



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2023 – 03:03 PM JST

PDB ID : 7YEV  
EMDB ID : EMD-33778  
Title : In situ structure of polymerase complex of mammalian reovirus in the pre-elongation state  
Authors : Bao, K.Y.; Zhang, X.L.; Li, D.Y.; Zhu, P.  
Deposited on : 2022-07-06  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

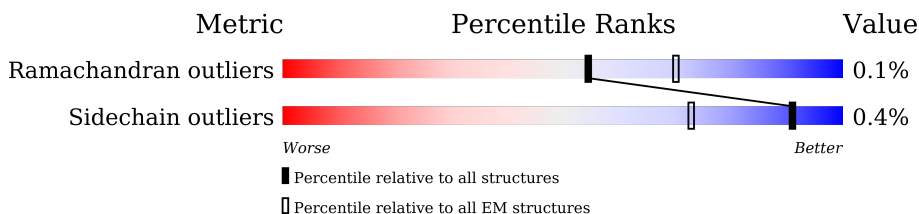
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.




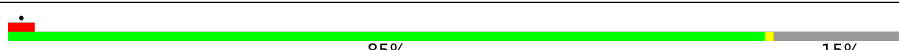
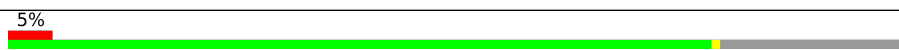


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	1	1275	
1	2	1275	
1	3	1275	
1	4	1275	
1	5	1275	
1	A	1275	
1	B	1275	
1	C	1275	
1	D	1275	

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Mol	Chain	Length	Quality of chain
1	E	1275	 82% 17%
1	a	1275	 84% 15%
1	b	1275	 85% 15%
1	c	1275	 85% 15%
1	d	1275	 85% 15%
1	e	1275	 85% 15%
2	H	1289	 79% 21% 6%
2	I	1289	 79% 21% 6%
2	J	1289	 79% 21% 5%
2	K	1289	 79% 21% 5%
2	L	1289	 79% 21% 6%
3	R	1267	 98% 22%
4	U	736	 89% 9% 15%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 146613 atoms, of which 220 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 RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	140	1041	619	198	221	3	0	0
1	2	139	1035	616	197	219	3	0	0
1	3	138	1030	613	196	218	3	0	0
1	4	131	967	574	183	207	3	0	0
1	5	140	1041	619	198	221	3	0	0
1	A	1128	8868	5654	1510	1651	53	0	0
1	B	1073	8442	5389	1431	1571	51	0	0
1	C	1088	8583	5480	1454	1598	51	0	0
1	D	1050	8300	5306	1403	1542	49	0	0
1	E	1061	8385	5356	1420	1560	49	0	0
1	a	1087	8571	5473	1455	1592	51	0	0
1	b	1087	8571	5473	1455	1592	51	0	0
1	c	1082	8539	5455	1452	1581	51	0	0
1	d	1087	8571	5473	1455	1592	51	0	0
1	e	1087	8571	5473	1455	1592	51	0	0

- Molecule 2 is a protein called Lambda-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	I	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	J	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	K	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	L	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		

- Molecule 3 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	1253	Total	C	N	O	S	0	0
			9913	6327	1697	1824	65		

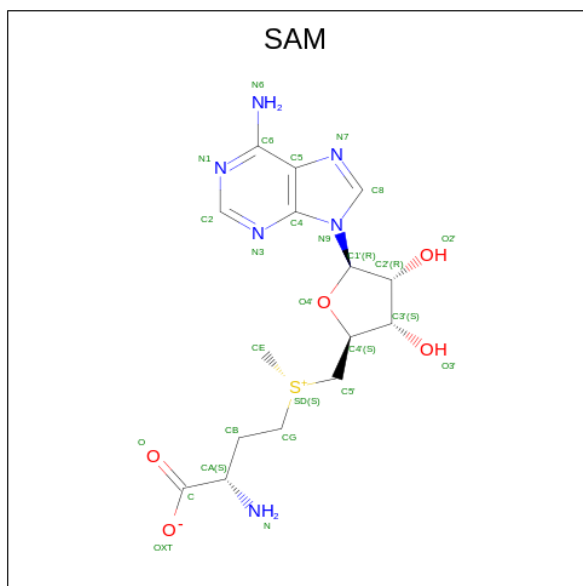
- Molecule 4 is a protein called Mu-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	668	Total	C	N	O	S	0	0
			5322	3413	901	979	29		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	a	1	Total	Zn	0
			1	1	
5	b	1	Total	Zn	0
			1	1	
5	c	1	Total	Zn	0
			1	1	
5	d	1	Total	Zn	0
			1	1	
5	e	1	Total	Zn	0
			1	1	

- Molecule 6 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		S
6	H	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	H	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	I	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	I	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	J	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	J	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	K	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	K	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	L	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	
6	L	1	Total	C	H	N	O	S	0
			49	15	22	6	5	1	











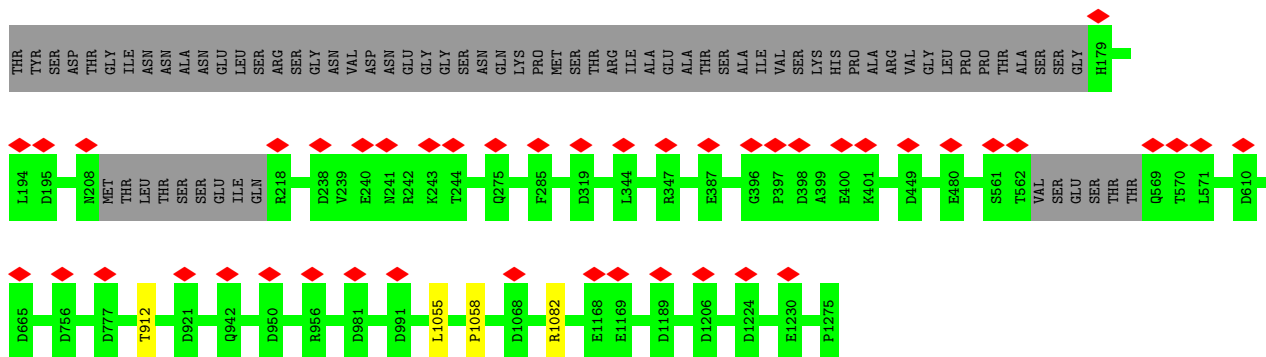




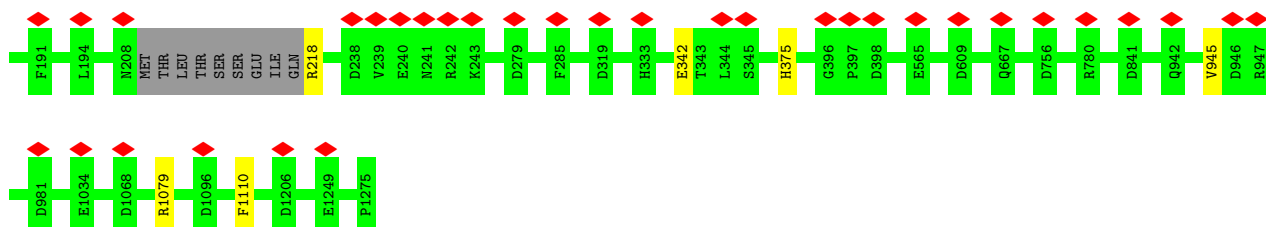
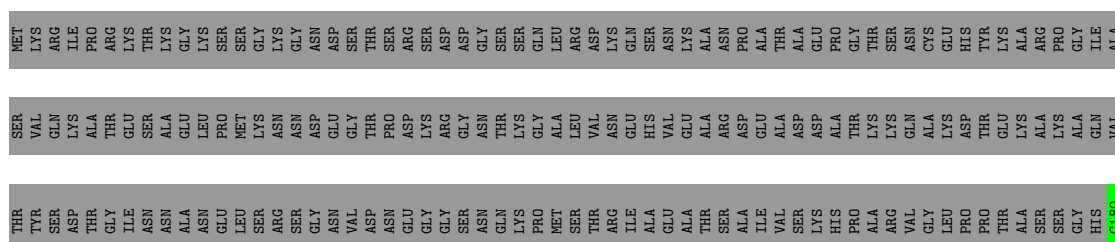
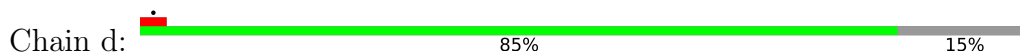




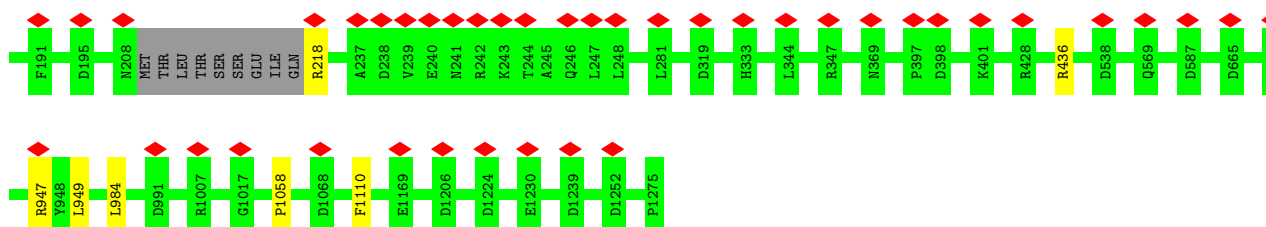
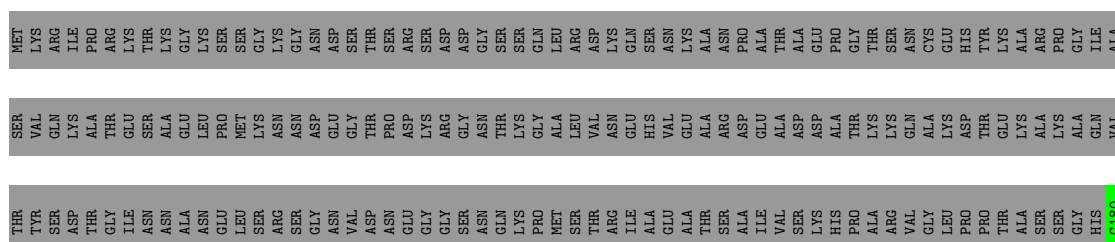
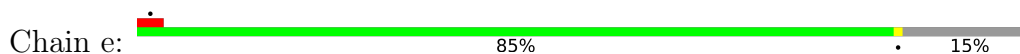




