Full wwPDB EM Validation Report (i)

Oct 3, 2024 – 12:27 PM JST

PDB ID	:	8YSX
EMDB ID	:	EMD-39565
Title	:	canine immunoproteasome 20S subunit in complex with compound 2
Authors	:	Kashima, A.; Arai, Y.
Deposited on	:	2024-03-24
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

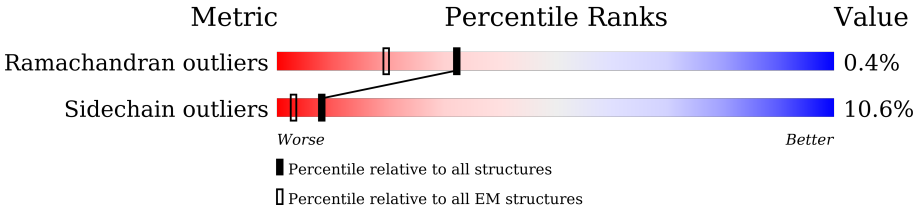
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	199	• 90% 10%
1	F	199	• 90% 10%
2	G	263	11% 79% 10% 11%
2	L	263	10% 79% 10% 11%
3	H	241	8% 83% 13% •
3	M	241	9% 83% 13% •
4	I	248	12% 81% 12% 7%
4	N	248	11% 81% 12% 7%
5	O	261	12% 87% 6% 7%

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Mol	Chain	Length	Quality of chain
5	Z	261	11% 87% 6% 7%
6	K	246	24% 87% 7% 6%
6	R	246	22% 87% 7% 6%
7	T	201	91% 7%
7	V	201	91% 7%
8	U	205	95% 5%
8	Y	205	95% 5%
9	W	264	76% 5% 19%
9	a	264	76% 5% 19%
10	C	204	89% 10%
10	D	204	89% 10%
11	P	234	12% 91% 6%
11	b	234	12% 91% 6%
12	S	241	82% 6% 12%
12	X	241	82% 6% 12%
13	J	255	12% 82% 11% 7%
13	Q	255	12% 82% 11% 7%
14	B	234	82% 11% 6%
14	E	234	82% 11% 6%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 47878 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 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	199	1488	934	254	290	10	0	0
1	A	199	1488	934	254	290	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	234	1832	1148	329	344	11	0	0
2	G	234	1832	1148	329	344	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	231	1761	1106	292	352	11	0	0
3	H	231	1761	1106	292	352	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	231	1815	1144	321	345	5	0	0
4	I	231	1815	1144	321	345	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	O	242	1904	1204	326	364	10	0	0
5	Z	242	1904	1204	326	364	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	232	1783	1129	297	344	13	0	0
6	K	232	1783	1129	297	344	13	0	0

- Molecule 7 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	T	196	1567	1004	264	290	9	0	0
7	V	196	1567	1004	264	290	9	0	0

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	U	204	1593	1014	265	295	19	0	0
8	Y	204	1593	1014	265	295	19	0	0

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	a	214	1673	1056	288	317	12	0	0
9	W	214	1673	1056	288	317	12	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	201	1568	980	269	306	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	201	1568	980	269	306	13	0	0

- Molecule 11 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	b	226	1769	1132	298	333	6	0	0
11	P	226	1769	1132	298	333	6	0	0

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	X	212	1644	1041	280	313	10	0	0
12	S	212	1644	1041	280	313	10	0	0

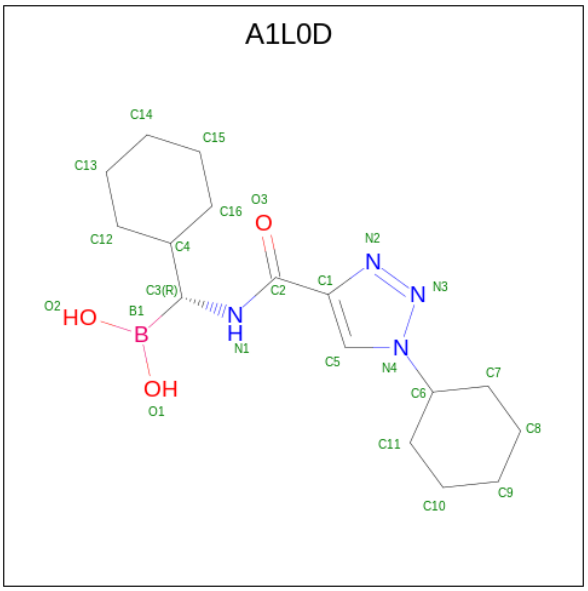
- Molecule 13 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	238	1866	1185	318	352	11	0	0
13	Q	238	1866	1185	318	352	11	0	0

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	219	1622	1014	286	313	9	0	0
14	B	219	1622	1014	286	313	9	0	0

- Molecule 15 is [({R})-cyclohexyl-[(1-cyclohexyl-1,2,3-triazol-4-yl)carbonylamino]methyl]boronic acid (three-letter code: A1L0D) (formula: $C_{16}H_{27}BN_4O_3$).



Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	B	C	N	O	0
			23	1	16	4	2	
15	C	1	Total	B	C	N	O	0
			23	1	16	4	2	
15	A	1	Total	B	C	N	O	0
			23	1	16	4	2	
15	D	1	Total	B	C	N	O	0
			23	1	16	4	2	

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	F	3	Total	O	0
			3	3	
16	C	2	Total	O	0
			2	2	
16	X	1	Total	O	0
			1	1	
16	E	2	Total	O	0
			2	2	
16	B	2	Total	O	0
			2	2	
16	A	3	Total	O	0
			3	3	
16	D	2	Total	O	0
			2	2	
16	S	1	Total	O	0
			1	1	

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: Proteasome subunit beta

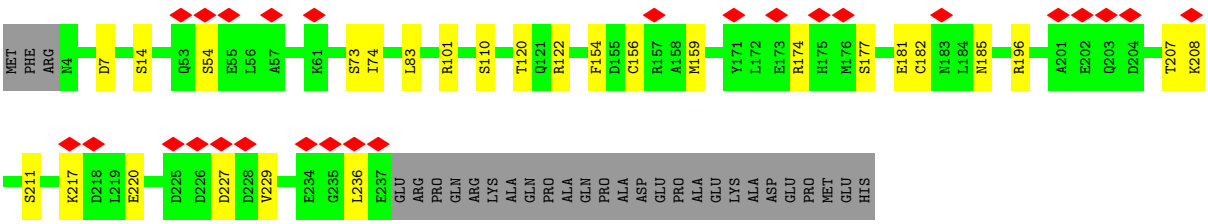
Chain F:

• Molecule 1: Proteasome subunit beta

Chain A:

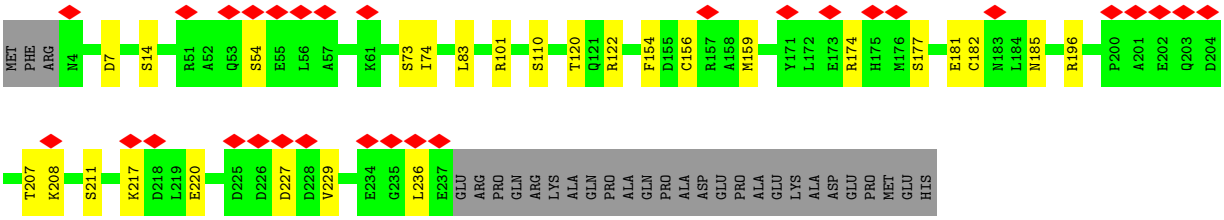
• Molecule 2: Proteasome subunit alpha type

Chain L:



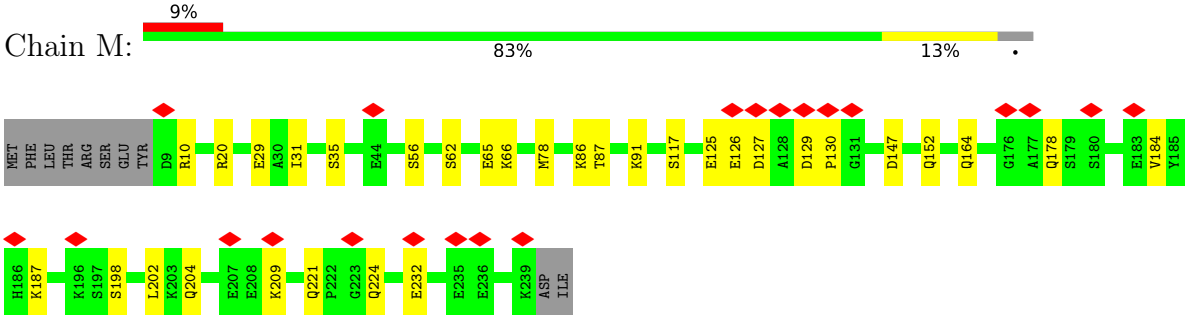
• Molecule 2: Proteasome subunit alpha type

Chain G:



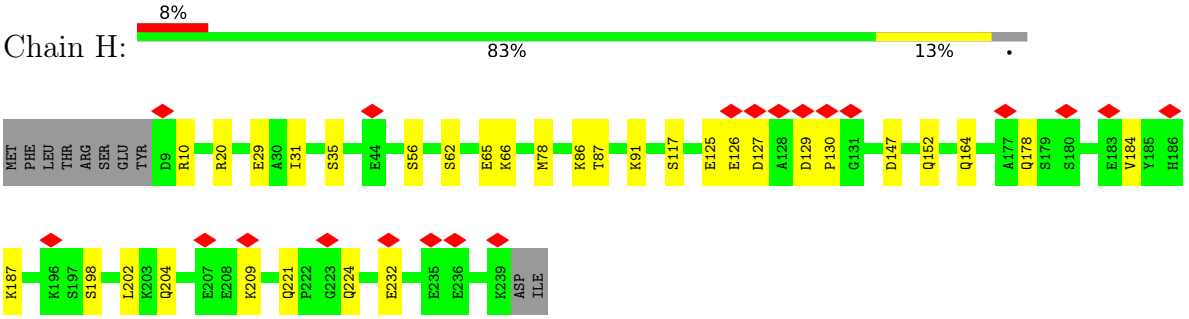
• Molecule 3: Proteasome subunit alpha type

Chain M:



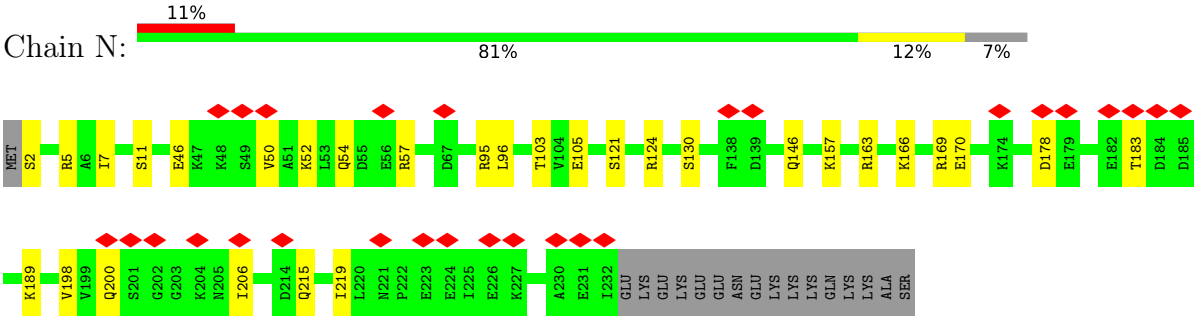
• Molecule 3: Proteasome subunit alpha type

Chain H:



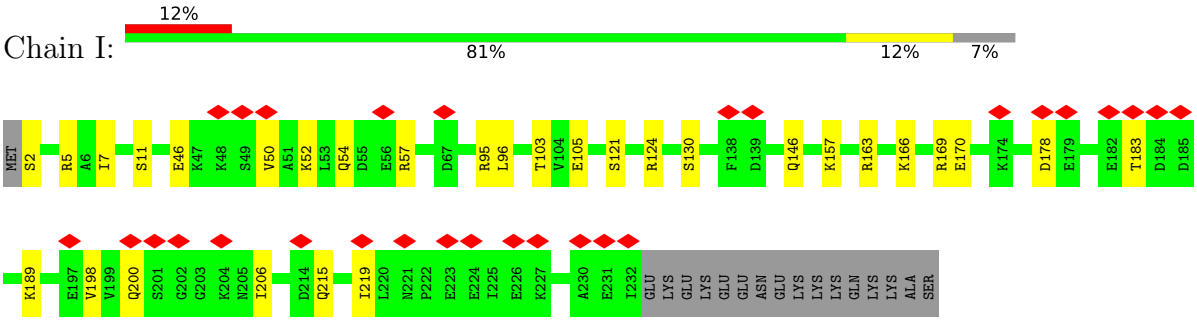
• Molecule 4: Proteasome subunit alpha type

Chain N:



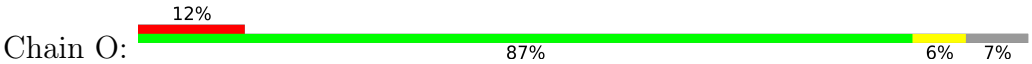
• Molecule 4: Proteasome subunit alpha type

