



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 02:34 AM UTC

PDB ID : 9RLT / pdb_00009rlt
EMDB ID : EMD-54045
Title : dimerised 13S-13S+Beta5 proteasome precursor complexes
Authors : Mark, E.; Ramos, P.C.; Nunes, M.M.; Dohmen, R.J.; Wendler, P.
Deposited on : 2025-06-17
Resolution : 3.09 Å(reported)
Based on initial model : 8RVL

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:

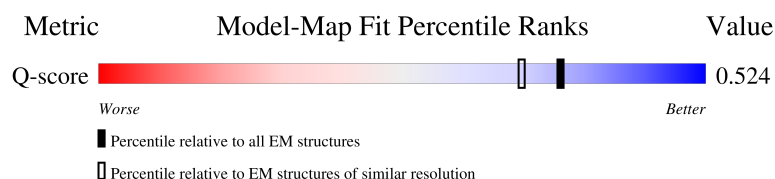
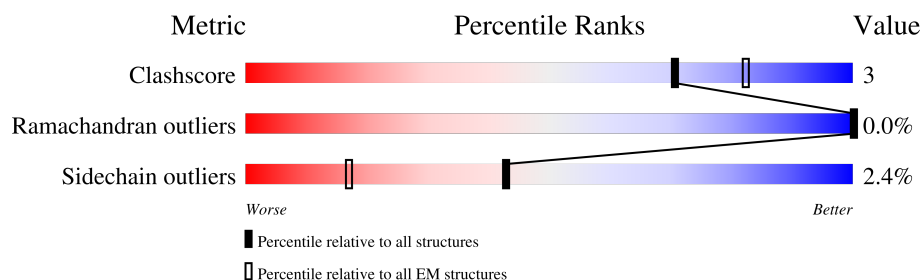
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.09 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	14003 (2.59 - 3.59)

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	252	 88% 10% .
1	O	252	 88% 10% .
2	D	254	 8% 85% 12% .
2	R	254	 6% 86% 12% .

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Mol	Chain	Length	Quality of chain
3	E	260	
3	S	260	
4	F	234	
4	T	234	
5	3	162	
5	6	162	
6	B	250	
6	P	250	
7	C	258	
7	Q	258	
8	G	288	
8	U	288	
9	I	261	
9	W	261	
10	J	205	
10	X	205	
11	K	198	
11	Y	198	
12	Z	287	
13	4	276	
13	7	276	
14	5	267	
14	8	267	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 47532 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	246	Total	C	N	O	S	0	0
			1921	1221	324	368	8		
1	O	246	Total	C	N	O	S	0	0
			1918	1221	321	368	8		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	249	Total	C	N	O	S	0	0
			1957	1220	343	389	5		
2	R	249	Total	C	N	O	S	0	0
			1949	1214	341	389	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	247	Total	C	N	O	S	0	0
			1914	1198	322	386	8		
3	S	247	Total	C	N	O	S	0	0
			1914	1198	322	386	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		
4	T	234	Total	C	N	O	S	0	0
			1802	1134	313	350	5		

- Molecule 5 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	111	Total	C	N	O	S	0	0
			911	557	167	181	6		
5	6	124	Total	C	N	O	S	0	0
			989	610	176	197	6		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-14	ASP	-	expression tag	UNP P38293
3	-13	TYR	-	expression tag	UNP P38293
3	-12	LYS	-	expression tag	UNP P38293
3	-11	ASP	-	expression tag	UNP P38293
3	-10	ASP	-	expression tag	UNP P38293
3	-9	ASP	-	expression tag	UNP P38293
3	-8	ASP	-	expression tag	UNP P38293
3	-7	LYS	-	expression tag	UNP P38293
3	-6	HIS	-	expression tag	UNP P38293
3	-5	HIS	-	expression tag	UNP P38293
3	-4	HIS	-	expression tag	UNP P38293
3	-3	HIS	-	expression tag	UNP P38293
3	-2	HIS	-	expression tag	UNP P38293
3	-1	HIS	-	expression tag	UNP P38293
6	-13	ASP	-	expression tag	UNP P38293
6	-12	TYR	-	expression tag	UNP P38293
6	-11	LYS	-	expression tag	UNP P38293
6	-10	ASP	-	expression tag	UNP P38293
6	-9	ASP	-	expression tag	UNP P38293
6	-8	ASP	-	expression tag	UNP P38293
6	-7	ASP	-	expression tag	UNP P38293
6	-6	LYS	-	expression tag	UNP P38293
6	-5	HIS	-	expression tag	UNP P38293
6	-4	HIS	-	expression tag	UNP P38293
6	-3	HIS	-	expression tag	UNP P38293
6	-2	HIS	-	expression tag	UNP P38293
6	-1	HIS	-	expression tag	UNP P38293
6	0	HIS	-	expression tag	UNP P38293

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	248	Total	C	N	O	S	0	0
			1900	1210	313	373	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	249	Total	C	N	O	S	0	0
			1906	1213	314	375	4		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	238	Total	C	N	O	S	0	0
			1868	1182	314	369	3		
7	Q	238	Total	C	N	O	S	0	0
			1868	1182	314	369	3		

- Molecule 8 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	244	Total	C	N	O	S	0	0
			1888	1200	328	356	4		
8	U	244	Total	C	N	O	S	0	0
			1892	1203	329	356	4		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	224	Total	C	N	O	S	0	0
			1701	1067	294	334	6		
9	W	224	Total	C	N	O	S	0	0
			1694	1064	291	333	6		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	189	Total	C	N	O	S	0	0
			1473	950	237	278	8		
10	X	186	Total	C	N	O	S	0	0
			1444	935	230	271	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	176	Total	C	N	O	S	0	0
			1401	889	240	269	3		
11	Y	195	Total	C	N	O	S	0	0
			1549	983	262	299	5		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	172	Total	C	N	O	S	0	0
			1319	841	220	250	8		

- Molecule 13 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	276	Total	C	N	O	S	0	0
			2108	1362	332	401	13		
13	4	276	Total	C	N	O	S	0	0
			2122	1369	333	407	13		


- Molecule 14 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	8	266	Total	C	N	O	S	0	0
			2161	1396	347	410	8		
14	5	266	Total	C	N	O	S	0	0
			2161	1396	347	410	8		

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.

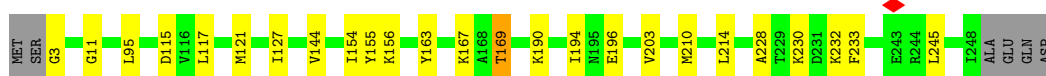
- Molecule 1: Proteasome subunit alpha type-1

Chain A: 




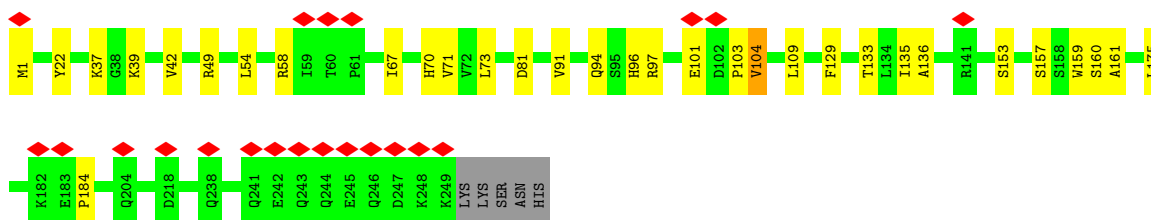
- Molecule 1: Proteasome subunit alpha type-1

Chain O: 




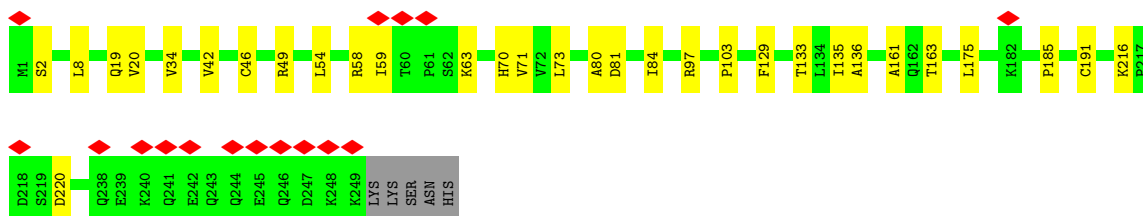
- Molecule 2: Proteasome subunit alpha type-4

Chain D: 

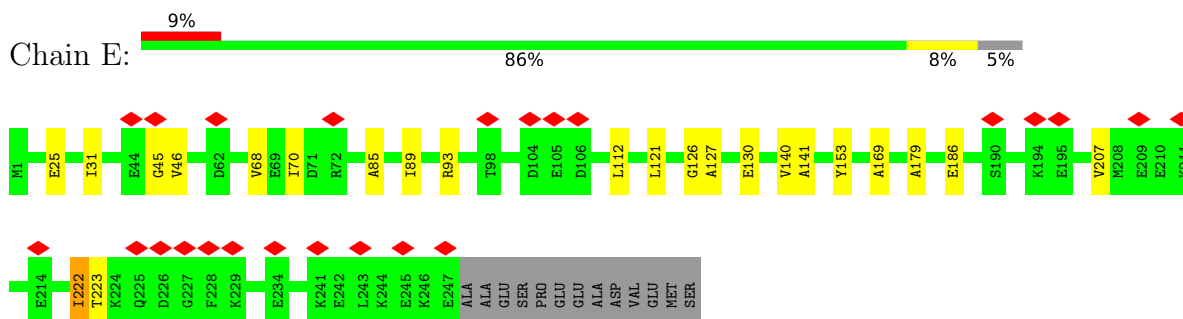


- Molecule 2: Proteasome subunit alpha type-4

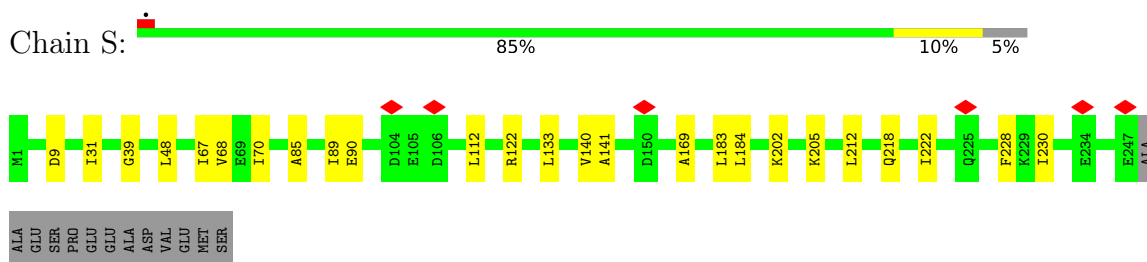
Chain R: 



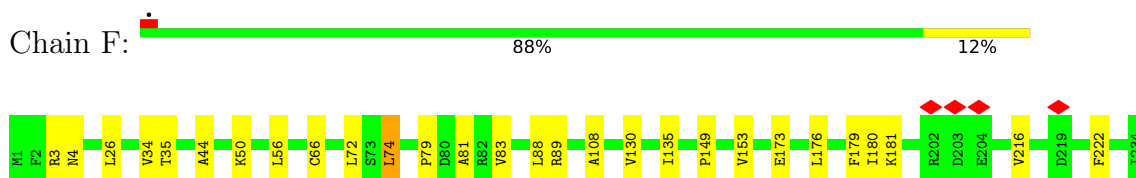
- Molecule 3: Proteasome subunit alpha type-5



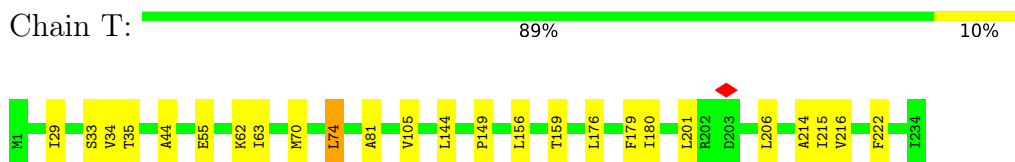
- Molecule 3: Proteasome subunit alpha type-5



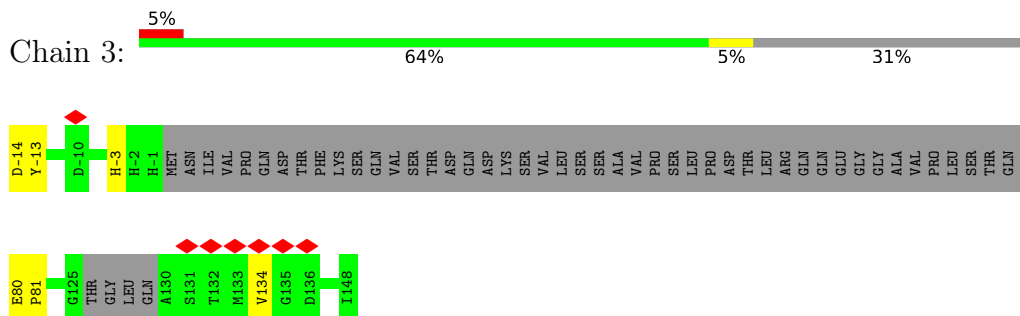
- Molecule 4: Proteasome subunit alpha type-6