• Molecule 1: RNA helicase



• Molecule 1: RNA helicase



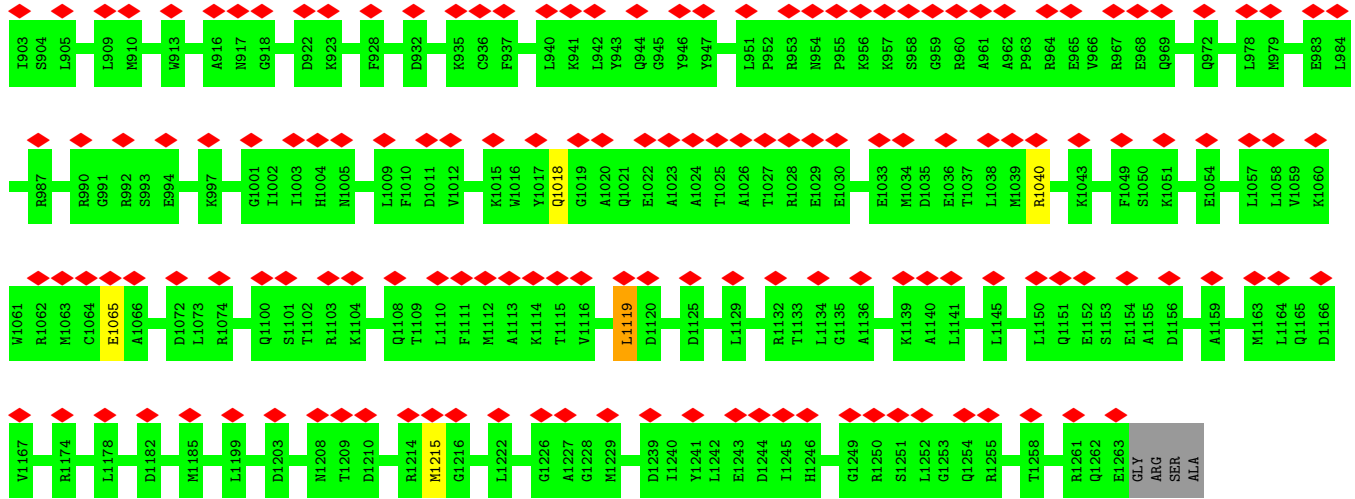
• Molecule 2: Lambda-2 protein



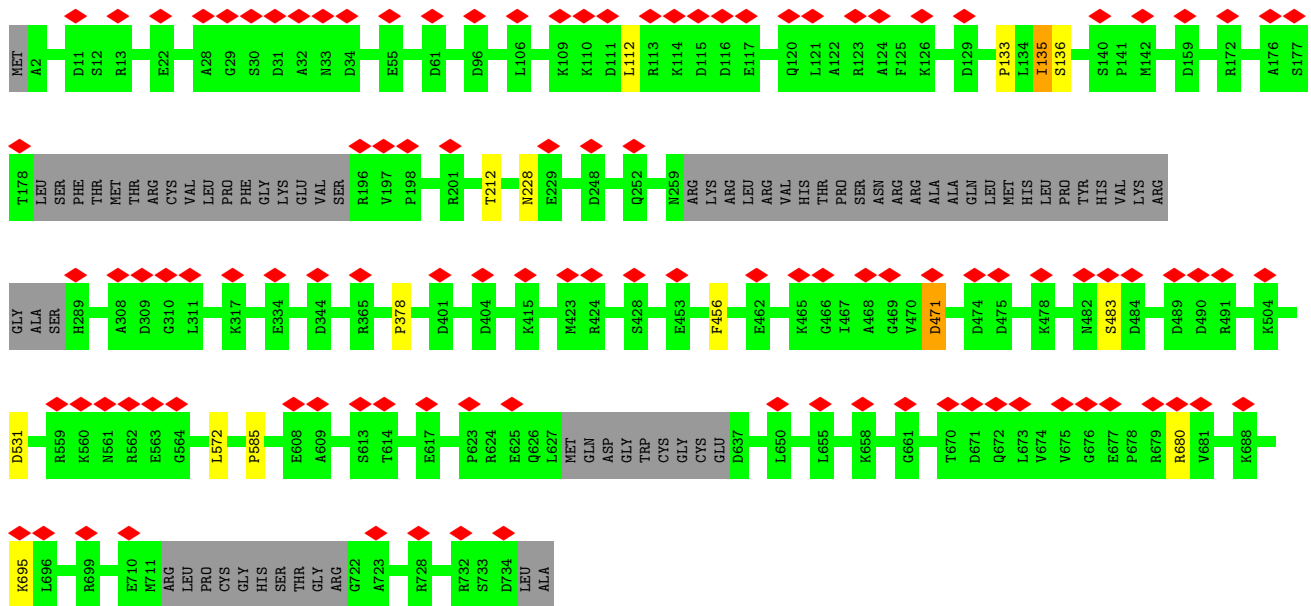
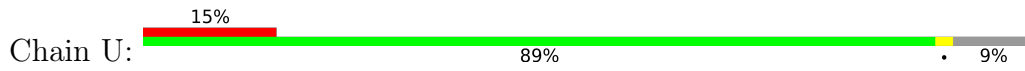








• Molecule 4: Mu-2 protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.634	Depositor
Minimum map value	-1.369	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.6	Depositor
Map size ( $\text{\AA}$ )	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.36, 1.36, 1.36	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: ZN, SAM

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	1	0.32	0/1052	0.58	0/1413
1	2	0.31	0/1046	0.56	0/1405
1	3	0.31	0/1041	0.57	0/1398
1	4	0.31	0/976	0.58	0/1308
1	5	0.32	0/1052	0.61	0/1413
1	A	0.34	0/9107	0.59	2/12474 (0.0%)
1	B	0.35	1/8671 (0.0%)	0.60	2/11878 (0.0%)
1	C	0.34	0/8814	0.59	3/12074 (0.0%)
1	D	0.34	0/8526	0.59	4/11680 (0.0%)
1	E	0.34	0/8612	0.59	3/11798 (0.0%)
1	a	0.34	0/8804	0.58	2/12061 (0.0%)
1	b	0.33	0/8804	0.56	0/12061
1	c	0.33	0/8772	0.57	1/12015 (0.0%)
1	d	0.34	0/8804	0.56	0/12061
1	e	0.34	0/8804	0.57	2/12061 (0.0%)
2	H	0.29	0/8275	0.58	4/11284 (0.0%)
2	I	0.29	0/8275	0.58	4/11284 (0.0%)
2	J	0.29	0/8275	0.57	4/11284 (0.0%)
2	K	0.29	0/8275	0.58	4/11284 (0.0%)
2	L	0.30	0/8275	0.58	4/11284 (0.0%)
3	R	0.34	0/10166	0.63	3/13806 (0.0%)
4	U	0.34	0/5439	0.66	3/7385 (0.0%)
All	All	0.33	1/149865 (0.0%)	0.59	45/204711 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	2
1	a	0	3
1	b	0	2
1	c	0	1
1	d	0	4
1	e	0	2
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
3	R	0	3
4	U	0	3
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1215	SER	C-N	-5.90	1.20	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	295	ASP	CB-CG-OD1	9.32	126.69	118.30
2	L	295	ASP	CB-CG-OD1	9.32	126.69	118.30
2	J	295	ASP	CB-CG-OD1	9.28	126.66	118.30
2	K	295	ASP	CB-CG-OD1	9.27	126.64	118.30
1	C	587	ASP	CB-CG-OD1	9.26	126.64	118.30
2	I	295	ASP	CB-CG-OD1	9.24	126.61	118.30
3	R	555	LEU	CA-CB-CG	8.82	135.60	115.30
4	U	112	LEU	CA-CB-CG	7.09	131.60	115.30
1	E	549	LEU	CA-CB-CG	6.93	131.24	115.30
1	B	549	LEU	CA-CB-CG	6.27	129.72	115.30
1	E	797	LEU	CA-CB-CG	6.09	129.30	115.30
4	U	471	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	616	ASP	CB-CG-OD1	6.06	123.76	118.30
1	E	714	PRO	C-N-CA	6.03	136.77	121.70
1	D	984	LEU	CA-CB-CG	5.98	129.05	115.30
1	D	714	PRO	C-N-CA	5.81	136.22	121.70
1	a	538	ASP	CB-CG-OD1	5.81	123.53	118.30
2	L	63	LEU	CA-CB-CG	5.63	128.24	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	63	LEU	CA-CB-CG	5.63	128.24	115.30
2	J	63	LEU	CA-CB-CG	5.61	128.21	115.30
2	I	63	LEU	CA-CB-CG	5.61	128.21	115.30
2	K	63	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	359	LEU	CA-CB-CG	5.55	128.07	115.30
1	C	714	PRO	C-N-CA	5.44	135.30	121.70
1	C	984	LEU	CA-CB-CG	5.41	127.74	115.30
4	U	572	LEU	CA-CB-CG	5.37	127.65	115.30
1	D	457	LEU	CA-CB-CG	5.33	127.56	115.30
2	L	860	CYS	CA-CB-SG	5.32	123.58	114.00
2	I	860	CYS	CA-CB-SG	5.32	123.57	114.00
2	J	860	CYS	CA-CB-SG	5.30	123.54	114.00
2	H	860	CYS	CA-CB-SG	5.29	123.53	114.00
2	K	860	CYS	CA-CB-SG	5.29	123.51	114.00
2	L	153	LEU	CA-CB-CG	5.27	127.42	115.30
2	K	153	LEU	CA-CB-CG	5.26	127.39	115.30
2	J	153	LEU	CA-CB-CG	5.25	127.39	115.30
2	I	153	LEU	CA-CB-CG	5.25	127.38	115.30
2	H	153	LEU	CA-CB-CG	5.25	127.36	115.30
1	D	983	LEU	CA-CB-CG	5.20	127.27	115.30
1	c	1055	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	732	LEU	CA-CB-CG	5.17	127.18	115.30
1	a	949	LEU	CA-CB-CG	5.15	127.15	115.30
1	e	949	LEU	CA-CB-CG	5.15	127.15	115.30
3	R	1119	LEU	CA-CB-CG	5.05	126.93	115.30
1	e	984	LEU	CA-CB-CG	5.02	126.84	115.30
3	R	1215	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	793	MET	Peptide
1	C	276	VAL	Peptide
1	E	376	THR	Peptide
1	E	981	ASP	Peptide
2	H	1002	SER	Peptide
2	I	1002	SER	Peptide
2	J	1002	SER	Peptide
2	K	1002	SER	Peptide
2	L	1002	SER	Peptide
3	R	1065	GLU	Peptide

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Mol	Chain	Res	Type	Group
3	R	1119	LEU	Peptide
3	R	97	CYS	Peptide
4	U	135	ILE	Peptide
4	U	378	PRO	Peptide
4	U	483	SER	Peptide
1	a	1110	PHE	Peptide
1	a	285	PHE	Peptide
1	a	945	VAL	Peptide
1	b	1110	PHE	Peptide
1	b	945	VAL	Peptide
1	c	912	THR	Peptide
1	d	1110	PHE	Peptide
1	d	342	GLU	Peptide
1	d	375	HIS	Peptide
1	d	945	VAL	Peptide
1	e	1110	PHE	Peptide
1	e	947	ARG	Peptide

## 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	1	136/1275 (11%)	123 (90%)	13 (10%)	0	100	100
1	2	135/1275 (11%)	125 (93%)	10 (7%)	0	100	100
1	3	134/1275 (10%)	124 (92%)	10 (8%)	0	100	100
1	4	125/1275 (10%)	115 (92%)	10 (8%)	0	100	100
1	5	136/1275 (11%)	126 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1126/1275 (88%)	1045 (93%)	80 (7%)	1 (0%)	51	83
1	B	1069/1275 (84%)	991 (93%)	76 (7%)	2 (0%)	47	79
1	C	1084/1275 (85%)	1016 (94%)	67 (6%)	1 (0%)	51	83
1	D	1046/1275 (82%)	974 (93%)	72 (7%)	0	100	100
1	E	1059/1275 (83%)	992 (94%)	66 (6%)	1 (0%)	51	83
1	a	1083/1275 (85%)	1002 (92%)	79 (7%)	2 (0%)	47	79
1	b	1083/1275 (85%)	1015 (94%)	68 (6%)	0	100	100
1	c	1076/1275 (84%)	1016 (94%)	59 (6%)	1 (0%)	51	83
1	d	1083/1275 (85%)	1017 (94%)	66 (6%)	0	100	100
1	e	1083/1275 (85%)	1002 (92%)	80 (7%)	1 (0%)	51	83
2	H	1022/1289 (79%)	950 (93%)	72 (7%)	0	100	100
2	I	1022/1289 (79%)	950 (93%)	72 (7%)	0	100	100
2	J	1022/1289 (79%)	949 (93%)	73 (7%)	0	100	100
2	K	1022/1289 (79%)	950 (93%)	72 (7%)	0	100	100
2	L	1022/1289 (79%)	946 (93%)	76 (7%)	0	100	100
3	R	1249/1267 (99%)	1166 (93%)	82 (7%)	1 (0%)	51	83
4	U	658/736 (89%)	591 (90%)	60 (9%)	7 (1%)	14	53
All	All	18475/27573 (67%)	17185 (93%)	1273 (7%)	17 (0%)	54	83

