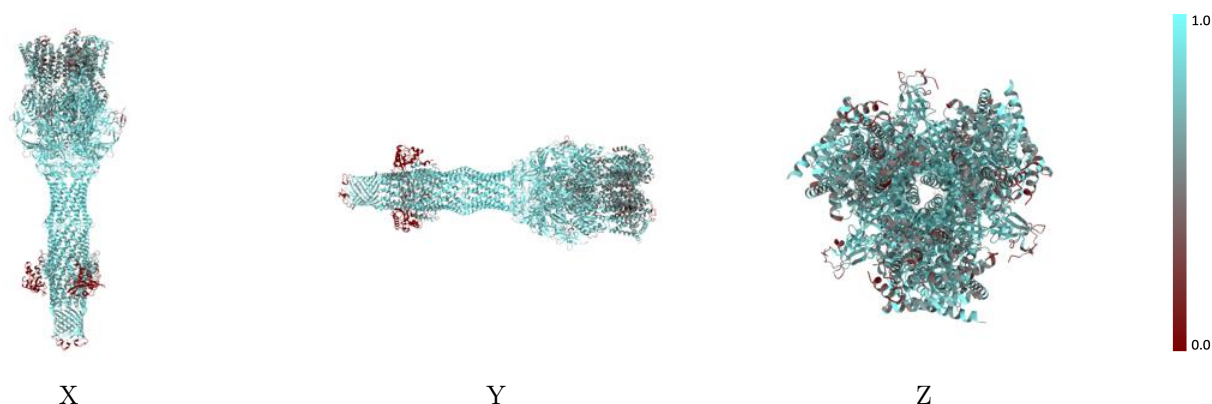
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



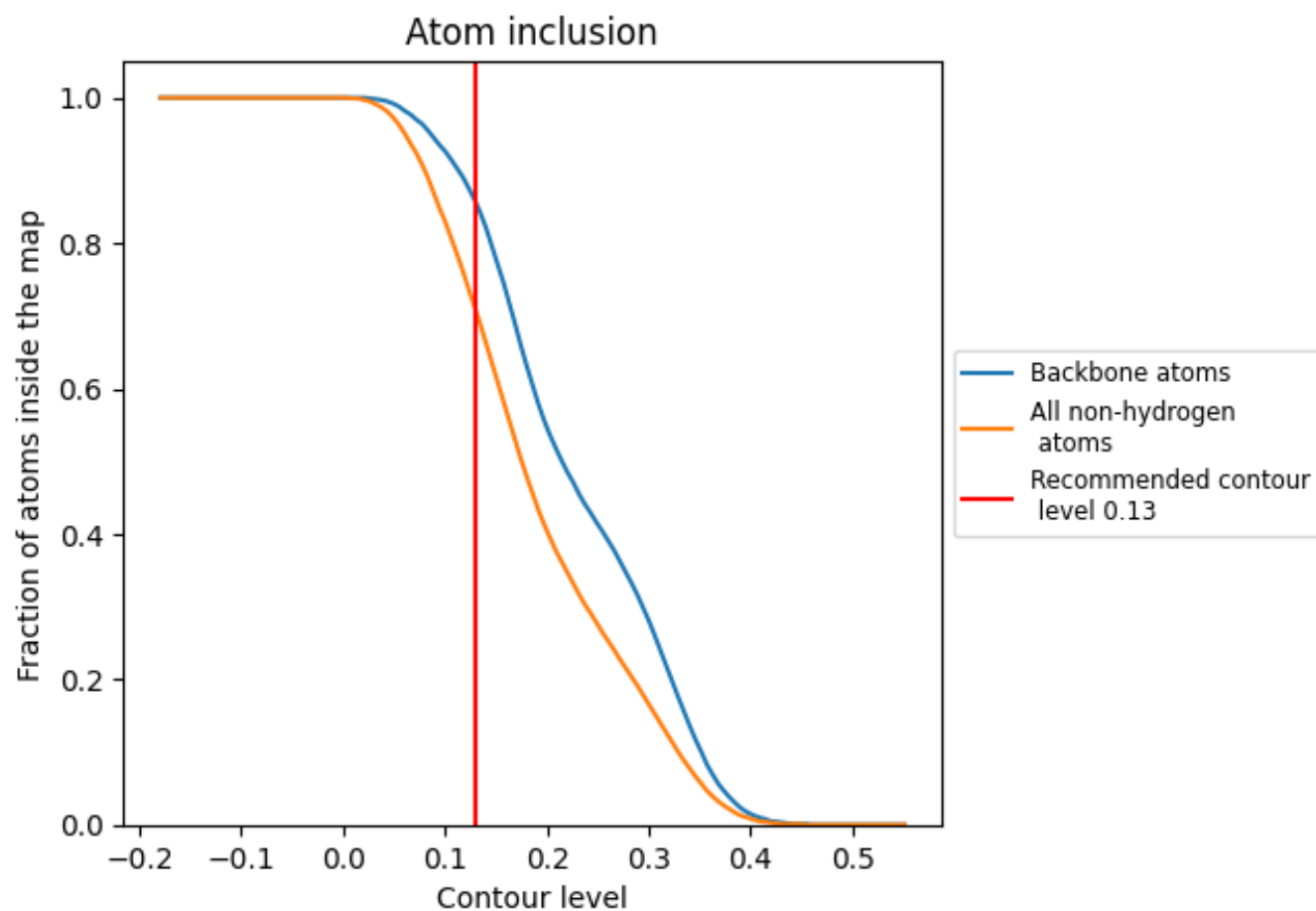
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7090	<div></div> 0.4800
A	<div></div> 0.7570	<div></div> 0.4860
B	<div></div> 0.7520	<div></div> 0.4860
C	<div></div> 0.7520	<div></div> 0.4820
D	<div></div> 0.8120	<div></div> 0.5160
E	<div></div> 0.8500	<div></div> 0.5340
F	<div></div> 0.8230	<div></div> 0.5180
G	<div></div> 0.8550	<div></div> 0.5330
H	<div></div> 0.8140	<div></div> 0.5140
I	<div></div> 0.8550	<div></div> 0.5330
J	<div></div> 0.7150	<div></div> 0.4610
K	<div></div> 0.7180	<div></div> 0.4590
L	<div></div> 0.7180	<div></div> 0.4580
M	<div></div> 0.5360	<div></div> 0.3940
N	<div></div> 0.5390	<div></div> 0.3820
O	<div></div> 0.5290	<div></div> 0.3860
P	<div></div> 0.0300	<div></div> 0.4240
Q	<div></div> 0.0310	<div></div> 0.4330
R	<div></div> 0.0320	<div></div> 0.4370

1.0

0.0

<0.0