- Molecule 4: Proteasome subunit alpha type-6

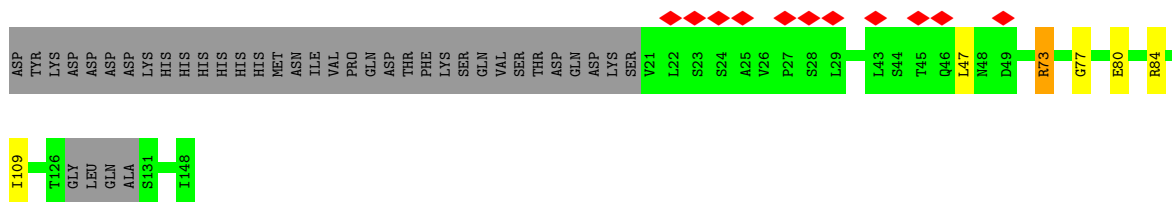


- Molecule 5: Proteasome maturation factor UMP1



- Molecule 5: Proteasome maturation factor UMP1





- Molecule 6: Proteasome subunit alpha type-2

Chain B: 90% 10%



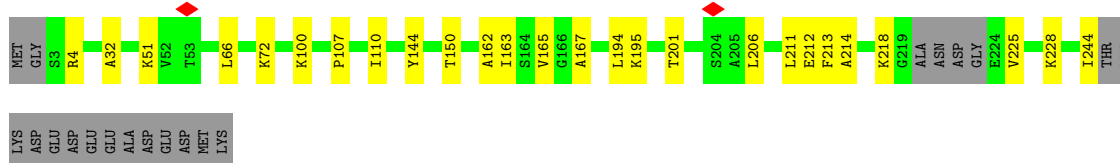
- Molecule 6: Proteasome subunit alpha type-2

Chain P: 88% 11%



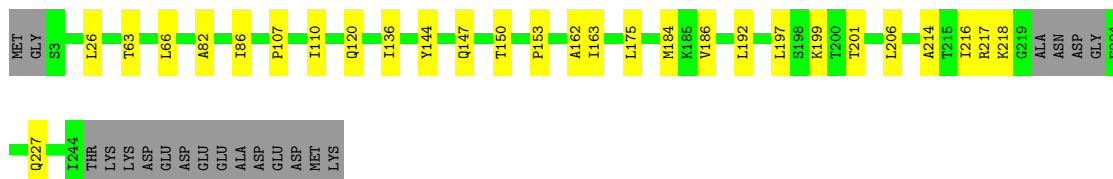
- Molecule 7: Proteasome subunit alpha type-3

Chain C: 82% 10% 8%



- Molecule 7: Proteasome subunit alpha type-3

Chain Q: 81% 11% 8%



- Molecule 8: Probable proteasome subunit alpha type-7

Chain G: 77% 6% 15%



MET
SER
SER
ASP
ASP
GLU
ASN
ALA
PRO
VAL
ALA
THR
THR
ALA
ASN
ALA
ALA
THR
THR
ASP
GLN
GLY
GLY
ILE
HIS
LEU
GLU

- Molecule 8: Probable proteasome subunit alpha type-7

Chain U: 75% 9% 15%

MET
T2
V24
M43
K82
L53
I54
T55
S56
K57
L58
L59
Q62
K66
V70
C76
H87
L88
R91
Y103
Y104
F112
L116
S128
S154
G186
K194
I200
Y201
E205
D206
N207
K208
E209
K210
D211
F212
E213
L214
C219
K232
Q233
Q237
K245
GLU
ILE
ASN
GLY
ASP
ASP
GLU
ASP
GLU
ASP
ASP
SER
SER
ASP
ASN
VAL
MET
SER
SER
GLN
ASP
ASP
GLU
ASN
ALA
ALA
PRO
VAL
ALA
VAL
LYS
CYS
THR
ASN
ALA
ASN
L34
K33
S38
P39
K40
I41
A44
I63
R75
A79
D104
S112
L125
A151
G162
N165
G168
S169
G170
S171
N172
C176
V177
M178
N189
T192
PRO
ASN
VAL
ARG
GLU
GLY
LYS
GLN
LYS
SER
TYR
PHE
PRO
ARG
GLY
THR
ALA
VAL
LEU
LYS
GLU
S216
N219
Q227
T231
ALA

- Molecule 9: Proteasome subunit beta type-2

Chain I: 76% 9% 14%

MET
A-28
D-23
F-16
H-10
T-9
Q-8
K-6
A-5
I3
K7
F8
V12
R19
S20
THR
GLN
GLY
PRO
ILE
VAL
ALA
ASP
LYS
ASN
CYS
ALA
K33
L34
S38
P39
K40
I41
A44
I63
R75
A79
D104
S112
L125
A151
G162
N165
G168
S169
G170
S171
N172
C176
V177
M178
N189
T192
PRO
ASN
VAL
ARG
GLU
GLY
LYS
GLN
LYS
SER
TYR
PHE
PRO
ARG
GLY
THR
ALA
VAL
LEU
LYS
GLU
S216
N219
Q227
T231
ALA

- Molecule 9: Proteasome subunit beta type-2

Chain W: 6% 78% 7% 14%

MET
A-28
D-23
E-13
H-10
T-9
Q-8
T-4
F8
V12
V13
R19
THR
GLN
GLY
PRO
ILE
VAL
ALA
ASP
LYS
ASN
CYS
A32
S38
I41
L80
D104
P105
F111
V121
D145
A151
I163
W164
N165
D166
L167
G168
S169
G170
S171
V177
M178
L191
T192
PRO
ASN
VAL
ARG
GLU
GLY
LYS
GLN
LYS
SER
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VAL
LEU
LYS
GLU
S216
N219
Q227
T231
ALA

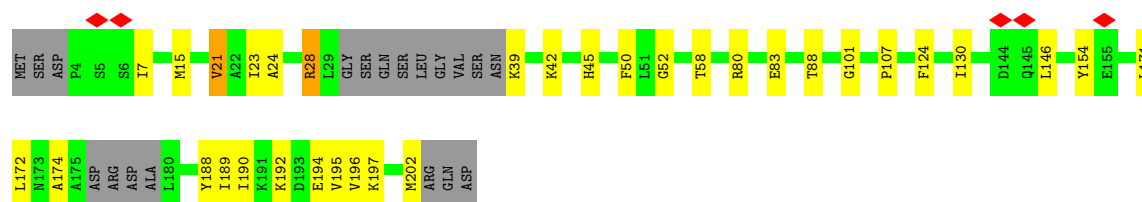
- Molecule 10: Proteasome subunit beta type-3

Chain J: 7% 82% 10% 8%

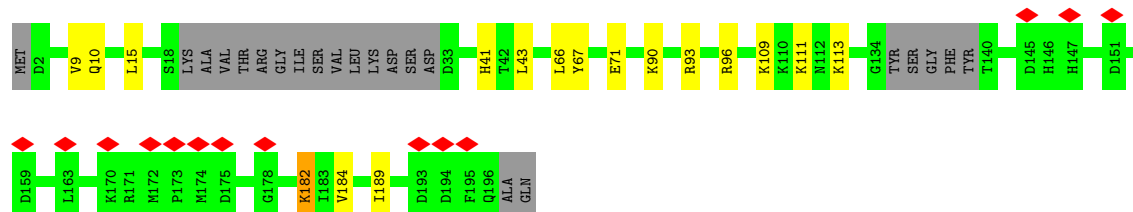
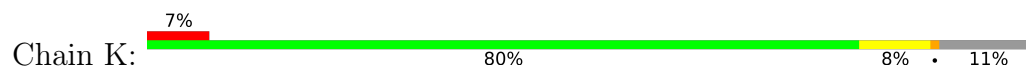
MET
SER
ASP
PRO
S5
M15
V21
R29
L29
GLY
SER
GLN
SER
LEU
GLY
VAL
SER
ASN
K39
H45
F50
L63
K70
T88
Q89
L90
G101
V105
G106
P107
F124
D125
L126
E132
T141
A142
S143
D144
E155
I167
A175
D176
R177
D178
A179
L180
S181
G182
I190
K191
V195
W202
ARG
GLN
ASP

- Molecule 10: Proteasome subunit beta type-3

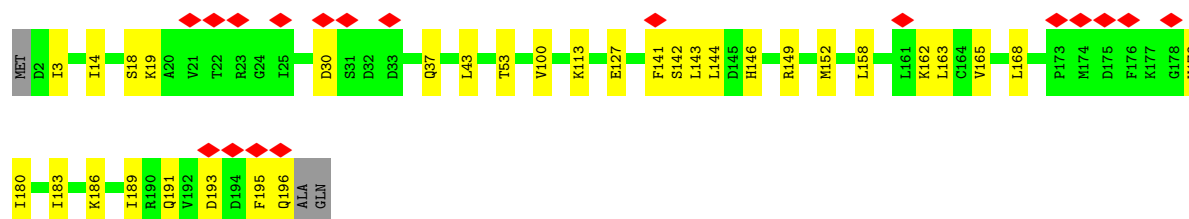
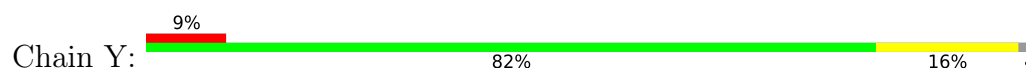
Chain X: 75% 15% 9%



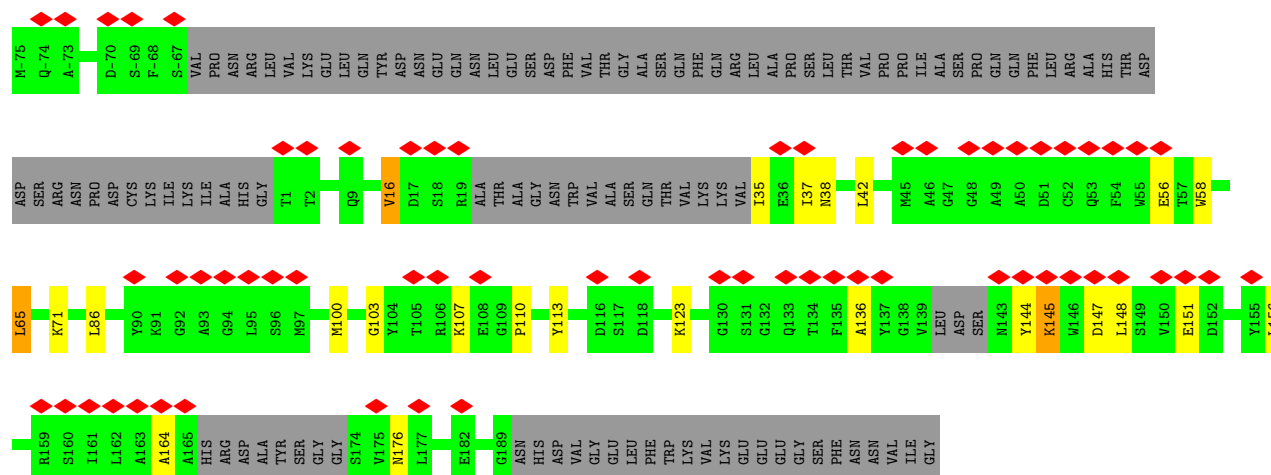
• Molecule 11: Proteasome subunit beta type-4



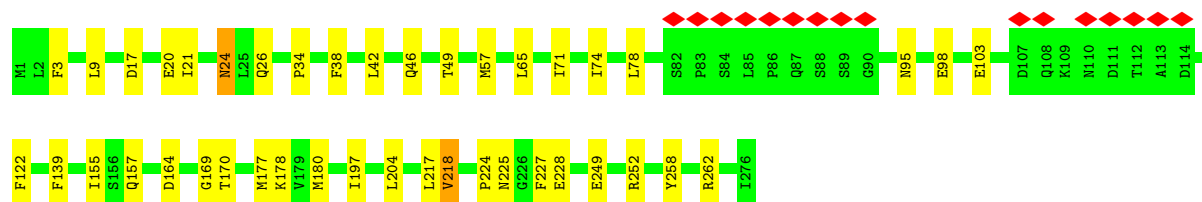
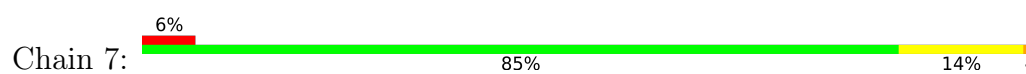
• Molecule 11: Proteasome subunit beta type-4



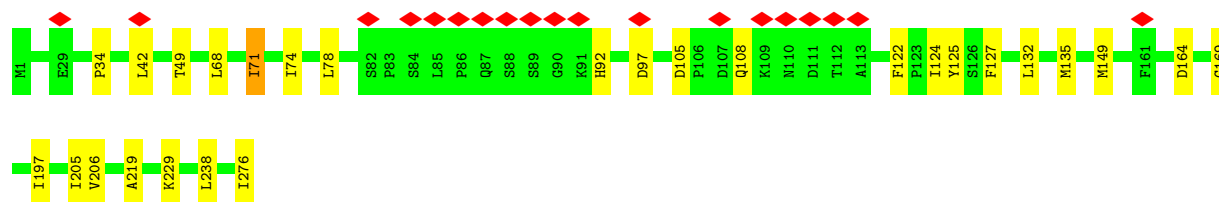
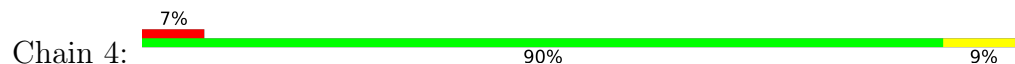
• Molecule 12: Proteasome subunit beta type-5



