



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 03:36 AM UTC

PDB ID : 9VJ8 / pdb\_00009vj8  
EMDB ID : EMD-65106  
Title : Type II-A CRISPR integrase complex, apo form  
Authors : Li, Z.; Li, Y.; Wu, Q.; Lu, M.; Xiao, Y.  
Deposited on : 2025-06-19  
Resolution : 3.90 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](mailto: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>.

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

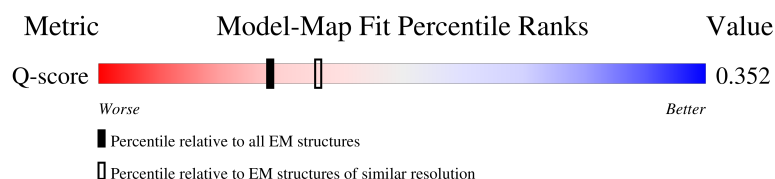
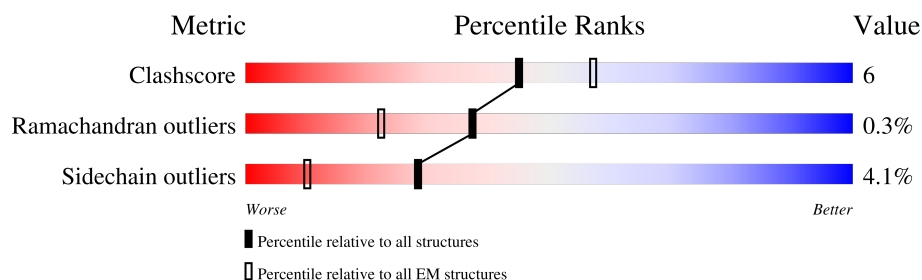
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.90 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.




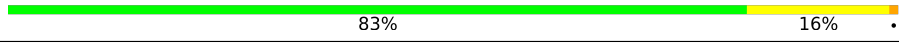
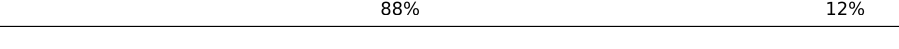




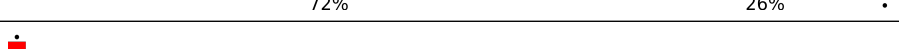


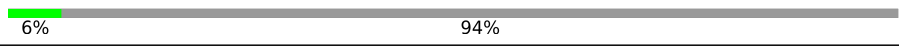
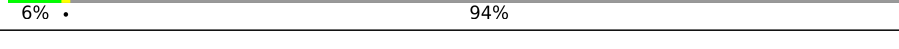
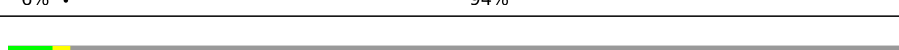





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 ( 3.40 - 4.40 )

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  $\geq 3$ , 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	219	
1	B	219	
1	C	219	
1	D	219	

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Mol	Chain	Length	Quality of chain
1	E	219	
1	F	219	
1	G	219	
1	H	219	
2	I	288	
2	J	288	
2	K	288	
2	L	288	
2	O	288	
2	P	288	
2	Q	288	
2	R	288	
3	M	109	
3	N	109	
3	U	109	
3	V	109	
4	S	1337	
4	T	1337	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 36995 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 Type II-A CRISPR-associated protein Csn2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
1	B	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
1	C	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
1	D	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
1	E	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
1	F	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
1	G	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
1	H	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	286	Total	C	N	O	S	0	0
			2347	1508	407	423	9		
2	J	287	Total	C	N	O	S	0	0
			2351	1510	408	424	9		
2	K	286	Total	C	N	O	S	0	0
			2347	1508	407	423	9		
2	L	287	Total	C	N	O	S	0	0
			2351	1510	408	424	9		
2	O	287	Total	C	N	O	S	0	0
			2351	1510	408	424	9		
2	P	287	Total	C	N	O	S	0	0
			2351	1510	408	424	9		
2	Q	286	Total	C	N	O	S	0	0
			2347	1508	407	423	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	287	Total	C	N	O	S	0	0
			2351	1510	408	424	9		

- Molecule 3 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	6	Total	C	N	O	0	0
			49	34	9	6		
3	N	7	Total	C	N	O	0	0
			54	37	10	7		
3	U	7	Total	C	N	O	0	0
			54	37	10	7		
3	V	7	Total	C	N	O	0	0
			54	37	10	7		

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	220	Total	C	N	O	S	0	0
			1828	1170	312	343	3		
4	T	220	Total	C	N	O	S	0	0
			1828	1170	312	343	3		

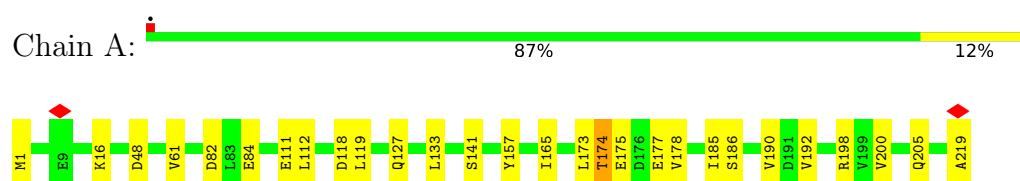
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	2	Total	Ca	0
			2	2	
5	C	1	Total	Ca	0
			1	1	
5	D	2	Total	Ca	0
			2	2	
5	E	1	Total	Ca	0
			1	1	
5	F	2	Total	Ca	0
			2	2	
5	G	1	Total	Ca	0
			1	1	
5	H	2	Total	Ca	0
			2	2	

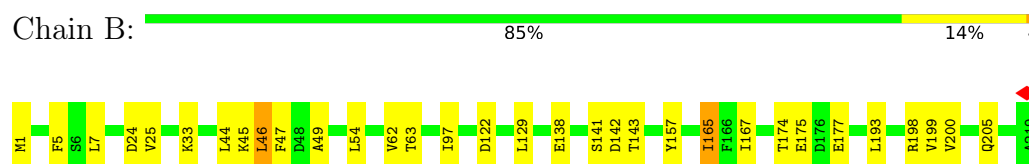
### 3 Residue-property plots [i](#)

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.

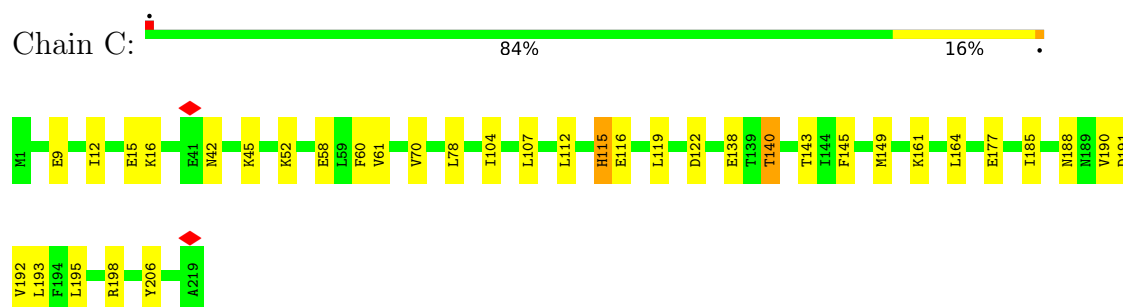
- Molecule 1: Type II-A CRISPR-associated protein Csn2



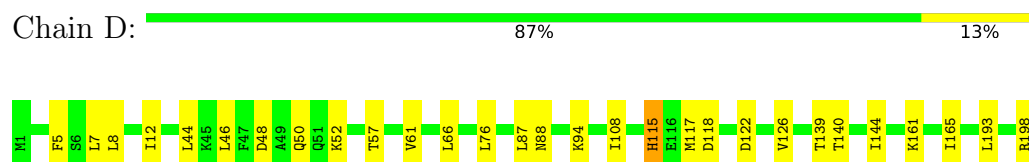
- Molecule 1: Type II-A CRISPR-associated protein Csn2



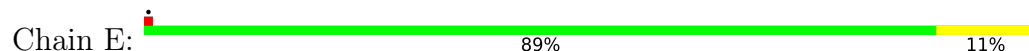
- Molecule 1: Type II-A CRISPR-associated protein Csn2



- Molecule 1: Type II-A CRISPR-associated protein Csn2



- Molecule 1: Type II-A CRISPR-associated protein Csn2





- Molecule 1: Type II-A CRISPR-associated protein Csn2

Chain F: 83% 16%



- Molecule 1: Type II-A CRISPR-associated protein Csn2

Chain G: 88% 12%



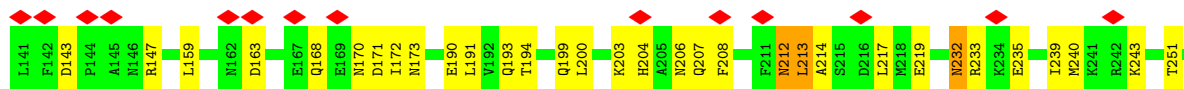
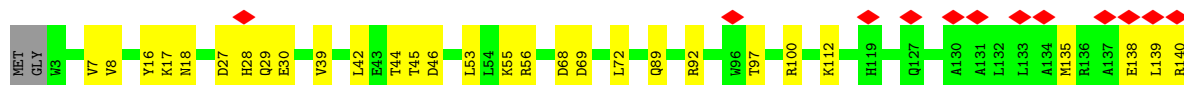
- Molecule 1: Type II-A CRISPR-associated protein Csn2

Chain H: 85% 15%



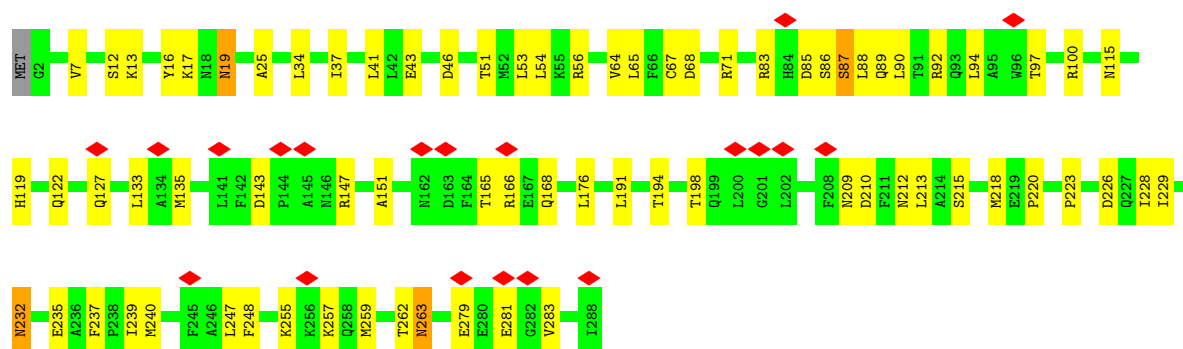
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain I: 10% 74% 24%

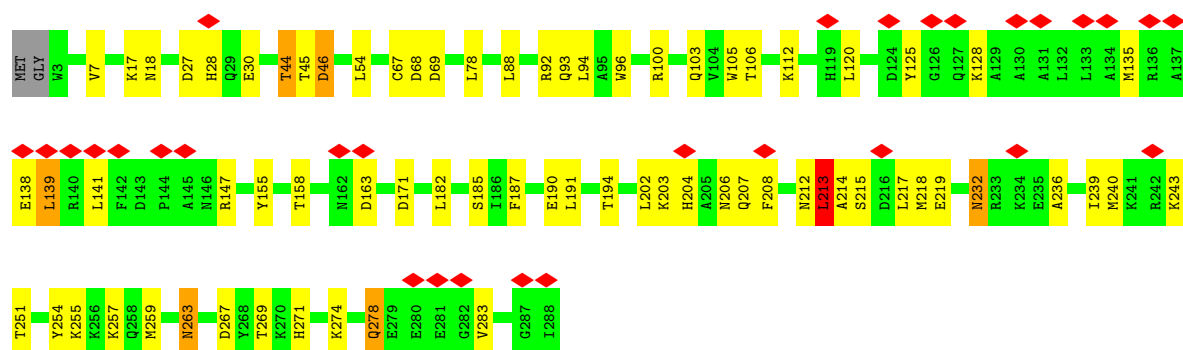


- Molecule 2: CRISPR-associated endonuclease Cas1

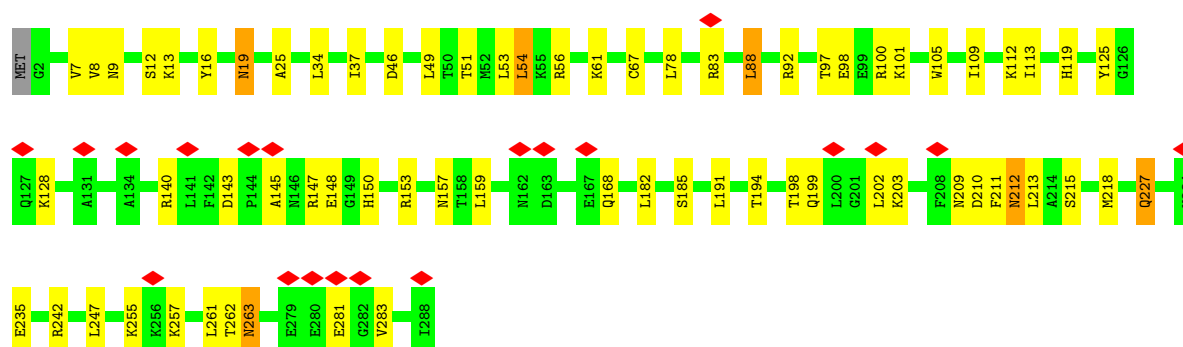
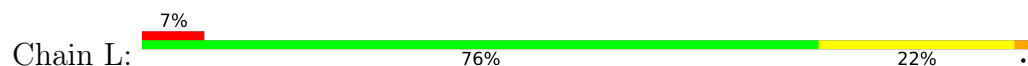
Chain J: 7% 74% 24%