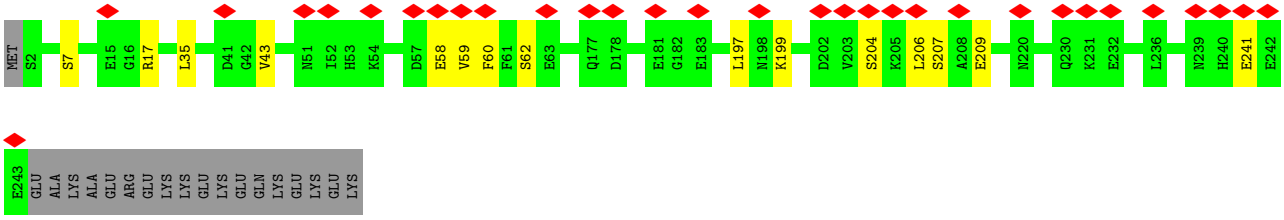
Chain I:



• Molecule 5: Proteasome subunit alpha type

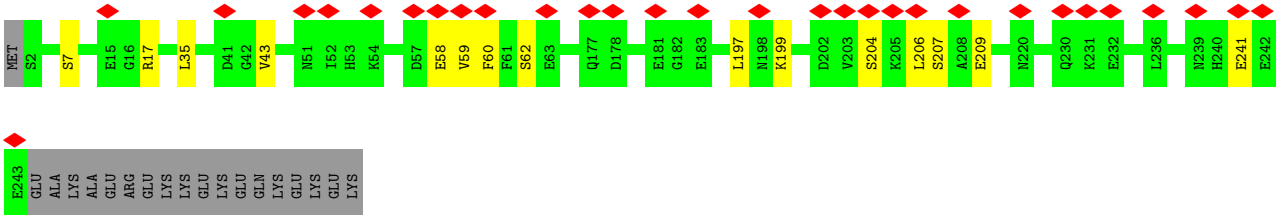
Chain O:





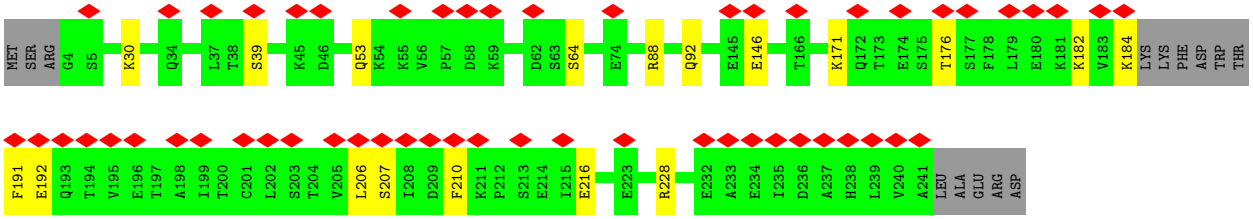
• Molecule 5: Proteasome subunit alpha type

Chain Z:



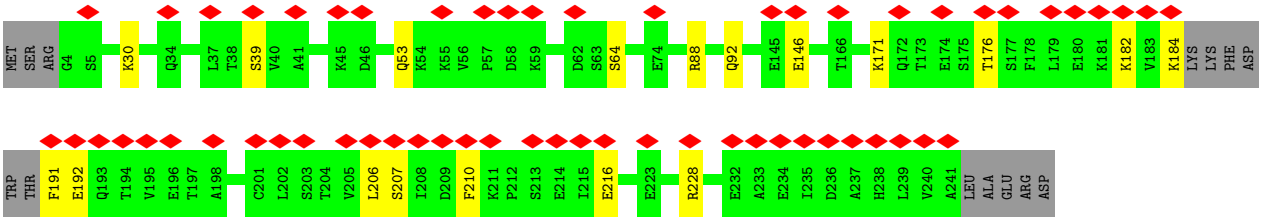
• Molecule 6: Proteasome subunit alpha type

Chain R:



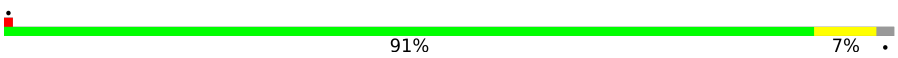
• Molecule 6: Proteasome subunit alpha type

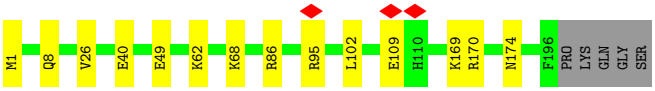
Chain K:



• Molecule 7: Proteasome subunit beta

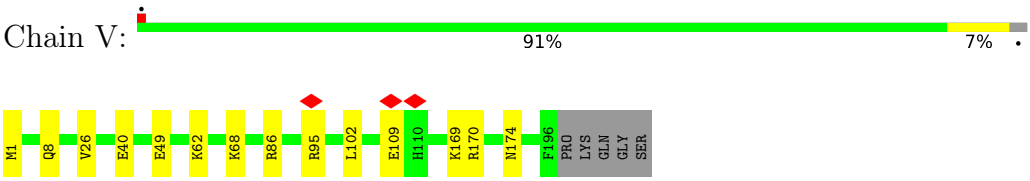
Chain T:





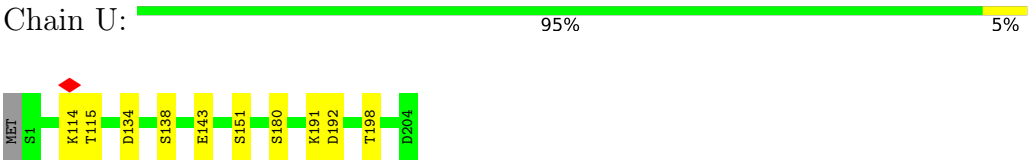
• Molecule 7: Proteasome subunit beta

Chain V:



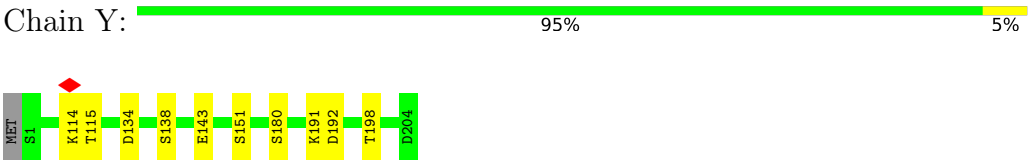
• Molecule 8: Proteasome subunit beta

Chain U:



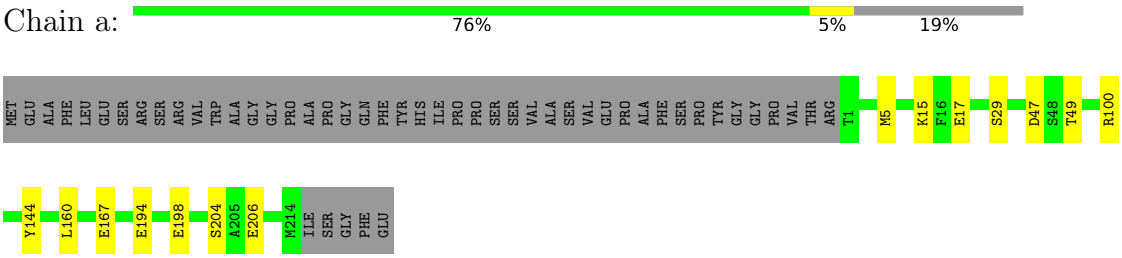
• Molecule 8: Proteasome subunit beta

Chain Y:



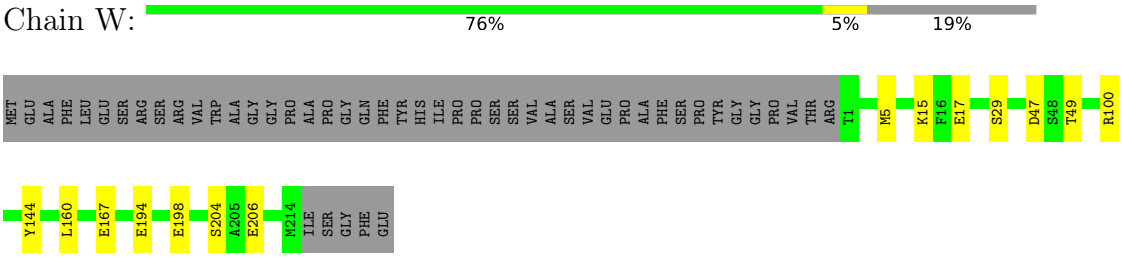
• Molecule 9: Proteasome subunit beta

Chain a:



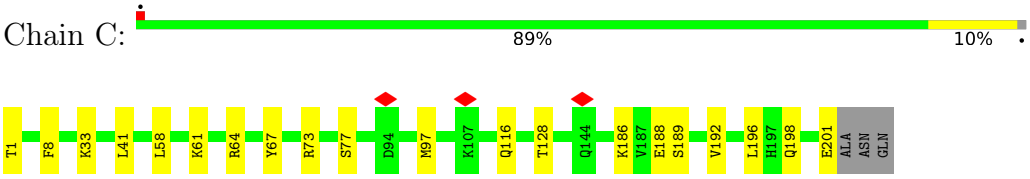
• Molecule 9: Proteasome subunit beta

Chain W:



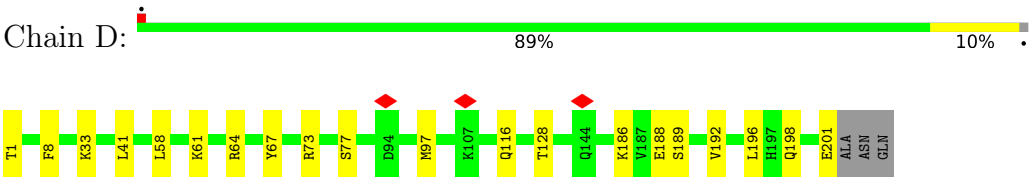
• Molecule 10: Proteasome subunit beta type-8

Chain C:



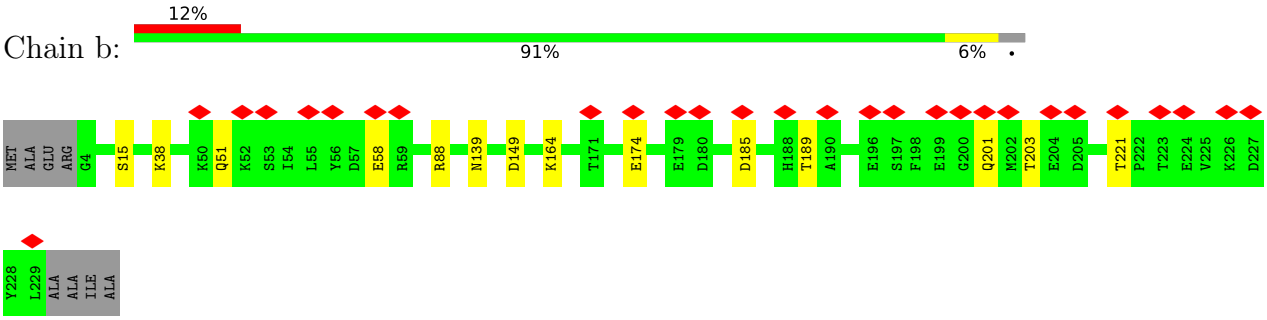
• Molecule 10: Proteasome subunit beta type-8

Chain D:



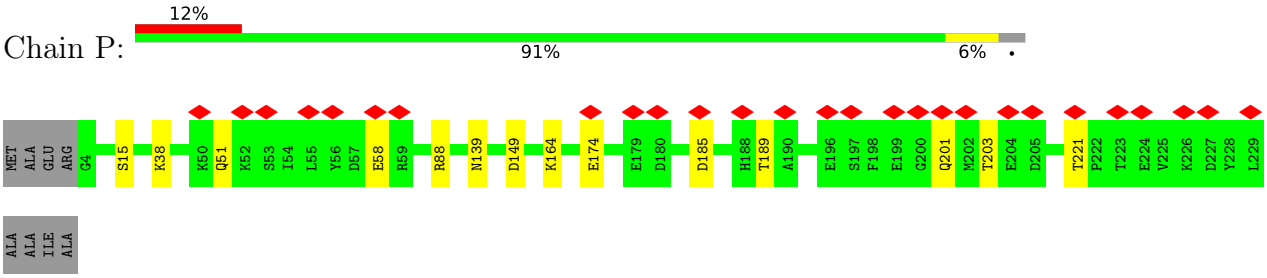
• Molecule 11: Proteasome subunit alpha type

Chain b:



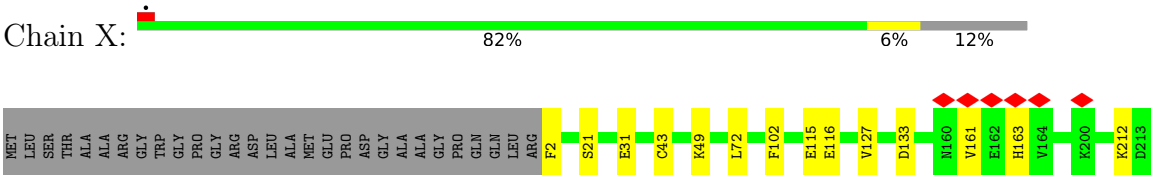
• Molecule 11: Proteasome subunit alpha type

Chain P:



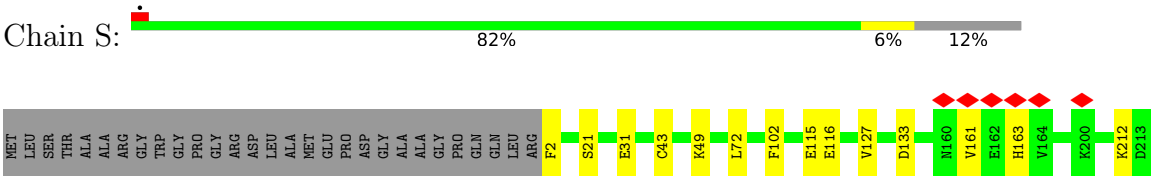
• Molecule 12: Proteasome subunit beta

Chain X:



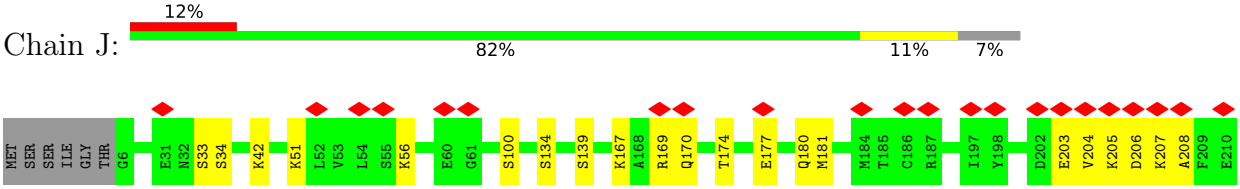
• Molecule 12: Proteasome subunit beta

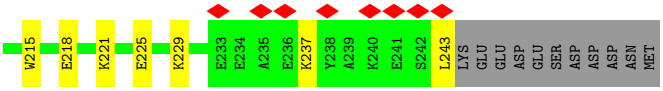
Chain S:



• Molecule 13: Proteasome subunit alpha type

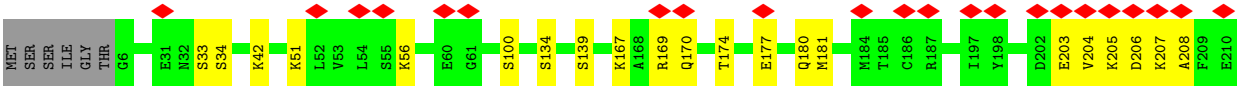
Chain J:

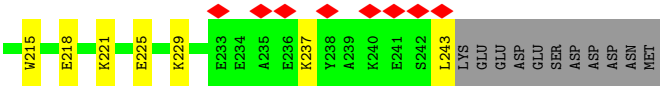




• Molecule 13: Proteasome subunit alpha type

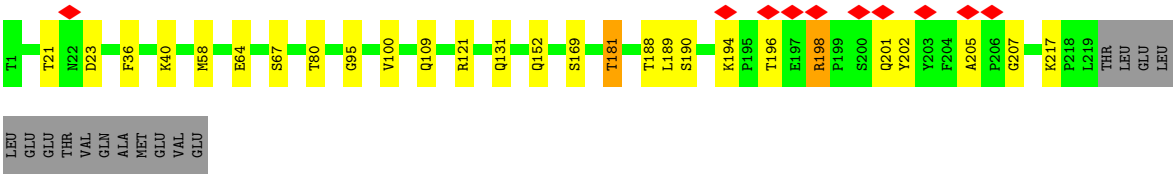
Chain Q:





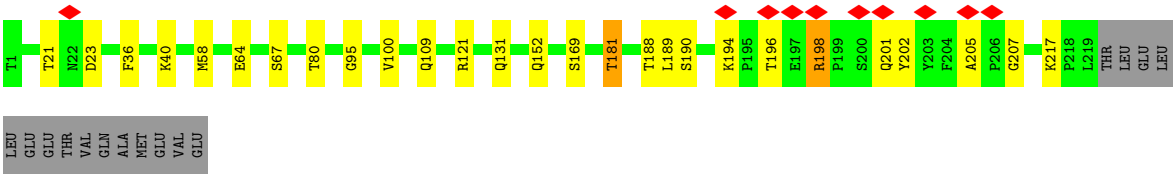
• Molecule 14: Proteasome subunit beta

Chain E:



• Molecule 14: Proteasome subunit beta

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	304965	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56.70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	292.16, 292.16, 292.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1L0D

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	0.27	0/1517	0.46	1/2058 (0.0%)
1	F	0.27	0/1517	0.46	1/2058 (0.0%)
2	G	0.23	0/1866	0.45	0/2522
2	L	0.23	0/1866	0.45	0/2522
3	H	0.24	0/1788	0.43	0/2415
3	M	0.24	0/1788	0.43	0/2415
4	I	0.23	0/1842	0.45	0/2489
4	N	0.23	0/1842	0.45	0/2489
5	O	0.55	0/1934	0.96	0/2608
5	Z	0.55	0/1934	0.96	0/2608
6	K	0.24	0/1813	0.45	0/2452
6	R	0.23	0/1813	0.44	0/2452
7	T	0.25	0/1599	0.47	0/2163
7	V	0.25	0/1599	0.47	0/2163
8	U	0.27	0/1622	0.49	0/2186
8	Y	0.27	0/1622	0.49	0/2186
9	W	0.25	0/1706	0.49	0/2308
9	a	0.25	0/1706	0.49	0/2308
10	C	0.65	0/1600	0.82	1/2160 (0.0%)
10	D	0.65	0/1600	0.82	1/2160 (0.0%)
11	P	0.57	0/1808	0.97	0/2449
11	b	0.57	0/1808	0.97	0/2449
12	S	0.66	0/1675	0.80	0/2258
12	X	0.66	0/1675	0.80	0/2258
13	J	0.23	0/1901	0.44	0/2559
13	Q	0.23	0/1901	0.44	0/2559
14	B	0.25	0/1650	0.49	0/2242
14	E	0.25	0/1650	0.49	0/2242
All	All	0.39	0/48642	0.62	4/65738 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	THR	O-C-N	5.91	132.16	122.70
1	F	1	THR	O-C-N	5.88	132.12	122.70
10	C	1	THR	O-C-N	5.83	132.02	122.70
10	D	1	THR	O-C-N	5.83	132.02	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/199 (99%)	192 (98%)	4 (2%)	1 (0%)	25	28
1	F	197/199 (99%)	192 (98%)	4 (2%)	1 (0%)	25	28
2	G	232/263 (88%)	223 (96%)	9 (4%)	0	100	100
2	L	232/263 (88%)	223 (96%)	9 (4%)	0	100	100
3	H	229/241 (95%)	219 (96%)	9 (4%)	1 (0%)	30	34
3	M	229/241 (95%)	219 (96%)	9 (4%)	1 (0%)	30	34
4	I	229/248 (92%)	221 (96%)	8 (4%)	0	100	100
4	N	229/248 (92%)	221 (96%)	8 (4%)	0	100	100
5	O	240/261 (92%)	229 (95%)	7 (3%)	4 (2%)	7	5
5	Z	240/261 (92%)	229 (95%)	7 (3%)	4 (2%)	7	5
6	K	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
6	R	228/246 (93%)	221 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	194/201 (96%)	190 (98%)	4 (2%)	0	100	100
7	V	194/201 (96%)	190 (98%)	4 (2%)	0	100	100
8	U	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
8	Y	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	212/264 (80%)	199 (94%)	13 (6%)	0	100	100
9	a	212/264 (80%)	199 (94%)	13 (6%)	0	100	100
10	C	199/204 (98%)	190 (96%)	9 (4%)	0	100	100
10	D	199/204 (98%)	190 (96%)	9 (4%)	0	100	100
11	P	224/234 (96%)	212 (95%)	12 (5%)	0	100	100
11	b	224/234 (96%)	212 (95%)	12 (5%)	0	100	100
12	S	210/241 (87%)	206 (98%)	4 (2%)	0	100	100
12	X	210/241 (87%)	206 (98%)	4 (2%)	0	100	100
13	J	236/255 (92%)	224 (95%)	11 (5%)	1 (0%)	30	34
13	Q	236/255 (92%)	224 (95%)	11 (5%)	1 (0%)	30	34
14	B	217/234 (93%)	204 (94%)	7 (3%)	6 (3%)	4	2
14	E	217/234 (93%)	204 (94%)	7 (3%)	6 (3%)	4	2
All	All	6098/6592 (92%)	5852 (96%)	220 (4%)	26 (0%)	32	34

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	O	59	VAL
5	Z	59	VAL
5	O	204	SER
5	Z	204	SER
5	O	60	PHE
5	Z	60	PHE
1	F	9	ASP
3	M	130	PRO
3	H	130	PRO
14	E	23	ASP
14	E	181	THR
14	B	23	ASP
14	B	181	THR
1	A	9	ASP
5	O	207	SER

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Mol	Chain	Res	Type
13	J	208	ALA
5	Z	207	SER
14	E	205	ALA
14	E	207	GLY
14	B	205	ALA
14	B	207	GLY
13	Q	208	ALA
14	E	198	ARG
14	B	198	ARG
14	E	95	GLY
14	B	95	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	152/152 (100%)	134 (88%)	18 (12%)	4 4
1	F	152/152 (100%)	134 (88%)	18 (12%)	4 4
2	G	199/223 (89%)	172 (86%)	27 (14%)	3 2
2	L	199/223 (89%)	172 (86%)	27 (14%)	3 2
3	H	193/203 (95%)	162 (84%)	31 (16%)	2 1
3	M	193/203 (95%)	162 (84%)	31 (16%)	2 1
4	I	195/211 (92%)	165 (85%)	30 (15%)	2 2
4	N	195/211 (92%)	165 (85%)	30 (15%)	2 2
5	O	204/221 (92%)	193 (95%)	11 (5%)	18 23
5	Z	204/221 (92%)	193 (95%)	11 (5%)	18 23
6	K	194/210 (92%)	176 (91%)	18 (9%)	7 7
6	R	194/210 (92%)	176 (91%)	18 (9%)	7 7
7	T	167/171 (98%)	153 (92%)	14 (8%)	9 9
7	V	167/171 (98%)	153 (92%)	14 (8%)	9 9
8	U	174/175 (99%)	164 (94%)	10 (6%)	17 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Y	174/175 (99%)	164 (94%)	10 (6%)	17	21
9	W	176/215 (82%)	162 (92%)	14 (8%)	10	10
9	a	176/215 (82%)	162 (92%)	14 (8%)	10	10
10	C	168/170 (99%)	149 (89%)	19 (11%)	4	4
10	D	168/170 (99%)	149 (89%)	19 (11%)	4	4
11	P	187/191 (98%)	173 (92%)	14 (8%)	11	12
11	b	187/191 (98%)	173 (92%)	14 (8%)	11	12
12	S	178/197 (90%)	164 (92%)	14 (8%)	10	11
12	X	178/197 (90%)	164 (92%)	14 (8%)	10	11
13	J	196/212 (92%)	169 (86%)	27 (14%)	3	2
13	Q	196/212 (92%)	169 (86%)	27 (14%)	3	2
14	B	174/188 (93%)	151 (87%)	23 (13%)	3	2
14	E	174/188 (93%)	151 (87%)	23 (13%)	3	2
All	All	5114/5478 (93%)	4574 (89%)	540 (11%)	8	5

All (540) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	14	VAL
1	F	39	GLN
1	F	48	SER
1	F	64	GLU
1	F	65	LEU
1	F	70	LEU
1	F	84	ARG
1	F	95	SER
1	F	105	ARG
1	F	106	ARG
1	F	110	GLN
1	F	115	MET
1	F	118	MET
1	F	143	LYS
1	F	184	ASP
1	F	185	TYR
1	F	191	ASN
1	F	195	LYS
2	L	7	ASP

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Mol	Chain	Res	Type
2	L	14	SER
2	L	54	SER
2	L	73	SER
2	L	74	ILE
2	L	83	LEU
2	L	101	ARG
2	L	110	SER
2	L	120	THR
2	L	122	ARG
2	L	154	PHE
2	L	156	CYS
2	L	159	MET
2	L	174	ARG
2	L	177	SER
2	L	181	GLU
2	L	182	CYS
2	L	185	ASN
2	L	196	ARG
2	L	207	THR
2	L	208	LYS
2	L	211	SER
2	L	217	LYS
2	L	220	GLU
2	L	227	ASP
2	L	229	VAL
2	L	236	LEU
3	M	10	ARG
3	M	20	ARG
3	M	29	GLU
3	M	31	ILE
3	M	35	SER
3	M	56	SER
3	M	62	SER
3	M	65	GLU
3	M	66	LYS
3	M	78	MET
3	M	86	LYS
3	M	87	THR
3	M	91	LYS
3	M	117	SER
3	M	125	GLU
3	M	126	GLU

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Mol	Chain	Res	Type
3	M	127	ASP
3	M	129	ASP
3	M	147	ASP
3	M	152	GLN
3	M	164	GLN
3	M	178	GLN
3	M	184	VAL
3	M	187	LYS
3	M	198	SER
3	M	202	LEU
3	M	204	GLN
3	M	209	LYS
3	M	221	GLN
3	M	224	GLN
3	M	232	GLU
4	N	2	SER
4	N	5	ARG
4	N	7	ILE
4	N	11	SER
4	N	46	GLU
4	N	50	VAL
4	N	52	LYS
4	N	54	GLN
4	N	57	ARG
4	N	95	ARG
4	N	96	LEU
4	N	103	THR
4	N	105	GLU
4	N	121	SER
4	N	124	ARG
4	N	130	SER
4	N	146	GLN
4	N	157	LYS
4	N	163	ARG
4	N	166	LYS
4	N	169	ARG
4	N	170	GLU
4	N	178	ASP
4	N	183	THR
4	N	189	LYS
4	N	198	VAL
4	N	200	GLN