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	TRP
1	B	310	TRP
3	R	287	GLU
1	a	310	TRP
1	B	1214	SER
4	U	585	PRO
4	U	136	SER
4	U	471	ASP
1	e	1058	PRO
4	U	456	PHE
4	U	531	ASP
1	C	586	SER
4	U	133	PRO
4	U	135	ILE

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Mol	Chain	Res	Type
1	E	583	PRO
1	a	346	VAL
1	c	1058	PRO

### 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	1	112/1113 (10%)	112 (100%)	0	100	100
1	2	111/1113 (10%)	110 (99%)	1 (1%)	78	90
1	3	111/1113 (10%)	111 (100%)	0	100	100
1	4	104/1113 (9%)	103 (99%)	1 (1%)	76	88
1	5	112/1113 (10%)	108 (96%)	4 (4%)	35	67
1	A	994/1113 (89%)	994 (100%)	0	100	100
1	B	945/1113 (85%)	939 (99%)	6 (1%)	86	94
1	C	963/1113 (86%)	963 (100%)	0	100	100
1	D	931/1113 (84%)	930 (100%)	1 (0%)	93	98
1	E	940/1113 (84%)	936 (100%)	4 (0%)	91	97
1	a	960/1113 (86%)	955 (100%)	5 (0%)	88	95
1	b	960/1113 (86%)	960 (100%)	0	100	100
1	c	955/1113 (86%)	954 (100%)	1 (0%)	93	98
1	d	960/1113 (86%)	958 (100%)	2 (0%)	93	98
1	e	960/1113 (86%)	958 (100%)	2 (0%)	93	98
2	H	884/1118 (79%)	878 (99%)	6 (1%)	84	93
2	I	884/1118 (79%)	878 (99%)	6 (1%)	84	93
2	J	884/1118 (79%)	878 (99%)	6 (1%)	84	93
2	K	884/1118 (79%)	878 (99%)	6 (1%)	84	93
2	L	884/1118 (79%)	877 (99%)	7 (1%)	81	91
3	R	1074/1084 (99%)	1070 (100%)	4 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	U	592/650 (91%)	588 (99%)	4 (1%)	84 93
All	All	16204/24019 (68%)	16138 (100%)	66 (0%)	91 97

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	146	ASN
1	4	146	ASN
1	5	3	ARG
1	5	6	ARG
1	5	9	LYS
1	5	13	SER
1	B	503	ARG
1	B	567	THR
1	B	752	THR
1	B	774	ASN
1	B	837	ARG
1	B	1120	ARG
1	D	524	ASN
1	E	582	ARG
1	E	720	ARG
1	E	780	ARG
1	E	794	ARG
2	H	8	ARG
2	H	21	ARG
2	H	23	ARG
2	H	476	ARG
2	H	738	ARG
2	H	758	ARG
2	I	8	ARG
2	I	21	ARG
2	I	23	ARG
2	I	476	ARG
2	I	738	ARG
2	I	758	ARG
2	J	8	ARG
2	J	21	ARG
2	J	23	ARG
2	J	476	ARG
2	J	738	ARG
2	J	758	ARG
2	K	8	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	K	21	ARG
2	K	23	ARG
2	K	476	ARG
2	K	738	ARG
2	K	758	ARG
2	L	8	ARG
2	L	21	ARG
2	L	23	ARG
2	L	476	ARG
2	L	578	VAL
2	L	738	ARG
2	L	758	ARG
3	R	524	ARG
3	R	880	VAL
3	R	1018	GLN
3	R	1040	ARG
4	U	212	THR
4	U	228	ASN
4	U	680	ARG
4	U	695	LYS
1	a	241	ASN
1	a	242	ARG
1	a	313	ASN
1	a	338	LEU
1	a	1079	ARG
1	c	1082	ARG
1	d	218	ARG
1	d	1079	ARG
1	e	218	ARG
1	e	436	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	141	ASN
1	1	146	ASN
1	2	76	ASN
1	2	86	ASN
1	3	146	ASN
1	4	109	GLN
1	4	131	ASN
1	5	52	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	131	ASN
1	A	278	GLN
1	A	331	ASN
1	A	357	ASN
1	A	382	HIS
1	A	527	ASN
1	A	692	GLN
1	A	812	GLN
1	A	1000	GLN
1	A	1123	ASN
1	B	278	GLN
1	B	357	ASN
1	B	441	ASN
1	B	692	GLN
1	B	1000	GLN
1	B	1003	GLN
1	B	1116	GLN
1	B	1123	ASN
1	B	1233	ASN
1	B	1244	GLN
1	C	340	ASN
1	C	357	ASN
1	C	375	HIS
1	C	527	ASN
1	C	692	GLN
1	C	749	ASN
1	C	763	ASN
1	C	1036	ASN
1	C	1116	GLN
1	C	1123	ASN
1	D	278	GLN
1	D	357	ASN
1	D	524	ASN
1	D	654	ASN
1	D	692	GLN
1	D	715	ASN
1	D	787	GLN
1	D	937	GLN
1	D	1123	ASN
1	D	1233	ASN
1	D	1244	GLN
1	E	217	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	246	GLN
1	E	278	GLN
1	E	357	ASN
1	E	382	HIS
1	E	527	ASN
1	E	585	ASN
1	E	692	GLN
1	E	763	ASN
1	E	774	ASN
1	E	1000	GLN
1	E	1246	GLN
2	H	108	HIS
2	H	310	ASN
2	H	634	ASN
2	I	108	HIS
2	I	310	ASN
2	I	634	ASN
2	J	28	HIS
2	J	108	HIS
2	J	310	ASN
2	J	634	ASN
2	K	108	HIS
2	K	310	ASN
2	K	634	ASN
2	L	108	HIS
2	L	310	ASN
2	L	634	ASN
3	R	22	GLN
3	R	183	HIS
3	R	493	GLN
3	R	535	GLN
3	R	536	GLN
3	R	646	ASN
3	R	754	GLN
3	R	864	GLN
3	R	944	GLN
3	R	1085	ASN
3	R	1195	HIS
3	R	1206	HIS
4	U	149	ASN
4	U	203	ASN
4	U	451	GLN

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Mol	Chain	Res	Type
1	a	241	ASN
1	a	357	ASN
1	a	524	ASN
1	a	667	GLN
1	a	731	ASN
1	a	745	HIS
1	a	1036	ASN
1	b	357	ASN
1	b	415	ASN
1	b	731	ASN
1	b	1036	ASN
1	b	1205	ASN
1	b	1233	ASN
1	b	1244	GLN
1	c	184	HIS
1	c	524	ASN
1	c	898	ASN
1	c	937	GLN
1	d	234	GLN
1	d	357	ASN
1	d	537	GLN
1	d	569	GLN
1	d	859	GLN
1	d	1075	HIS
1	d	1197	GLN
1	e	488	GLN
1	e	524	ASN
1	e	745	HIS
1	e	868	ASN
1	e	1125	GLN
1	e	1205	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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
6	SAM	L	1302	-	24,29,29	1.03	1 (4%)	23,42,42	1.45	5 (21%)
6	SAM	J	1301	-	24,29,29	1.04	2 (8%)	23,42,42	1.59	4 (17%)
6	SAM	J	1302	-	24,29,29	1.05	1 (4%)	23,42,42	1.58	4 (17%)
6	SAM	K	1302	-	24,29,29	1.03	1 (4%)	23,42,42	1.62	4 (17%)
6	SAM	H	1302	-	24,29,29	1.03	2 (8%)	23,42,42	1.48	4 (17%)
6	SAM	H	1301	-	24,29,29	1.04	1 (4%)	23,42,42	1.47	4 (17%)
6	SAM	I	1301	-	24,29,29	1.05	1 (4%)	23,42,42	1.62	5 (21%)
6	SAM	L	1301	-	24,29,29	1.05	1 (4%)	23,42,42	1.53	5 (21%)
6	SAM	K	1301	-	24,29,29	1.06	2 (8%)	23,42,42	1.48	5 (21%)
6	SAM	I	1302	2	24,29,29	1.07	2 (8%)	23,42,42	1.44	4 (17%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SAM	L	1302	-	-	3/12/33/33	0/3/3/3
6	SAM	J	1301	-	-	6/12/33/33	0/3/3/3
6	SAM	J	1302	-	-	6/12/33/33	0/3/3/3
6	SAM	K	1302	-	-	2/12/33/33	0/3/3/3
6	SAM	H	1302	-	-	6/12/33/33	0/3/3/3
6	SAM	H	1301	-	-	4/12/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SAM	I	1301	-	-	0/12/33/33	0/3/3/3
6	SAM	L	1301	-	-	6/12/33/33	0/3/3/3
6	SAM	K	1301	-	-	6/12/33/33	0/3/3/3
6	SAM	I	1302	2	-	6/12/33/33	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	1302	SAM	OXT-C	-2.30	1.23	1.30
6	K	1301	SAM	C5-C4	2.30	1.47	1.40
6	L	1302	SAM	C5-C4	2.24	1.46	1.40
6	J	1301	SAM	C5-C4	2.20	1.46	1.40
6	I	1301	SAM	C5-C4	2.15	1.46	1.40
6	L	1301	SAM	C5-C4	2.15	1.46	1.40
6	I	1302	SAM	C5-C4	2.12	1.46	1.40
6	H	1302	SAM	C5-C4	2.08	1.46	1.40
6	K	1302	SAM	C5-C4	2.08	1.46	1.40
6	J	1302	SAM	C5-C4	2.08	1.46	1.40
6	H	1301	SAM	C5-C4	2.08	1.46	1.40
6	K	1301	SAM	CE-SD	-2.02	1.66	1.78
6	H	1302	SAM	CE-SD	-2.02	1.66	1.78
6	J	1301	SAM	CE-SD	-2.00	1.66	1.78