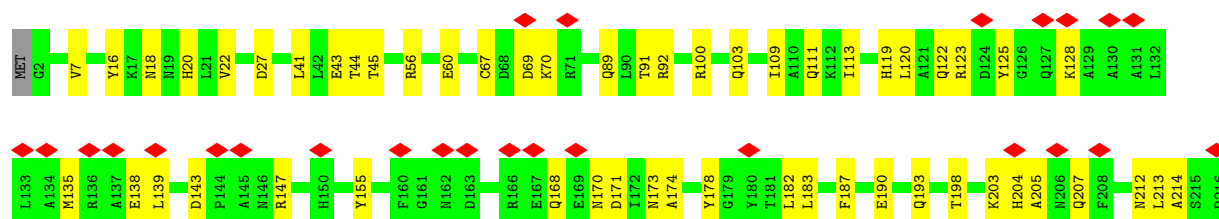
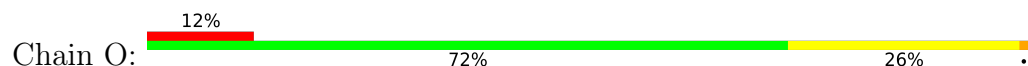
• Molecule 2: CRISPR-associated endonuclease Cas1



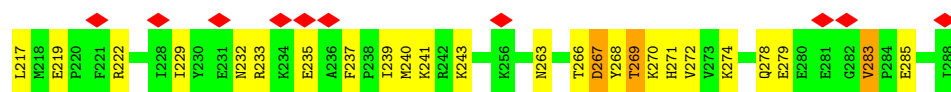
• Molecule 2: CRISPR-associated endonuclease Cas1



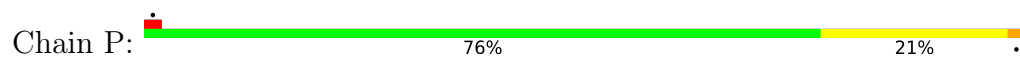
• Molecule 2: CRISPR-associated endonuclease Cas1



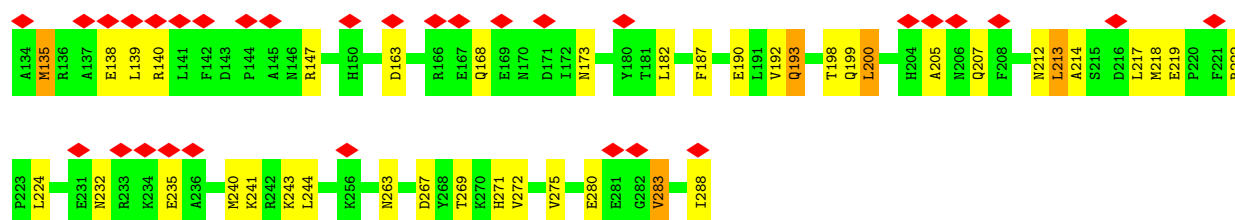
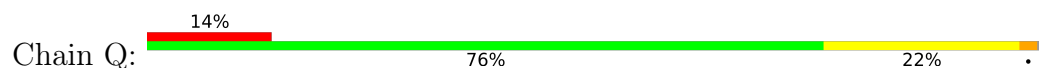




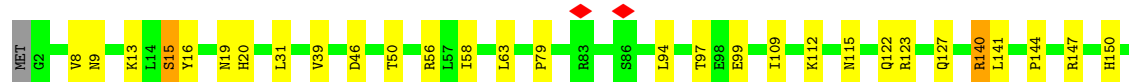
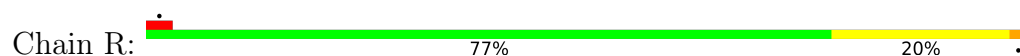
• Molecule 2: CRISPR-associated endonuclease Cas1



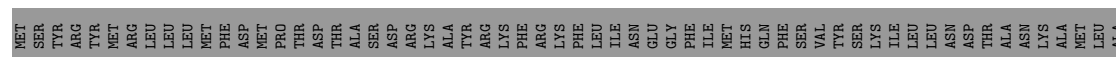
• Molecule 2: CRISPR-associated endonuclease Cas1



• Molecule 2: CRISPR-associated endonuclease Cas1



• Molecule 3: CRISPR-associated endonuclease Cas2









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52810	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.752	Depositor
Minimum map value	-0.245	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	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: CA

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	0.16	0/1817	0.31	0/2456
1	B	0.15	0/1817	0.35	0/2456
1	C	0.16	0/1817	0.35	0/2456
1	D	0.15	0/1817	0.35	0/2456
1	E	0.15	0/1817	0.30	0/2456
1	F	0.15	0/1817	0.32	0/2456
1	G	0.16	0/1817	0.32	0/2456
1	H	0.15	0/1817	0.32	0/2456
2	I	0.15	0/2395	0.37	0/3232
2	J	0.15	0/2399	0.38	1/3237 (0.0%)
2	K	0.14	0/2395	0.35	0/3232
2	L	0.15	0/2399	0.37	0/3237
2	O	0.13	0/2399	0.37	0/3237
2	P	0.14	0/2399	0.35	0/3237
2	Q	0.13	0/2395	0.38	0/3232
2	R	0.14	0/2399	0.35	0/3237
3	M	0.13	0/49	0.25	0/64
3	N	0.13	0/54	0.44	0/71
3	U	0.14	0/54	0.27	0/71
3	V	0.20	0/54	0.35	0/71
4	S	0.14	0/1861	0.30	0/2491
4	T	0.15	0/1861	0.32	0/2491
All	All	0.15	0/37649	0.35	1/50788 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	87	SER	CB-CA-C	-5.44	110.32	116.63