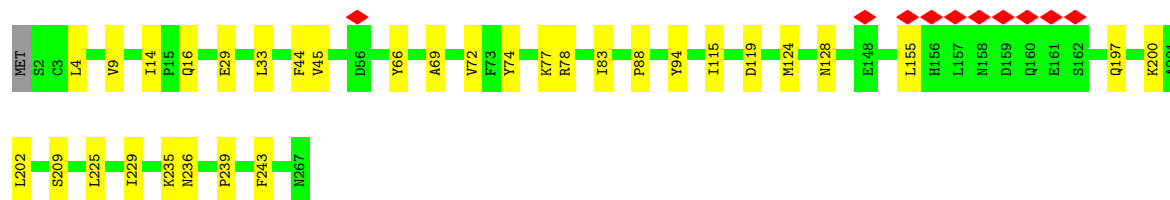
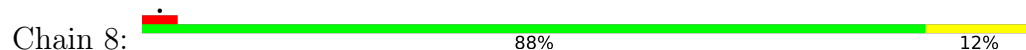
• Molecule 13: Proteasome chaperone 1



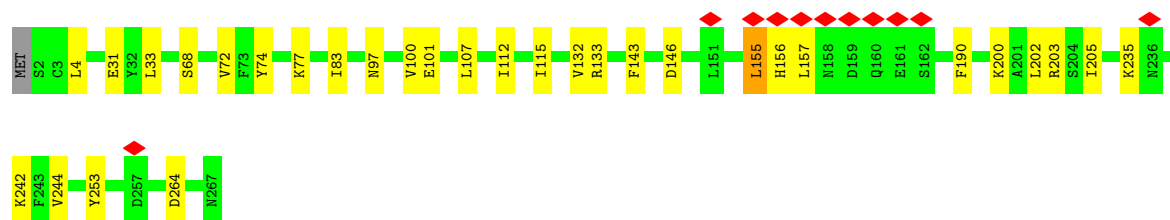
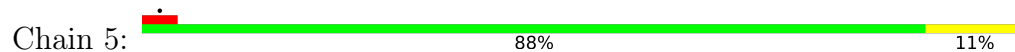
• Molecule 13: Proteasome chaperone 1



• Molecule 14: Proteasome assembly chaperone 2



• Molecule 14: Proteasome assembly chaperone 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	156855	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.195	Depositor
Minimum map value	-0.726	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.134	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.996, 0.996, 0.996	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/1959	0.26	0/2654
1	O	0.13	0/1956	0.28	0/2651
2	D	0.11	0/1986	0.24	0/2685
2	R	0.12	0/1978	0.25	0/2677
3	E	0.09	0/1941	0.23	0/2614
3	S	0.10	0/1941	0.22	0/2614
4	F	0.10	0/1830	0.25	0/2473
4	T	0.11	0/1830	0.25	0/2473
5	3	0.11	0/929	0.26	0/1252
5	6	0.11	0/1005	0.25	0/1359
6	B	0.13	0/1936	0.24	0/2620
6	P	0.13	0/1943	0.26	0/2631
7	C	0.13	0/1897	0.24	0/2566
7	Q	0.13	0/1897	0.24	0/2566
8	G	0.12	0/1928	0.27	0/2605
8	U	0.12	0/1932	0.27	0/2609
9	I	0.10	0/1730	0.26	0/2346
9	W	0.10	0/1723	0.24	0/2338
10	J	0.11	0/1501	0.25	0/2025
10	X	0.11	0/1472	0.25	0/1986
11	K	0.09	0/1424	0.23	0/1921
11	Y	0.10	0/1577	0.24	0/2127
12	Z	0.09	0/1343	0.23	0/1812
13	4	0.10	0/2175	0.25	0/2961
13	7	0.10	0/2160	0.26	0/2941
14	5	0.10	0/2214	0.24	0/3010
14	8	0.10	0/2214	0.23	0/3010
All	All	0.11	0/48421	0.25	0/65526

There are no bond length outliers.

There are no bond angle outliers.