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1302	SAM	CG-SD-C5'	3.97	113.53	103.40
6	H	1301	SAM	N3-C2-N1	-3.83	122.69	128.68
6	L	1301	SAM	N3-C2-N1	-3.77	122.79	128.68
6	I	1301	SAM	N3-C2-N1	-3.74	122.84	128.68
6	L	1302	SAM	N3-C2-N1	-3.72	122.86	128.68
6	K	1302	SAM	N3-C2-N1	-3.71	122.89	128.68
6	I	1301	SAM	CG-SD-C5'	3.69	112.81	103.40
6	J	1301	SAM	N3-C2-N1	-3.69	122.91	128.68
6	H	1302	SAM	N3-C2-N1	-3.67	122.94	128.68
6	J	1302	SAM	N3-C2-N1	-3.66	122.95	128.68
6	I	1302	SAM	N3-C2-N1	-3.61	123.03	128.68
6	J	1302	SAM	CG-SD-C5'	3.60	112.58	103.40
6	K	1301	SAM	N3-C2-N1	-3.59	123.07	128.68
6	I	1302	SAM	C3'-C2'-C1'	3.23	105.85	100.98
6	I	1301	SAM	C3'-C2'-C1'	2.89	105.33	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1301	SAM	CG-SD-C5'	2.87	110.72	103.40
6	J	1301	SAM	C4-C5-N7	-2.85	106.42	109.40
6	L	1301	SAM	C3'-C2'-C1'	2.84	105.26	100.98
6	J	1302	SAM	C4-C5-N7	-2.81	106.47	109.40
6	L	1301	SAM	C4-C5-N7	-2.71	106.58	109.40
6	I	1301	SAM	C4-C5-N7	-2.70	106.58	109.40
6	I	1302	SAM	C4-C5-N7	-2.65	106.64	109.40
6	K	1302	SAM	C4-C5-N7	-2.65	106.64	109.40
6	H	1302	SAM	C4-C5-N7	-2.62	106.67	109.40
6	K	1301	SAM	CG-SD-C5'	2.59	110.01	103.40
6	H	1302	SAM	C3'-C2'-C1'	2.58	104.86	100.98
6	J	1301	SAM	C3'-C2'-C1'	2.54	104.80	100.98
6	H	1301	SAM	C4-C5-N7	-2.52	106.77	109.40
6	L	1302	SAM	C3'-C2'-C1'	2.49	104.72	100.98
6	K	1301	SAM	O4'-C1'-C2'	-2.45	103.35	106.93
6	K	1302	SAM	C3'-C2'-C1'	2.44	104.66	100.98
6	J	1301	SAM	CG-SD-C5'	2.42	109.57	103.40
6	H	1302	SAM	CG-SD-C5'	2.36	109.43	103.40
6	L	1302	SAM	C2-N1-C6	2.20	122.52	118.75
6	H	1301	SAM	C3'-C2'-C1'	2.19	104.28	100.98
6	L	1302	SAM	C4-C5-N7	-2.19	107.11	109.40
6	K	1301	SAM	C1'-N9-C4	2.18	130.47	126.64
6	L	1302	SAM	CG-SD-C5'	2.13	108.84	103.40
6	I	1302	SAM	CG-SD-C5'	2.11	108.78	103.40
6	J	1302	SAM	C1'-N9-C4	-2.08	122.99	126.64
6	H	1301	SAM	C2-N1-C6	2.07	122.30	118.75
6	K	1301	SAM	C4-C5-N7	-2.04	107.27	109.40
6	I	1301	SAM	C2-N1-C6	2.02	122.21	118.75
6	L	1301	SAM	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1301	SAM	C3'-C4'-C5'-SD
6	H	1302	SAM	C-CA-CB-CG
6	H	1302	SAM	CB-CG-SD-CE
6	H	1302	SAM	CB-CG-SD-C5'
6	H	1302	SAM	O4'-C4'-C5'-SD
6	H	1302	SAM	C3'-C4'-C5'-SD
6	I	1302	SAM	N-CA-CB-CG
6	I	1302	SAM	C-CA-CB-CG

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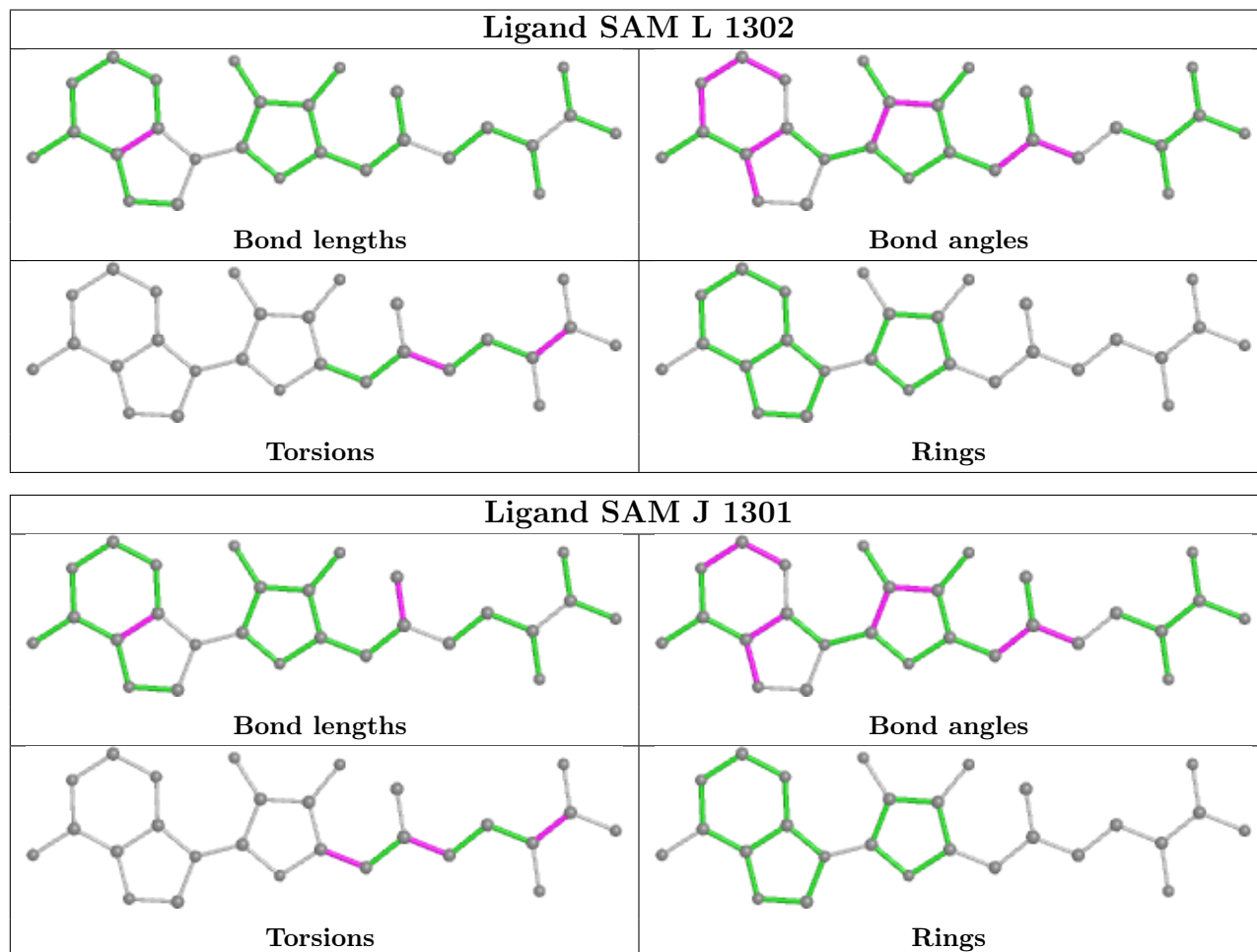
Mol	Chain	Res	Type	Atoms
6	I	1302	SAM	CA-CB-CG-SD
6	I	1302	SAM	C3'-C4'-C5'-SD
6	J	1301	SAM	CB-CG-SD-CE
6	J	1302	SAM	N-CA-CB-CG
6	J	1302	SAM	C-CA-CB-CG
6	K	1301	SAM	N-CA-CB-CG
6	K	1301	SAM	C-CA-CB-CG
6	L	1301	SAM	N-CA-CB-CG
6	L	1301	SAM	C-CA-CB-CG
6	L	1301	SAM	CB-CG-SD-CE
6	L	1301	SAM	CB-CG-SD-C5'
6	L	1301	SAM	O4'-C4'-C5'-SD
6	L	1301	SAM	C3'-C4'-C5'-SD
6	L	1302	SAM	CB-CG-SD-CE
6	L	1302	SAM	CB-CG-SD-C5'
6	H	1301	SAM	OXT-C-CA-N
6	J	1302	SAM	CB-CG-SD-CE
6	H	1301	SAM	O-C-CA-N
6	J	1302	SAM	OXT-C-CA-CB
6	I	1302	SAM	O4'-C4'-C5'-SD
6	J	1301	SAM	CB-CG-SD-C5'
6	J	1301	SAM	O4'-C4'-C5'-SD
6	J	1302	SAM	CB-CG-SD-C5'
6	H	1302	SAM	CA-CB-CG-SD
6	J	1301	SAM	C3'-C4'-C5'-SD
6	K	1301	SAM	CA-CB-CG-SD
6	K	1302	SAM	CA-CB-CG-SD
6	J	1302	SAM	O-C-CA-CB
6	J	1301	SAM	O-C-CA-N
6	L	1302	SAM	O-C-CA-N
6	K	1301	SAM	CB-CG-SD-CE
6	K	1302	SAM	OXT-C-CA-N
6	J	1301	SAM	OXT-C-CA-N
6	I	1302	SAM	OXT-C-CA-CB
6	H	1301	SAM	O4'-C4'-C5'-SD
6	K	1301	SAM	CB-CG-SD-C5'
6	K	1301	SAM	C4'-C5'-SD-CG

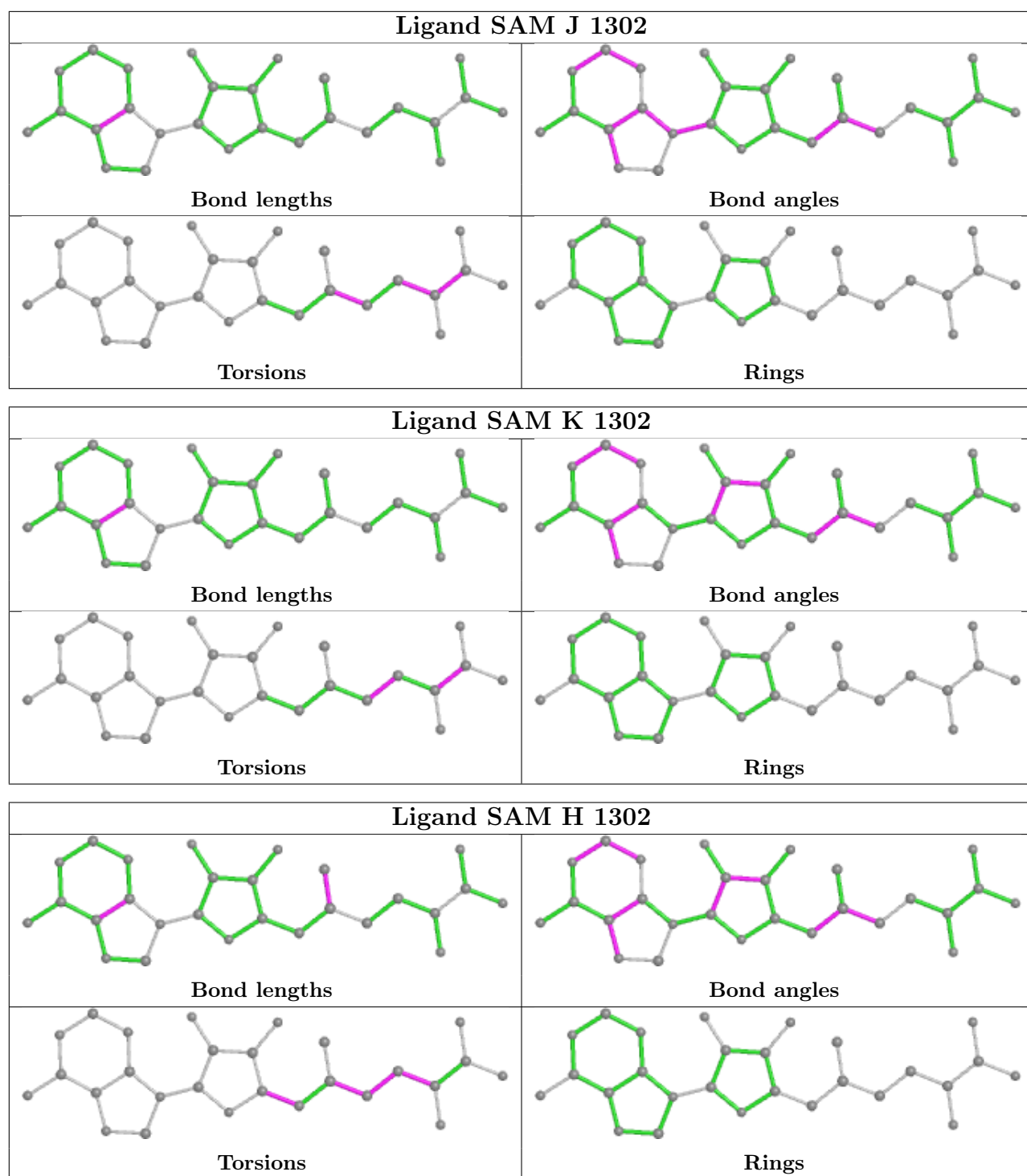
There are no ring outliers.