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	1790	0	1811	16	0
1	B	1790	0	1811	15	0
1	C	1790	0	1811	20	0
1	D	1790	0	1811	16	0
1	E	1790	0	1811	12	0
1	F	1790	0	1811	15	0
1	G	1790	0	1811	14	0
1	H	1790	0	1811	20	0
2	I	2347	0	2371	46	0
2	J	2351	0	2374	42	0
2	K	2347	0	2371	43	0
2	L	2351	0	2374	42	0
2	O	2351	0	2374	48	0
2	P	2351	0	2374	44	0
2	Q	2347	0	2371	37	0
2	R	2351	0	2374	41	0
3	M	49	0	55	0	0
3	N	54	0	57	1	0
3	U	54	0	57	0	0
3	V	54	0	57	1	0
4	S	1828	0	1849	6	0
4	T	1828	0	1849	12	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
All	All	36995	0	37395	469	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 (469) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:58:ILE:HD11	2:R:79:PRO:HG3	1.74	0.69
2:Q:275:VAL:HG22	2:Q:280:GLU:HB3	1.74	0.69
1:A:173:LEU:HB3	1:A:177:GLU:HB2	1.76	0.68
2:O:272:VAL:HG12	2:O:283:VAL:HG21	1.76	0.68
2:P:93:GLN:O	2:P:96:TRP:NE1	2.27	0.68
2:P:200:LEU:O	2:P:212:ASN:ND2	2.19	0.68
1:E:173:LEU:HB3	1:E:177:GLU:HB2	1.76	0.67
2:O:229:ILE:O	2:O:233:ARG:NH1	2.27	0.67
2:I:135:MET:O	2:I:147:ARG:NH2	2.29	0.66
2:O:111:GLN:HB2	2:O:285:GLU:HG2	1.78	0.66
2:P:92:ARG:O	2:P:92:ARG:NH1	2.29	0.66
2:R:170:ASN:OD1	2:R:173:ASN:ND2	2.29	0.65
2:J:16:TYR:OH	2:J:56:ARG:NH1	2.30	0.65
2:L:16:TYR:OH	2:L:56:ARG:NH1	2.29	0.65
2:L:215:SER:HA	2:L:218:MET:HE3	1.78	0.65
2:R:200:LEU:O	2:R:212:ASN:ND2	2.29	0.65
1:C:198:ARG:HB2	1:D:198:ARG:HH22	1.62	0.65
2:I:172:ILE:HD11	2:I:233:ARG:HG3	1.78	0.64
2:O:100:ARG:HG2	2:O:278:GLN:HE22	1.63	0.64
2:O:214:ALA:HA	2:O:217:LEU:HB2	1.80	0.63
1:D:139:THR:HG23	1:D:140:THR:HG23	1.80	0.63
2:K:263:ASN:OD1	2:K:263:ASN:N	2.27	0.63
2:L:263:ASN:OD1	2:L:263:ASN:N	2.21	0.63
1:E:185:ILE:HD13	1:E:192:VAL:HG11	1.80	0.62
2:K:135:MET:O	2:K:147:ARG:NH2	2.33	0.62
2:Q:125:TYR:HB3	2:Q:128:LYS:HE2	1.81	0.62
2:P:11:HIS:HD2	2:P:46:ASP:HB2	1.65	0.62
2:P:63:LEU:HB2	2:P:189:ARG:HG3	1.81	0.62
2:Q:214:ALA:HA	2:Q:217:LEU:HB2	1.81	0.62
1:C:9:GLU:OE2	2:P:13:LYS:NZ	2.33	0.62
1:A:185:ILE:HD13	1:A:192:VAL:HG11	1.82	0.61
1:H:165:ILE:HG22	1:H:193:LEU:HB3	1.81	0.61
2:O:45:THR:HG23	2:P:52:MET:HE3	1.82	0.61
2:Q:199:GLN:HG2	2:Q:200:LEU:HD22	1.81	0.61
2:R:235:GLU:HB2	2:R:239:ILE:HD13	1.80	0.61
1:G:9:GLU:OE2	2:R:13:LYS:NZ	2.34	0.61
2:J:215:SER:HA	2:J:218:MET:HE3	1.83	0.60
1:A:61:VAL:HG12	1:A:165:ILE:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLN:NE2	1:H:114:GLU:OE1	2.34	0.60
2:P:191:LEU:O	2:P:194:THR:OG1	2.20	0.59
2:P:46:ASP:OD1	2:P:46:ASP:N	2.35	0.59
2:J:43:GLU:HG2	2:J:71:ARG:HD2	1.84	0.59
1:G:197:GLN:OE1	1:H:198:ARG:NH1	2.33	0.59
1:A:174:THR:OG1	1:A:175:GLU:N	2.34	0.59
2:K:44:THR:OG1	2:K:45:THR:N	2.34	0.59
2:K:125:TYR:HB3	2:K:128:LYS:HE3	1.84	0.59
2:Q:275:VAL:HG21	2:Q:283:VAL:HB	1.84	0.59
2:I:206:ASN:O	2:I:208:PHE:N	2.36	0.59
2:P:211:PHE:O	2:P:215:SER:N	2.32	0.58
2:Q:232:ASN:HD22	2:Q:235:GLU:HB2	1.69	0.58
2:O:267:ASP:O	2:O:271:HIS:ND1	2.34	0.58
2:J:263:ASN:OD1	2:J:263:ASN:N	2.22	0.58
2:P:263:ASN:N	2:P:263:ASN:OD1	2.35	0.57
1:D:61:VAL:HG22	1:D:165:ILE:HD11	1.84	0.57
2:R:255:LYS:O	2:R:257:LYS:NZ	2.37	0.57
2:P:19:ASN:O	2:P:20:HIS:ND1	2.38	0.57
2:R:63:LEU:HB3	2:R:189:ARG:HG3	1.86	0.57
2:J:165:THR:H	2:J:168:GLN:HG2	1.70	0.57
2:K:46:ASP:N	2:K:46:ASP:OD1	2.38	0.57
2:O:232:ASN:O	2:O:233:ARG:NH1	2.37	0.57
2:R:140:ARG:NH1	2:R:141:LEU:O	2.38	0.56
2:R:211:PHE:HB3	2:R:214:ALA:HB3	1.86	0.56
1:F:24:ASP:OD1	1:F:25:VAL:N	2.39	0.56
2:R:273:VAL:O	2:R:277:ASN:ND2	2.39	0.56
2:R:257:LYS:HD2	2:R:259:MET:HE3	1.87	0.56
1:G:185:ILE:HG23	1:G:190:VAL:HG23	1.87	0.56
2:I:232:ASN:N	2:I:232:ASN:OD1	2.38	0.56
2:K:191:LEU:O	2:K:194:THR:OG1	2.24	0.56
2:R:263:ASN:OD1	2:R:263:ASN:N	2.29	0.56
2:L:8:VAL:HG12	3:N:106:LEU:HB2	1.88	0.56
1:F:75:THR:HG22	1:F:158:LEU:HD11	1.88	0.56
1:G:191:ASP:N	1:G:191:ASP:OD1	2.38	0.56
1:B:1:MET:HG3	1:B:49:ALA:HB2	1.87	0.56
2:J:100:ARG:NH2	2:J:281:GLU:OE2	2.39	0.56
2:J:232:ASN:OD1	2:J:232:ASN:N	2.38	0.55
4:T:540:ASP:N	4:T:540:ASP:OD1	2.39	0.55
2:J:235:GLU:HG3	2:J:239:ILE:HD12	1.88	0.55
2:P:157:ASN:HD22	2:P:162:ASN:HA	1.71	0.55
2:Q:37:ILE:HB	2:Q:62:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:584:ILE:HD12	4:T:587:LEU:HD21	1.89	0.55
1:A:16:LYS:HD2	1:A:186:SER:HA	1.87	0.55
2:I:46:ASP:OD1	2:I:46:ASP:N	2.40	0.55
2:J:115:ASN:ND2	2:J:220:PRO:O	2.39	0.55
1:D:165:ILE:HG22	1:D:193:LEU:HB3	1.87	0.55
2:I:44:THR:OG1	2:I:45:THR:N	2.39	0.55
2:K:232:ASN:N	2:K:232:ASN:OD1	2.39	0.55
2:Q:240:MET:HA	2:Q:243:LYS:HG2	1.89	0.55
2:Q:63:LEU:HD11	2:Q:76:LYS:HE2	1.89	0.54
4:S:569:LYS:HG3	4:S:587:LEU:HD12	1.89	0.54
2:I:140:ARG:HH12	2:I:143:ASP:HB2	1.70	0.54
2:R:191:LEU:O	2:R:194:THR:OG1	2.24	0.54
1:B:24:ASP:OD1	1:B:25:VAL:N	2.40	0.54
2:L:191:LEU:O	2:L:194:THR:OG1	2.22	0.54
4:T:568:LYS:HD2	4:T:570:LYS:HE2	1.89	0.54
1:H:118:ASP:OD1	1:H:118:ASP:N	2.41	0.54
2:J:210:ASP:OD1	2:J:210:ASP:N	2.39	0.54
2:J:135:MET:HE1	2:J:147:ARG:HE	1.72	0.54
1:H:8:LEU:HD21	1:H:12:ILE:HG12	1.90	0.54
1:D:8:LEU:HD21	1:D:12:ILE:HG12	1.88	0.54
2:L:51:THR:HA	2:L:54:LEU:HD23	1.90	0.54
1:A:1:MET:HB3	1:A:48:ASP:HA	1.89	0.53
1:B:129:LEU:HD21	1:C:104:ILE:HD11	1.89	0.53
1:C:191:ASP:OD1	1:C:191:ASP:N	2.41	0.53
4:S:564:ARG:HD2	4:S:567:VAL:HG12	1.90	0.53
2:Q:25:ALA:O	2:Q:29:GLN:NE2	2.41	0.53
1:E:174:THR:OG1	1:E:175:GLU:N	2.41	0.53
2:K:203:LYS:HG2	2:K:204:HIS:H	1.74	0.53
4:S:556:ILE:HD11	4:S:572:ILE:HD12	1.90	0.53
1:E:82:ASP:OD2	1:E:157:TYR:OH	2.27	0.53
1:F:84:GLU:OE2	1:F:88:ASN:ND2	2.42	0.53
2:I:138:GLU:OE2	2:I:147:ARG:NE	2.40	0.53
2:O:125:TYR:HB3	2:O:128:LYS:HE2	1.91	0.53
2:L:140:ARG:HH22	2:L:145:ALA:H	1.57	0.53
2:O:43:GLU:HA	2:O:67:CYS:HB2	1.89	0.53
2:L:125:TYR:HB3	2:L:128:LYS:HE2	1.90	0.53
2:Q:119:HIS:O	2:Q:123:ARG:NH1	2.41	0.53
1:C:112:LEU:HD11	1:C:119:LEU:HD12	1.91	0.52
1:F:66:LEU:HD13	1:F:147:LYS:HG3	1.91	0.52
2:K:27:ASP:N	2:K:27:ASP:OD1	2.42	0.52
2:P:255:LYS:O	2:P:257:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:168:GLN:O	2:P:173:ASN:ND2	2.42	0.52
2:J:191:LEU:O	2:J:194:THR:OG1	2.25	0.52
2:Q:163:ASP:O	2:Q:168:GLN:NE2	2.42	0.52
2:P:160:PHE:HE1	2:P:233:ARG:HD2	1.74	0.52
2:Q:187:PHE:HB3	2:Q:214:ALA:HB1	1.90	0.52
2:I:203:LYS:HG2	2:I:204:HIS:H	1.75	0.52
1:B:97:ILE:HD11	1:C:107:LEU:HD22	1.91	0.52
2:K:88:LEU:HB3	2:K:92:ARG:HH21	1.74	0.52
2:O:44:THR:OG1	2:O:45:THR:N	2.37	0.52
1:A:82:ASP:OD2	1:A:157:TYR:OH	2.26	0.52
2:Q:218:MET:HG3	2:Q:222:ARG:HH21	1.74	0.52
2:I:112:LYS:HD2	2:I:219:GLU:HB3	1.91	0.52
2:J:237:PHE:HA	2:J:240:MET:HE2	1.90	0.52
2:Q:241:LYS:HD3	2:Q:244:LEU:HD21	1.91	0.52
1:D:88:ASN:OD1	1:D:94:LYS:NZ	2.43	0.52
1:E:142:ASP:O	1:F:33:LYS:NZ	2.32	0.52
2:K:251:THR:OG1	2:K:259:MET:O	2.27	0.52
2:L:98:GLU:HA	2:L:101:LYS:HE2	1.92	0.52
2:Q:267:ASP:O	2:Q:271:HIS:ND1	2.33	0.52
2:R:140:ARG:HH22	2:R:144:PRO:HD2	1.74	0.51
2:K:78:LEU:HD22	2:L:78:LEU:HD22	1.93	0.51
2:O:138:GLU:OE1	2:O:138:GLU:N	2.43	0.51
2:R:211:PHE:O	2:R:215:SER:N	2.40	0.51
2:L:140:ARG:HH22	2:L:145:ALA:HB3	1.76	0.51
2:R:97:THR:OG1	2:R:99:GLU:OE1	2.28	0.51
2:L:101:LYS:HB2	2:L:202:LEU:HD12	1.93	0.51
4:S:713:GLN:HG2	4:S:714:LEU:HD22	1.91	0.51
2:L:109:ILE:O	2:L:112:LYS:HG3	2.11	0.51
2:P:115:ASN:HB3	2:P:288:ILE:HG12	1.90	0.51
2:P:16:TYR:OH	2:P:56:ARG:NH1	2.43	0.51
2:K:236:ALA:H	2:K:239:ILE:HD12	1.76	0.51
1:A:112:LEU:HD21	1:A:119:LEU:HB2	1.93	0.51
2:I:39:VAL:HG11	2:I:193:GLN:HE21	1.76	0.51
2:L:210:ASP:OD1	2:L:210:ASP:N	2.43	0.51
2:I:16:TYR:OH	2:I:56:ARG:NH1	2.44	0.51
2:L:255:LYS:O	2:L:257:LYS:NZ	2.39	0.51
2:P:253:MET:HE1	2:P:256:LYS:HA	1.93	0.51
2:I:68:ASP:OD1	2:I:72:LEU:N	2.34	0.50
1:C:164:LEU:HB3	1:C:192:VAL:HG12	1.93	0.50
2:I:140:ARG:HH22	2:I:143:ASP:HA	1.76	0.50
2:L:12:SER:OG	2:L:13:LYS:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:271:HIS:HA	2:O:274:LYS:HZ2	1.76	0.50
1:D:48:ASP:OD1	1:D:52:LYS:N	2.35	0.50
1:H:61:VAL:HG22	1:H:165:ILE:HD11	1.92	0.50
2:I:89:GLN:HA	2:I:92:ARG:HB2	1.93	0.50
2:I:191:LEU:O	2:I:194:THR:OG1	2.25	0.50
2:P:227:GLN:NE2	2:P:231:GLU:OE2	2.43	0.50
2:Q:135:MET:O	2:Q:147:ARG:NH1	2.44	0.50
2:J:51:THR:HA	2:J:54:LEU:HD23	1.92	0.50
2:Q:109:ILE:O	2:Q:112:LYS:HG3	2.12	0.50
2:R:46:ASP:N	2:R:46:ASP:OD1	2.44	0.50
4:T:556:ILE:HD11	4:T:572:ILE:HD12	1.93	0.50
1:A:205:GLN:HE21	1:A:219:ALA:HB3	1.76	0.50
2:P:228:ILE:HG13	2:P:247:LEU:HD12	1.94	0.50
1:H:57:THR:O	1:H:161:LYS:NZ	2.40	0.50
2:K:267:ASP:O	2:K:271:HIS:ND1	2.41	0.50
2:O:170:ASN:H	2:O:173:ASN:HD21	1.59	0.50
2:R:16:TYR:OH	2:R:56:ARG:NH1	2.45	0.50
1:D:118:ASP:OD1	1:D:118:ASP:N	2.45	0.50
2:K:240:MET:HA	2:K:243:LYS:HE3	1.93	0.50
2:J:143:ASP:OD2	2:J:147:ARG:N	2.44	0.49
2:O:203:LYS:NZ	2:O:205:ALA:O	2.44	0.49
2:Q:83:ARG:NH1	2:Q:87:SER:OG	2.45	0.49
2:Q:118:LEU:HD11	2:Q:288:ILE:HG23	1.93	0.49
1:B:199:VAL:HG13	1:B:205:GLN:HE22	1.77	0.49
1:H:88:ASN:HA	1:H:94:LYS:HD2	1.94	0.49
2:I:168:GLN:OE1	2:I:170:ASN:ND2	2.45	0.49
2:P:210:ASP:OD1	2:P:210:ASP:N	2.44	0.49
1:D:66:LEU:HD11	1:D:144:ILE:HG12	1.92	0.49
2:I:44:THR:OG1	2:I:46:ASP:OD1	2.21	0.49
2:L:209:ASN:HD21	2:L:211:PHE:HD2	1.59	0.49
2:O:123:ARG:NH1	2:O:125:TYR:OH	2.45	0.49
1:H:174:THR:HG22	1:H:177:GLU:HG2	1.95	0.49
2:Q:112:LYS:HB3	2:Q:219:GLU:HB2	1.95	0.49
2:P:215:SER:HA	2:P:218:MET:HE2	1.94	0.49
2:I:27:ASP:OD1	2:I:27:ASP:N	2.42	0.49
1:E:2:ARG:HH11	1:E:13:GLU:HG2	1.78	0.49
2:Q:71:ARG:HH22	2:Q:182:LEU:HD22	1.78	0.49
2:O:143:ASP:OD1	2:O:143:ASP:N	2.38	0.48
2:J:212:ASN:OD1	2:J:213:LEU:N	2.42	0.48
2:O:190:GLU:O	2:O:193:GLN:HG3	2.14	0.48
2:J:255:LYS:O	2:J:257:LYS:NZ	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:143:ASP:OD1	2:L:147:ARG:N	2.41	0.48
2:O:27:ASP:OD1	2:O:27:ASP:N	2.45	0.48
2:P:140:ARG:NH1	2:P:141:LEU:H	2.11	0.48
2:Q:240:MET:HG2	2:Q:243:LYS:HE3	1.95	0.48
2:J:16:TYR:HB2	2:J:53:LEU:HD13	1.96	0.48
2:Q:190:GLU:O	2:Q:193:GLN:HG3	2.14	0.48
2:Q:205:ALA:O	2:Q:207:GLN:NE2	2.46	0.48
1:C:185:ILE:HG23	1:C:190:VAL:HG23	1.94	0.48
1:E:170:CYS:HB2	1:E:196:GLU:HG2	1.96	0.48
2:O:7:VAL:HG22	2:O:41:LEU:HB2	1.95	0.48
2:R:156:PHE:HB3	2:R:164:PHE:HD2	1.79	0.48
1:C:42:ASN:O	1:C:45:LYS:NZ	2.46	0.48
1:G:82:ASP:OD2	1:G:157:TYR:OH	2.32	0.48
2:J:12:SER:OG	2:J:13:LYS:N	2.46	0.48
2:I:100:ARG:HE	2:I:278:GLN:NE2	2.12	0.48
2:L:9:ASN:N	2:L:9:ASN:OD1	2.45	0.48
2:O:16:TYR:OH	2:O:56:ARG:NH1	2.47	0.48
2:O:212:ASN:O	2:O:214:ALA:N	2.47	0.48
2:P:213:LEU:HD12	2:P:216:ASP:HB2	1.97	0.47
2:L:199:GLN:HA	2:L:212:ASN:HD21	1.79	0.47
1:B:45:LYS:HE3	1:B:47:PHE:HB2	1.97	0.47
1:E:185:ILE:HG23	1:E:190:VAL:HG23	1.96	0.47
2:I:251:THR:OG1	2:I:259:MET:O	2.31	0.47
2:K:106:THR:HG21	2:K:141:LEU:HA	1.96	0.47
2:Q:27:ASP:OD1	2:Q:27:ASP:N	2.46	0.47
1:C:60:PHE:HB2	1:C:161:LYS:HD3	1.96	0.47
1:G:15:GLU:HG2	1:G:16:LYS:HG2	1.97	0.47
2:I:199:GLN:O	2:I:212:ASN:ND2	2.46	0.47
2:O:171:ASP:OD1	2:O:171:ASP:N	2.41	0.47
1:A:84:GLU:OE1	1:A:127:GLN:NE2	2.47	0.47
1:F:165:ILE:HD12	1:F:193:LEU:HD23	1.96	0.47
2:K:163:ASP:N	2:K:163:ASP:OD1	2.48	0.47
2:L:140:ARG:NH2	2:L:145:ALA:H	2.11	0.47
2:Q:168:GLN:O	2:Q:173:ASN:ND2	2.47	0.47
1:A:141:SER:O	1:B:33:LYS:NZ	2.37	0.47
1:E:21:THR:HB	1:E:207:ILE:HD13	1.97	0.47
1:E:39:ASP:OD1	1:E:39:ASP:N	2.47	0.47
1:H:200:VAL:O	1:H:205:GLN:NE2	2.48	0.47