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	1921	0	1911	11	0
1	O	1918	0	1909	16	0
2	D	1957	0	1969	19	0
2	R	1949	0	1947	19	0
3	E	1914	0	1892	14	0
3	S	1914	0	1892	12	0
4	F	1802	0	1809	16	0
4	T	1802	0	1809	13	0
5	3	911	0	841	3	0
5	6	989	0	971	3	0
6	B	1900	0	1912	11	0
6	P	1906	0	1918	12	0
7	C	1868	0	1872	12	0
7	Q	1868	0	1872	17	0
8	G	1888	0	1875	11	0
8	U	1892	0	1886	13	0
9	I	1701	0	1671	14	0
9	W	1694	0	1660	10	0
10	J	1473	0	1474	11	0
10	X	1444	0	1444	20	0
11	K	1401	0	1389	10	0
11	Y	1549	0	1533	15	0
12	Z	1319	0	1284	11	0
13	4	2122	0	2069	16	0
13	7	2108	0	2048	22	0
14	5	2161	0	2115	16	0
14	8	2161	0	2115	18	0
All	All	47532	0	47087	327	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 3.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:85:ALA:HB2	3:E:140:VAL:HG21	1.68	0.74
7:C:150:THR:HG21	7:C:163:ILE:HG12	1.71	0.73
9:W:-10:HIS:HB3	9:W:-8:GLN:HE22	1.55	0.71
2:D:73:LEU:HD11	2:D:133:THR:HB	1.72	0.70
13:4:49:THR:HG22	13:4:164:ASP:HB2	1.73	0.70
3:S:85:ALA:HB2	3:S:140:VAL:HG21	1.73	0.69
10:J:21:VAL:HG23	10:J:190:ILE:HB	1.74	0.69
6:B:46:ALA:HB1	6:B:196:LEU:HD11	1.74	0.68
13:7:74:ILE:HB	13:7:122:PHE:HB3	1.75	0.68
10:X:21:VAL:HG23	10:X:190:ILE:HB	1.77	0.67
14:5:72:VAL:HG22	14:5:83:ILE:HG12	1.77	0.66
8:U:200:ILE:HG21	8:U:214:LEU:HD13	1.78	0.66
12:Z:103:GLY:O	12:Z:110:PRO:HA	1.97	0.65
13:7:178:LYS:HB2	13:7:218:VAL:HG23	1.79	0.65
13:4:74:ILE:HB	13:4:122:PHE:HB3	1.79	0.65
12:Z:16:VAL:HG23	12:Z:176:ASN:HB2	1.78	0.64
13:4:205:ILE:HG22	13:4:206:VAL:HG13	1.79	0.63
11:Y:180:ILE:HG23	11:Y:191:GLN:HE21	1.64	0.63
4:T:74:LEU:HD22	4:T:81:ALA:HB1	1.81	0.62
2:R:73:LEU:HD13	2:R:135:ILE:HG12	1.80	0.62
2:D:54:LEU:HD13	7:C:162:ALA:HB3	1.82	0.61
2:R:73:LEU:HD11	2:R:133:THR:HB	1.82	0.61
2:D:73:LEU:HD13	2:D:135:ILE:HG12	1.81	0.61
1:A:228:ALA:HB2	1:A:233:PHE:HD1	1.65	0.61
10:X:24:ALA:HB1	10:X:171:LEU:HD11	1.83	0.61
11:Y:14:ILE:HG12	11:Y:183:ILE:HG12	1.83	0.60
3:S:31:ILE:HD13	3:S:141:ALA:HB2	1.84	0.60
13:7:49:THR:HG22	13:7:164:ASP:HB2	1.83	0.60
4:T:201:LEU:HD11	4:T:206:LEU:HG	1.84	0.60
11:Y:165:VAL:HG21	11:Y:196:GLN:HG2	1.84	0.59
3:E:31:ILE:HD13	3:E:141:ALA:HB2	1.84	0.59
6:B:174:PHE:HA	6:B:177:LYS:HE2	1.84	0.59
14:8:29:GLU:HG2	14:8:77:LYS:HD2	1.84	0.58
3:E:126:GLY:HA3	3:E:130:GLU:HB2	1.85	0.58
13:4:169:GLY:HA3	13:4:197:ILE:HG13	1.84	0.58
10:X:107:PRO:HG2	10:X:124:PHE:HB2	1.86	0.58
4:F:74:LEU:HD13	4:F:81:ALA:HB1	1.85	0.58
14:5:33:LEU:HD22	14:5:74:TYR:HB2	1.86	0.57
7:Q:184:MET:HE1	7:Q:192:LEU:HD22	1.86	0.57
13:4:74:ILE:HG13	13:4:124:ILE:HD11	1.87	0.57
14:5:132:VAL:HG23	14:5:133:ARG:HG2	1.86	0.57
14:8:225:LEU:HD23	14:8:243:PHE:HE1	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:LYS:HE2	2:D:160:SER:HA	1.86	0.56
2:R:161:ALA:HB1	2:R:175:LEU:HD13	1.87	0.56
3:E:70:ILE:HG21	3:E:112:LEU:HD21	1.87	0.56
5:3:-14:ASP:HB3	8:G:229:LYS:HD2	1.88	0.56
13:7:65:LEU:HD13	13:7:252:ARG:HE	1.71	0.56
14:5:4:LEU:HD11	14:5:83:ILE:HG13	1.87	0.56
13:7:139:PHE:HB3	13:7:225:ASN:HB3	1.87	0.56
7:Q:175:LEU:HD13	7:Q:199:LYS:HE3	1.88	0.56
3:E:45:GLY:HA3	3:E:223:THR:HG22	1.87	0.56
11:K:111:LYS:HG3	11:K:113:LYS:HG2	1.87	0.56
14:8:4:LEU:HD11	14:8:83:ILE:HG13	1.88	0.56
12:Z:136:ALA:HB2	12:Z:164:ALA:HB2	1.87	0.55
10:J:15:MET:HE2	10:J:167:ILE:HB	1.89	0.55
13:7:34:PRO:HB3	13:7:78:LEU:HB2	1.88	0.55
13:7:224:PRO:HG2	13:7:227:PHE:HB2	1.87	0.55
1:A:119:LYS:HE3	6:B:83:ARG:HD2	1.89	0.55
3:S:122:ARG:HH11	3:S:133:LEU:HB2	1.71	0.55
2:R:49:ARG:HH21	13:7:103:GLU:H	1.55	0.55
14:5:242:LYS:HG3	14:5:244:VAL:HG23	1.88	0.55
10:X:15:MET:HE3	10:X:154:TYR:HD1	1.72	0.55
2:R:81:ASP:HB3	2:R:129:PHE:HD1	1.72	0.54
6:P:94:HIS:HA	6:P:98:LYS:HB3	1.89	0.54
4:F:180:ILE:HG23	4:F:181:LYS:HG3	1.90	0.54
3:S:169:ALA:HB1	3:S:183:LEU:HD22	1.90	0.53
14:8:119:ASP:O	14:8:209:SER:HA	2.08	0.53
3:S:122:ARG:HB3	3:S:133:LEU:HB3	1.90	0.53
4:T:176:LEU:HD23	8:U:57:LYS:HE2	1.88	0.53
13:4:68:LEU:HD23	13:4:127:PHE:HB3	1.90	0.53
10:J:107:PRO:HG2	10:J:124:PHE:HB2	1.91	0.53
10:X:7:ILE:HG22	10:X:28:ARG:HH12	1.73	0.53
7:C:66:LEU:HD12	7:C:212:GLU:HG2	1.90	0.53
10:J:63:LEU:HD11	10:J:105:VAL:HG21	1.91	0.53
13:7:24:ASN:HB2	13:7:26:GLN:HE22	1.74	0.53
6:P:10:THR:HG22	6:P:18:LEU:HD22	1.91	0.53
2:D:91:VAL:HG11	5:3:134:VAL:HG13	1.90	0.52
6:B:183:LEU:HD21	6:B:191:ILE:HD12	1.92	0.52
9:I:63:ILE:HD11	9:I:79:ALA:HB2	1.91	0.52
1:O:11:GLY:HA3	14:8:124:MET:HE2	1.92	0.52
11:K:184:VAL:HG22	11:K:189:ILE:HG13	1.92	0.51
14:8:72:VAL:HG22	14:8:83:ILE:HG12	1.92	0.51
2:D:39:LYS:HG2	2:D:184:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:63:ILE:HG21	4:T:214:ALA:HB2	1.92	0.51
9:W:13:VAL:HG22	9:W:177:VAL:HG13	1.92	0.51
2:D:94:GLN:HG3	11:K:66:LEU:HB2	1.93	0.51
9:I:7:LYS:HG2	9:I:12:VAL:HG23	1.93	0.51
14:5:100:VAL:HG13	14:5:101:GLU:HG3	1.93	0.51
14:5:146:ASP:HB3	14:5:203:ARG:HH21	1.74	0.51
7:Q:144:TYR:HB2	7:Q:147:GLN:HE21	1.75	0.51
12:Z:145:LYS:HZ3	12:Z:148:LEU:HD21	1.76	0.51
1:O:127:ILE:HD11	5:6:109:ILE:HB	1.91	0.51
8:U:52:LYS:HB3	8:U:66:LYS:HG3	1.93	0.51
10:X:23:ILE:HG23	10:X:188:TYR:HB2	1.92	0.51
2:D:81:ASP:HB3	2:D:129:PHE:HD1	1.76	0.51
9:I:75:ARG:HA	9:I:104:ASP:HB3	1.93	0.51
2:R:54:LEU:HD13	7:Q:162:ALA:HB3	1.91	0.51
7:C:194:LEU:HB3	7:C:244:ILE:HD11	1.92	0.51
2:D:67:ILE:HG21	2:D:109:LEU:HD21	1.92	0.51
3:E:70:ILE:HA	3:E:93:ARG:HE	1.77	0.50
13:7:258:TYR:CZ	13:7:262:ARG:HD2	2.47	0.50
14:8:9:VAL:HG11	14:8:88:PRO:HB3	1.93	0.50
11:K:9:VAL:HG23	11:K:10:GLN:H	1.77	0.50
13:7:21:ILE:HG13	14:8:94:TYR:HE2	1.76	0.50
1:A:115:ASP:HB3	1:A:155:TYR:CZ	2.47	0.50
4:F:66:CYS:HA	4:F:89:ARG:HG2	1.92	0.50
8:G:50:VAL:HG11	8:G:66:LYS:HG2	1.94	0.50
6:P:42:GLY:HA3	6:P:185:LEU:HD13	1.93	0.50
6:P:74:VAL:HG12	6:P:135:LEU:HB2	1.93	0.50
8:U:128:SER:HB3	13:7:3:PHE:HA	1.93	0.50
10:J:70:LYS:HD3	10:J:90:LEU:HD11	1.94	0.49
14:5:107:LEU:HD23	14:5:112:ILE:HD13	1.92	0.49
2:R:34:VAL:HG13	2:R:163:THR:HG22	1.93	0.49
2:D:96:HIS:ND1	2:D:104:VAL:HG12	2.27	0.49
7:C:107:PRO:HD2	7:C:110:ILE:HD12	1.94	0.49
13:7:42:LEU:HD13	13:7:71:ILE:HG21	1.93	0.49
4:F:44:ALA:HB3	4:F:216:VAL:HG12	1.93	0.49
7:C:206:LEU:HD11	7:C:211:LEU:HD21	1.93	0.49
12:Z:37:ILE:HG22	12:Z:38:ASN:HD22	1.77	0.49
8:G:50:VAL:HG12	8:G:51:GLU:H	1.76	0.49
4:T:156:LEU:HD22	4:T:159:THR:HB	1.94	0.49
6:P:161:ALA:HB1	6:P:175:LEU:HD13	1.95	0.49
14:8:115:ILE:HG22	14:8:202:LEU:HD11	1.94	0.49
14:5:115:ILE:HG22	14:5:202:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:18:SER:HA	11:Y:179:VAL:HG12	1.94	0.48
9:W:38:SER:HB3	9:W:41:ILE:HB	1.94	0.48
9:I:-16:PHE:HD1	11:K:96:ARG:HE	1.62	0.48
2:D:58:ARG:HH12	7:C:144:TYR:HB3	1.79	0.48
6:B:75:TYR:HB3	6:B:82:TYR:CD1	2.49	0.48
9:I:-7:PRO:HG2	10:J:126:LEU:HD13	1.96	0.48
7:Q:136:ILE:HG12	7:Q:150:THR:HG22	1.96	0.48
7:Q:144:TYR:HB2	7:Q:147:GLN:NE2	2.27	0.48
1:O:228:ALA:HB2	1:O:233:PHE:HD1	1.79	0.48
4:F:176:LEU:HD23	8:G:57:LYS:HE2	1.95	0.48
10:J:190:ILE:HG23	10:J:195:VAL:HG22	1.95	0.48
2:R:2:SER:HB2	13:7:17:ASP:HB3	1.95	0.48
13:4:34:PRO:HG2	13:4:149:MET:HG3	1.94	0.48
4:F:26:LEU:HD23	4:F:149:PRO:HG2	1.94	0.47
4:F:173:GLU:HA	8:G:58:LEU:HD21	1.97	0.47
6:B:94:HIS:HA	6:B:98:LYS:HB3	1.95	0.47
11:Y:142:SER:O	11:Y:146:HIS:HB2	2.14	0.47
7:Q:150:THR:HG21	7:Q:163:ILE:HG12	1.96	0.47
3:S:205:LYS:HB2	3:S:212:LEU:HD22	1.97	0.47
5:3:80:GLU:HB3	5:3:81:PRO:HD3	1.95	0.47
14:8:155:LEU:HD23	14:8:155:LEU:H	1.79	0.47
4:F:88:LEU:HD11	4:F:108:ALA:HB1	1.96	0.47
9:I:172:ASN:HB3	9:I:189:ASN:HA	1.97	0.47
4:T:70:MET:HE2	4:T:105:VAL:HG22	1.97	0.47
7:Q:201:THR:HG21	7:Q:206:LEU:HD13	1.96	0.47
7:Q:216:ILE:HG13	7:Q:227:GLN:HG2	1.97	0.47
12:Z:35:ILE:HG12	12:Z:56:GLU:HB3	1.96	0.47
3:S:184:LEU:HD22	4:T:55:GLU:HG2	1.96	0.47
2:R:80:ALA:HB1	7:Q:120:GLN:HG3	1.97	0.47
10:X:190:ILE:HG23	10:X:195:VAL:HG22	1.97	0.47
1:A:46:ARG:HD2	1:A:152:PRO:HB2	1.97	0.47
9:I:-23:ASP:O	10:J:101:GLY:HA3	2.14	0.47
4:T:144:LEU:HD21	4:T:159:THR:HG22	1.97	0.47
3:E:68:VAL:HG11	3:E:89:ILE:HD13	1.97	0.46
2:R:97:ARG:HG2	2:R:103:PRO:HA	1.97	0.46
9:I:12:VAL:HG13	9:I:178:MET:HE3	1.97	0.46
10:X:45:HIS:HB3	10:X:50:PHE:CE2	2.51	0.46
8:U:52:LYS:HG3	8:U:213:GLU:HB2	1.97	0.46
11:Y:19:LYS:HB2	11:Y:180:ILE:HG13	1.96	0.46
13:7:38:PHE:CG	13:7:157:GLN:HG3	2.51	0.46
6:B:21:ILE:HG21	6:B:153:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:149:GLN:O	6:P:156:TYR:HA	2.15	0.46
3:S:67:ILE:HG22	3:S:228:PHE:HZ	1.80	0.46
9:W:-23:ASP:O	10:X:101:GLY:HA3	2.16	0.46
4:F:3:ARG:HB2	14:5:253:TYR:HA	1.98	0.46
4:F:176:LEU:HA	4:F:179:PHE:CE2	2.51	0.46
9:W:111:PHE:HD1	9:W:121:VAL:HG22	1.81	0.46
13:4:206:VAL:HG21	14:5:68:SER:HB3	1.97	0.46
1:A:214:LEU:HD12	1:A:218:PHE:HZ	1.81	0.46
2:R:58:ARG:HG3	2:R:59:ILE:HG23	1.96	0.46
9:W:104:ASP:HB2	9:W:105:PRO:HD2	1.97	0.46
4:T:44:ALA:HB3	4:T:216:VAL:HG12	1.98	0.45
9:W:8:PHE:HB3	9:W:151:ALA:HB2	1.98	0.45
11:Y:53:THR:HG23	11:Y:100:VAL:HG23	1.99	0.45
2:R:42:VAL:HG11	2:R:136:ALA:HB1	1.97	0.45
1:A:210:MET:HE3	1:A:214:LEU:HD11	1.99	0.45
7:Q:186:VAL:HG21	7:Q:217:ARG:HG3	1.98	0.45
11:Y:158:LEU:O	11:Y:162:LYS:HG3	2.17	0.45
3:E:25:GLU:HB3	13:4:229:LYS:HE3	1.98	0.45
3:E:46:VAL:HB	3:E:222:ILE:HG23	1.97	0.45
7:Q:217:ARG:HG2	7:Q:218:LYS:H	1.82	0.45
13:4:105:ASP:HB3	13:4:108:GLN:HB3	1.99	0.45
6:B:122:THR:HG22	6:B:129:PRO:HB3	1.99	0.45
8:G:232:LYS:HE2	8:G:232:LYS:HB2	1.82	0.45
6:P:122:THR:HG22	6:P:129:PRO:HB3	1.98	0.45
8:U:24:VAL:HG11	8:U:154:SER:HB3	1.97	0.45
4:T:29:ILE:HD11	4:T:149:PRO:HD3	1.99	0.44
10:X:88:THR:HG23	10:X:124:PHE:CZ	2.52	0.44
1:O:115:ASP:HB3	1:O:155:TYR:CZ	2.53	0.44
6:P:75:TYR:HB3	6:P:82:TYR:CD1	2.52	0.44
5:6:80:GLU:O	5:6:84:ARG:HG2	2.17	0.44
8:U:201:TYR:O	8:U:205:GLU:HG2	2.17	0.44
3:E:127:ALA:HA	4:F:83:VAL:HG22	1.98	0.44
8:G:53:LEU:HD11	8:G:209:GLU:HB3	1.99	0.44
9:I:3:ILE:HG21	9:I:44:ALA:HB3	1.99	0.44
8:U:43:ASN:HD21	8:U:186:GLY:HA3	1.83	0.44
10:X:80:ARG:HH21	10:X:83:GLU:HG2	1.82	0.44
11:Y:43:LEU:HB2	11:Y:189:ILE:HD13	1.98	0.44
2:D:161:ALA:HB1	2:D:175:LEU:HD13	1.98	0.44
6:B:140:ASP:OD1	6:B:143:ASN:HB2	2.18	0.44
13:7:95:ASN:OD1	13:7:98:GLU:HB3	2.17	0.44
9:I:112:SER:HB2	9:I:125:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:149:ARG:HB2	11:Y:152:MET:HG3	2.00	0.44
14:8:229:ILE:HG21	14:8:239:PRO:HA	1.98	0.44
2:D:97:ARG:HD3	2:D:103:PRO:HB3	1.99	0.44
9:I:38:SER:HB3	9:I:41:ILE:HB	1.98	0.44
2:R:46:CYS:HB3	2:R:63:LYS:HD3	2.00	0.44
2:R:216:LYS:HB2	2:R:220:ASP:HB3	1.99	0.44
10:X:124:PHE:CE2	10:X:130:ILE:HG12	2.53	0.44
7:C:66:LEU:HD13	7:C:214:ALA:HB2	2.00	0.44
7:Q:197:LEU:O	7:Q:201:THR:HG23	2.18	0.44
4:F:135:ILE:HD11	4:F:222:PHE:HE1	1.83	0.43
5:6:73:ARG:HA	5:6:77:GLY:O	2.17	0.43
13:4:42:LEU:HD13	13:4:71:ILE:HD12	2.00	0.43
14:5:157:LEU:HD23	14:5:190:PHE:HZ	1.83	0.43
12:Z:65:LEU:HD13	12:Z:65:LEU:HA	1.88	0.43
2:D:49:ARG:HH12	13:4:97:ASP:HA	1.83	0.43
2:D:70:HIS:ND1	2:D:71:VAL:HG23	2.33	0.43
7:Q:82:ALA:O	7:Q:86:ILE:HG12	2.18	0.43
3:S:70:ILE:HG21	3:S:112:LEU:HD21	1.99	0.43
1:A:117:LEU:O	1:A:121:MET:HG2	2.19	0.43
13:7:57:MET:HE2	13:7:170:THR:HG23	2.00	0.43
11:K:41:HIS:CD2	11:K:109:LYS:HD2	2.54	0.43
7:Q:26:LEU:HD23	7:Q:153:PRO:HD2	2.01	0.43
11:Y:143:LEU:HD21	11:Y:163:LEU:HB3	2.00	0.43
13:7:169:GLY:HA3	13:7:197:ILE:HG13	2.01	0.43
10:J:45:HIS:HB3	10:J:50:PHE:CE2	2.53	0.43
13:4:125:TYR:HB2	13:4:132:LEU:HB3	2.01	0.43
1:O:156:LYS:HE3	1:O:169:THR:HG21	2.01	0.42
1:O:194:ILE:HG22	1:O:196:GLU:HG2	2.01	0.42
12:Z:144:TYR:HA	12:Z:156:LEU:HD11	2.01	0.42
8:G:208:LYS:HG3	8:G:209:GLU:H	1.84	0.42
11:K:182:LYS:HE2	11:K:182:LYS:HB3	1.82	0.42
1:O:144:VAL:HG12	1:O:154:ILE:HG12	2.01	0.42
4:T:176:LEU:HA	4:T:179:PHE:CE1	2.54	0.42
11:Y:141:PHE:HA	11:Y:144:LEU:HB2	2.00	0.42
7:C:32:ALA:O	7:C:167:ALA:HB2	2.19	0.42
11:K:90:LYS:O	11:K:93:ARG:HG2	2.19	0.42
8:U:116:LEU:HD23	8:U:116:LEU:HA	1.89	0.42
2:D:157:SER:HB3	2:D:159:TRP:HE1	1.85	0.42
11:K:15:LEU:HD12	11:K:43:LEU:HD23	2.01	0.42
3:S:39:GLY:HA2	3:S:48:LEU:HD23	2.00	0.42
9:I:8:PHE:HB3	9:I:151:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:50:PHE:CZ	10:X:195:VAL:HG11	2.54	0.42
10:X:124:PHE:HE2	10:X:130:ILE:HG12	1.84	0.42
13:7:177:MET:HE3	13:7:217:LEU:HD11	2.02	0.42
2:R:216:LYS:HB2	2:R:216:LYS:HE2	1.92	0.42
6:P:213:ILE:HD11	6:P:236:ARG:HH11	1.84	0.42
11:Y:191:GLN:HE22	11:Y:193:ASP:HB3	1.84	0.42
13:7:9:LEU:HD12	14:8:124:MET:HE1	2.01	0.42
1:O:203:VAL:HG11	1:O:245:LEU:HD13	2.02	0.42
8:U:70:VAL:HG11	8:U:112:PHE:CZ	2.54	0.42
14:8:9:VAL:HG22	14:8:16:GLN:NE2	2.34	0.42
1:A:83:VAL:HG13	1:A:141:LEU:HD23	2.00	0.42
10:J:107:PRO:HG2	10:J:124:PHE:CD2	2.55	0.42
1:O:3:GLY:HA3	14:8:128:ASN:HA	2.02	0.42
12:Z:100:MET:HE2	12:Z:100:MET:HB2	1.90	0.42
14:8:78:ARG:HB3	14:8:236:ASN:HB3	2.02	0.42
9:W:12:VAL:HG13	9:W:178:MET:HE3	2.00	0.42
3:E:179:ALA:HB2	3:E:207:VAL:HG11	2.02	0.42
8:G:24:VAL:HG11	8:G:154:SER:HB3	2.01	0.42
9:I:-6:LYS:HD3	9:I:-5:ALA:N	2.35	0.42
10:X:39:LYS:NZ	11:Y:127:GLU:H	2.18	0.42
6:B:149:GLN:O	6:B:156:TYR:HA	2.19	0.41
1:O:156:LYS:O	1:O:163:TYR:HA	2.19	0.41
8:U:87:HIS:O	8:U:91:ARG:HG2	2.20	0.41
13:4:219:ALA:HB2	13:4:238:LEU:HD21	2.02	0.41
2:D:1:MET:HG2	2:D:22:TYR:OH	2.21	0.41
11:K:67:TYR:CZ	11:K:71:GLU:HG3	2.55	0.41
10:X:146:LEU:HD13	10:X:174:ALA:HB2	2.02	0.41
3:E:169:ALA:HB3	4:F:56:LEU:HD13	2.02	0.41
10:J:88:THR:HG23	10:J:124:PHE:CZ	2.55	0.41
2:R:70:HIS:CD2	2:R:71:VAL:HG13	2.56	0.41
10:X:42:LYS:O	10:X:52:GLY:HA2	2.21	0.41
2:D:58:ARG:NH1	7:C:144:TYR:HB3	2.36	0.41
2:R:185:PRO:HB2	2:R:191:CYS:SG	2.60	0.41
3:S:68:VAL:HG21	3:S:89:ILE:HD13	2.02	0.41
13:7:155:ILE:HD12	13:7:204:LEU:HD21	2.03	0.41
7:C:4:ARG:HA	7:C:4:ARG:HH11	1.86	0.41
8:G:205:GLU:C	8:G:207:ASN:H	2.27	0.41
1:O:117:LEU:O	1:O:121:MET:HG2	2.21	0.41
1:O:210:MET:HE3	1:O:214:LEU:HD11	2.03	0.41
2:R:80:ALA:O	2:R:84:ILE:HG12	2.21	0.41
12:Z:58:TRP:CE3	12:Z:86:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:VAL:HG11	2:D:136:ALA:HB1	2.03	0.41
9:I:34:LEU:HD13	9:I:176:CYS:HB2	2.02	0.41
1:O:190:LYS:HE2	1:O:190:LYS:HB2	1.88	0.41
2:R:8:LEU:HD23	2:R:19:GLN:HB3	2.03	0.41
7:Q:66:LEU:HD13	7:Q:214:ALA:HB2	2.02	0.41
8:U:103:TYR:O	8:U:104:LYS:HG2	2.21	0.41
9:W:111:PHE:CD1	9:W:121:VAL:HG22	2.56	0.41
10:X:172:LEU:HD21	10:X:202:MET:SD	2.61	0.41
10:X:189:ILE:HB	10:X:196:VAL:HG23	2.02	0.41
11:Y:37:GLN:HG3	11:Y:189:ILE:HD12	2.02	0.41
12:Z:113:TYR:CE2	12:Z:123:LYS:HB2	2.56	0.41
14:8:33:LEU:HD22	14:8:74:TYR:HB2	2.02	0.41
3:S:218:GLN:HE21	3:S:230:ILE:HG21	1.86	0.41
7:Q:107:PRO:HD2	7:Q:110:ILE:HD12	2.03	0.41
14:8:44:PHE:HB3	14:8:69:ALA:HB2	2.03	0.41
13:4:122:PHE:HE2	13:4:135:MET:HA	1.85	0.41
1:A:164:VAL:HG13	1:A:166:TYR:CE2	2.56	0.40
3:E:45:GLY:HA2	3:E:153:TYR:CE2	2.56	0.40
4:F:81:ALA:HB2	4:F:130:VAL:HG21	2.02	0.40
1:A:190:LYS:HE2	1:A:190:LYS:HB2	1.82	0.40
4:F:153:VAL:H	8:G:86:ARG:HH12	1.69	0.40
14:5:143:PHE:HB3	14:5:205:ILE:HB	2.02	0.40
14:5:155:LEU:HB3	14:5:156:HIS:H	1.59	0.40
1:A:194:ILE:HG22	1:A:196:GLU:HG2	2.04	0.40
6:B:66:LEU:HD12	6:B:235:PHE:CD2	2.57	0.40
1:O:167:LYS:HG2	6:P:55:LEU:O	2.22	0.40
4:T:215:ILE:O	4:T:222:PHE:HA	2.21	0.40
9:W:227:GLN:HE22	10:X:194:GLU:HG3	1.86	0.40
13:7:180:MET:HE3	14:8:66:TYR:HE2	1.86	0.40
13:4:34:PRO:HB3	13:4:78:LEU:HB2	2.02	0.40
7:C:218:LYS:HB2	7:C:225:VAL:HG22	2.04	0.40
1:O:95:LEU:HD23	1:O:95:LEU:HA	1.86	0.40
14:5:97:ASN:HA	14:5:100:VAL:HG12	2.03	0.40
3:E:121:LEU:HD22	4:F:79:PRO:HB3	2.03	0.40
1:O:167:LYS:HB3	6:P:57:MET:HE3	2.03	0.40
4:T:33:SER:HB2	4:T:62:LYS:NZ	2.36	0.40
6:P:46:ALA:HB1	6:P:196:LEU:HD11	2.03	0.40
8:U:88:LEU:HA	8:U:88:LEU:HD23	1.85	0.40
14:5:146:ASP:HB3	14:5:203:ARG:NH2	2.37	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	244/252 (97%)	236 (97%)	8 (3%)	0	100	100
1	O	244/252 (97%)	238 (98%)	6 (2%)	0	100	100
2	D	247/254 (97%)	240 (97%)	6 (2%)	1 (0%)	30	61
2	R	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
3	E	245/260 (94%)	240 (98%)	5 (2%)	0	100	100
3	S	245/260 (94%)	239 (98%)	6 (2%)	0	100	100
4	F	232/234 (99%)	226 (97%)	6 (3%)	0	100	100
4	T	232/234 (99%)	223 (96%)	9 (4%)	0	100	100
5	3	105/162 (65%)	96 (91%)	9 (9%)	0	100	100
5	6	120/162 (74%)	111 (92%)	9 (8%)	0	100	100
6	B	244/250 (98%)	240 (98%)	4 (2%)	0	100	100
6	P	247/250 (99%)	244 (99%)	3 (1%)	0	100	100
7	C	234/258 (91%)	225 (96%)	9 (4%)	0	100	100
7	Q	234/258 (91%)	230 (98%)	4 (2%)	0	100	100
8	G	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
8	U	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
9	I	218/261 (84%)	207 (95%)	11 (5%)	0	100	100
9	W	218/261 (84%)	213 (98%)	5 (2%)	0	100	100
10	J	185/205 (90%)	175 (95%)	10 (5%)	0	100	100
10	X	180/205 (88%)	172 (96%)	8 (4%)	0	100	100
11	K	170/198 (86%)	162 (95%)	8 (5%)	0	100	100
11	Y	193/198 (98%)	184 (95%)	9 (5%)	0	100	100
12	Z	162/287 (56%)	160 (99%)	1 (1%)	1 (1%)	21	52
13	4	274/276 (99%)	258 (94%)	16 (6%)	0	100	100
13	7	274/276 (99%)	263 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5	264/267 (99%)	256 (97%)	8 (3%)	0	100	100
14	8	264/267 (99%)	259 (98%)	5 (2%)	0	100	100
All	All	6006/6617 (91%)	5805 (97%)	199 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	101	GLU
12	Z	107	LYS