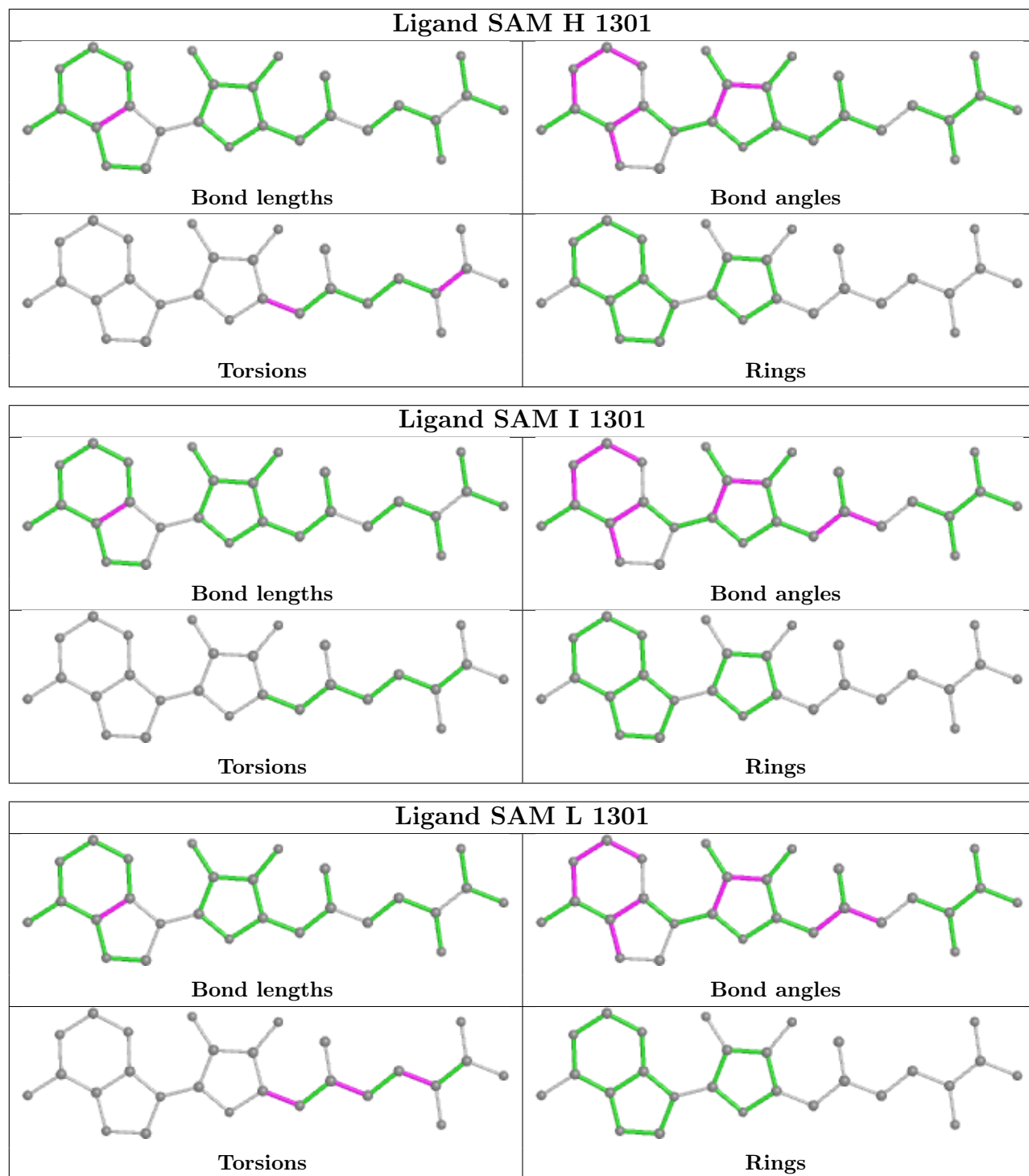
No monomer is involved in short contacts.

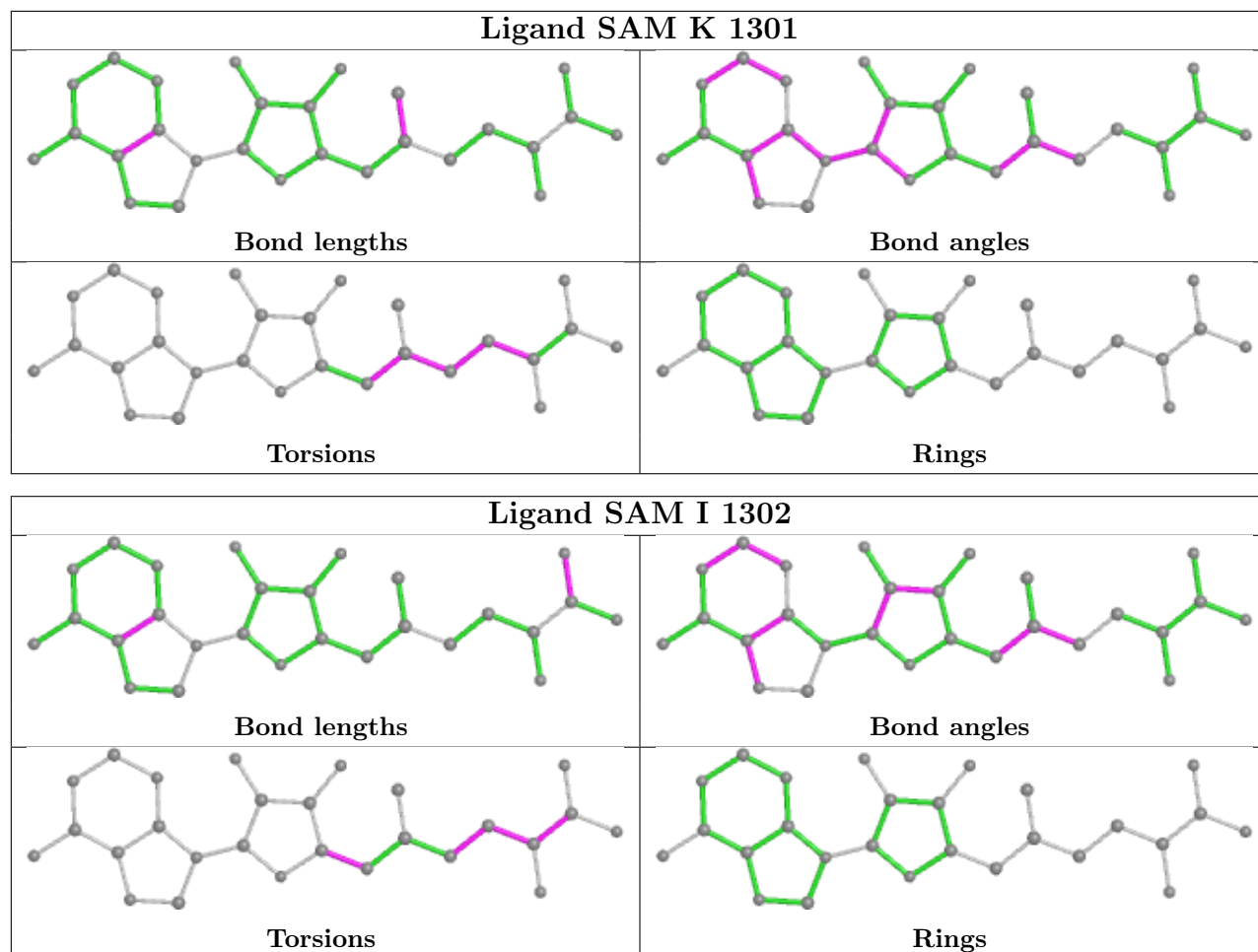
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.









## 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.



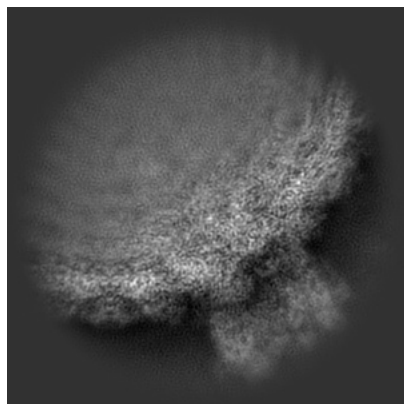
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33778. These allow visual inspection of the internal detail of the map and identification of artifacts.

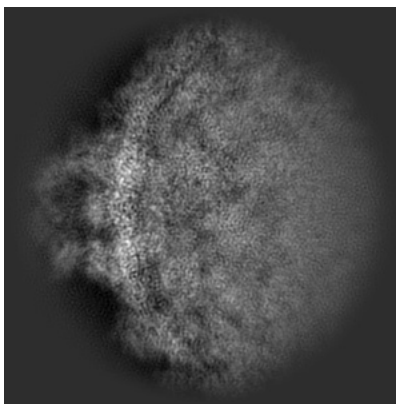
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

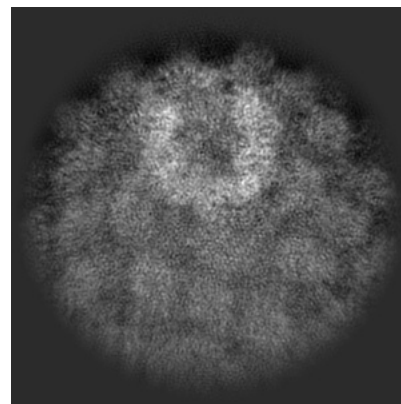
#### 6.1.1 Primary map



X

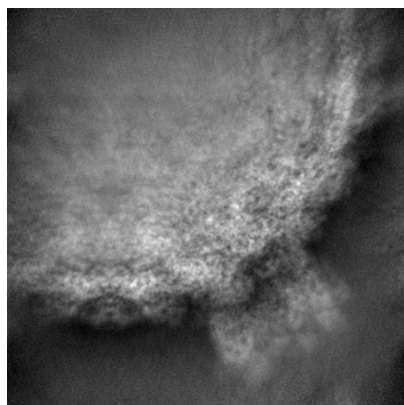


Y

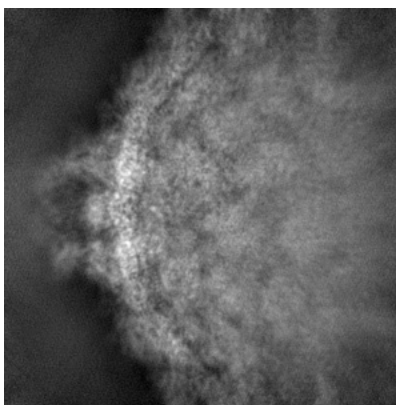


Z

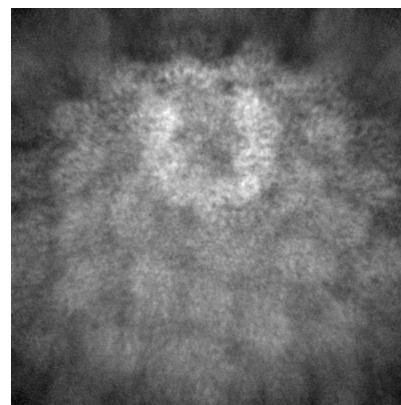
#### 6.1.2 Raw map



X



Y

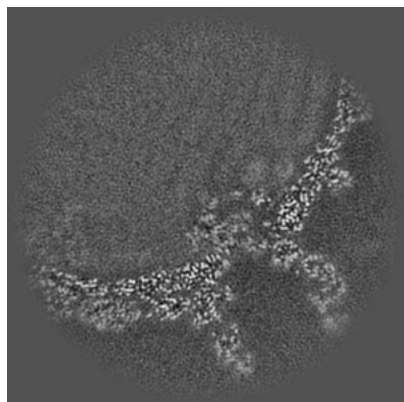


Z

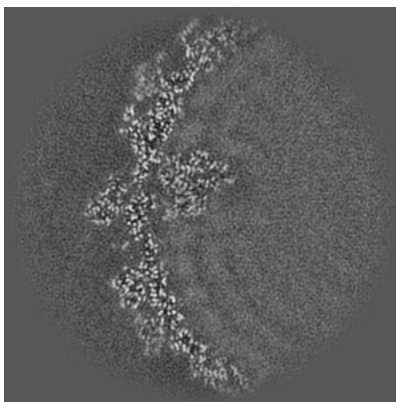
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