2:I:17:LYS:HG3	2:I:18:ASN:ND2	2.30	0.47
2:I:163:ASP:OD1	2:I:163:ASP:N	2.47	0.47
2:J:34:LEU:HD12	2:J:37:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:198:THR:O	2:J:198:THR:OG1	2.32	0.47
2:O:203:LYS:HZ3	2:O:205:ALA:H	1.63	0.47
2:P:223:PRO:HG2	2:P:288:ILE:HG21	1.97	0.47
1:D:48:ASP:OD2	1:D:52:LYS:NZ	2.48	0.46
2:P:223:PRO:HB2	2:P:288:ILE:HD13	1.97	0.46
2:P:223:PRO:HA	2:P:226:ASP:HB2	1.96	0.46
2:L:49:LEU:HD11	2:L:53:LEU:HD22	1.97	0.46
2:P:43:GLU:CD	2:P:71:ARG:HE	2.24	0.46
2:P:139:LEU:HD23	2:P:139:LEU:H	1.81	0.46
1:G:145:PHE:O	1:G:149:MET:HG2	2.15	0.46
2:J:67:CYS:SG	2:J:68:ASP:N	2.88	0.46
2:R:260:PHE:H	2:R:263:ASN:HD21	1.62	0.46
2:I:240:MET:HA	2:I:243:LYS:HE3	1.97	0.46
2:O:235:GLU:HB3	2:O:239:ILE:HB	1.97	0.46
1:A:198:ARG:HB2	1:B:198:ARG:HH21	1.80	0.46
1:H:21:THR:HG21	1:H:199:VAL:HG12	1.98	0.46
2:J:89:GLN:HB2	2:J:92:ARG:HH21	1.80	0.46
2:K:120:LEU:HD11	2:K:155:TYR:HA	1.98	0.46
2:L:150:HIS:CD2	2:L:153:ARG:HH22	2.33	0.46
1:C:177:GLU:H	1:C:177:GLU:CD	2.24	0.46
2:O:269:THR:HA	2:O:272:VAL:HG22	1.96	0.46
2:R:39:VAL:HG12	2:R:63:LEU:HD21	1.96	0.46
2:R:251:THR:OG1	2:R:259:MET:O	2.26	0.46
4:S:537:SER:HB2	4:S:545:LYS:HD2	1.97	0.46
1:B:46:LEU:HB3	1:B:54:LEU:HD12	1.98	0.46
2:I:212:ASN:OD1	2:I:212:ASN:N	2.49	0.46
2:L:34:LEU:HD12	2:L:37:ILE:HD12	1.97	0.46
2:L:143:ASP:OD2	2:L:148:GLU:N	2.47	0.46
2:P:15:SER:OG	2:P:16:TYR:N	2.48	0.46
2:I:212:ASN:O	2:I:214:ALA:N	2.49	0.45
2:L:153:ARG:O	2:L:157:ASN:ND2	2.37	0.45
2:Q:73:PRO:HG3	2:Q:192:VAL:HG21	1.97	0.45
2:O:178:TYR:CG	2:O:241:LYS:HE3	2.51	0.45
2:P:234:LYS:HB2	2:P:234:LYS:HE2	1.69	0.45
1:C:15:GLU:HG2	1:C:16:LYS:HG2	1.98	0.45
1:F:141:SER:OG	1:F:142:ASP:N	2.44	0.45
2:O:89:GLN:HA	2:O:92:ARG:HG2	1.99	0.45
2:R:122:GLN:HG3	2:R:123:ARG:HH21	1.82	0.45
1:C:185:ILE:HD13	1:C:192:VAL:HG21	1.98	0.45
2:I:199:GLN:OE1	2:I:199:GLN:N	2.47	0.45
2:Q:69:ASP:OD1	2:Q:70:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:135:MET:HB2	2:K:147:ARG:HH21	1.82	0.45
2:J:41:LEU:HD12	2:J:65:LEU:HB2	1.99	0.45
2:O:91:THR:OG1	2:P:206:ASN:ND2	2.39	0.45
2:O:100:ARG:O	2:O:103:GLN:HG3	2.16	0.45
2:P:50:THR:OG1	2:P:51:THR:N	2.49	0.45
1:A:185:ILE:HG23	1:A:190:VAL:HG23	1.98	0.45
2:J:19:ASN:OD1	2:J:19:ASN:N	2.50	0.45
2:K:254:TYR:O	2:K:255:LYS:HG3	2.17	0.45
2:J:257:LYS:HD2	2:J:259:MET:HE3	1.99	0.45
2:L:88:LEU:HD12	2:L:92:ARG:HG3	1.99	0.45
2:Q:212:ASN:O	2:Q:214:ALA:N	2.50	0.45
1:H:2:ARG:HH21	1:H:11:PRO:HG3	1.82	0.45
2:K:105:TRP:CH2	2:K:203:LYS:HG3	2.52	0.45
2:O:263:ASN:HA	2:O:266:THR:HG22	1.99	0.45
1:C:145:PHE:O	1:C:149:MET:HG2	2.16	0.45
1:D:139:THR:OG1	1:D:140:THR:N	2.49	0.44
1:G:12:ILE:HG23	1:G:206:TYR:HE2	1.82	0.44
2:I:170:ASN:OD1	2:I:173:ASN:ND2	2.50	0.44
2:I:235:GLU:HB2	2:I:239:ILE:HD12	2.00	0.44
2:K:69:ASP:OD1	2:K:69:ASP:N	2.49	0.44
2:K:278:GLN:HE21	2:K:278:GLN:HB3	1.53	0.44
2:L:105:TRP:CE2	2:L:203:LYS:HE2	2.52	0.44
2:R:147:ARG:H	2:R:147:ARG:HD3	1.82	0.44
1:C:188:ASN:OD1	4:S:661:ARG:NH2	2.47	0.44
1:G:177:GLU:CD	1:G:177:GLU:H	2.25	0.44
1:G:198:ARG:HB2	1:H:198:ARG:HH22	1.82	0.44
2:K:44:THR:OG1	2:K:46:ASP:OD1	2.22	0.44
2:O:138:GLU:OE2	2:O:147:ARG:NH2	2.51	0.44
2:P:43:GLU:OE2	2:P:71:ARG:NE	2.47	0.44
2:I:254:TYR:O	2:I:255:LYS:HG3	2.17	0.44
2:J:191:LEU:HD21	2:J:213:LEU:HD23	1.99	0.44
2:L:191:LEU:HD11	2:L:213:LEU:HD23	2.00	0.44
2:O:240:MET:HA	2:O:243:LYS:HG2	1.98	0.44
2:Q:198:THR:HA	2:Q:213:LEU:HD12	2.00	0.44
2:K:139:LEU:HD13	2:K:139:LEU:HA	1.87	0.44
2:K:240:MET:HE3	2:K:240:MET:HB3	1.81	0.44
2:R:109:ILE:HA	2:R:112:LYS:HG2	1.99	0.44
1:F:174:THR:OG1	1:F:175:GLU:N	2.48	0.44
2:J:83:ARG:NH1	2:J:85:ASP:O	2.50	0.44
2:K:17:LYS:HG3	2:K:18:ASN:ND2	2.33	0.44
1:F:125:THR:OG1	1:F:126:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:9:ASN:OD1	2:P:9:ASN:N	2.51	0.44
2:P:165:THR:OG1	2:P:166:ARG:N	2.51	0.44
4:T:553:LYS:NZ	4:T:691:LEU:O	2.51	0.44
2:J:12:SER:HB2	2:J:25:ALA:HB2	2.00	0.44
2:K:191:LEU:HD21	2:K:213:LEU:HD22	1.99	0.44
2:Q:263:ASN:OD1	2:Q:263:ASN:N	2.51	0.44
2:L:182:LEU:O	2:L:185:SER:OG	2.28	0.44
2:O:203:LYS:HG2	2:O:204:HIS:H	1.82	0.44
2:I:200:LEU:HG	2:J:90:LEU:HD23	2.00	0.43
2:O:18:ASN:O	2:O:20:HIS:ND1	2.41	0.43
1:B:5:PHE:HE2	1:B:7:LEU:HB2	1.83	0.43
2:J:17:LYS:HE3	2:J:17:LYS:HB3	1.87	0.43
2:J:166:ARG:HH12	2:J:176:LEU:HD13	1.82	0.43
4:T:711:ASP:OD1	4:T:712:SER:N	2.51	0.43
1:H:5:PHE:HE2	1:H:7:LEU:HB2	1.84	0.43
2:L:112:LYS:HZ1	2:L:148:GLU:HG3	1.82	0.43
2:R:9:ASN:OD1	2:R:9:ASN:N	2.51	0.43
4:T:541:ASP:OD2	4:T:542:ARG:NH1	2.51	0.43
1:B:174:THR:OG1	1:B:175:GLU:N	2.50	0.43
2:J:176:LEU:HG	2:J:229:ILE:HD13	2.01	0.43
2:J:223:PRO:HA	2:J:226:ASP:HB2	2.00	0.43
1:C:12:ILE:HG23	1:C:206:TYR:HE2	1.83	0.43
2:I:69:ASP:OD1	2:I:69:ASP:N	2.52	0.43
2:I:28:HIS:O	2:I:30:GLU:N	2.51	0.43
2:I:214:ALA:HA	2:I:217:LEU:HB3	2.00	0.43
2:O:109:ILE:O	2:O:113:ILE:HG13	2.18	0.43
2:O:119:HIS:HD2	2:O:155:TYR:HE1	1.66	0.43
1:C:138:GLU:HG2	1:C:140:THR:HG22	2.01	0.43
1:F:112:LEU:HD11	1:F:119:LEU:HD12	2.01	0.43
2:P:109:ILE:HA	2:P:112:LYS:HG2	1.99	0.43
2:R:150:HIS:CG	2:R:153:ARG:HH21	2.36	0.43
1:F:206:TYR:HD2	1:F:214:LEU:HD11	1.83	0.43
2:I:251:THR:OG1	2:I:258:GLN:OE1	2.18	0.43
2:J:119:HIS:O	2:J:122:GLN:NE2	2.51	0.42
2:P:17:LYS:HE3	2:P:17:LYS:HB3	1.90	0.42
2:R:58:ILE:HD12	2:R:58:ILE:HA	1.80	0.42
2:Q:90:LEU:HD21	2:R:199:GLN:HB3	2.01	0.42
4:T:631:LEU:HD22	4:T:664:TYR:HD2	1.84	0.42
1:A:133:LEU:HD13	1:D:108:ILE:HG21	2.01	0.42
2:R:156:PHE:HB3	2:R:164:PHE:CD2	2.54	0.42
2:K:100:ARG:O	2:K:103:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:15:SER:OG	2:R:16:TYR:N	2.52	0.42
1:H:115:HIS:HE1	1:H:117:MET:HE2	1.84	0.42
2:I:55:LYS:HD3	2:I:56:ARG:HD2	2.02	0.42
2:P:203:LYS:HD3	2:P:203:LYS:HA	1.91	0.42
2:R:8:VAL:HG12	3:V:106:LEU:HD12	2.01	0.42
2:R:115:ASN:HB3	2:R:288:ILE:HG12	2.00	0.42
2:O:263:ASN:OD1	2:O:263:ASN:N	2.51	0.42
2:P:212:ASN:OD1	2:P:212:ASN:N	2.52	0.42
2:R:209:ASN:O	2:R:211:PHE:N	2.51	0.42
2:I:257:LYS:HD2	2:I:257:LYS:HA	1.88	0.42
2:I:274:LYS:HE2	2:I:280:GLU:HG2	2.01	0.42
2:K:112:LYS:HD2	2:K:219:GLU:HB3	2.00	0.42
2:O:173:ASN:OD1	2:O:174:ALA:N	2.52	0.42
2:P:163:ASP:OD1	2:P:163:ASP:N	2.51	0.42
1:F:72:SER:O	1:F:75:THR:OG1	2.37	0.42
2:K:28:HIS:O	2:K:30:GLU:N	2.53	0.42
2:L:19:ASN:OD1	2:L:19:ASN:N	2.52	0.42
2:L:61:LYS:HD2	2:L:83:ARG:HG3	2.02	0.42
2:O:187:PHE:HB3	2:O:214:ALA:HB1	2.01	0.42
2:R:215:SER:HA	2:R:218:MET:HE3	2.01	0.42
1:G:206:TYR:HE1	1:G:216:TYR:HD2	1.68	0.42
2:O:168:GLN:NE2	2:O:170:ASN:OD1	2.47	0.42
2:P:123:ARG:NH1	2:P:123:ARG:HA	2.35	0.42
1:B:5:PHE:CE2	1:B:7:LEU:HB2	2.55	0.42
1:C:58:GLU:N	1:C:58:GLU:OE1	2.53	0.42
1:F:5:PHE:HE1	1:F:7:LEU:HB2	1.85	0.42
2:I:29:GLN:OE1	2:I:29:GLN:N	2.49	0.42
2:J:135:MET:HE2	2:J:151:ALA:HB2	2.02	0.42
2:K:93:GLN:HA	2:K:96:TRP:CZ2	2.55	0.42
2:K:182:LEU:O	2:K:185:SER:OG	2.29	0.41
2:K:257:LYS:HD2	2:K:257:LYS:HA	1.79	0.41
2:R:19:ASN:O	2:R:20:HIS:ND1	2.53	0.41
1:B:165:ILE:HD12	1:B:193:LEU:HD23	2.02	0.41
2:K:212:ASN:O	2:K:214:ALA:N	2.53	0.41
1:G:71:ASN:HD21	1:G:136:LYS:HG3	1.85	0.41
2:I:190:GLU:HG3	2:I:269:THR:HG21	2.01	0.41
2:K:171:ASP:OD1	2:K:171:ASP:N	2.52	0.41
2:L:100:ARG:NH1	2:L:281:GLU:OE2	2.53	0.41
2:P:156:PHE:HB3	2:P:164:PHE:HD2	1.83	0.41
2:Q:269:THR:HA	2:Q:272:VAL:HG22	2.02	0.41
2:R:20:HIS:CD2	2:R:31:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:170:ASN:H	2:I:173:ASN:HD22	1.68	0.41
2:K:190:GLU:HG3	2:K:269:THR:HG21	2.02	0.41
2:O:268:TYR:O	2:O:272:VAL:HG13	2.21	0.41
4:T:573:ILE:HG13	4:T:584:ILE:HG12	2.01	0.41
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.91	0.41
1:H:65:ILE:HD13	1:H:65:ILE:HA	1.90	0.41
2:L:112:LYS:HE3	2:L:113:ILE:HG13	2.03	0.41
2:O:219:GLU:HA	2:O:222:ARG:NH1	2.34	0.41
1:D:57:THR:O	1:D:161:LYS:NZ	2.46	0.41
2:I:240:MET:HA	2:I:243:LYS:HG2	2.03	0.41
2:L:12:SER:HB2	2:L:25:ALA:HB2	2.02	0.41
2:O:274:LYS:O	2:O:279:GLU:HB2	2.21	0.41
2:Q:85:ASP:OD1	2:Q:85:ASP:N	2.53	0.41
2:R:228:ILE:HG13	2:R:247:LEU:HD12	2.03	0.41
1:A:111:GLU:HG2	1:D:87:LEU:HD13	2.02	0.41
2:K:28:HIS:O	2:K:28:HIS:ND1	2.52	0.41
2:O:267:ASP:O	2:O:270:LYS:HG2	2.21	0.41
2:R:203:LYS:HD2	2:R:203:LYS:HA	1.74	0.41
1:H:146:GLU:OE1	1:H:146:GLU:N	2.54	0.41
1:H:205:GLN:HB2	1:H:207:ILE:HD11	2.03	0.41
2:I:263:ASN:OD1	2:I:263:ASN:N	2.54	0.41
2:O:69:ASP:OD1	2:O:70:LYS:NZ	2.53	0.41
2:O:237:PHE:HA	2:O:240:MET:HG2	2.02	0.41
2:R:223:PRO:HA	2:R:226:ASP:HB2	2.03	0.41
1:E:204:PHE:CE1	1:E:218:LYS:HB2	2.56	0.41
1:F:38:TYR:CZ	1:F:46:LEU:HD23	2.56	0.41
1:H:86:GLN:NE2	1:H:86:GLN:O	2.54	0.41
2:J:83:ARG:HH11	2:J:86:SER:HA	1.85	0.41
2:J:94:LEU:HD23	2:J:94:LEU:HA	1.91	0.41
2:K:206:ASN:O	2:K:208:PHE:N	2.53	0.41
2:L:150:HIS:HD2	2:L:153:ARG:HH22	1.68	0.41
4:T:637:ARG:HH12	4:T:661:ARG:HA	1.86	0.41
1:B:46:LEU:HD13	1:B:46:LEU:HA	1.87	0.41
1:F:129:LEU:HD21	1:G:104:ILE:HD11	2.02	0.41
2:J:191:LEU:HD11	2:J:213:LEU:HB3	2.02	0.41
2:K:271:HIS:HA	2:K:274:LYS:HE2	2.03	0.41
2:K:67:CYS:SG	2:K:68:ASP:N	2.94	0.40
1:C:115:HIS:CG	1:C:116:GLU:H	2.38	0.40
1:G:7:LEU:HD13	1:G:7:LEU:HA	1.95	0.40
2:J:46:ASP:N	2:J:46:ASP:OD1	2.51	0.40
2:K:215:SER:HA	2:K:218:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:163:ASP:OD1	2:R:163:ASP:N	2.46	0.40
1:D:5:PHE:HE2	1:D:7:LEU:HB2	1.85	0.40
2:L:119:HIS:ND1	2:L:227:GLN:OE1	2.54	0.40
2:L:242:ARG:HA	2:L:242:ARG:HD3	1.90	0.40
2:O:69:ASP:OD1	2:O:69:ASP:N	2.54	0.40
2:Q:138:GLU:HG3	2:Q:140:ARG:HH11	1.85	0.40
2:Q:163:ASP:OD1	2:Q:163:ASP:N	2.55	0.40
4:T:658:LYS:HE3	4:T:658:LYS:HB2	1.89	0.40
1:C:52:LYS:HE3	1:C:52:LYS:HB3	1.94	0.40
2:I:8:VAL:HG22	2:I:42:LEU:HA	2.03	0.40
2:I:171:ASP:OD1	2:I:171:ASP:N	2.54	0.40
2:J:87:SER:OG	2:J:88:LEU:N	2.53	0.40
2:L:46:ASP:OD1	2:L:46:ASP:N	2.53	0.40
2:L:198:THR:O	2:L:198:THR:OG1	2.36	0.40
1:A:118:ASP:OD1	1:A:118:ASP:N	2.53	0.40
1:B:141:SER:OG	1:B:142:ASP:N	2.54	0.40
1:H:204:PHE:HD1	1:H:204:PHE:HA	1.78	0.40
2:J:228:ILE:HG13	2:J:247:LEU:HD12	2.02	0.40
2:K:190:GLU:O	2:K:194:THR:HG23	2.22	0.40
2:L:261:LEU:HD13	2:L:261:LEU:HA	1.96	0.40
4:T:719:ALA:O	4:T:722:LYS:HG3	2.22	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	217/219 (99%)	201 (93%)	16 (7%)	0	100	100
1	B	217/219 (99%)	195 (90%)	22 (10%)	0	100	100
1	C	217/219 (99%)	202 (93%)	14 (6%)	1 (0%)	24	59
1	D	217/219 (99%)	193 (89%)	23 (11%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
1	F	217/219 (99%)	199 (92%)	18 (8%)	0	100	100
1	G	217/219 (99%)	201 (93%)	16 (7%)	0	100	100
1	H	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
2	I	284/288 (99%)	256 (90%)	26 (9%)	2 (1%)	18	53
2	J	285/288 (99%)	259 (91%)	24 (8%)	2 (1%)	18	53
2	K	284/288 (99%)	258 (91%)	24 (8%)	2 (1%)	18	53
2	L	285/288 (99%)	264 (93%)	21 (7%)	0	100	100
2	O	285/288 (99%)	259 (91%)	24 (8%)	2 (1%)	18	53
2	P	285/288 (99%)	257 (90%)	26 (9%)	2 (1%)	18	53
2	Q	284/288 (99%)	254 (89%)	29 (10%)	1 (0%)	30	64
2	R	285/288 (99%)	262 (92%)	23 (8%)	0	100	100
3	M	4/109 (4%)	4 (100%)	0	0	100	100
3	N	5/109 (5%)	4 (80%)	1 (20%)	0	100	100
3	U	5/109 (5%)	5 (100%)	0	0	100	100
3	V	5/109 (5%)	5 (100%)	0	0	100	100
4	S	218/1337 (16%)	201 (92%)	17 (8%)	0	100	100
4	T	218/1337 (16%)	204 (94%)	14 (6%)	0	100	100
All	All	4468/7166 (62%)	4088 (92%)	367 (8%)	13 (0%)	37	69