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	204/210 (97%)	198 (97%)	6 (3%)	37	66
1	O	204/210 (97%)	201 (98%)	3 (2%)	57	75
2	D	221/226 (98%)	219 (99%)	2 (1%)	70	80
2	R	219/226 (97%)	218 (100%)	1 (0%)	81	85
3	E	205/215 (95%)	203 (99%)	2 (1%)	68	79
3	S	205/215 (95%)	201 (98%)	4 (2%)	48	72
4	F	193/193 (100%)	187 (97%)	6 (3%)	35	64
4	T	193/193 (100%)	189 (98%)	4 (2%)	47	71
5	3	101/150 (67%)	97 (96%)	4 (4%)	28	60
5	6	114/150 (76%)	112 (98%)	2 (2%)	51	73
6	B	207/209 (99%)	204 (99%)	3 (1%)	59	76
6	P	208/209 (100%)	201 (97%)	7 (3%)	32	63
7	C	200/216 (93%)	192 (96%)	8 (4%)	28	60
7	Q	200/216 (93%)	199 (100%)	1 (0%)	81	85
8	G	200/239 (84%)	189 (94%)	11 (6%)	19	50
8	U	201/239 (84%)	194 (96%)	7 (4%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	183/214 (86%)	181 (99%)	2 (1%)	65	78
9	W	181/214 (85%)	176 (97%)	5 (3%)	38	66
10	J	159/173 (92%)	153 (96%)	6 (4%)	29	60
10	X	156/173 (90%)	151 (97%)	5 (3%)	34	64
11	K	153/175 (87%)	152 (99%)	1 (1%)	76	82
11	Y	169/175 (97%)	163 (96%)	6 (4%)	31	62
12	Z	135/235 (57%)	128 (95%)	7 (5%)	21	51
13	4	238/251 (95%)	235 (99%)	3 (1%)	61	77
13	7	233/251 (93%)	227 (97%)	6 (3%)	40	68
14	5	243/244 (100%)	237 (98%)	6 (2%)	42	69
14	8	243/244 (100%)	238 (98%)	5 (2%)	47	71
All	All	5168/5665 (91%)	5045 (98%)	123 (2%)	43	69

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	64	LEU
1	A	95	LEU
1	A	169	THR
1	A	216	THR
1	A	232	LYS
2	D	104	VAL
2	D	153	SER
3	E	186	GLU
3	E	222	ILE
4	F	4	ASN
4	F	34	VAL
4	F	35	THR
4	F	50	LYS
4	F	72	LEU
4	F	74	LEU
5	3	-13	TYR
5	3	-3	HIS
5	3	64	GLN
5	3	65	ARG
6	B	63	LYS
6	B	97	TYR

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Mol	Chain	Res	Type
6	B	99	ARG
7	C	51	LYS
7	C	72	LYS
7	C	100	LYS
7	C	165	VAL
7	C	195	LYS
7	C	201	THR
7	C	213	PHE
7	C	228	LYS
8	G	18	ASP
8	G	50	VAL
8	G	53	LEU
8	G	54	ILE
8	G	63	LYS
8	G	107	ILE
8	G	170	GLN
8	G	178	LYS
8	G	208	LYS
8	G	229	LYS
8	G	232	LYS
9	I	40	LYS
9	I	63	ILE
10	J	21	VAL
10	J	29	LEU
10	J	39	LYS
10	J	132	GLU
10	J	141	THR
10	J	191	LYS
11	K	182	LYS
1	O	169	THR
1	O	230	LYS
1	O	232	LYS
2	R	20	VAL
3	S	9	ASP
3	S	90	GLU
3	S	202	LYS
3	S	222	ILE
4	T	34	VAL
4	T	35	THR
4	T	74	LEU
4	T	180	ILE
5	6	47	LEU

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Mol	Chain	Res	Type
5	6	73	ARG
6	P	37	ILE
6	P	43	VAL
6	P	57	MET
6	P	63	LYS
6	P	169	VAL
6	P	211	LEU
6	P	230	ASP
7	Q	63	THR
8	U	52	LYS
8	U	54	ILE
8	U	59	LEU
8	U	76	CYS
8	U	194	LYS
8	U	210	LYS
8	U	219	CYS
9	W	-10	HIS
9	W	-4	THR
9	W	80	LEU
9	W	163	ILE
9	W	191	LEU
10	X	21	VAL
10	X	28	ARG
10	X	58	THR
10	X	192	LYS
10	X	197	LYS
11	Y	3	ILE
11	Y	30	ASP
11	Y	113	LYS
11	Y	168	LEU
11	Y	186	LYS
11	Y	195	PHE
12	Z	16	VAL
12	Z	42	LEU
12	Z	65	LEU
12	Z	71	LYS
12	Z	145	LYS
12	Z	147	ASP
12	Z	151	GLU
13	7	20	GLU
13	7	24	ASN
13	7	46	GLN

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Mol	Chain	Res	Type
13	7	218	VAL
13	7	228	GLU
13	7	249	GLU
14	8	14	ILE
14	8	45	VAL
14	8	197	GLN
14	8	200	LYS
14	8	235	LYS
13	4	71	ILE
13	4	92	HIS
13	4	276	ILE
14	5	31	GLU
14	5	77	LYS
14	5	155	LEU
14	5	200	LYS
14	5	235	LYS
14	5	264	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
3	E	147	HIS
3	E	218	GLN
4	F	91	GLN
5	3	-5	HIS
5	3	-1	HIS
6	B	143	ASN
6	B	190	HIS
7	C	21	GLN
7	C	168	ASN
8	G	33	ASN
8	G	64	ASN
9	I	10	ASN
10	J	8	ASN
10	J	64	ASN
1	O	37	GLN
3	S	154	GLN
3	S	180	GLN
4	T	90	GLN
4	T	110	HIS
5	6	36	GLN

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Mol	Chain	Res	Type
5	6	48	ASN
7	Q	227	GLN
8	U	123	HIS
8	U	207	ASN
9	W	219	ASN
9	W	227	GLN
10	X	8	ASN
11	Y	191	GLN
12	Z	143	ASN
12	Z	179	HIS
13	7	26	GLN
13	7	64	ASN
14	8	24	ASN
14	8	156	HIS
14	8	236	ASN
13	4	99	ASN
13	4	102	ASN
13	4	157	GLN
13	4	183	ASN
13	4	271	GLN
14	5	13	ASN
14	5	84	GLN
14	5	156	HIS
14	5	158	ASN
14	5	213	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

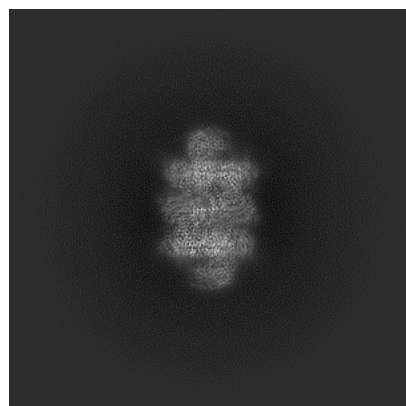
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54045. These allow visual inspection of the internal detail of the map and identification of artifacts.