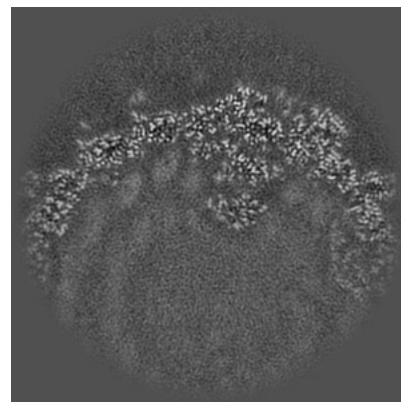
### 6.2.1 Primary map



X Index: 160

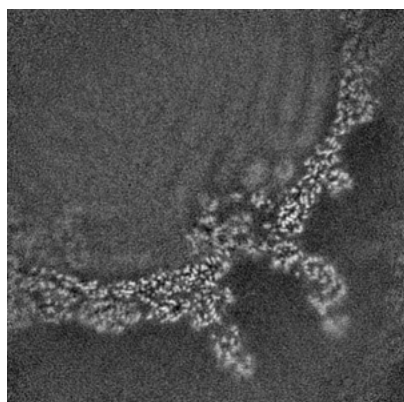


Y Index: 160

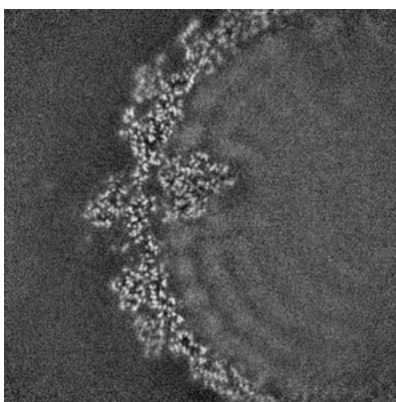


Z Index: 160

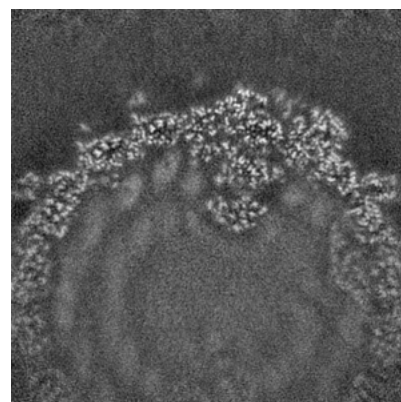
### 6.2.2 Raw map



X Index: 160



Y Index: 160

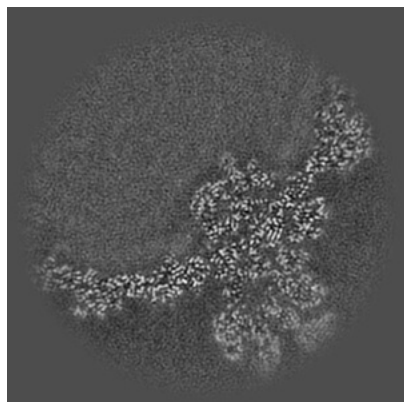


Z Index: 160

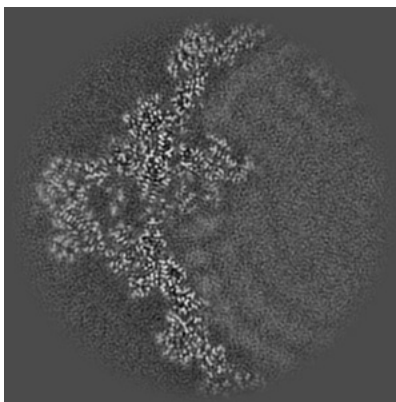
The images above show central slices of the map in three orthogonal directions.

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

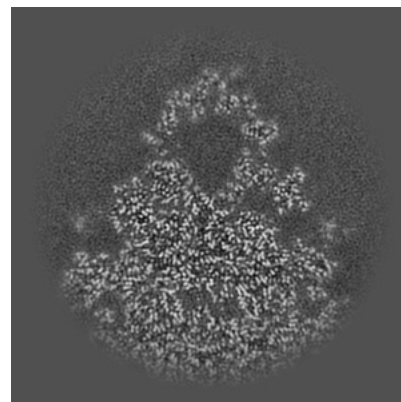
### 6.3.1 Primary map



X Index: 193

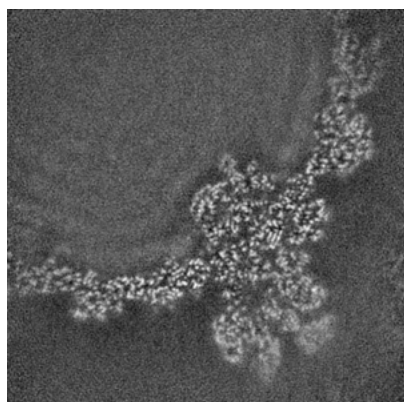


Y Index: 180

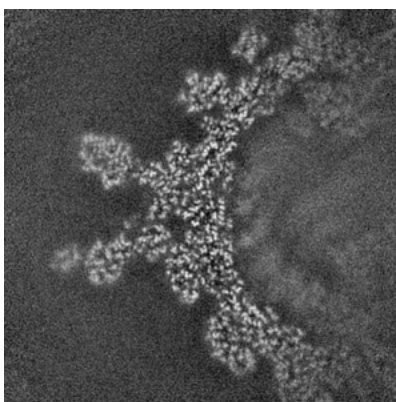


Z Index: 100

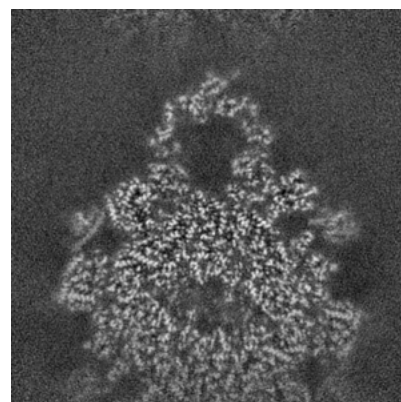
### 6.3.2 Raw map



X Index: 193



Y Index: 228

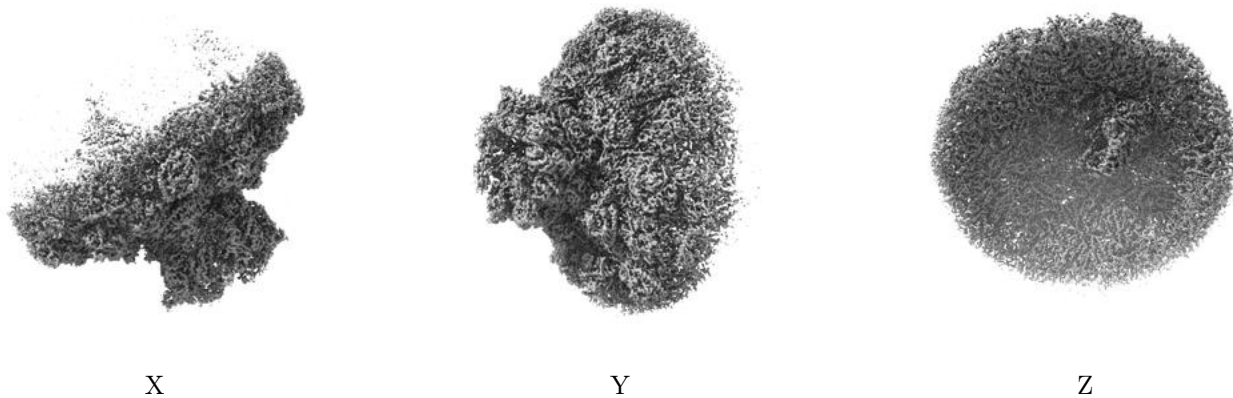


Z Index: 103

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

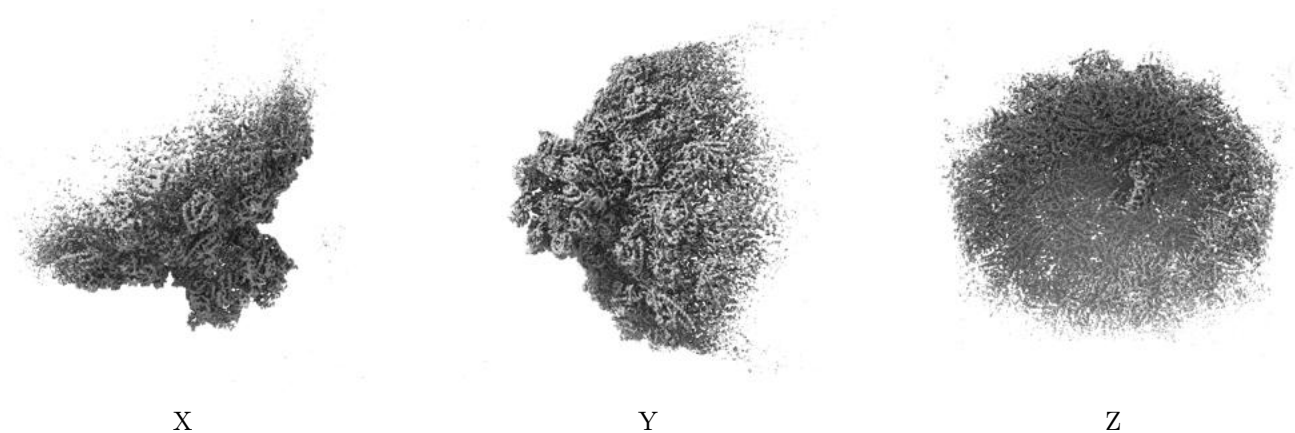
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