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	115	HIS
2	I	207	GLN
2	I	213	LEU
2	K	207	GLN
2	K	213	LEU
2	Q	213	LEU
2	O	213	LEU
2	O	207	GLN
1	C	115	HIS
2	J	209	ASN
2	J	279	GLU
2	P	209	ASN
2	P	278	GLN

### 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	202/202 (100%)	199 (98%)	3 (2%)	57	70
1	B	202/202 (100%)	190 (94%)	12 (6%)	18	44
1	C	202/202 (100%)	194 (96%)	8 (4%)	28	51
1	D	202/202 (100%)	195 (96%)	7 (4%)	32	54
1	E	202/202 (100%)	199 (98%)	3 (2%)	57	70
1	F	202/202 (100%)	190 (94%)	12 (6%)	18	44
1	G	202/202 (100%)	194 (96%)	8 (4%)	28	51
1	H	202/202 (100%)	197 (98%)	5 (2%)	42	62
2	I	254/255 (100%)	244 (96%)	10 (4%)	28	52
2	J	254/255 (100%)	243 (96%)	11 (4%)	26	49
2	K	254/255 (100%)	238 (94%)	16 (6%)	16	42
2	L	254/255 (100%)	239 (94%)	15 (6%)	18	44
2	O	254/255 (100%)	242 (95%)	12 (5%)	23	48
2	P	254/255 (100%)	245 (96%)	9 (4%)	32	54
2	Q	254/255 (100%)	243 (96%)	11 (4%)	26	49
2	R	254/255 (100%)	240 (94%)	14 (6%)	19	45
3	M	5/99 (5%)	5 (100%)	0	100	100
3	N	5/99 (5%)	5 (100%)	0	100	100
3	U	5/99 (5%)	4 (80%)	1 (20%)	1	9
3	V	5/99 (5%)	4 (80%)	1 (20%)	1	9
4	S	202/1192 (17%)	196 (97%)	6 (3%)	36	57
4	T	202/1192 (17%)	200 (99%)	2 (1%)	68	75
All	All	4072/6436 (63%)	3906 (96%)	166 (4%)	28	51

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	THR
1	A	178	VAL
1	A	200	VAL
1	B	44	LEU
1	B	46	LEU
1	B	62	VAL
1	B	63	THR
1	B	122	ASP
1	B	138	GLU
1	B	143	THR
1	B	157	TYR
1	B	165	ILE
1	B	167	ILE
1	B	177	GLU
1	B	200	VAL
1	C	61	VAL
1	C	70	VAL
1	C	78	LEU
1	C	122	ASP
1	C	140	THR
1	C	143	THR
1	C	193	LEU
1	C	195	LEU
1	D	44	LEU
1	D	46	LEU
1	D	50	GLN
1	D	115	HIS
1	D	117	MET
1	D	122	ASP
1	D	126	VAL
1	E	36	TYR
1	E	143	THR
1	E	187	LEU
1	F	44	LEU
1	F	46	LEU
1	F	62	VAL
1	F	63	THR
1	F	70	VAL
1	F	108	ILE
1	F	122	ASP
1	F	138	GLU
1	F	165	ILE
1	F	167	ILE

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Mol	Chain	Res	Type
1	F	177	GLU
1	F	200	VAL
1	G	78	LEU
1	G	112	LEU
1	G	122	ASP
1	G	140	THR
1	G	191	ASP
1	G	193	LEU
1	G	195	LEU
1	G	199	VAL
1	H	44	LEU
1	H	46	LEU
1	H	122	ASP
1	H	143	THR
1	H	204	PHE
2	I	7	VAL
2	I	53	LEU
2	I	97	THR
2	I	139	LEU
2	I	159	LEU
2	I	212	ASN
2	I	213	LEU
2	I	232	ASN
2	I	263	ASN
2	I	283	VAL
2	J	7	VAL
2	J	19	ASN
2	J	64	VAL
2	J	97	THR
2	J	127	GLN
2	J	133	LEU
2	J	232	ASN
2	J	248	PHE
2	J	262	THR
2	J	263	ASN
2	J	283	VAL
2	K	7	VAL
2	K	44	THR
2	K	46	ASP
2	K	54	LEU
2	K	94	LEU
2	K	138	GLU

*Continued on next page...*

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Mol	Chain	Res	Type
2	K	139	LEU
2	K	158	THR
2	K	187	PHE
2	K	202	LEU
2	K	213	LEU
2	K	217	LEU
2	K	232	ASN
2	K	263	ASN
2	K	278	GLN
2	K	283	VAL
2	L	7	VAL
2	L	19	ASN
2	L	54	LEU
2	L	67	CYS
2	L	88	LEU
2	L	97	THR
2	L	159	LEU
2	L	168	GLN
2	L	212	ASN
2	L	227	GLN
2	L	235	GLU
2	L	247	LEU
2	L	262	THR
2	L	263	ASN
2	L	283	VAL
2	O	22	VAL
2	O	60	GLU
2	O	120	LEU
2	O	122	GLN
2	O	135	MET
2	O	139	LEU
2	O	182	LEU
2	O	183	LEU
2	O	198	THR
2	O	267	ASP
2	O	269	THR
2	O	283	VAL
2	P	15	SER
2	P	50	THR
2	P	63	LEU
2	P	133	LEU
2	P	200	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	P	202	LEU
2	P	233	ARG
2	P	247	LEU
2	P	263	ASN
3	U	104	VAL
2	Q	33	HIS
2	Q	44	THR
2	Q	50	THR
2	Q	60	GLU
2	Q	97	THR
2	Q	135	MET
2	Q	139	LEU
2	Q	193	GLN
2	Q	200	LEU
2	Q	224	LEU
2	Q	283	VAL
2	R	15	SER
2	R	50	THR
2	R	94	LEU
2	R	127	GLN
2	R	140	ARG
2	R	202	LEU
2	R	203	LYS
2	R	233	ARG
2	R	235	GLU
2	R	247	LEU
2	R	263	ASN
2	R	276	LEU
2	R	279	GLU
2	R	288	ILE
3	V	104	VAL
4	S	515	LYS
4	S	566	LYS
4	S	585	VAL
4	S	630	ILE
4	S	701	TYR
4	S	716	PHE
4	T	624	LEU
4	T	716	PHE

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	86	GLN
1	B	71	ASN
1	B	155	HIS
1	B	188	ASN
1	B	201	GLN
1	B	205	GLN
1	B	211	ASN
1	C	88	ASN
1	C	127	GLN
1	C	168	ASN
1	C	201	GLN
1	C	211	ASN
1	D	37	GLN
1	D	180	GLN
1	D	189	ASN
1	E	115	HIS
1	E	179	GLN
1	F	155	HIS
1	G	127	GLN
1	G	168	ASN
1	G	202	ASN
1	H	37	GLN
1	H	50	GLN
1	H	86	GLN
1	H	211	ASN
2	I	11	HIS
2	I	93	GLN
2	I	111	GLN
2	I	173	ASN
2	I	193	GLN
2	I	278	GLN
2	J	29	GLN
2	J	93	GLN
2	J	127	GLN
2	J	258	GLN
2	K	111	GLN
2	K	173	ASN
2	K	227	GLN
2	K	278	GLN
2	L	116	GLN
2	L	127	GLN
2	L	173	ASN
2	L	258	GLN

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Mol	Chain	Res	Type
2	O	9	ASN
2	O	177	ASN
2	O	258	GLN
2	O	278	GLN
2	P	11	HIS
2	P	28	HIS
2	P	127	GLN
2	P	157	ASN
2	P	177	ASN
2	Q	11	HIS
2	Q	177	ASN
2	Q	193	GLN
2	R	116	GLN
2	R	122	GLN
2	R	127	GLN
2	R	170	ASN
2	R	173	ASN
2	R	204	HIS
2	R	232	ASN
4	S	724	GLN
4	T	650	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](#)

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 12 ligands modelled in this entry, 12 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

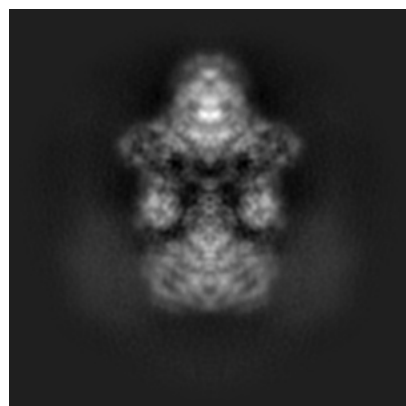
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65106. These allow visual inspection of the internal detail of the map and identification of artifacts.