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Mol	Chain	Res	Type
4	N	206	ILE
4	N	215	GLN
4	N	219	ILE
5	O	7	SER
5	O	17	ARG
5	O	35	LEU
5	O	43	VAL
5	O	58	GLU
5	O	62	SER
5	O	197	LEU
5	O	199	LYS
5	O	206	LEU
5	O	209	GLU
5	O	241	GLU
6	R	30	LYS
6	R	39	SER
6	R	53	GLN
6	R	64	SER
6	R	88	ARG
6	R	92	GLN
6	R	146	GLU
6	R	171	LYS
6	R	176	THR
6	R	182	LYS
6	R	184	LYS
6	R	191	PHE
6	R	192	GLU
6	R	206	LEU
6	R	207	SER
6	R	210	PHE
6	R	216	GLU
6	R	228	ARG
7	T	1	MET
7	T	8	GLN
7	T	26	VAL
7	T	40	GLU
7	T	49	GLU
7	T	62	LYS
7	T	68	LYS
7	T	86	ARG
7	T	95	ARG
7	T	102	LEU

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Mol	Chain	Res	Type
7	T	109	GLU
7	T	169	LYS
7	T	170	ARG
7	T	174	ASN
8	U	114	LYS
8	U	115	THR
8	U	134	ASP
8	U	138	SER
8	U	143	GLU
8	U	151	SER
8	U	180	SER
8	U	191	LYS
8	U	192	ASP
8	U	198	THR
9	a	5	MET
9	a	15	LYS
9	a	17	GLU
9	a	29	SER
9	a	47	ASP
9	a	49	THR
9	a	100	ARG
9	a	144	TYR
9	a	160	LEU
9	a	167	GLU
9	a	194	GLU
9	a	198	GLU
9	a	204	SER
9	a	206	GLU
10	C	8	PHE
10	C	33	LYS
10	C	41	LEU
10	C	58	LEU
10	C	61	LYS
10	C	64	ARG
10	C	67	TYR
10	C	73	ARG
10	C	77	SER
10	C	97	MET
10	C	116	GLN
10	C	128	THR
10	C	186	LYS
10	C	188	GLU

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Mol	Chain	Res	Type
10	C	189	SER
10	C	192	VAL
10	C	196	LEU
10	C	198	GLN
10	C	201	GLU
11	b	15	SER
11	b	38	LYS
11	b	51	GLN
11	b	58	GLU
11	b	88	ARG
11	b	139	ASN
11	b	149	ASP
11	b	164	LYS
11	b	174	GLU
11	b	185	ASP
11	b	189	THR
11	b	201	GLN
11	b	203	THR
11	b	221	THR
12	X	2	PHE
12	X	21	SER
12	X	31	GLU
12	X	43	CYS
12	X	49	LYS
12	X	72	LEU
12	X	102	PHE
12	X	115	GLU
12	X	116	GLU
12	X	127	VAL
12	X	133	ASP
12	X	161	VAL
12	X	163	HIS
12	X	212	LYS
3	H	10	ARG
3	H	20	ARG
3	H	29	GLU
3	H	31	ILE
3	H	35	SER
3	H	56	SER
3	H	62	SER
3	H	65	GLU
3	H	66	LYS

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Mol	Chain	Res	Type
3	H	78	MET
3	H	86	LYS
3	H	87	THR
3	H	91	LYS
3	H	117	SER
3	H	125	GLU
3	H	126	GLU
3	H	127	ASP
3	H	129	ASP
3	H	147	ASP
3	H	152	GLN
3	H	164	GLN
3	H	178	GLN
3	H	184	VAL
3	H	187	LYS
3	H	198	SER
3	H	202	LEU
3	H	204	GLN
3	H	209	LYS
3	H	221	GLN
3	H	224	GLN
3	H	232	GLU
4	I	2	SER
4	I	5	ARG
4	I	7	ILE
4	I	11	SER
4	I	46	GLU
4	I	50	VAL
4	I	52	LYS
4	I	54	GLN
4	I	57	ARG
4	I	95	ARG
4	I	96	LEU
4	I	103	THR
4	I	105	GLU
4	I	121	SER
4	I	124	ARG
4	I	130	SER
4	I	146	GLN
4	I	157	LYS
4	I	163	ARG
4	I	166	LYS

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Mol	Chain	Res	Type
4	I	169	ARG
4	I	170	GLU
4	I	178	ASP
4	I	183	THR
4	I	189	LYS
4	I	198	VAL
4	I	200	GLN
4	I	206	ILE
4	I	215	GLN
4	I	219	ILE
13	J	33	SER
13	J	34	SER
13	J	42	LYS
13	J	51	LYS
13	J	56	LYS
13	J	100	SER
13	J	134	SER
13	J	139	SER
13	J	167	LYS
13	J	169	ARG
13	J	170	GLN
13	J	174	THR
13	J	177	GLU
13	J	180	GLN
13	J	181	MET
13	J	203	GLU
13	J	204	VAL
13	J	205	LYS
13	J	206	ASP
13	J	207	LYS
13	J	215	TRP
13	J	218	GLU
13	J	221	LYS
13	J	225	GLU
13	J	229	LYS
13	J	237	LYS
13	J	243	LEU
7	V	1	MET
7	V	8	GLN
7	V	26	VAL
7	V	40	GLU
7	V	49	GLU

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Mol	Chain	Res	Type
7	V	62	LYS
7	V	68	LYS
7	V	86	ARG
7	V	95	ARG
7	V	102	LEU
7	V	109	GLU
7	V	169	LYS
7	V	170	ARG
7	V	174	ASN
8	Y	114	LYS
8	Y	115	THR
8	Y	134	ASP
8	Y	138	SER
8	Y	143	GLU
8	Y	151	SER
8	Y	180	SER
8	Y	191	LYS
8	Y	192	ASP
8	Y	198	THR
5	Z	7	SER
5	Z	17	ARG
5	Z	35	LEU
5	Z	43	VAL
5	Z	58	GLU
5	Z	62	SER
5	Z	197	LEU
5	Z	199	LYS
5	Z	206	LEU
5	Z	209	GLU
5	Z	241	GLU
2	G	7	ASP
2	G	14	SER
2	G	54	SER
2	G	73	SER
2	G	74	ILE
2	G	83	LEU
2	G	101	ARG
2	G	110	SER
2	G	120	THR
2	G	122	ARG
2	G	154	PHE
2	G	156	CYS

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Mol	Chain	Res	Type
2	G	159	MET
2	G	174	ARG
2	G	177	SER
2	G	181	GLU
2	G	182	CYS
2	G	185	ASN
2	G	196	ARG
2	G	207	THR
2	G	208	LYS
2	G	211	SER
2	G	217	LYS
2	G	220	GLU
2	G	227	ASP
2	G	229	VAL
2	G	236	LEU
14	E	21	THR
14	E	36	PHE
14	E	40	LYS
14	E	58	MET
14	E	64	GLU
14	E	67	SER
14	E	80	THR
14	E	100	VAL
14	E	109	GLN
14	E	121	ARG
14	E	131	GLN
14	E	152	GLN
14	E	169	SER
14	E	181	THR
14	E	188	THR
14	E	189	LEU
14	E	190	SER
14	E	194	LYS
14	E	196	THR
14	E	198	ARG
14	E	201	GLN
14	E	202	TYR
14	E	217	LYS
9	W	5	MET
9	W	15	LYS
9	W	17	GLU
9	W	29	SER

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Mol	Chain	Res	Type
9	W	47	ASP
9	W	49	THR
9	W	100	ARG
9	W	144	TYR
9	W	160	LEU
9	W	167	GLU
9	W	194	GLU
9	W	198	GLU
9	W	204	SER
9	W	206	GLU
14	B	21	THR
14	B	36	PHE
14	B	40	LYS
14	B	58	MET
14	B	64	GLU
14	B	67	SER
14	B	80	THR
14	B	100	VAL
14	B	109	GLN
14	B	121	ARG
14	B	131	GLN
14	B	152	GLN
14	B	169	SER
14	B	181	THR
14	B	188	THR
14	B	189	LEU
14	B	190	SER
14	B	194	LYS
14	B	196	THR
14	B	198	ARG
14	B	201	GLN
14	B	202	TYR
14	B	217	LYS
13	Q	33	SER
13	Q	34	SER
13	Q	42	LYS
13	Q	51	LYS
13	Q	56	LYS
13	Q	100	SER
13	Q	134	SER
13	Q	139	SER
13	Q	167	LYS

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Mol	Chain	Res	Type
13	Q	169	ARG
13	Q	170	GLN
13	Q	174	THR
13	Q	177	GLU
13	Q	180	GLN
13	Q	181	MET
13	Q	203	GLU
13	Q	204	VAL
13	Q	205	LYS
13	Q	206	ASP
13	Q	207	LYS
13	Q	215	TRP
13	Q	218	GLU
13	Q	221	LYS
13	Q	225	GLU
13	Q	229	LYS
13	Q	237	LYS
13	Q	243	LEU
1	A	14	VAL
1	A	39	GLN
1	A	48	SER
1	A	64	GLU
1	A	65	LEU
1	A	70	LEU
1	A	84	ARG
1	A	95	SER
1	A	105	ARG
1	A	106	ARG
1	A	110	GLN
1	A	115	MET
1	A	118	MET
1	A	143	LYS
1	A	184	ASP
1	A	185	TYR
1	A	191	ASN
1	A	195	LYS
6	K	30	LYS
6	K	39	SER
6	K	53	GLN
6	K	64	SER
6	K	88	ARG
6	K	92	GLN

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Mol	Chain	Res	Type
6	K	146	GLU
6	K	171	LYS
6	K	176	THR
6	K	182	LYS
6	K	184	LYS
6	K	191	PHE
6	K	192	GLU
6	K	206	LEU
6	K	207	SER
6	K	210	PHE
6	K	216	GLU
6	K	228	ARG
10	D	8	PHE
10	D	33	LYS
10	D	41	LEU
10	D	58	LEU
10	D	61	LYS
10	D	64	ARG
10	D	67	TYR
10	D	73	ARG
10	D	77	SER
10	D	97	MET
10	D	116	GLN
10	D	128	THR
10	D	186	LYS
10	D	188	GLU
10	D	189	SER
10	D	192	VAL
10	D	196	LEU
10	D	198	GLN
10	D	201	GLU
11	P	15	SER
11	P	38	LYS
11	P	51	GLN
11	P	58	GLU
11	P	88	ARG
11	P	139	ASN
11	P	149	ASP
11	P	164	LYS
11	P	174	GLU
11	P	185	ASP
11	P	189	THR

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Mol	Chain	Res	Type
11	P	201	GLN
11	P	203	THR
11	P	221	THR
12	S	2	PHE
12	S	21	SER
12	S	31	GLU
12	S	43	CYS
12	S	49	LYS
12	S	72	LEU
12	S	102	PHE
12	S	115	GLU
12	S	116	GLU
12	S	127	VAL
12	S	133	ASP
12	S	161	VAL
12	S	163	HIS
12	S	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	186	GLN
1	F	191	ASN
2	L	31	GLN
2	L	65	HIS
2	L	68	ASN
2	L	203	GLN
3	M	41	GLN
3	M	118	ASN
3	M	164	GLN
3	M	178	GLN
3	M	182	GLN
3	M	224	GLN
6	R	92	GLN
7	T	132	HIS
7	T	174	ASN
8	U	161	HIS
9	a	89	HIS
10	C	9	GLN
10	C	116	GLN
10	C	117	ASN
10	C	193	ASN

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Mol	Chain	Res	Type
11	b	165	ASN
11	b	168	ASN
12	X	131	GLN
12	X	151	ASN
12	X	152	GLN
12	X	157	ASN
3	H	41	GLN
3	H	118	ASN
3	H	164	GLN
3	H	178	GLN
3	H	182	GLN
3	H	224	GLN
13	J	143	ASN
7	V	132	HIS
7	V	174	ASN
8	Y	161	HIS
2	G	31	GLN
2	G	65	HIS
2	G	68	ASN
2	G	203	GLN
14	E	30	ASN
14	E	66	HIS
14	E	109	GLN
14	E	116	HIS
9	W	89	HIS
14	B	30	ASN
14	B	66	HIS
14	B	109	GLN
14	B	116	HIS
13	Q	143	ASN
1	A	81	ASN
1	A	186	GLN
1	A	191	ASN
6	K	92	GLN
10	D	9	GLN
10	D	53	GLN
10	D	116	GLN
10	D	117	ASN
10	D	193	ASN
11	P	165	ASN
11	P	168	ASN
12	S	131	GLN