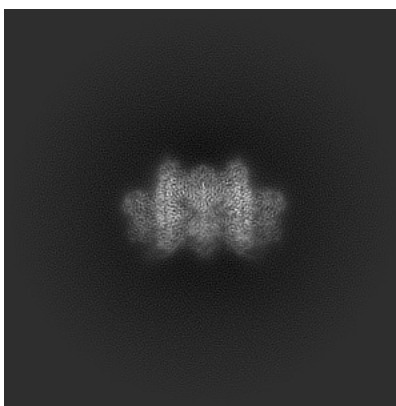
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

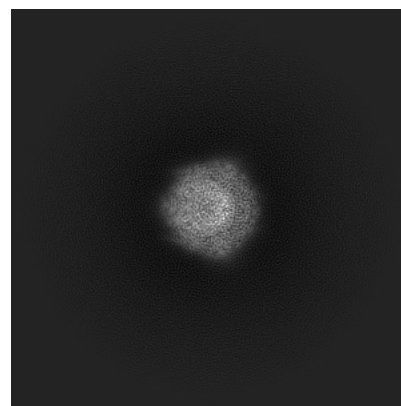
6.1.1 Primary map



X

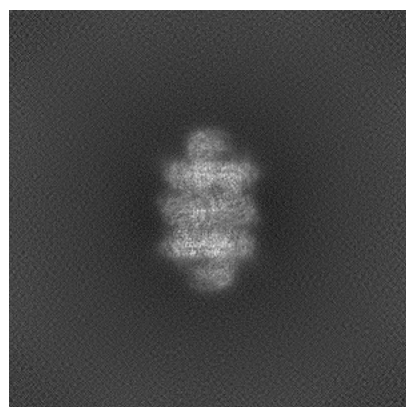


Y

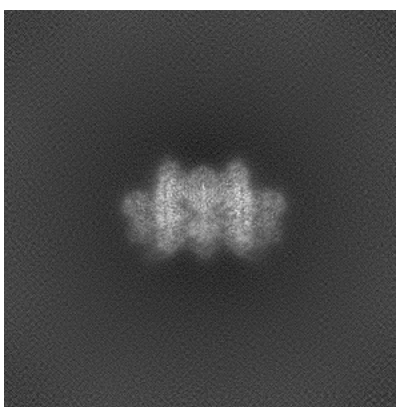


Z

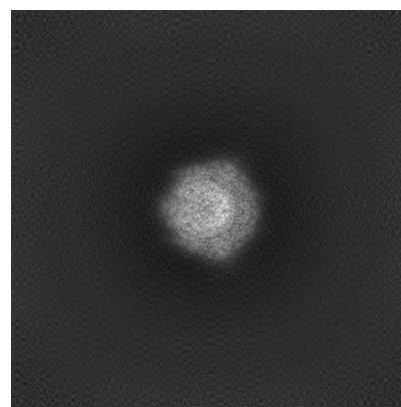
6.1.2 Raw map



X



Y

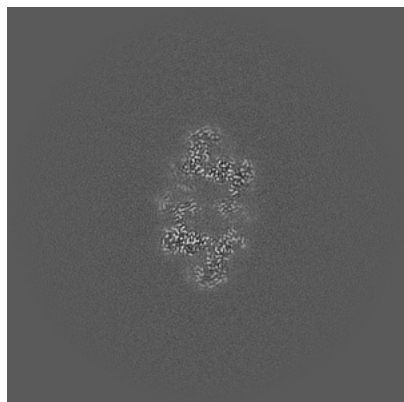


Z

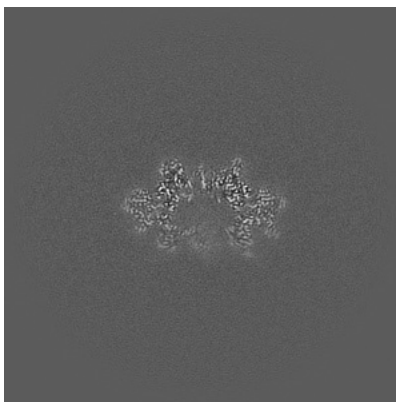
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

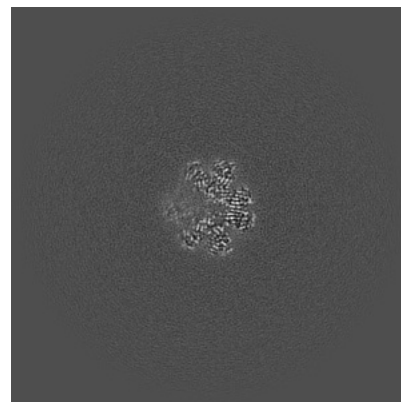
6.2.1 Primary map



X Index: 250

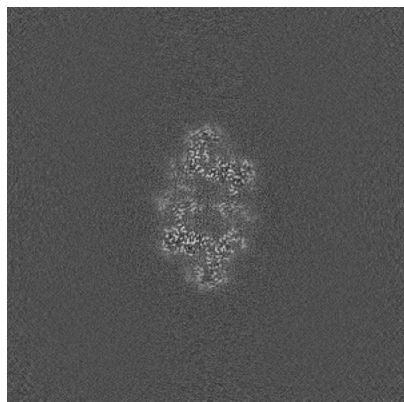


Y Index: 250

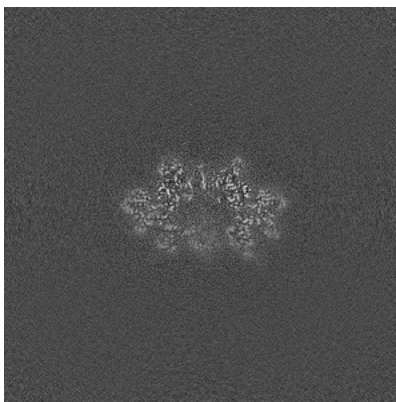


Z Index: 250

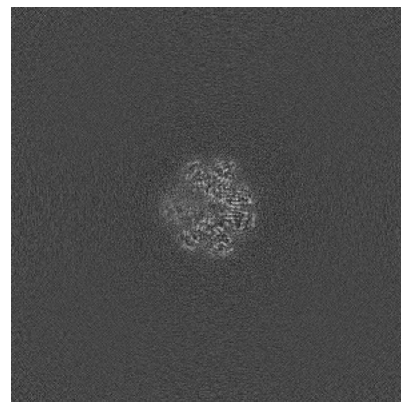
6.2.2 Raw map



X Index: 250



Y Index: 250

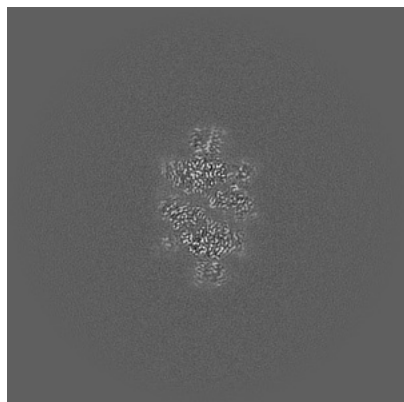


Z Index: 250

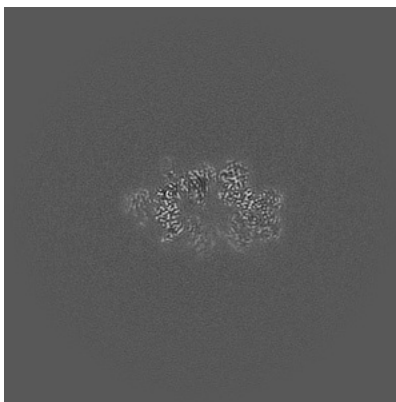
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

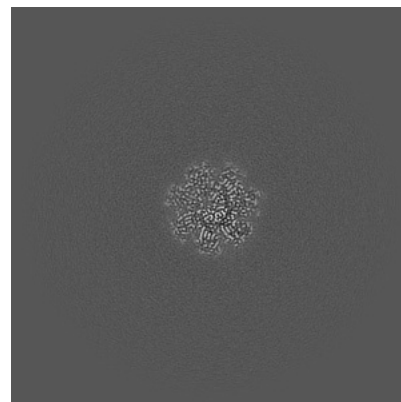
6.3.1 Primary map



X Index: 264

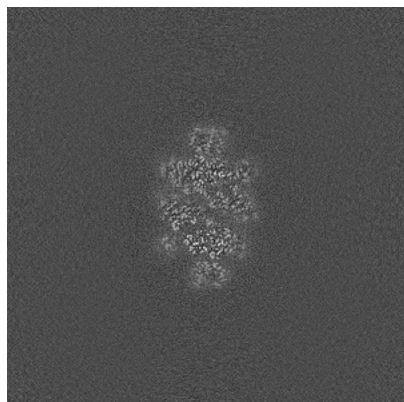


Y Index: 238

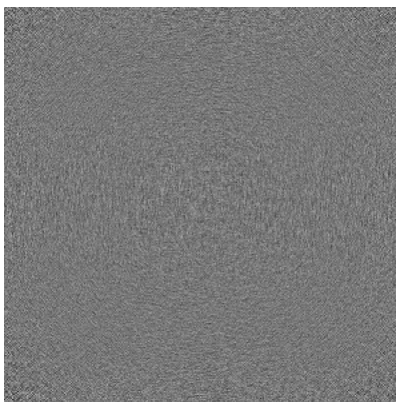


Z Index: 207

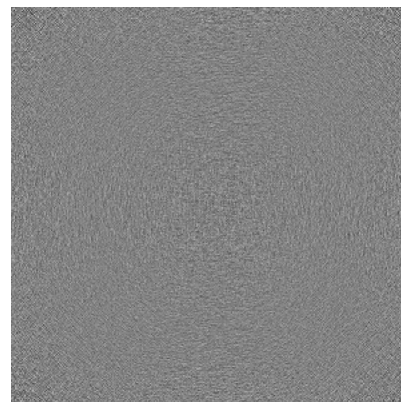
6.3.2 Raw map



X Index: 263



Y Index: 0

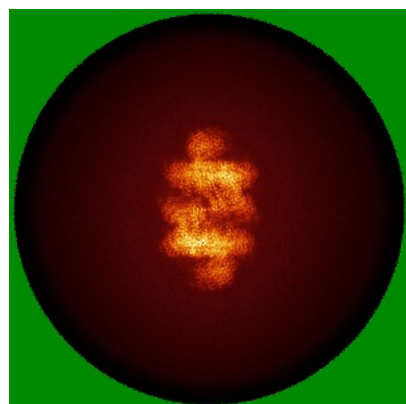


Z Index: 499

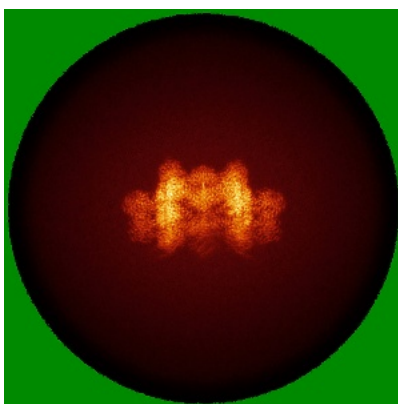
The images above show the largest variance slices of the map in three orthogonal directions.