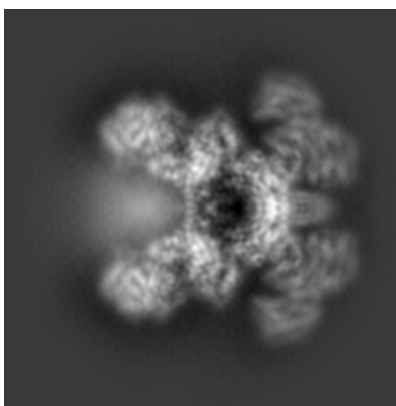
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

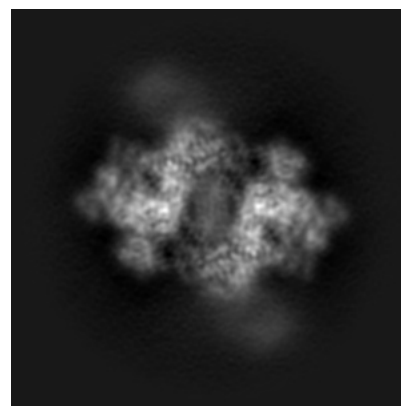
#### 6.1.1 Primary map



X

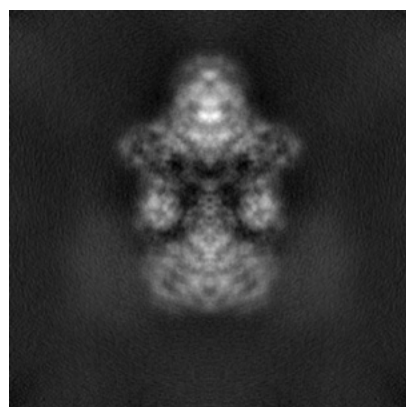


Y

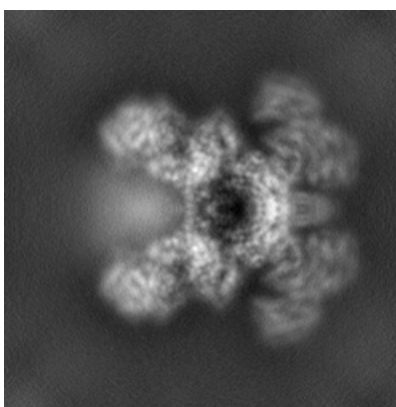


Z

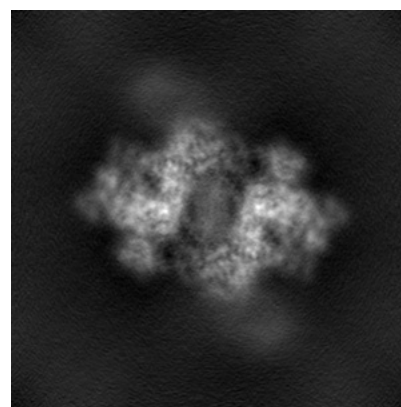
#### 6.1.2 Raw map



X



Y

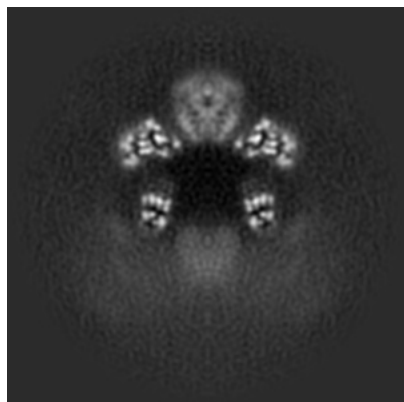


Z

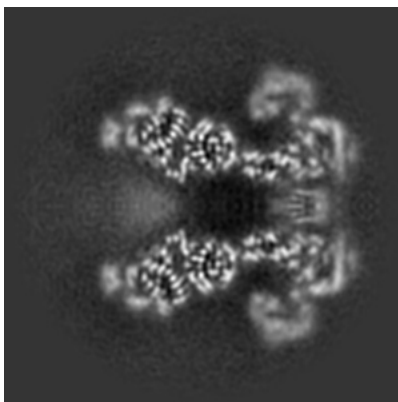
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

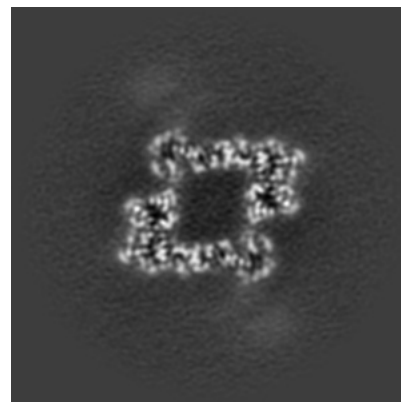
### 6.2.1 Primary map



X Index: 128

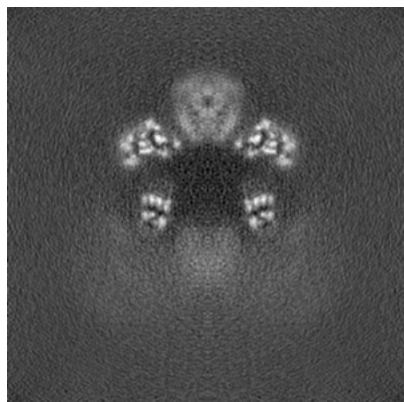


Y Index: 128

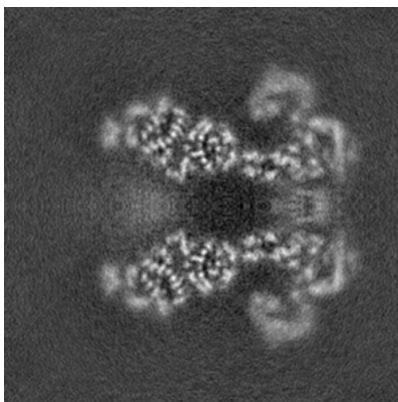


Z Index: 128

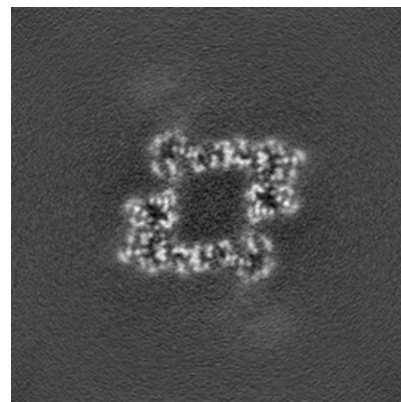
### 6.2.2 Raw map



X Index: 128



Y Index: 128

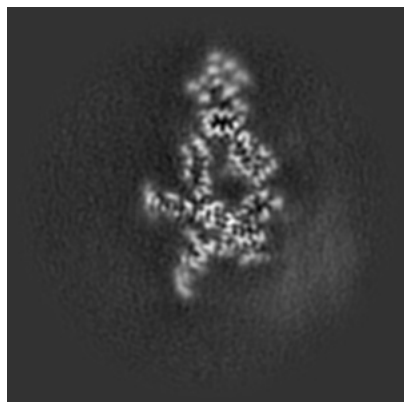


Z Index: 128

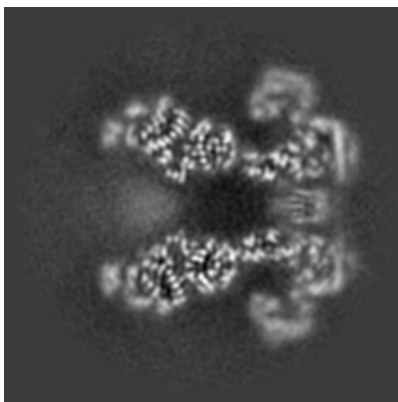
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

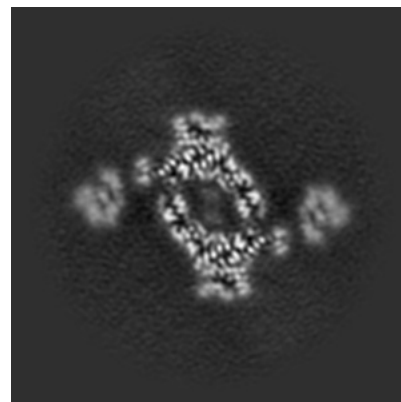
### 6.3.1 Primary map



X Index: 99

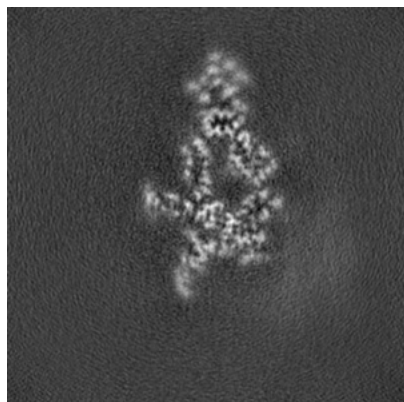


Y Index: 127

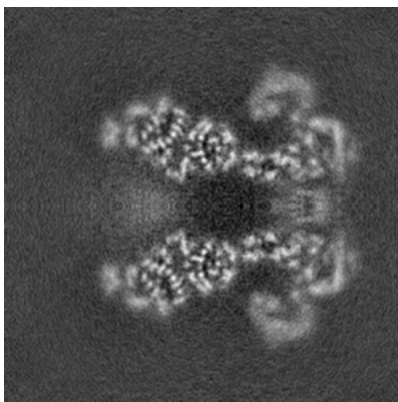


Z Index: 169

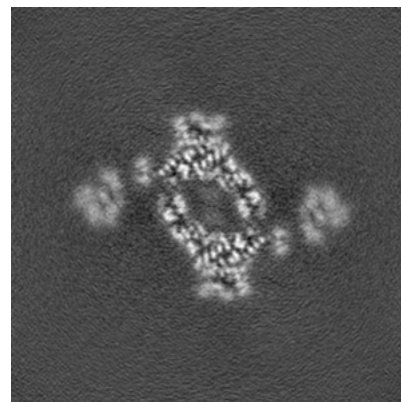
### 6.3.2 Raw map



X Index: 99



Y Index: 128



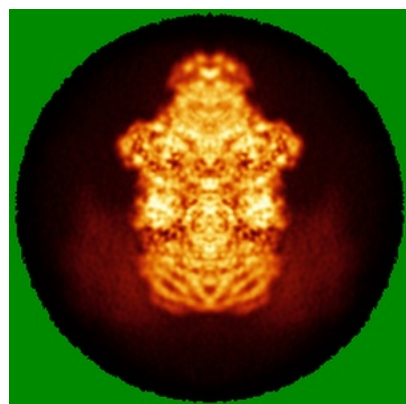
Z Index: 169

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

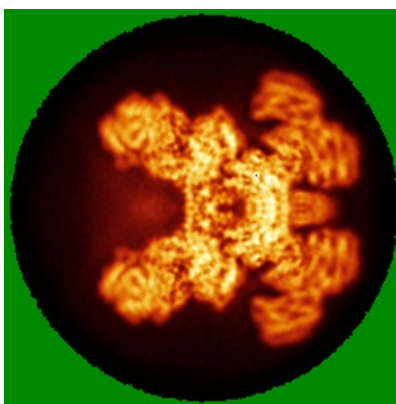


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

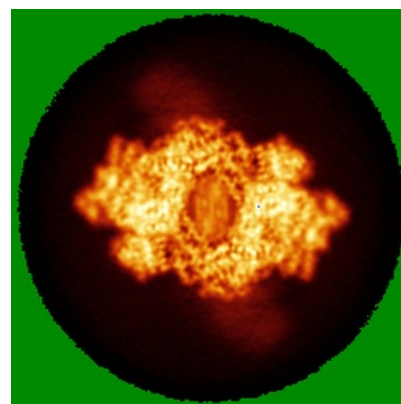
### 6.4.1 Primary map



X

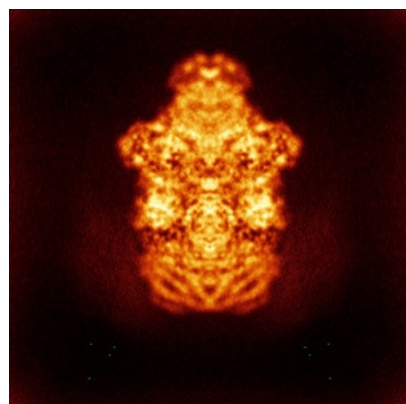


Y

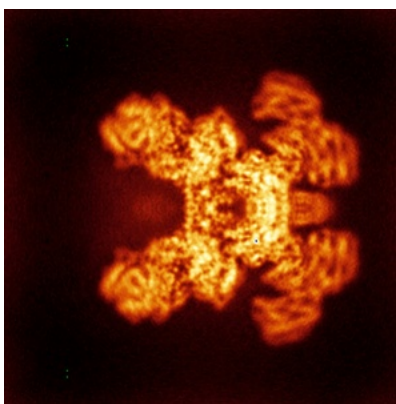


Z

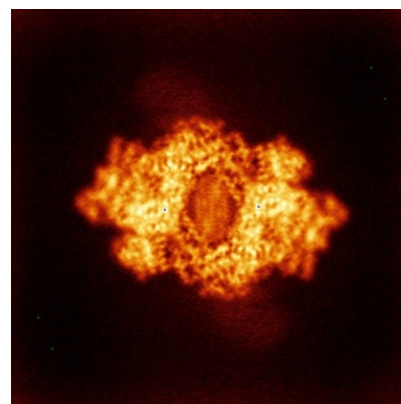
### 6.4.2 Raw map



X



Y



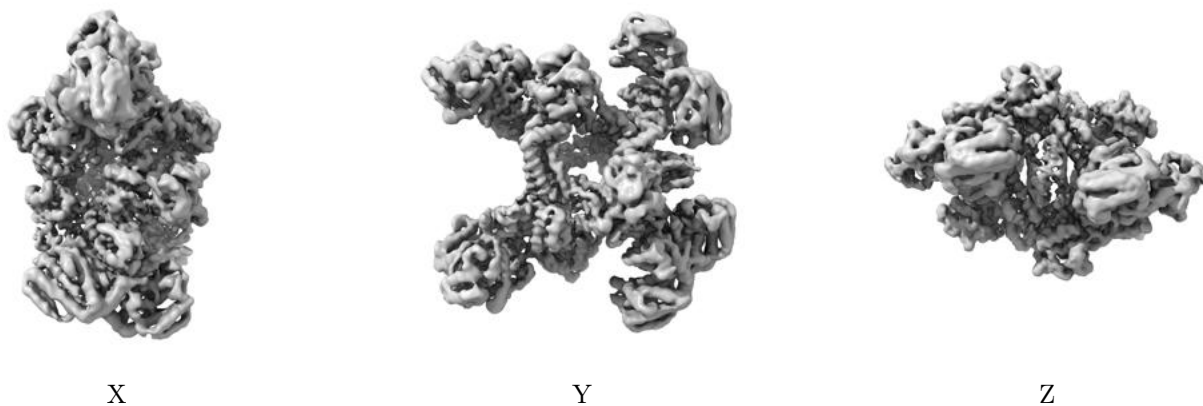
Z

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.