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Mol	Chain	Res	Type
12	S	151	ASN
12	S	152	GLN
12	S	157	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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	A1L0D	F	301	1	20,25,26	0.58	0	21,33,35	1.39	3 (14%)
15	A1L0D	C	401	10	20,25,26	0.91	1 (5%)	21,33,35	1.30	2 (9%)
15	A1L0D	D	401	10	20,25,26	0.91	1 (5%)	21,33,35	1.30	2 (9%)
15	A1L0D	A	301	1	20,25,26	0.58	0	21,33,35	1.38	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1L0D	F	301	1	-	0/5/34/36	0/3/3/3
15	A1L0D	C	401	10	-	0/5/34/36	0/3/3/3
15	A1L0D	D	401	10	-	0/5/34/36	0/3/3/3
15	A1L0D	A	301	1	-	0/5/34/36	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	401	A1L0D	N2-N3	-2.11	1.30	1.34
15	D	401	A1L0D	N2-N3	-2.11	1.30	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	301	A1L0D	C5-N4-C6	4.74	129.68	125.48
15	A	301	A1L0D	C5-N4-C6	4.71	129.65	125.48
15	A	301	A1L0D	C12-C4-C3	-2.76	109.44	112.16
15	F	301	A1L0D	C16-C4-C3	-2.75	109.45	112.16
15	C	401	A1L0D	C16-C4-C3	-2.46	109.74	112.16
15	D	401	A1L0D	C16-C4-C3	-2.46	109.74	112.16
15	C	401	A1L0D	C5-N4-C6	2.37	127.58	125.48
15	D	401	A1L0D	C5-N4-C6	2.37	127.58	125.48
15	A	301	A1L0D	C16-C4-C3	-2.12	110.07	112.16
15	F	301	A1L0D	C12-C4-C3	-2.12	110.07	112.16

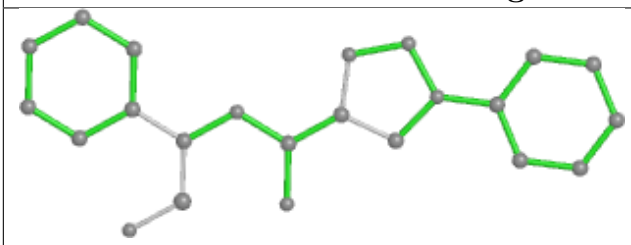
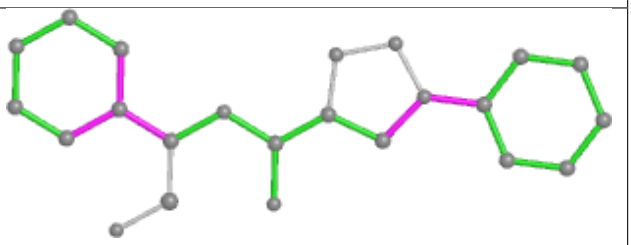
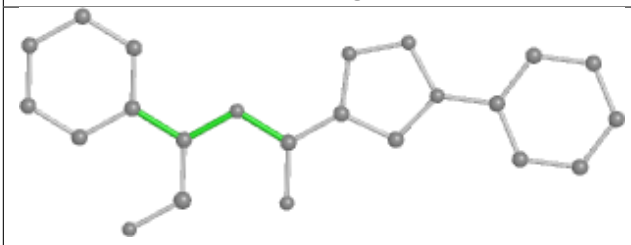
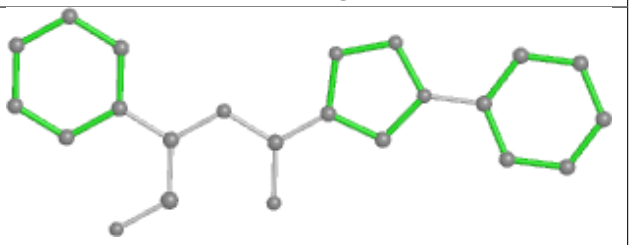
There are no chirality outliers.

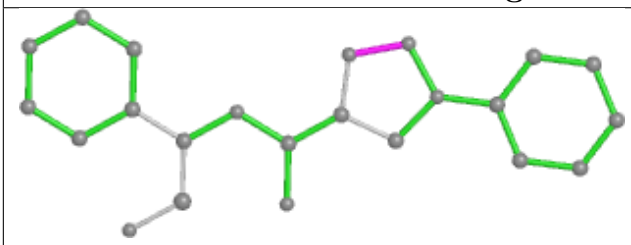
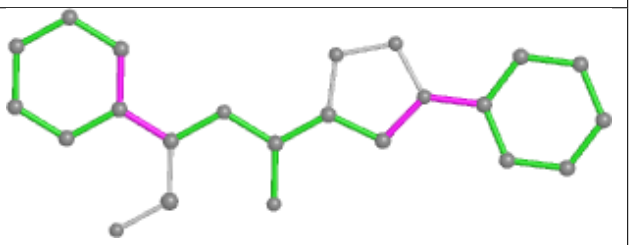
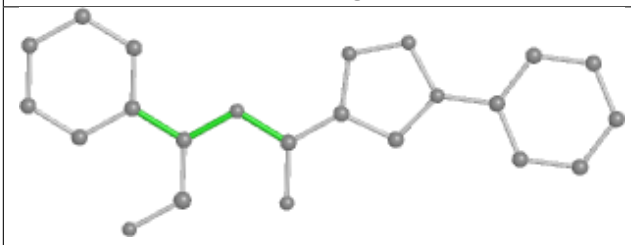
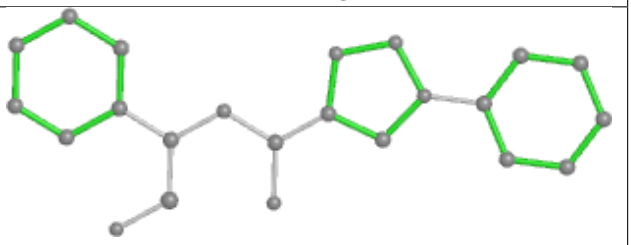
There are no torsion outliers.

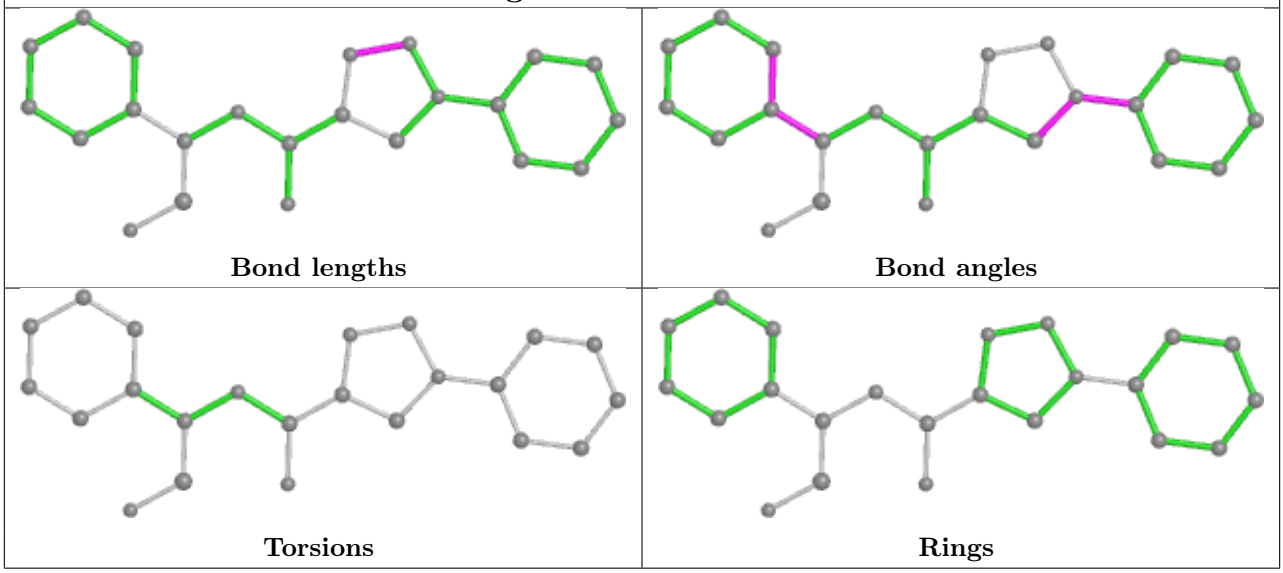
There are no ring outliers.

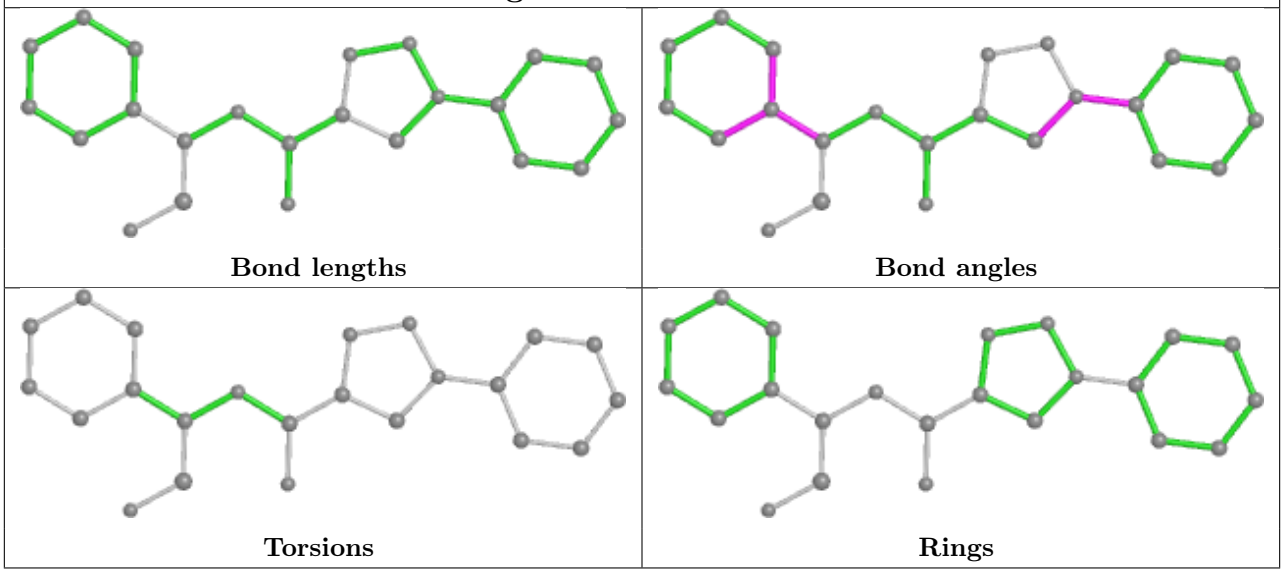
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1L0D F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1L0D C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1L0D D 401	
	
Bond lengths	Bond angles
Torsions	Rings

Ligand A1L0D A 301	
	
Bond lengths	Bond angles
Torsions	Rings

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.

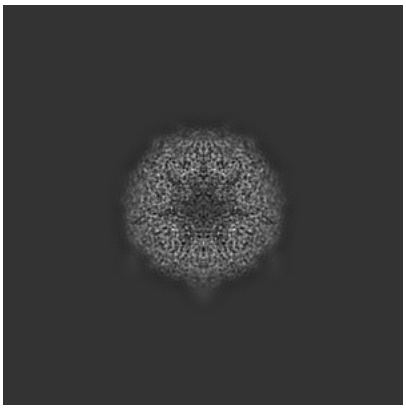
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-39565. These allow visual inspection of the internal detail of the map and identification of artifacts.

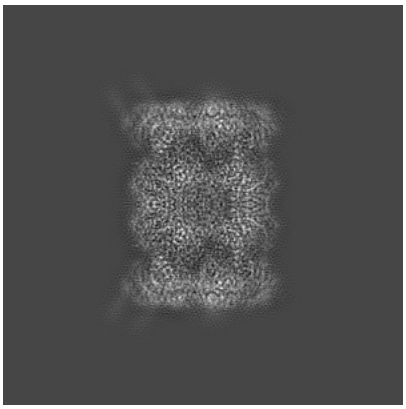
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