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

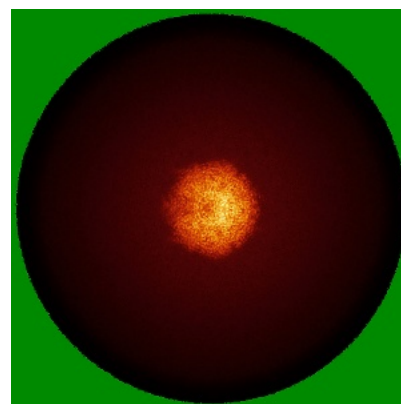
6.4.1 Primary map



X

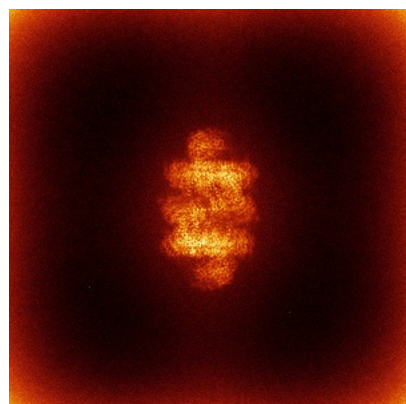


Y

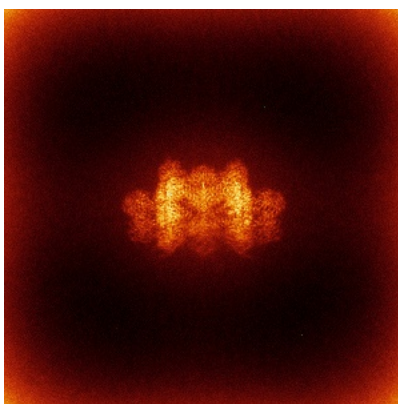


Z

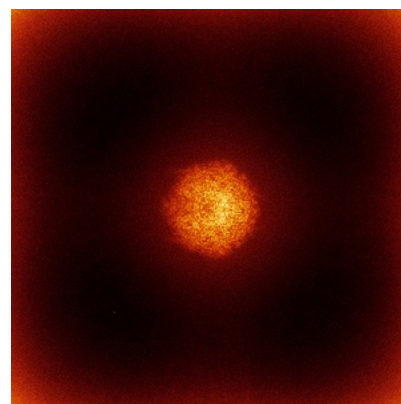
6.4.2 Raw map



X



Y

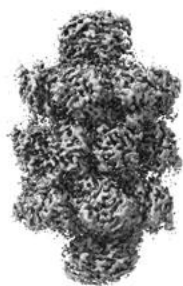


Z

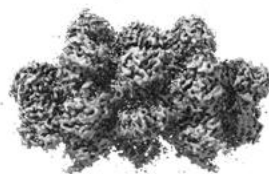
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

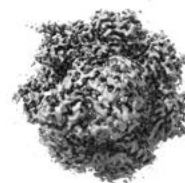
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.134. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

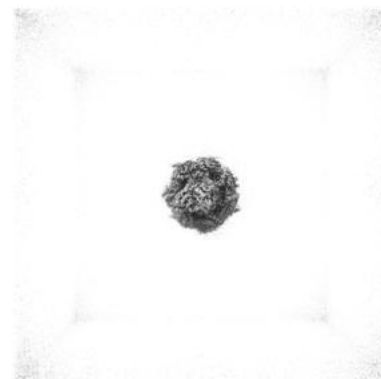
6.5.2 Raw map



X



Y



Z

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

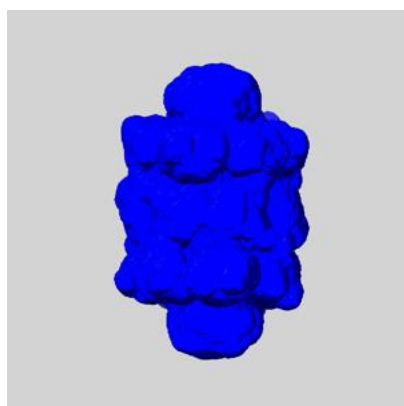
6.6 Mask visualisation [i](#)

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

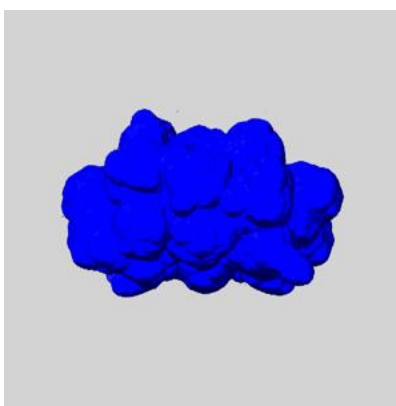
A mask typically either:

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

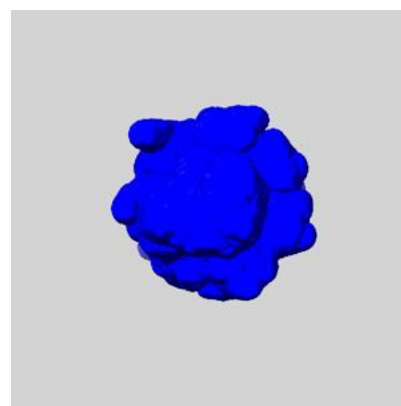
6.6.1 emd_54045_msk_1.map [i](#)



X



Y

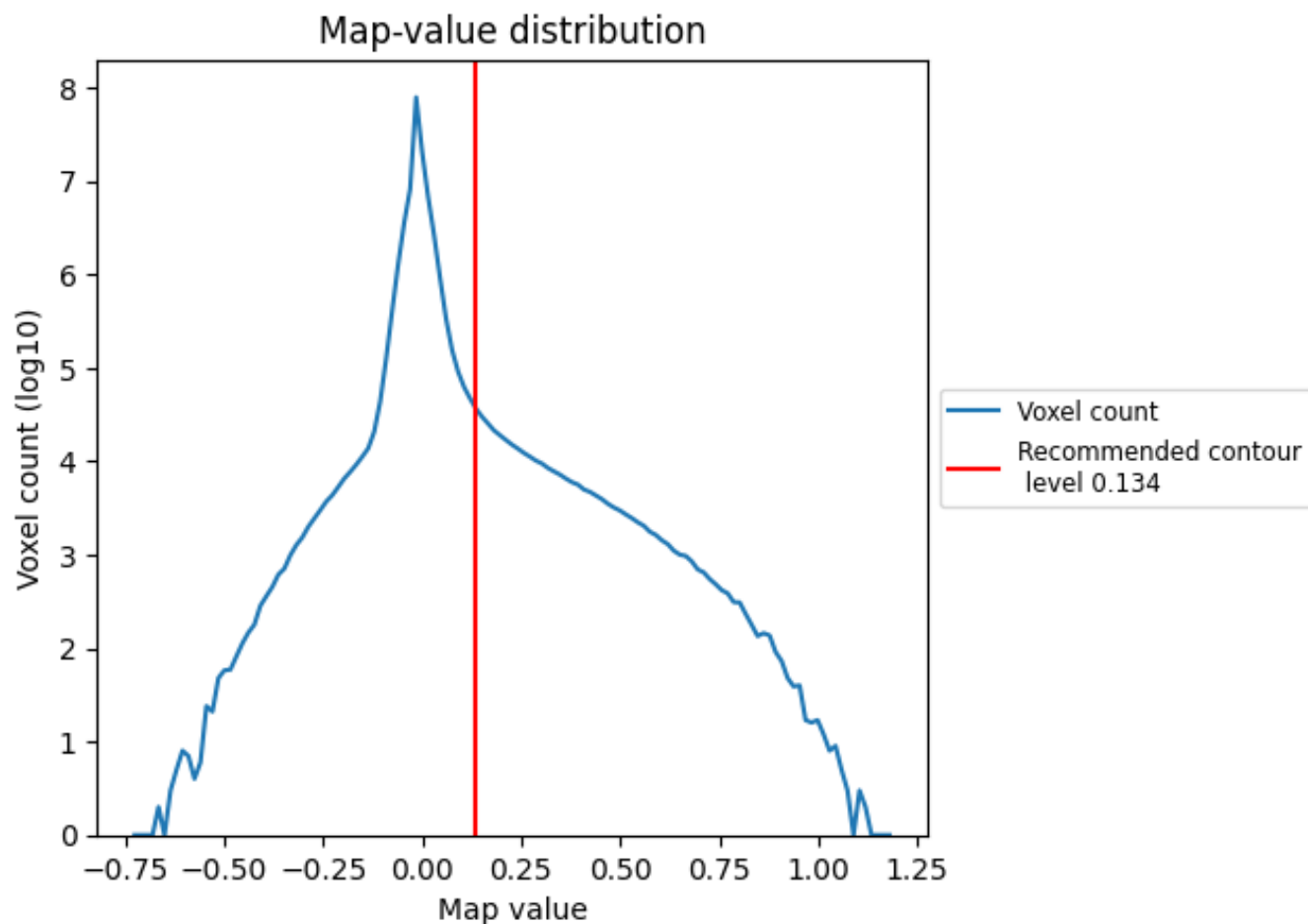


Z

7 Map analysis [i](#)

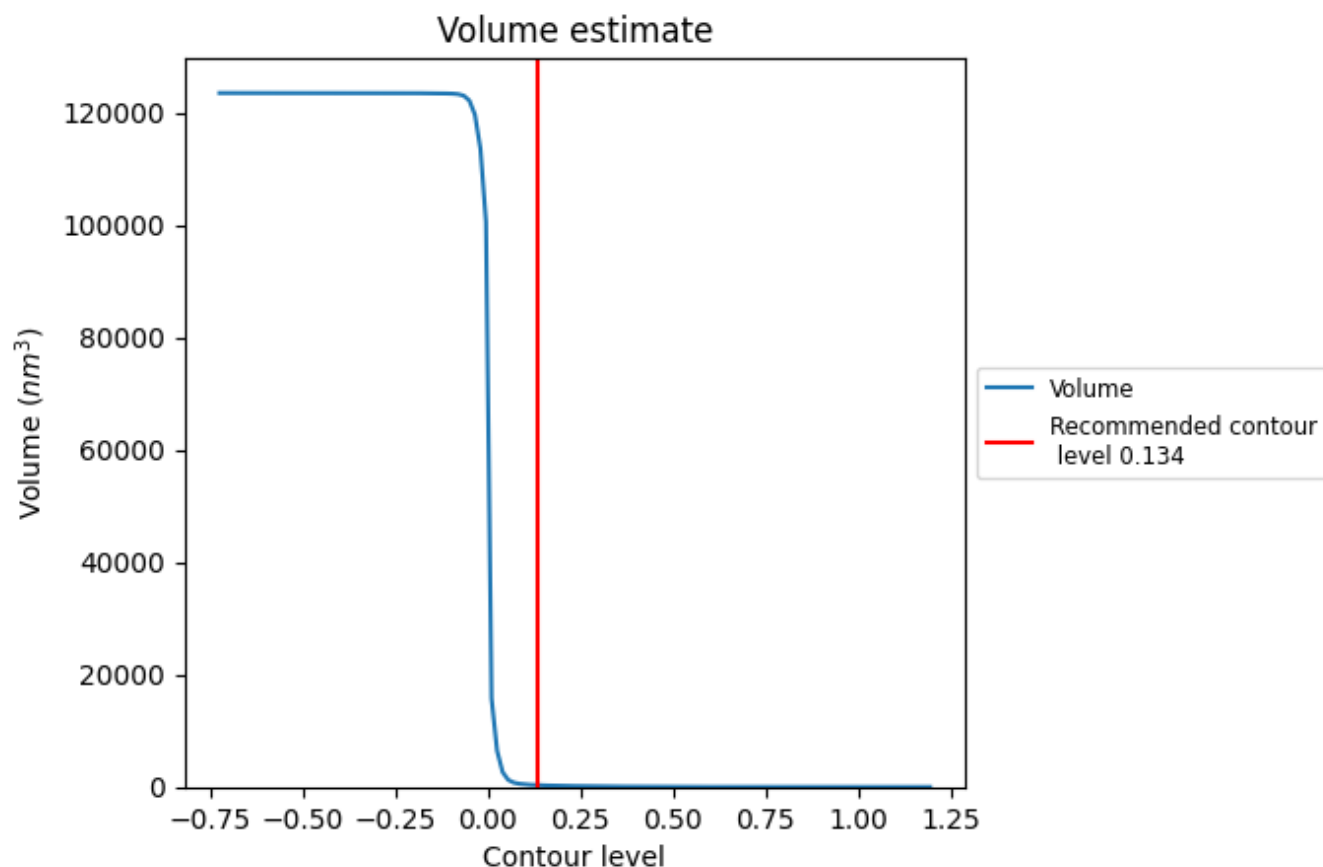
This section contains the results of statistical analysis of the map.

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.

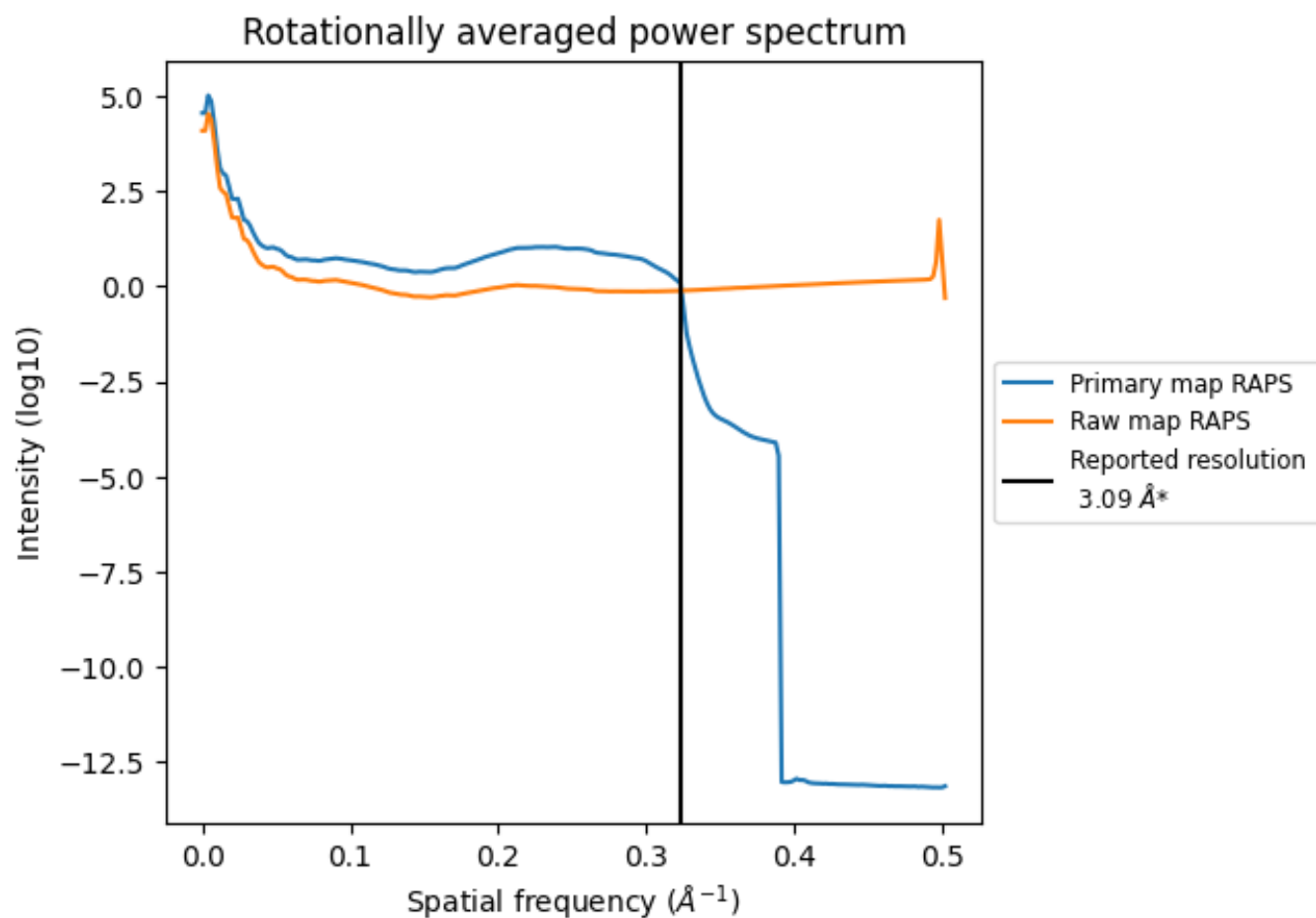
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 319 nm³; this corresponds to an approximate mass of 288 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 ⓘ