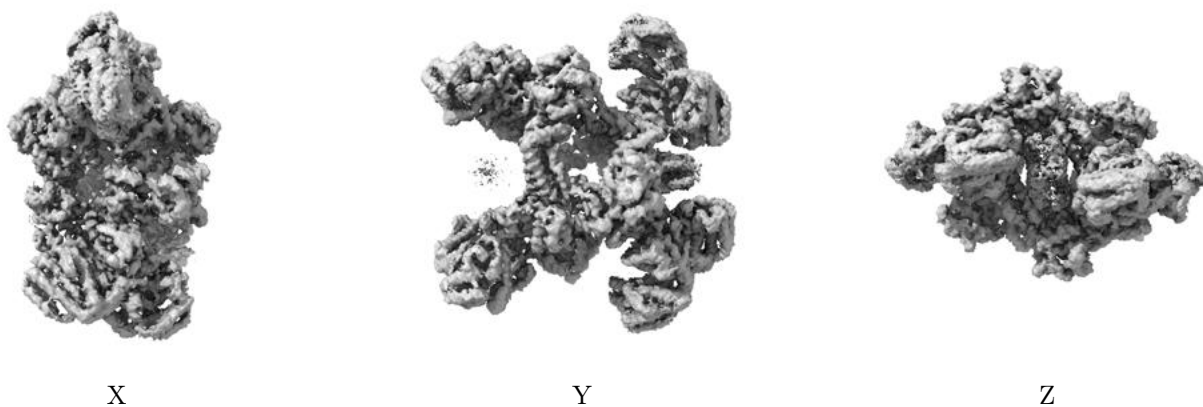
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

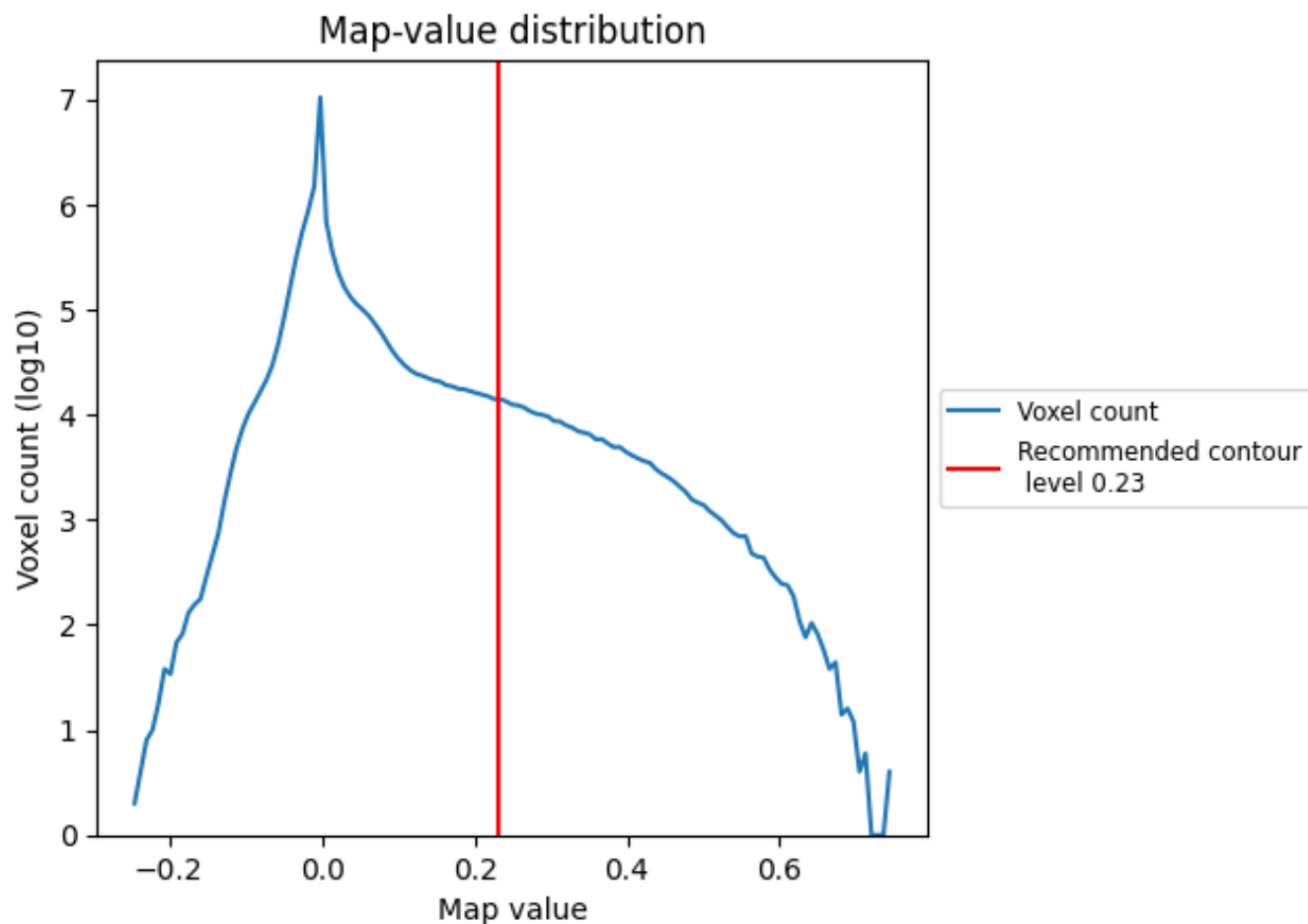
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

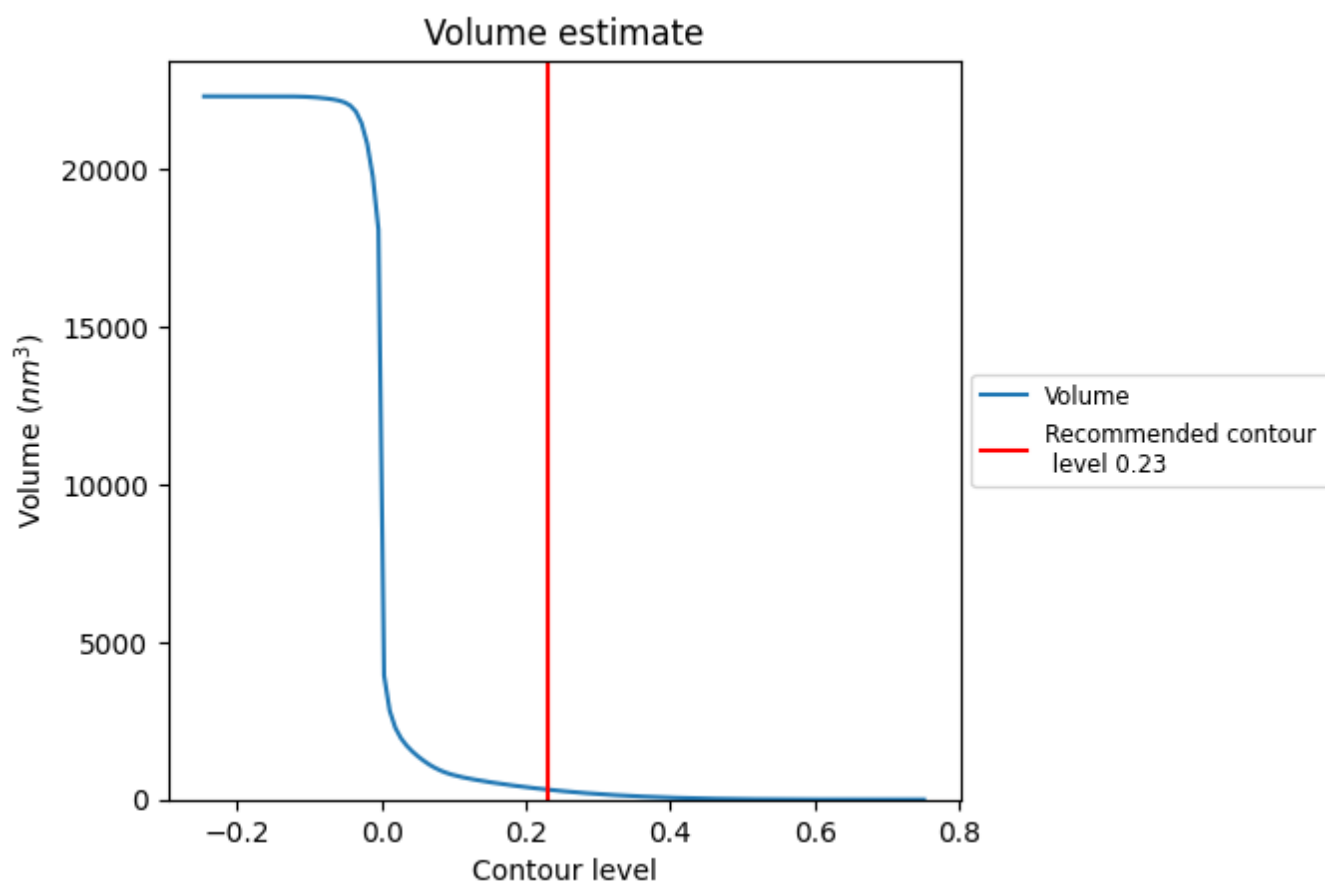
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

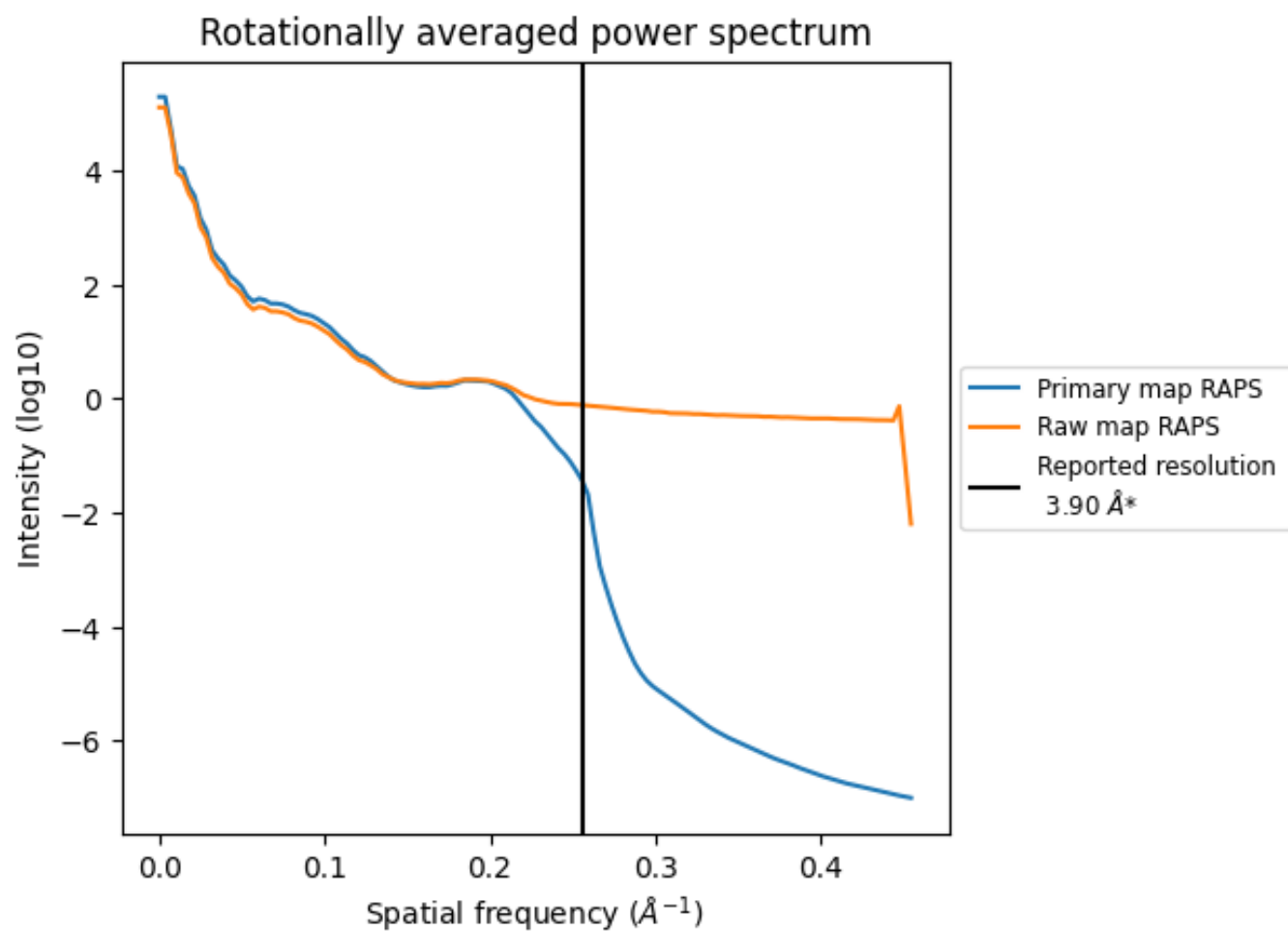
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm<sup>3</sup>; this corresponds to an approximate mass of 287 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