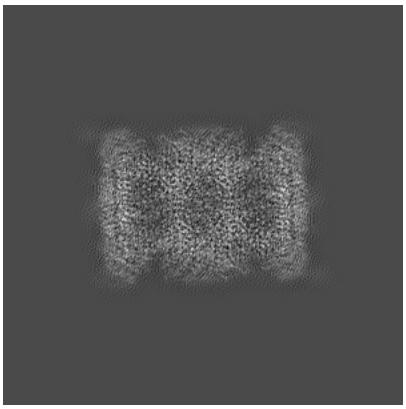
6.1.1 Primary map



X

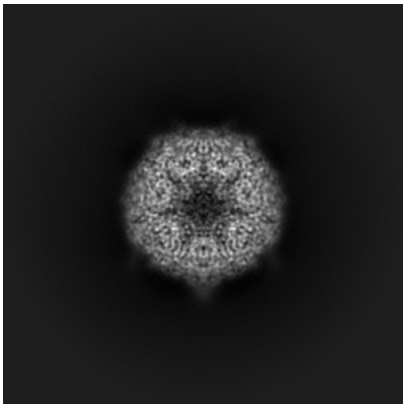


Y

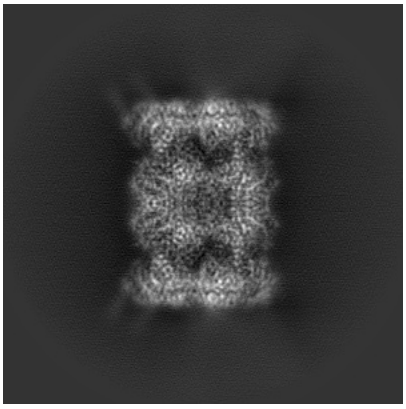


Z

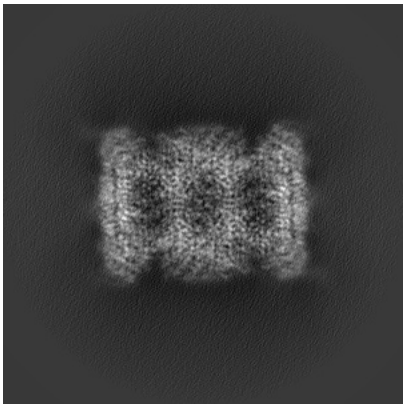
6.1.2 Raw map



X



Y

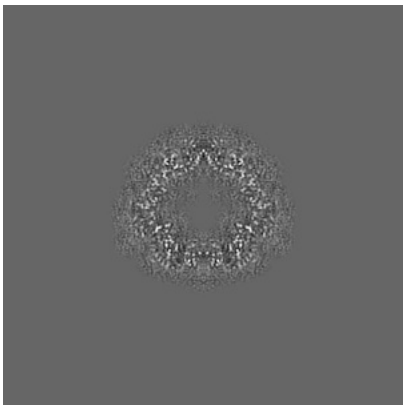


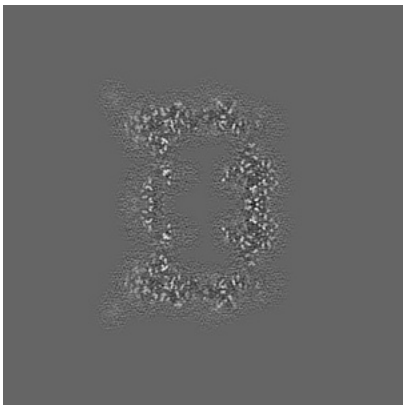
Z

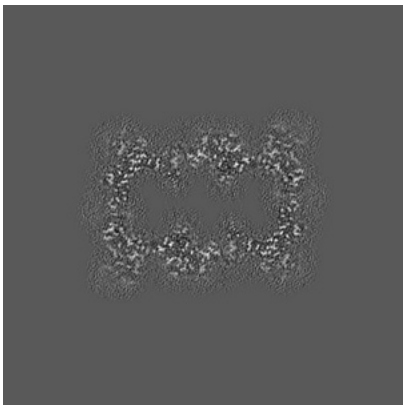
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

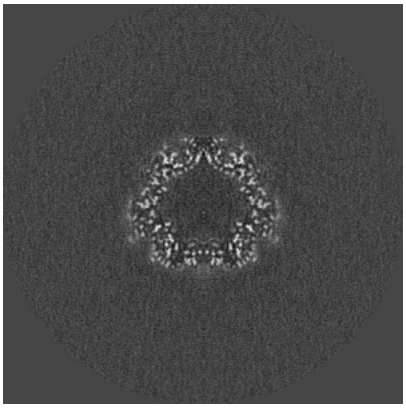
6.2.1 Primary map

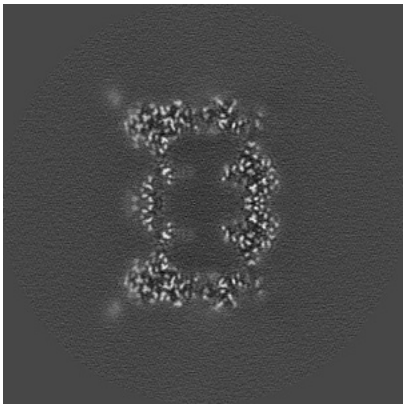

X Index: 176

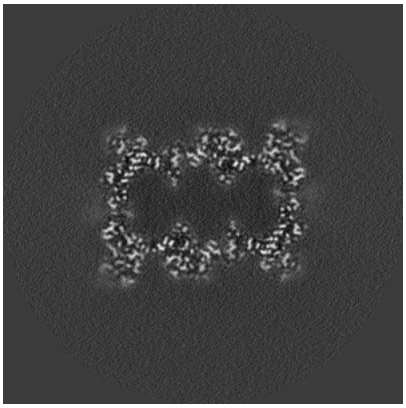

Y Index: 176


Z Index: 176

6.2.2 Raw map


X Index: 176

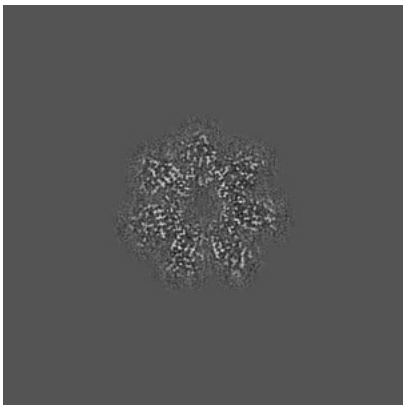

Y Index: 176


Z Index: 176

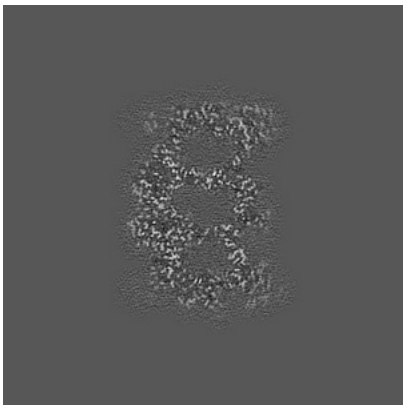
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

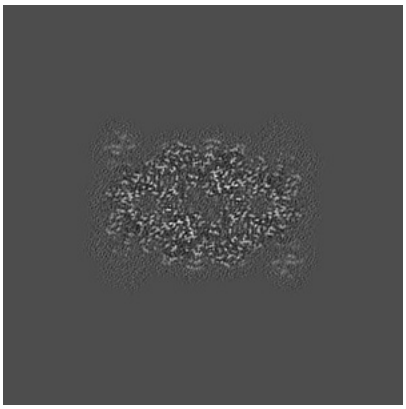
6.3.1 Primary map



X Index: 199

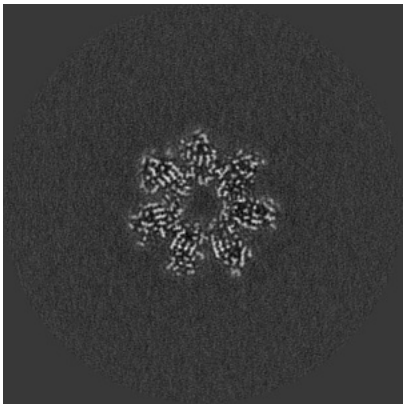


Y Index: 199

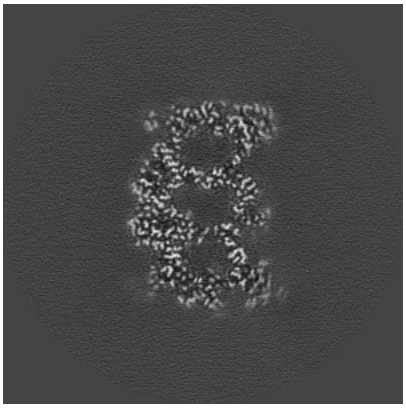


Z Index: 206

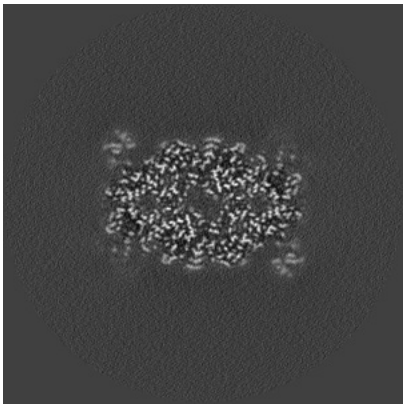
6.3.2 Raw map



X Index: 199



Y Index: 199

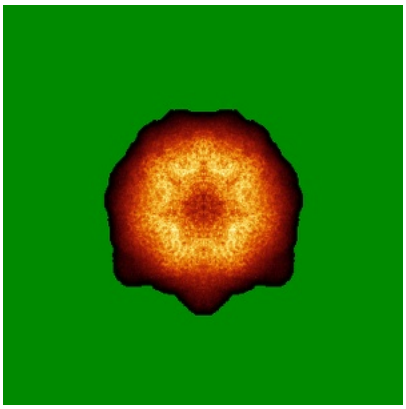


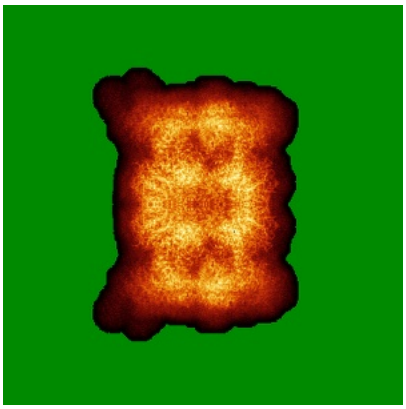
Z Index: 206

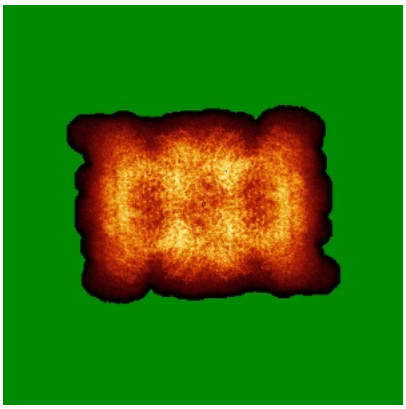
The images above show the largest variance slices of the map in three orthogonal directions.

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

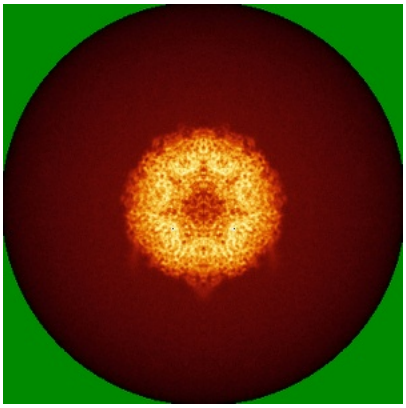
6.4.1 Primary map

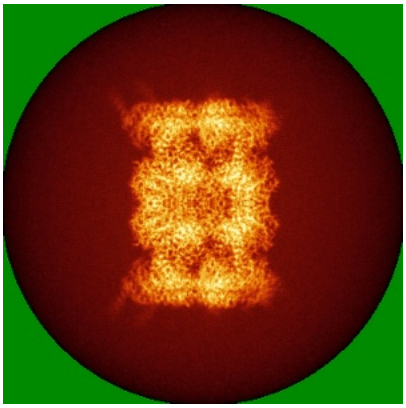

X

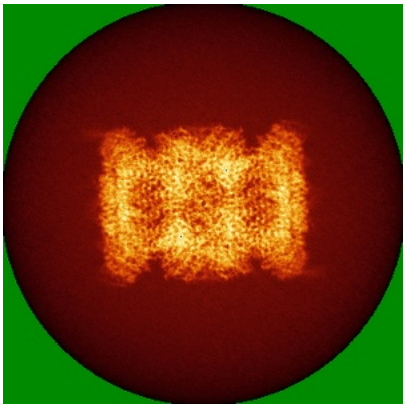

Y


Z

6.4.2 Raw map


X

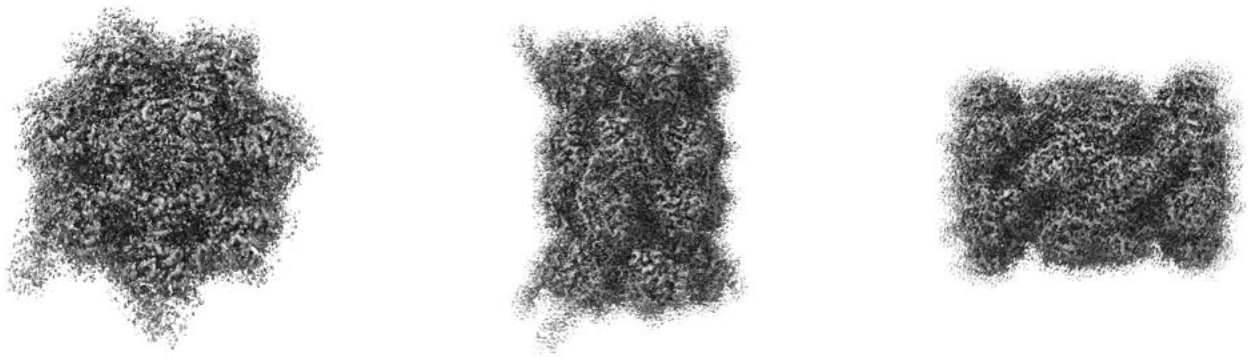

Y


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)

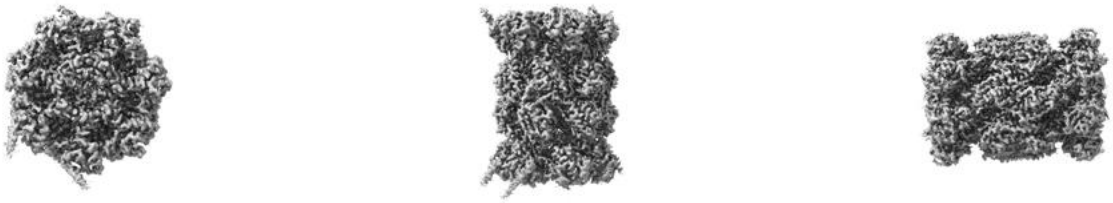
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. 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.