## 6.5 Mask visualisation [i](#)

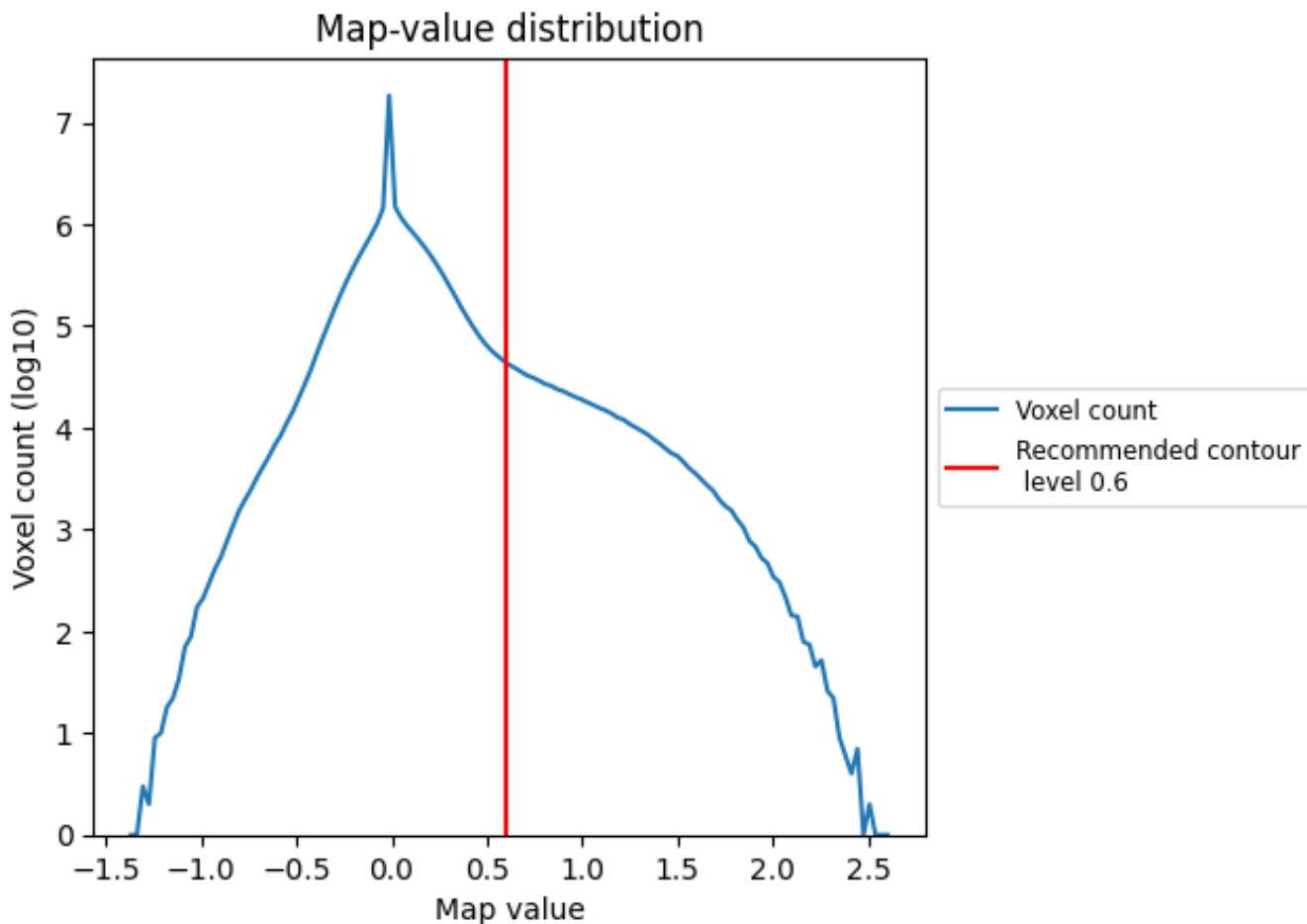
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

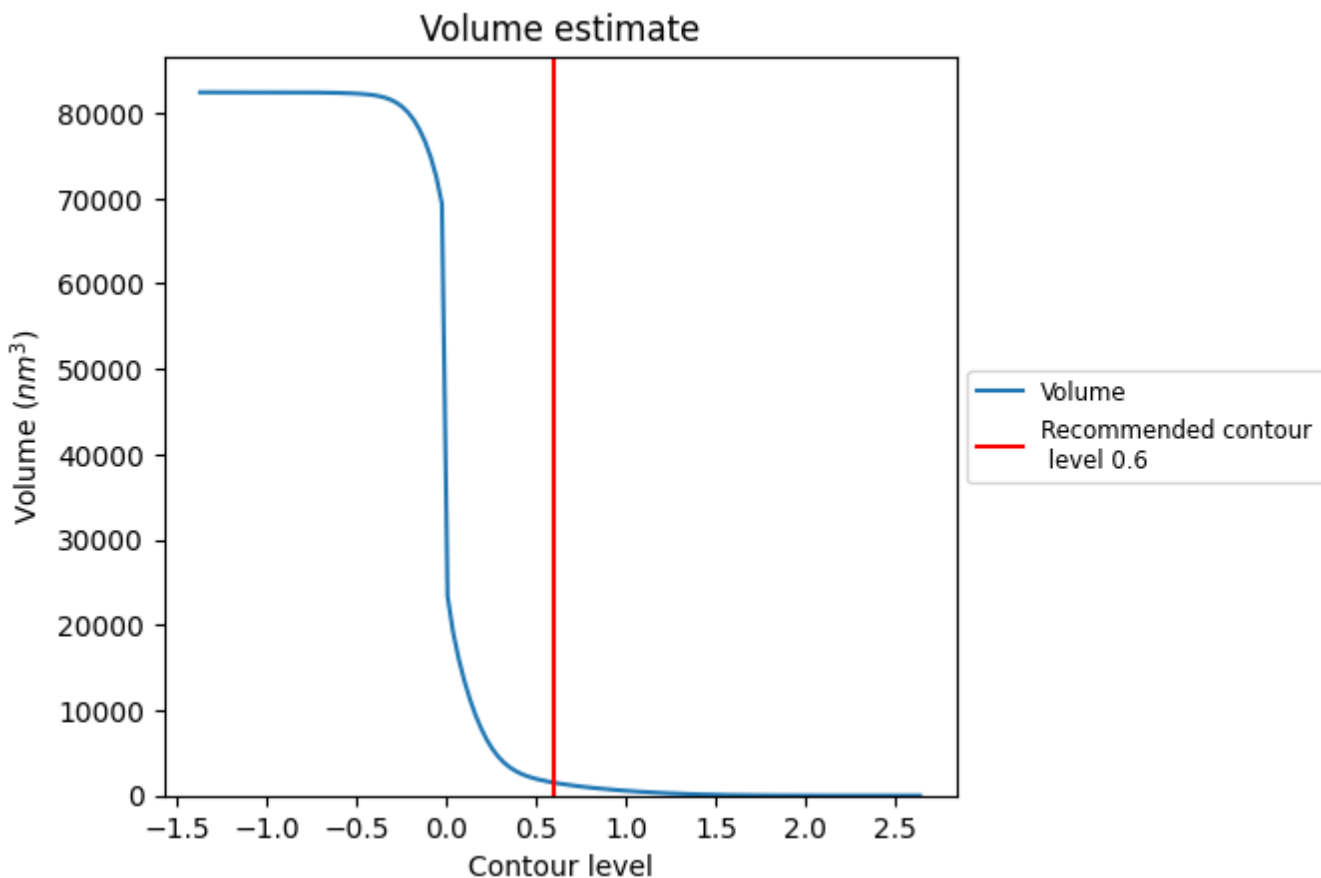
This section contains the results of statistical analysis of the map.

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



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

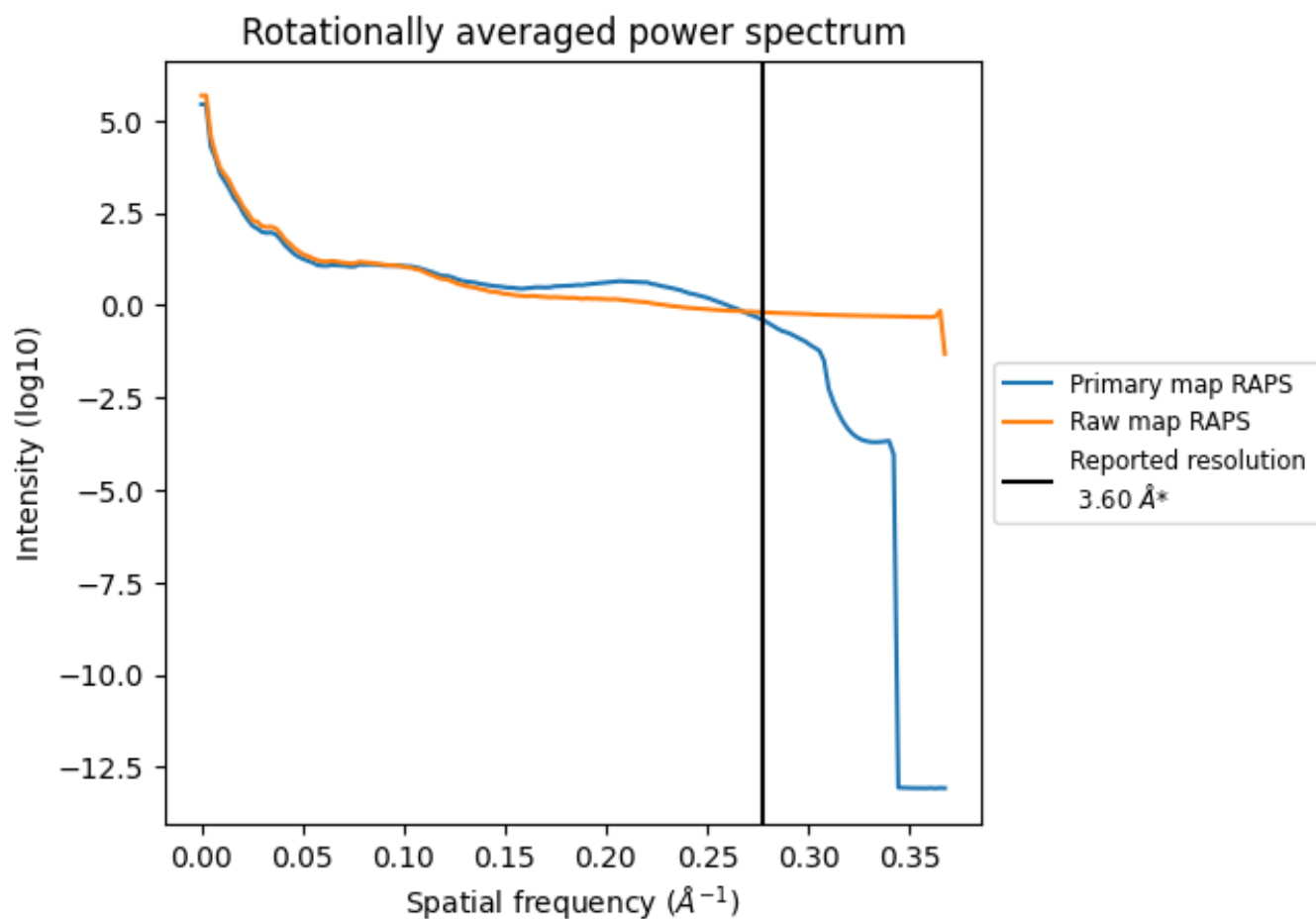
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1507 nm<sup>3</sup>; this corresponds to an approximate mass of 1361 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