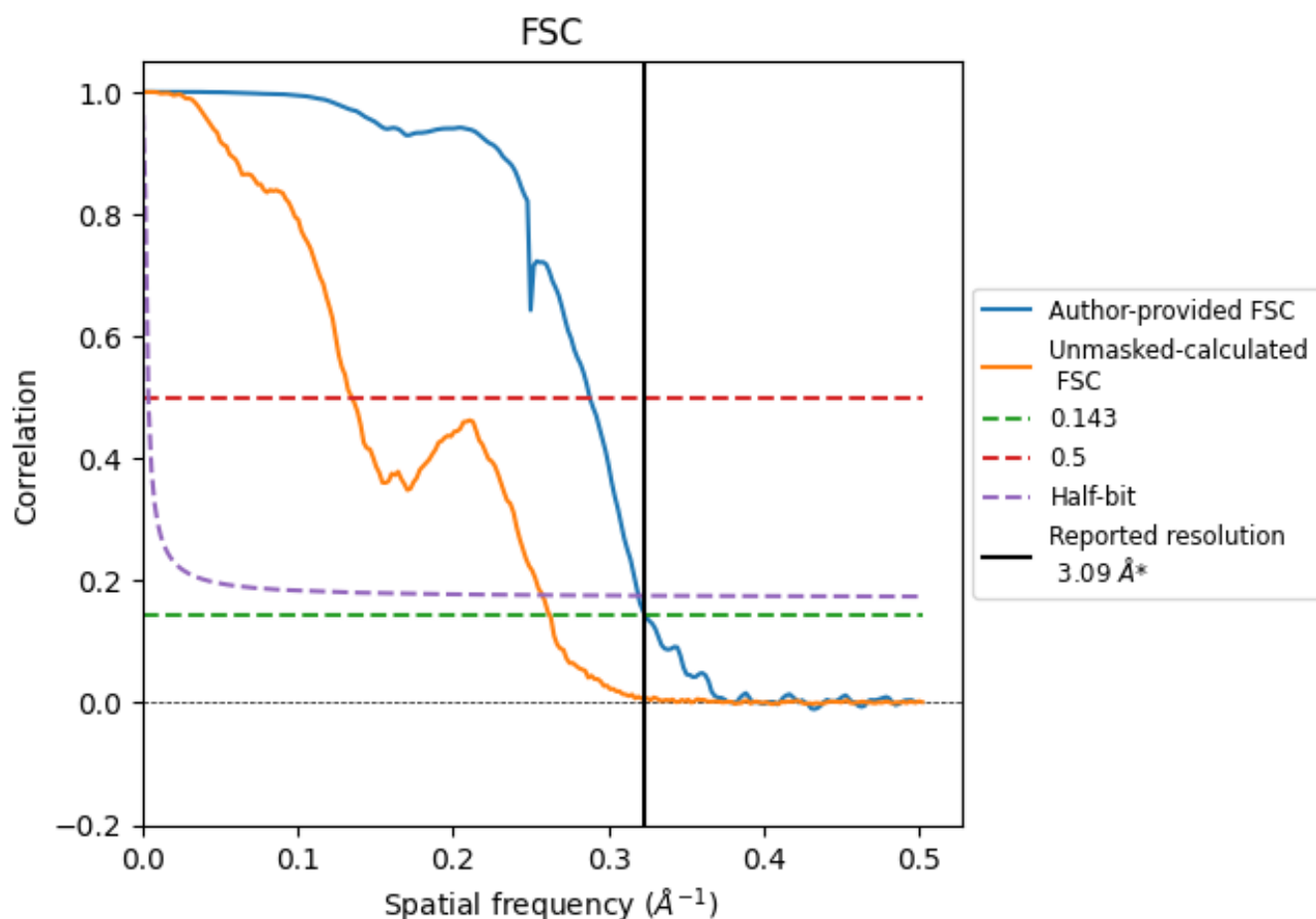


*Reported resolution corresponds to spatial frequency of 0.324 \AA^{-1}

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 0.324 \AA^{-1}

8.2 Resolution estimates [i](#)

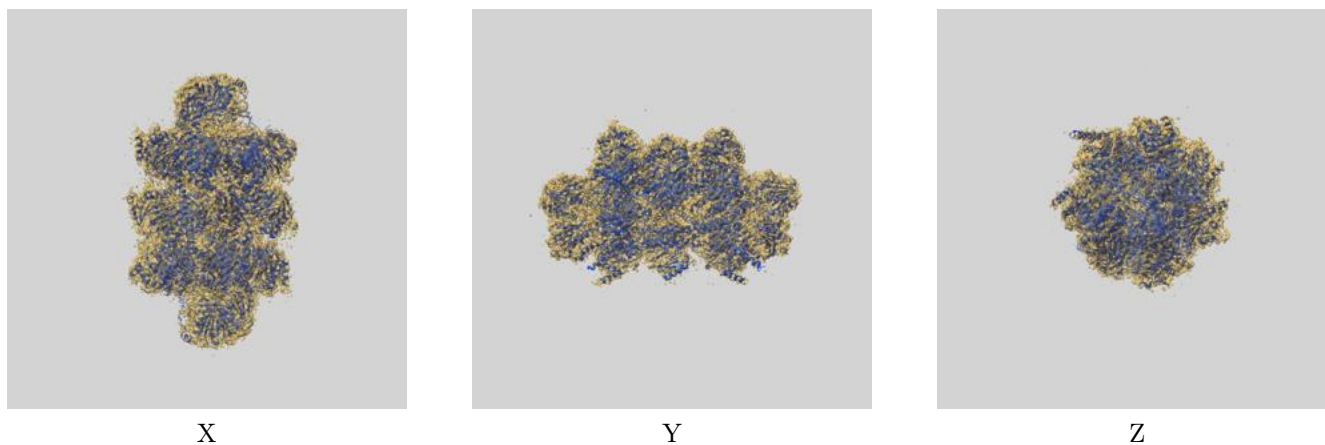
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.47	3.13
Unmasked-calculated*	3.81	7.41	3.88

*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 3.81 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

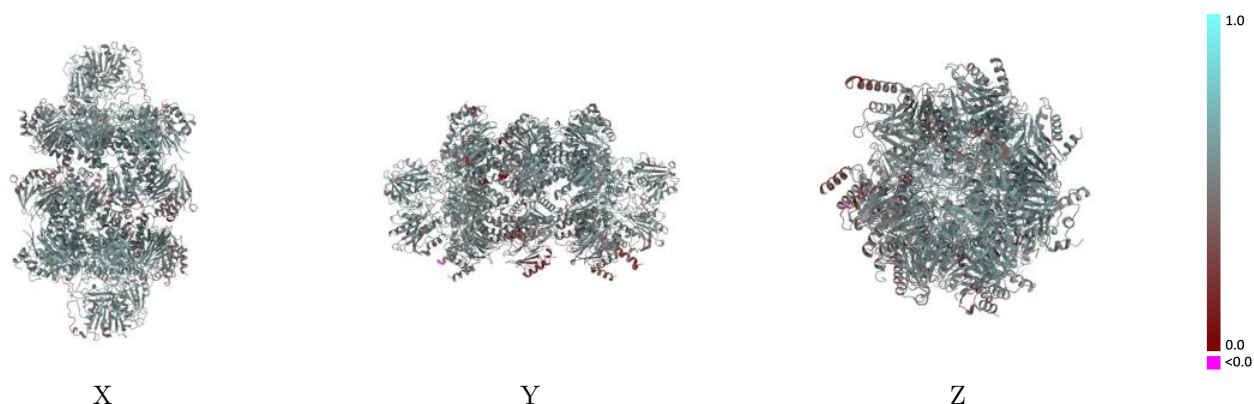
This section contains information regarding the fit between EMDB map EMD-54045 and PDB model 9RLT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.134 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](#)

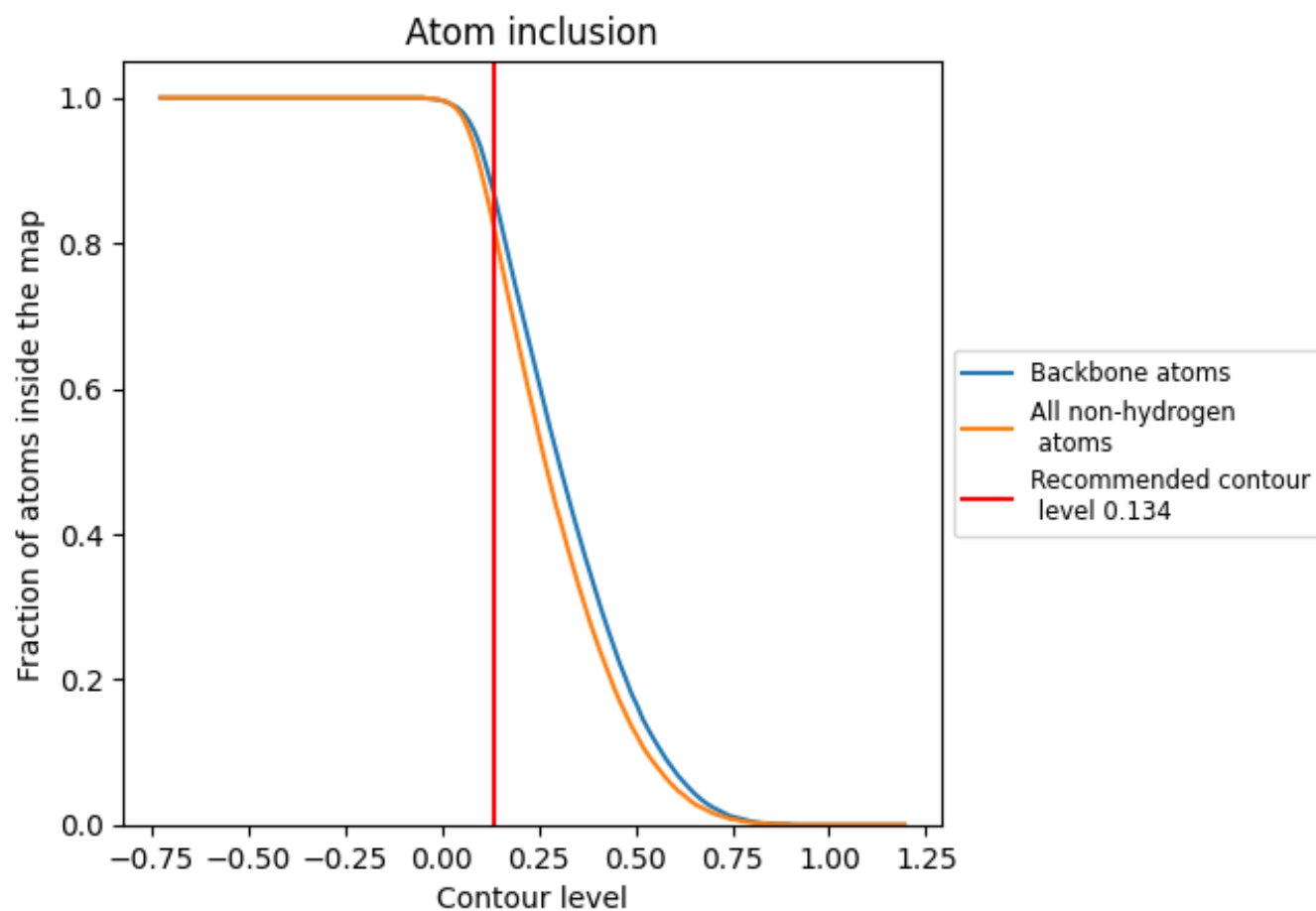


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.5240
3	 0.8330	 0.5300
4	 0.7930	 0.5040
5	 0.8420	 0.5250
6	 0.8010	 0.5360
7	 0.8160	 0.5110
8	 0.8390	 0.5170
A	 0.8940	 0.5610
B	 0.8970	 0.5690
C	 0.8710	 0.5490
D	 0.7930	 0.5040
E	 0.7180	 0.4680
F	 0.8410	 0.5290
G	 0.8560	 0.5320
I	 0.8230	 0.5250
J	 0.8180	 0.5200
K	 0.7580	 0.4950
O	 0.8940	 0.5590
P	 0.9080	 0.5740
Q	 0.8860	 0.5560
R	 0.8290	 0.5280
S	 0.8060	 0.5150
T	 0.8570	 0.5390
U	 0.8370	 0.5270
W	 0.8090	 0.5240
X	 0.8610	 0.5440
Y	 0.7380	 0.4820
Z	 0.5150	 0.3910