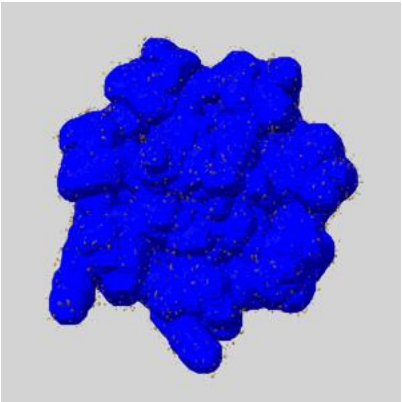
6.6 Mask visualisation (i)

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

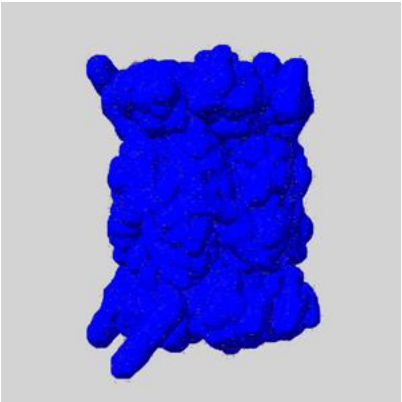
A mask typically either:

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

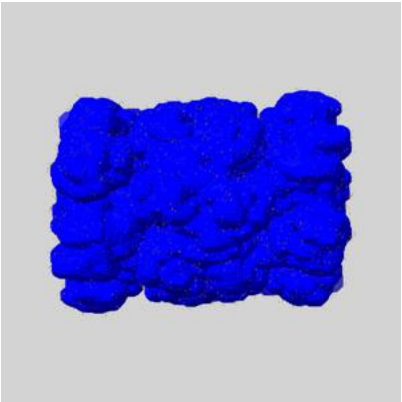
6.6.1 emd_39565_msk_1.map (i)



X



Y

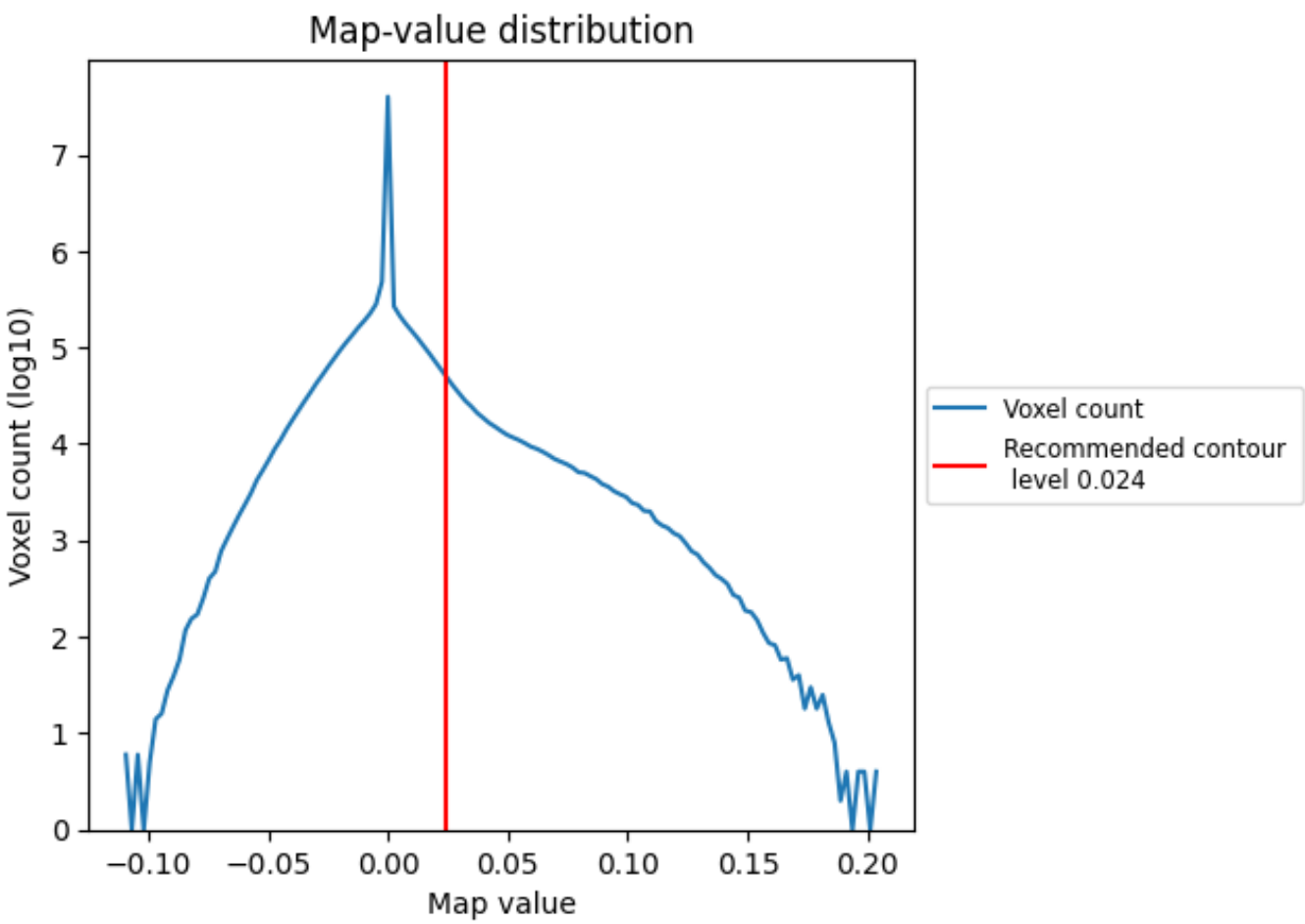


Z

7 Map analysis (i)

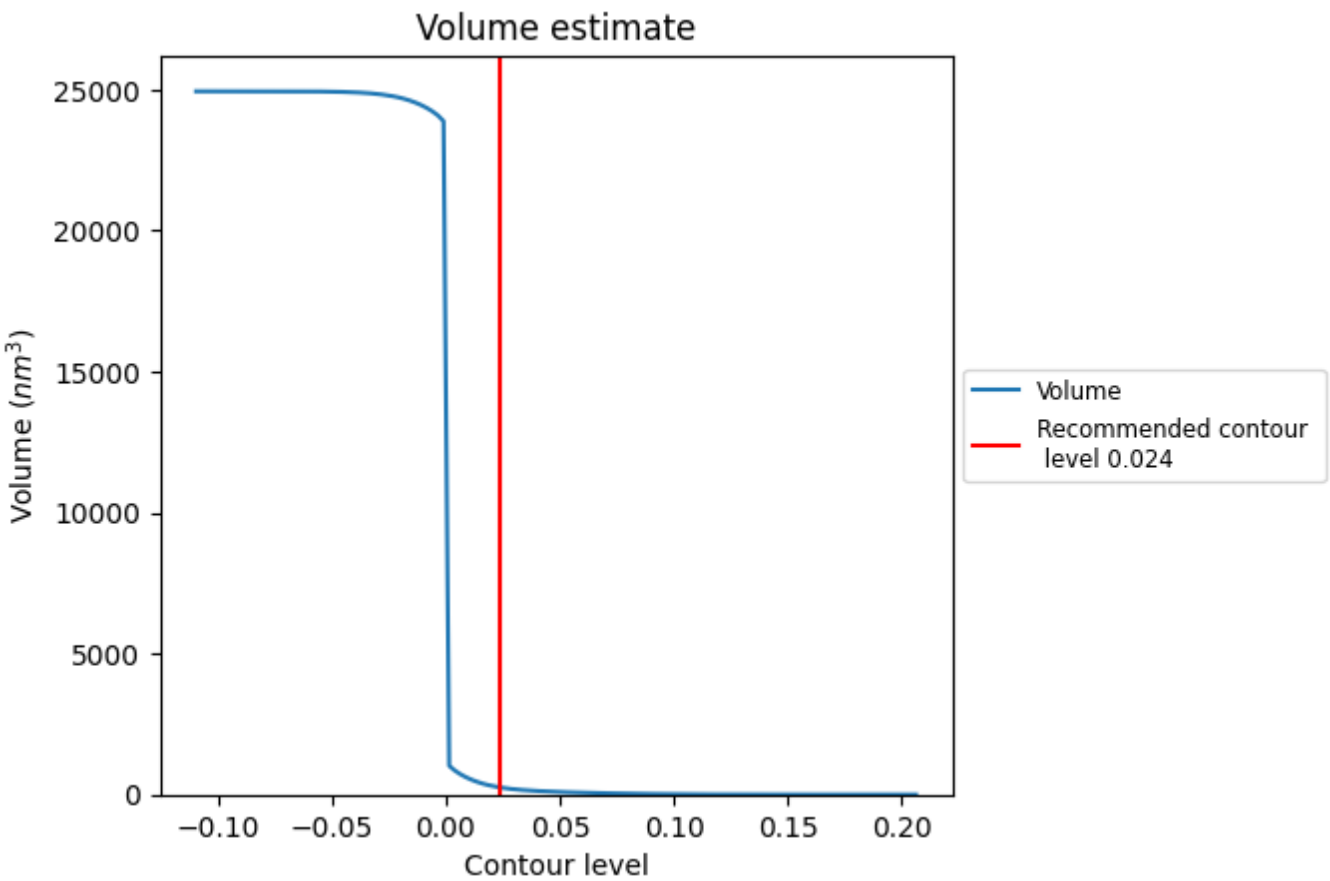
This section contains the results of statistical analysis of the map.

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.

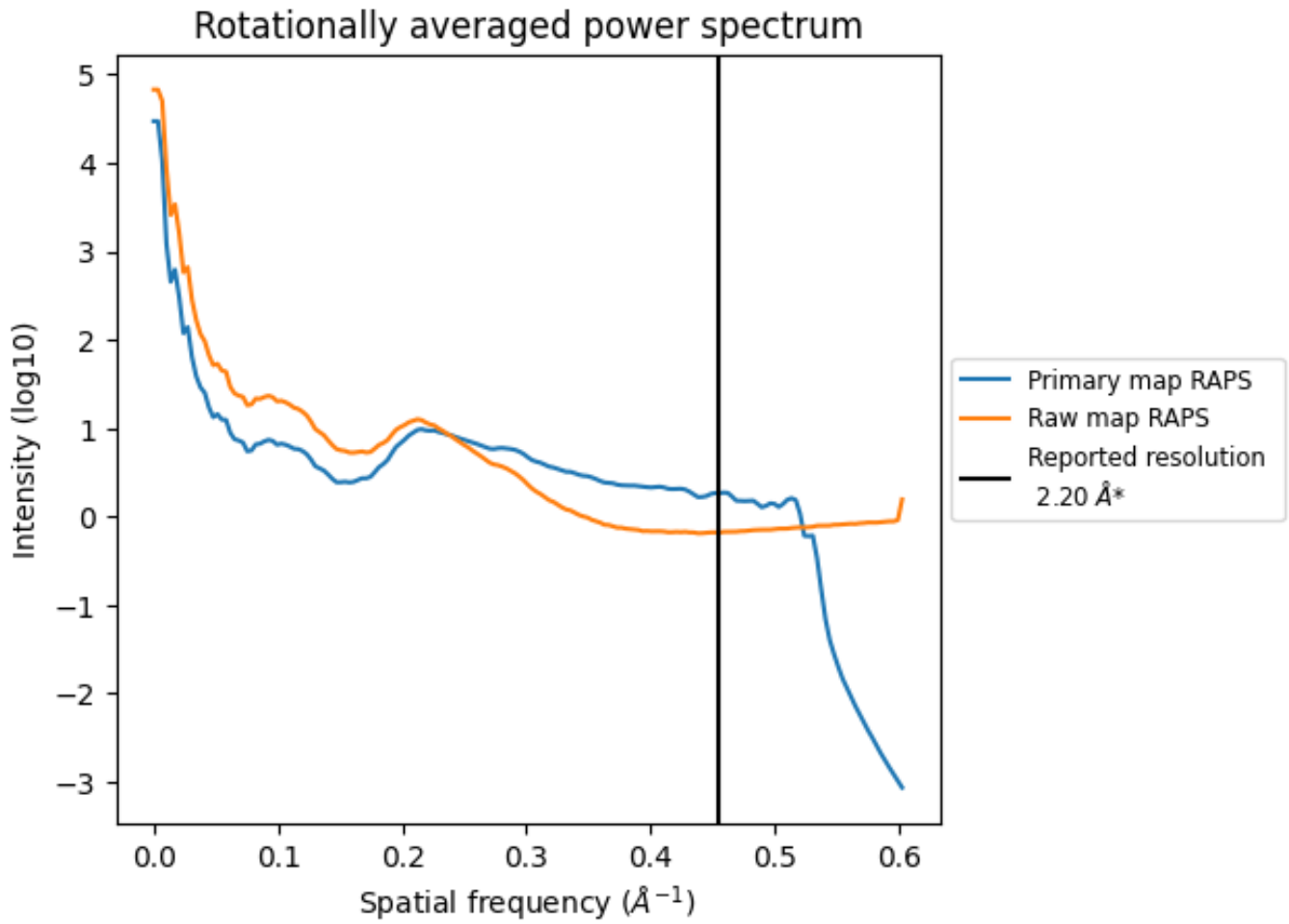
7.2 Volume estimate (i)



The volume at the recommended contour level is 250 nm^3; this corresponds to an approximate mass of 226 kDa.