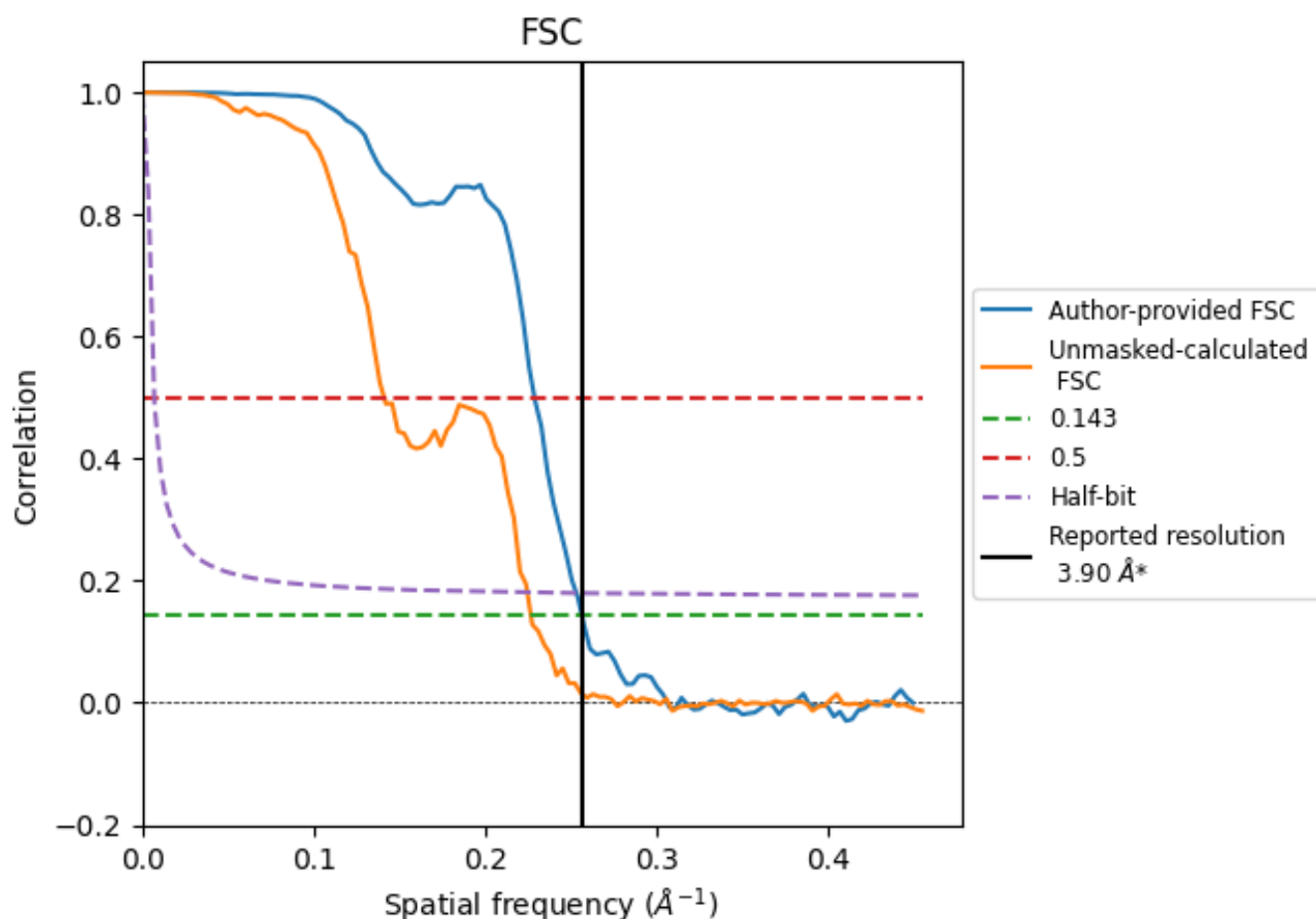


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

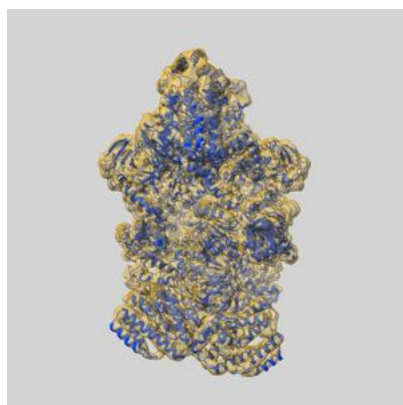
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	4.37	3.95
Unmasked-calculated*	4.42	7.09	4.46

\*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 4.42 differs from the reported value 3.9 by more than 10 %

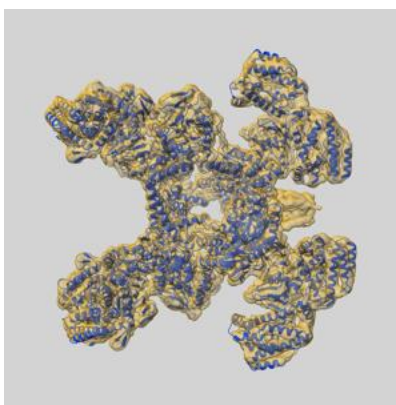
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65106 and PDB model 9VJ8. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

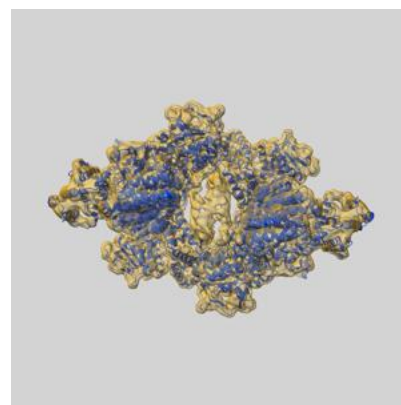
### 9.1 Map-model overlay [i](#)



X



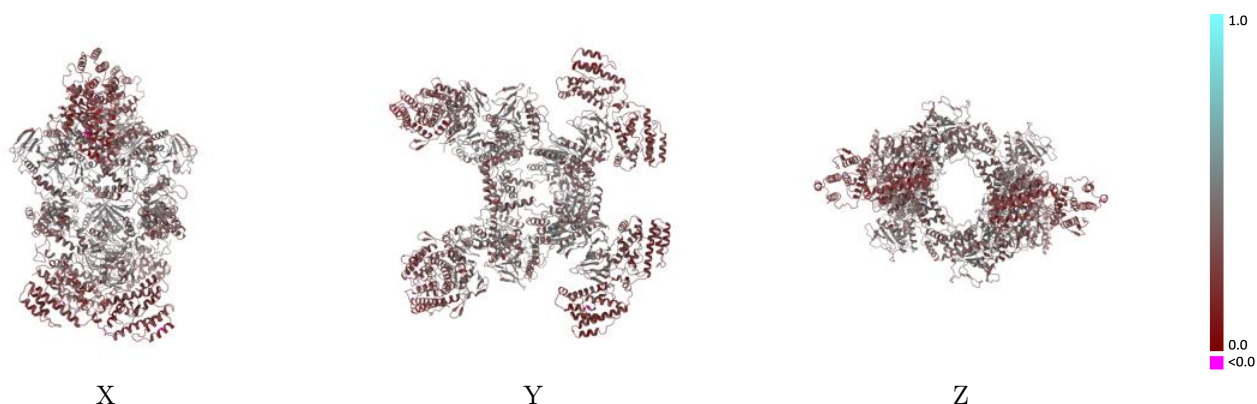
Y



Z

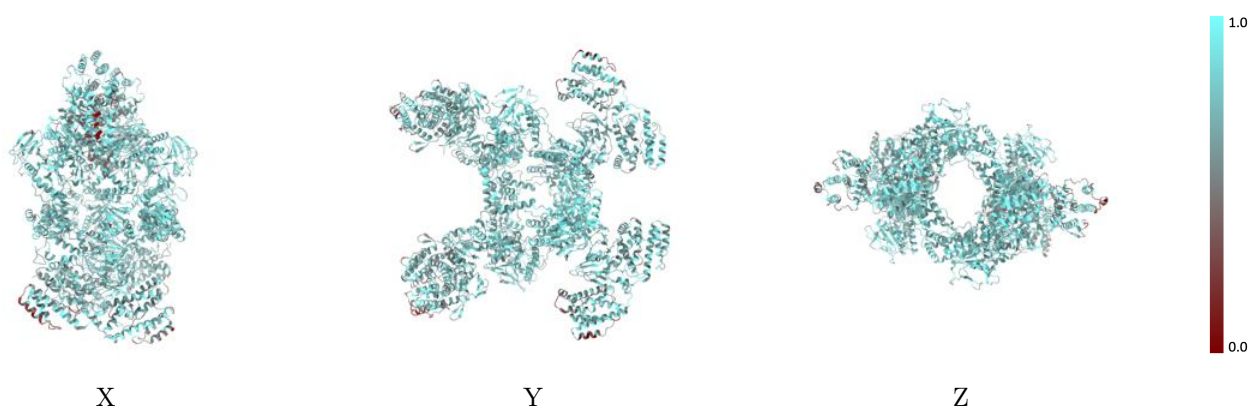
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

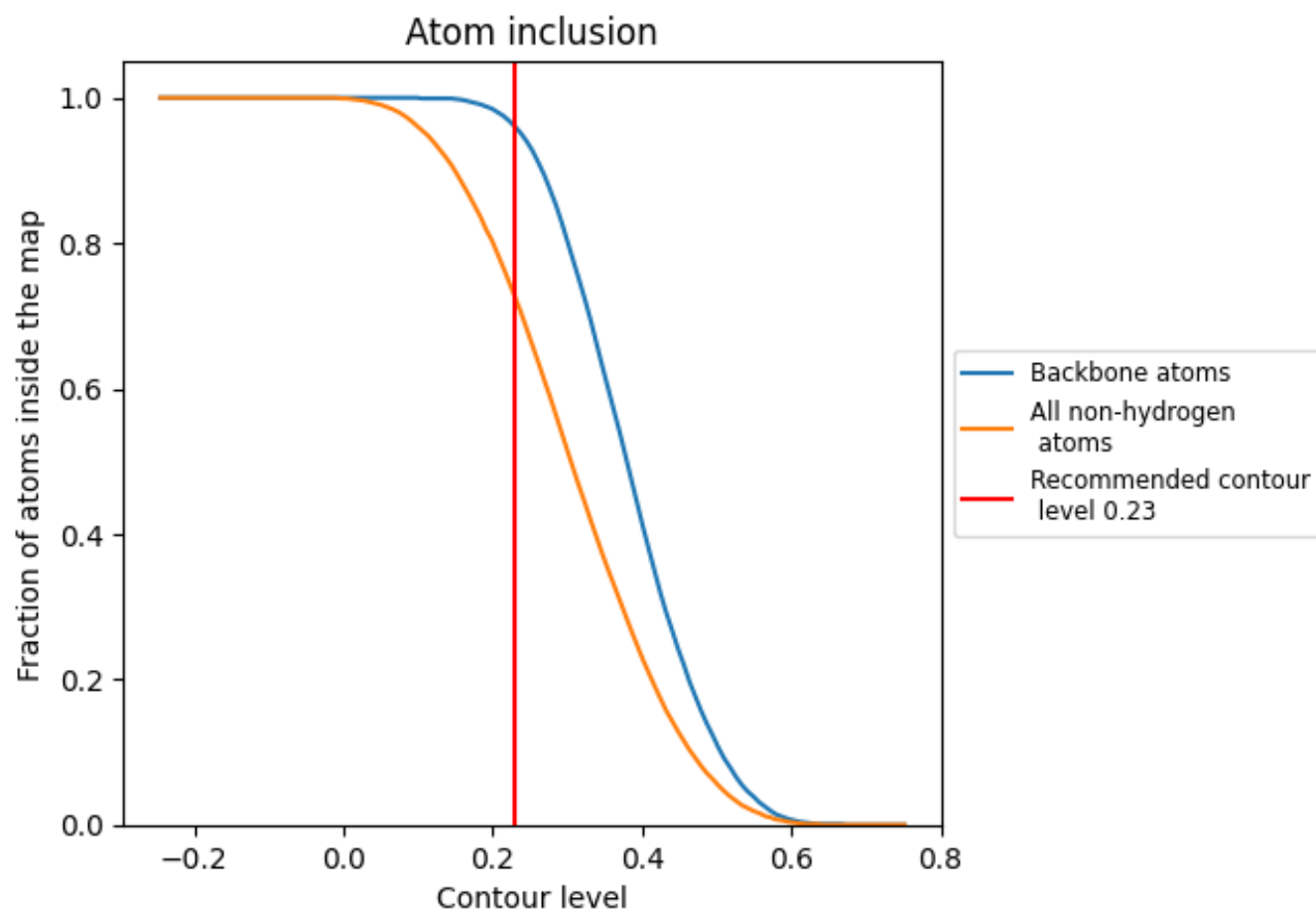
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.23).

















































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 72% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.3520
A	 0.7740	 0.4090
B	 0.7760	 0.3890
C	 0.7630	 0.4120
D	 0.7910	 0.3940
E	 0.7730	 0.4110
F	 0.7820	 0.3930
G	 0.7600	 0.4120
H	 0.7870	 0.3930
I	 0.6750	 0.3190
J	 0.6790	 0.3110
K	 0.6690	 0.3210
L	 0.6820	 0.3080
M	 0.7230	 0.4380
N	 0.7120	 0.4640
O	 0.6730	 0.2840
P	 0.7270	 0.3150
Q	 0.6650	 0.2790
R	 0.7240	 0.3110
S	 0.7230	 0.3930
T	 0.7290	 0.3940
U	 0.6920	 0.4400
V	 0.7310	 0.4340