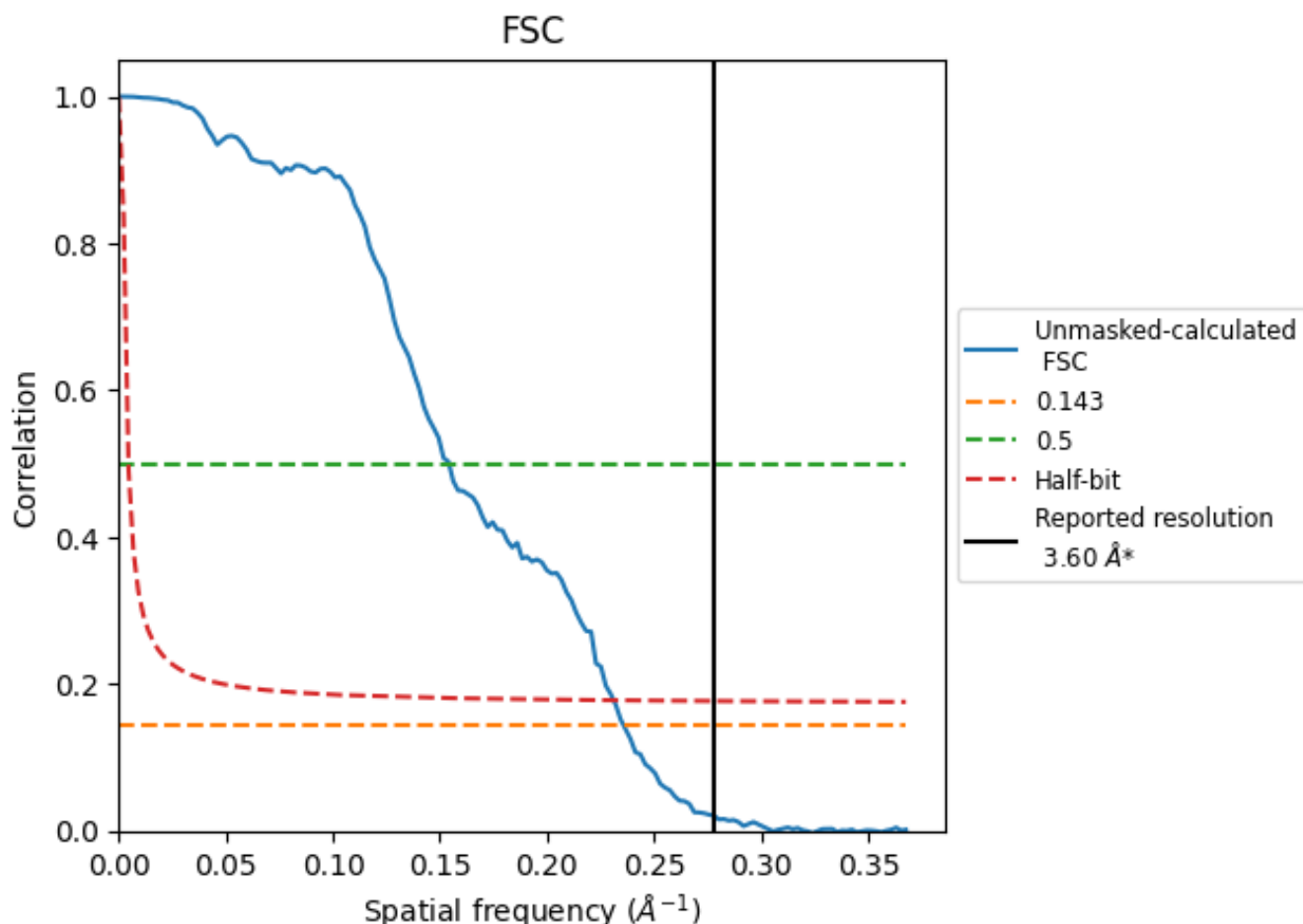


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

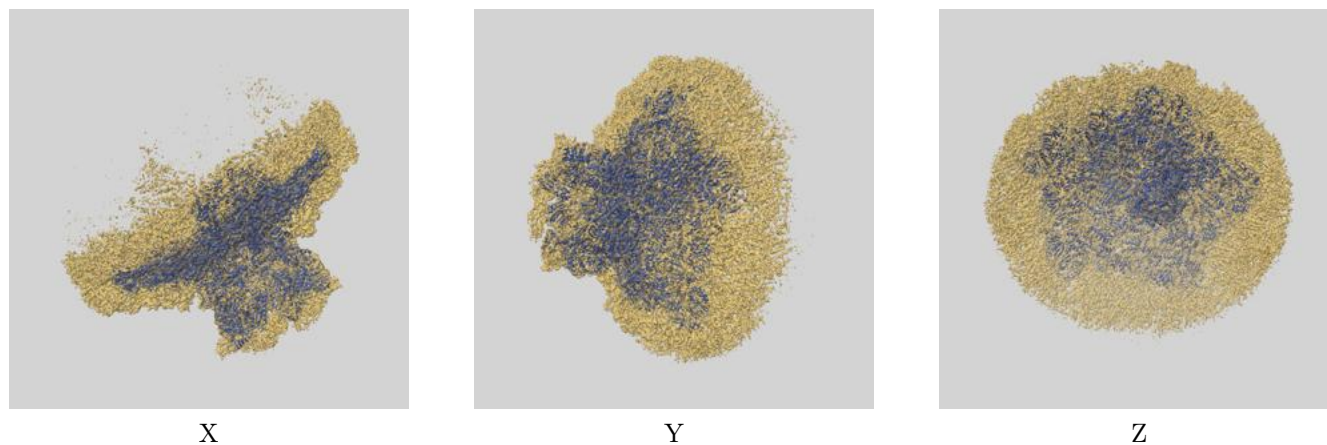
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	6.49	4.33

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.6 by more than 10 %

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

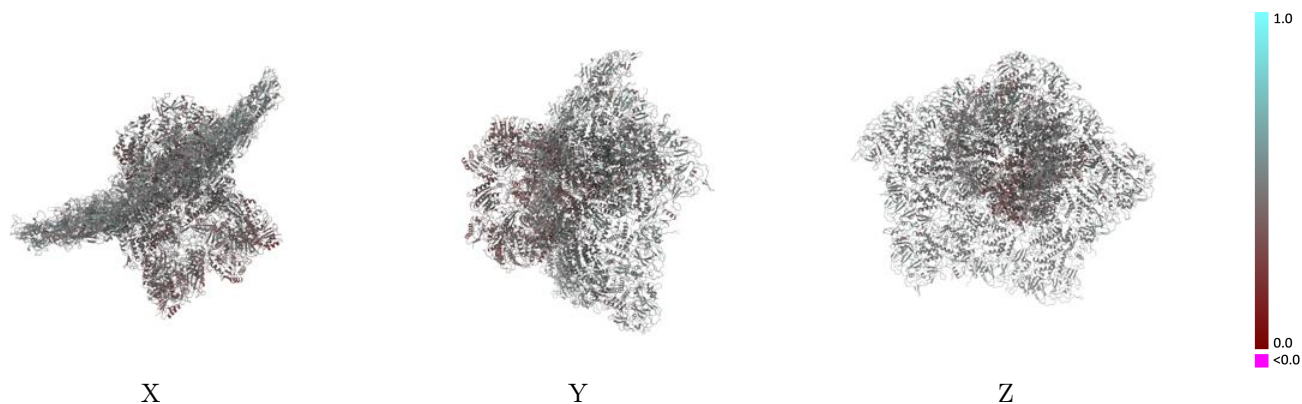
This section contains information regarding the fit between EMDB map EMD-33778 and PDB model 7YEV. Per-residue inclusion information can be found in section 3 on page 7.

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



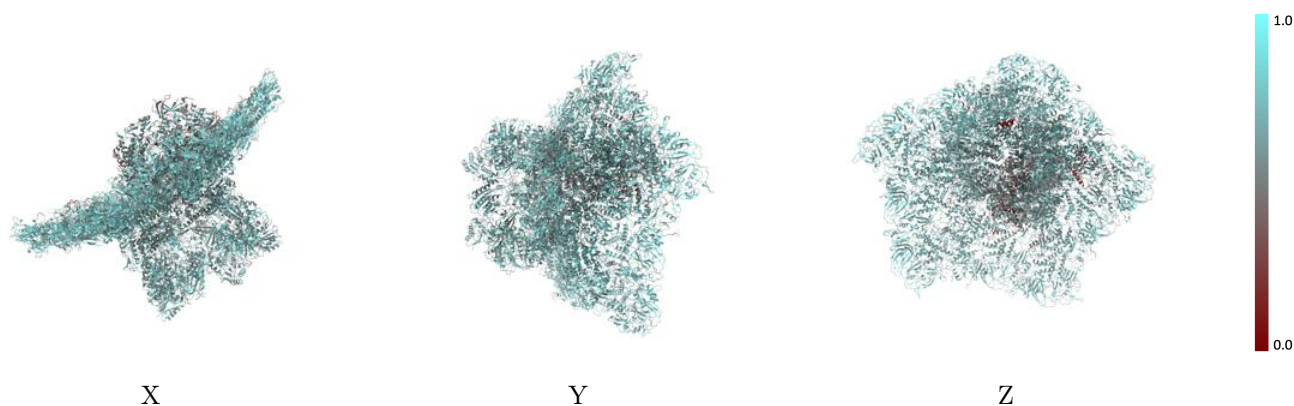
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



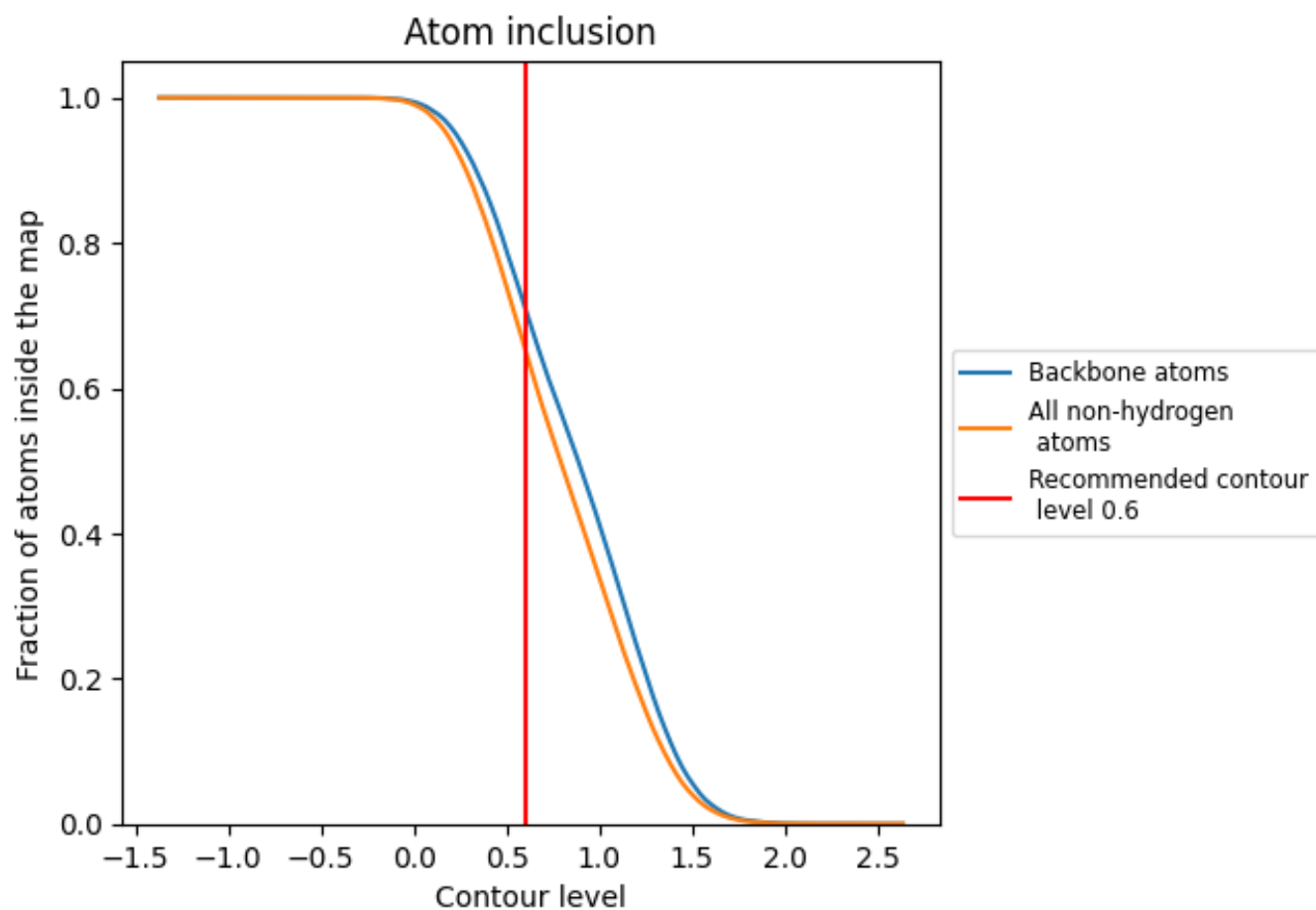
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6535	 0.4570
1	 0.5298	 0.4540
2	 0.5976	 0.4660
3	 0.6016	 0.4560
4	 0.4774	 0.4560
5	 0.3044	 0.4250
A	 0.6738	 0.4720
B	 0.6854	 0.4730
C	 0.6880	 0.4730
D	 0.7052	 0.4810
E	 0.6885	 0.4790
H	 0.6453	 0.4230
I	 0.6432	 0.4230
J	 0.6502	 0.4270
K	 0.6553	 0.4260
L	 0.6505	 0.4310
R	 0.5440	 0.4260
U	 0.5814	 0.4500
a	 0.6963	 0.4780
b	 0.7052	 0.4790
c	 0.7032	 0.4800
d	 0.7034	 0.4780
e	 0.6901	 0.4760