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

7.3 Rotationally averaged power spectrum (i)

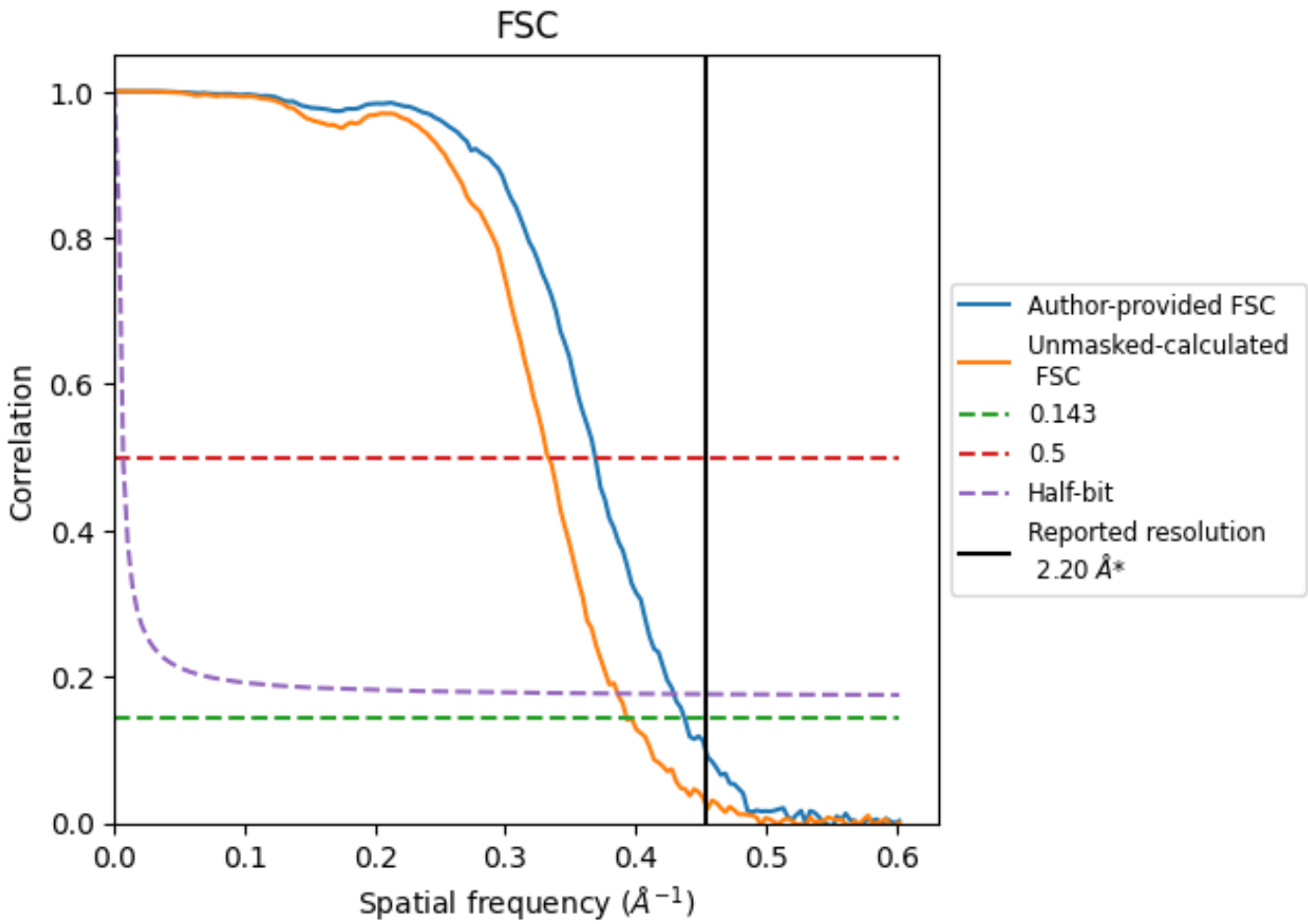


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

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 0.455 Å^{-1}

8.2 Resolution estimates (i)

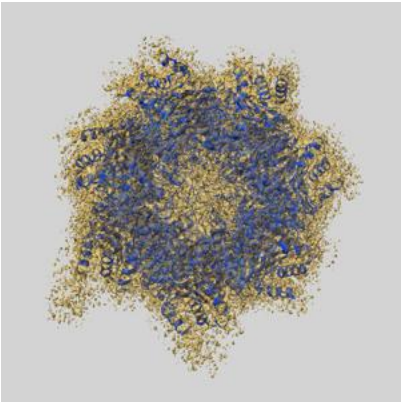
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.28	2.71	2.33
Unmasked-calculated*	2.54	3.00	2.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

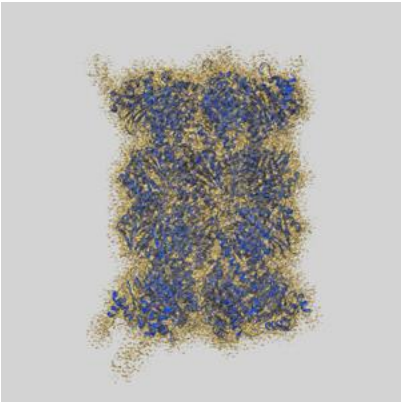
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-39565 and PDB model 8YSX. Per-residue inclusion information can be found in section 3 on page 8.

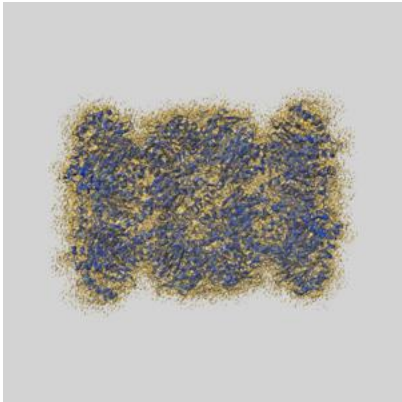
9.1 Map-model overlay (i)



X



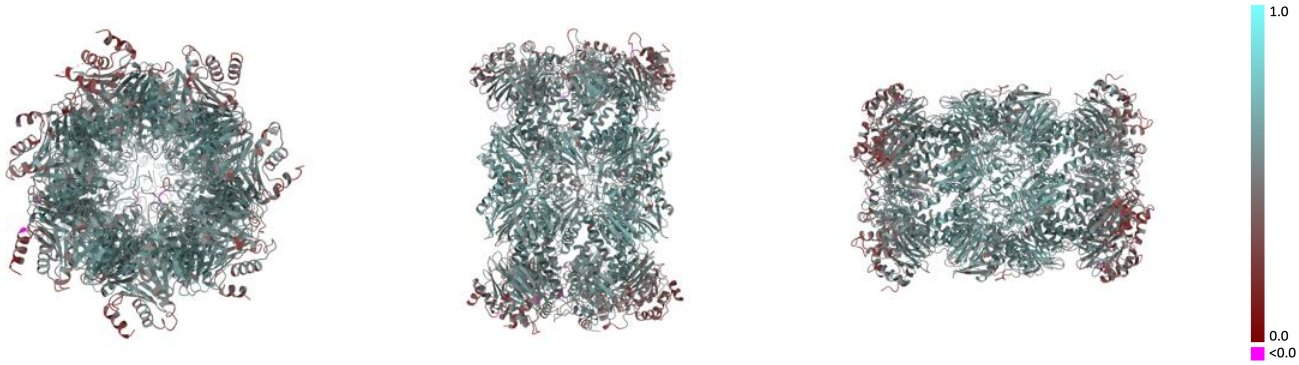
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

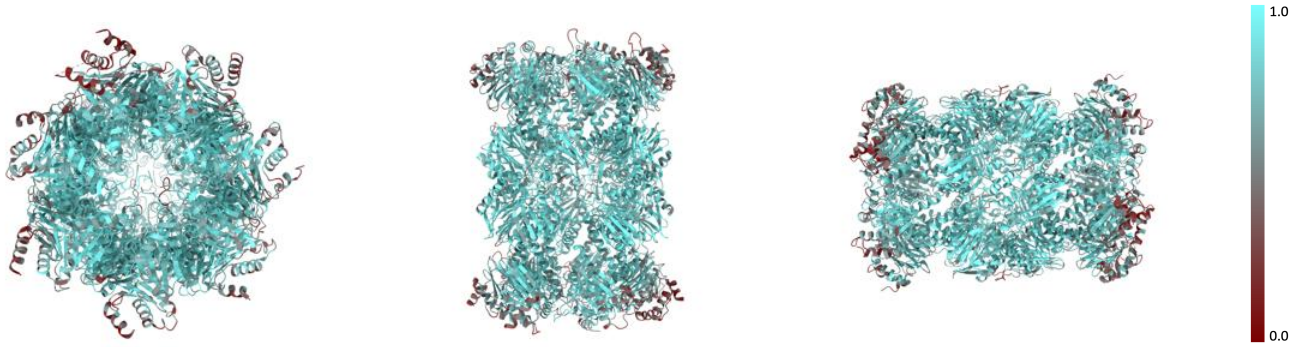
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

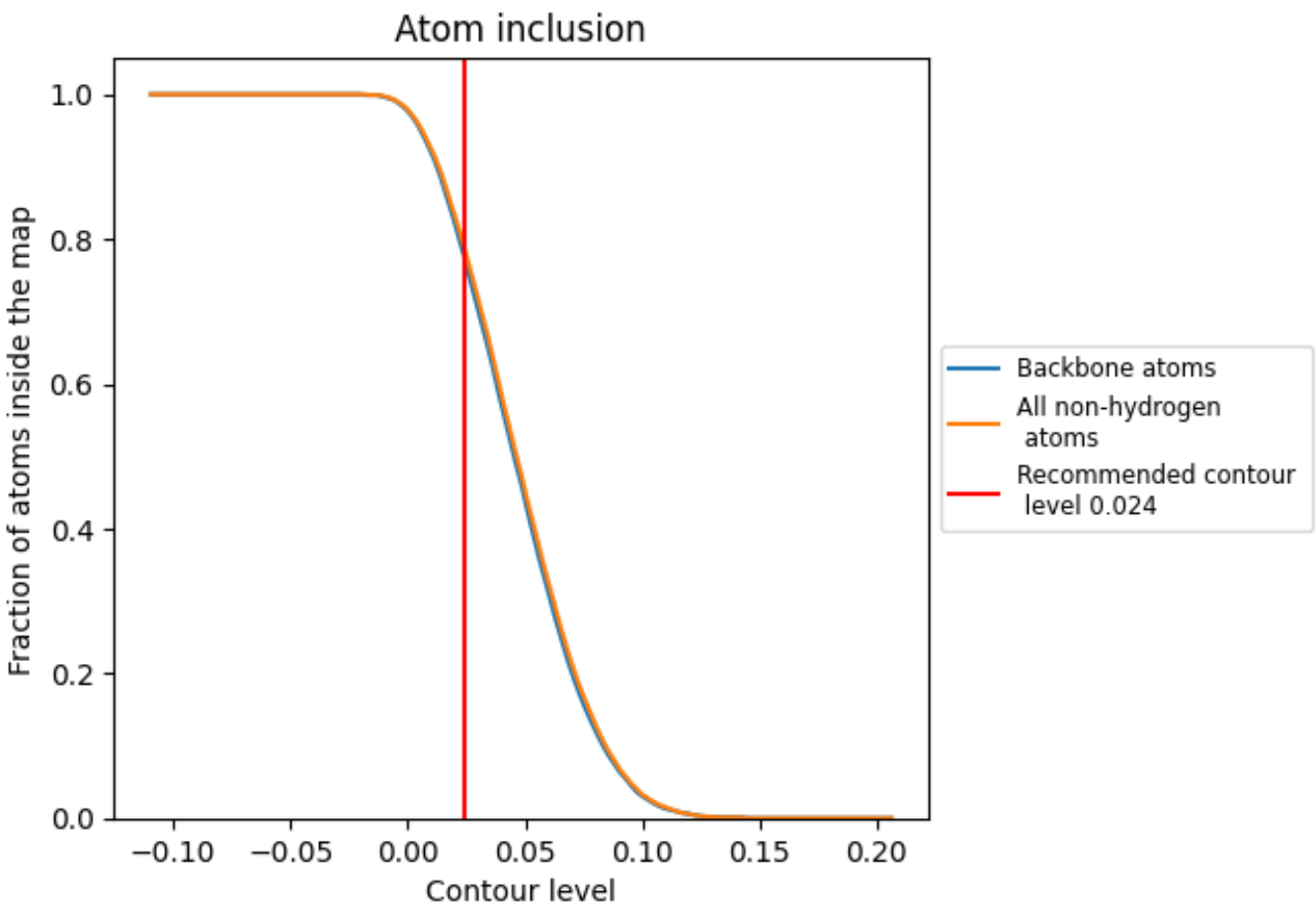
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.5410
A	0.8800	0.6060
B	0.8300	0.5720
C	0.8790	0.5970
D	0.8790	0.5980
E	0.8310	0.5710
F	0.8790	0.6050
G	0.7500	0.5140
H	0.7350	0.5070
I	0.7120	0.4940
J	0.7240	0.4990
K	0.6420	0.4490
L	0.7550	0.5130
M	0.7360	0.5100
N	0.7080	0.4930
O	0.7290	0.4920
P	0.7510	0.5050
Q	0.7240	0.4980
R	0.6520	0.4630
S	0.8700	0.5800
T	0.9080	0.6140
U	0.9000	0.5940
V	0.9060	0.6120
W	0.9060	0.5940
X	0.8700	0.5810
Y	0.9030	0.5990
Z	0.7290	0.4950
a	0.9050	0.5950
b	0.7500	0.5010