



## Full wwPDB EM Validation Report ⓘ

Sep 18, 2023 – 01:56 pm BST

PDB ID : 8B3D  
EMDB ID : EMD-15825  
Title : Structure of the Pol II-TCR-ELOF1 complex.  
Authors : Kokic, G.; Cramer, P.  
Deposited on : 2022-09-16  
Resolution : 2.60 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:

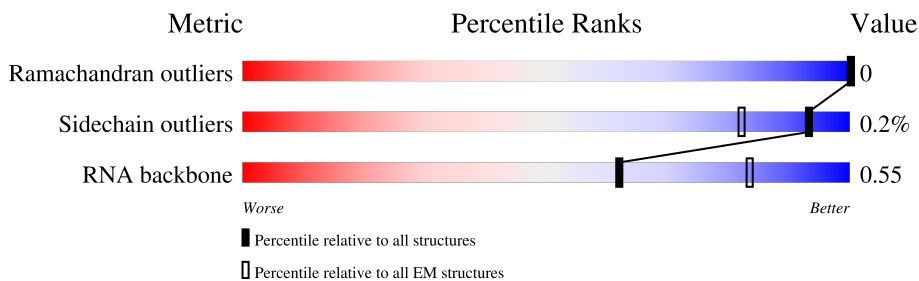
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

# 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 2.60 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
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1167	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	254	
8	H	150	

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	83	
14	N	52	
15	P	10	
16	T	52	
17	a	396	
18	b	1493	
19	c	709	
20	d	1140	

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 95808 atoms, of which 46954 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1409	22460	7022	11299	1998	2070	71	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1130	18131	5725	9083	1591	1668	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	260	4120	1309	2031	359	415	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	128	1985	636	972	172	201	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	209	3457	1089	1737	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	82	1341	418	684	113	121	5	0	0

- Molecule 7 is a protein called RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	171	2665	867	1331	216	243	8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	148	2333	750	1147	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	117	1827	587	878	169	182	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	67	1086	345	553	90	92	6	0	0

- Molecule 11 is a protein called RNA\_pol\_L\_2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	115	1862	593	942	152	173	2	0	0

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	46	781	241	393	75	66	6	0	0

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	M	64	968	312	463	81	105	7	0	0

- Molecule 14 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
14	N	40	913	393	84	162	234	40	0	0

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
15	P	10	330	98	110	45	67	10	0	0

- Molecule 16 is a DNA chain called TS.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
16	T	52	1078	476	87	160	303	52	0	0

- Molecule 17 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	a	365	5624	1775	2775	507	548	19	0	0

- Molecule 18 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	b	520	8561	2746	4302	746	746	21	0	0

- Molecule 19 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	c	264	3910	1237	1911	390	363	9	0	0

- Molecule 20 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	d	781	12321	3916	6160	1038	1173	34	0	0

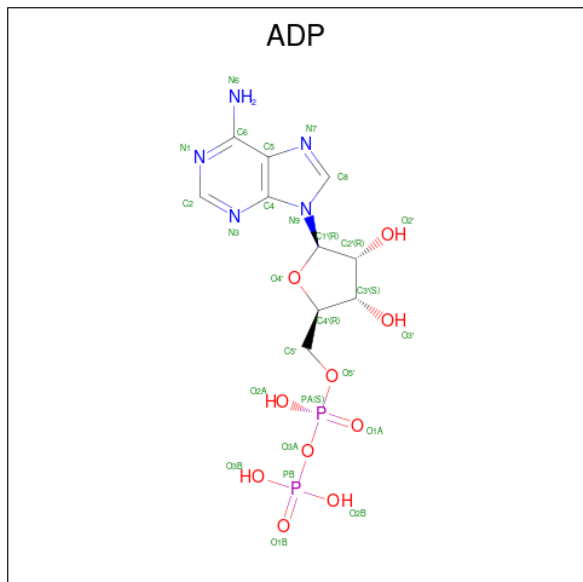
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total	Zn	0
			2	2	
21	B	1	Total	Zn	0
			1	1	
21	C	1	Total	Zn	0
			1	1	
21	I	2	Total	Zn	0
			2	2	
21	J	1	Total	Zn	0
			1	1	
21	L	1	Total	Zn	0
			1	1	
21	M	1	Total	Zn	0
			1	1	
21	c	1	Total	Zn	0
			1	1	

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

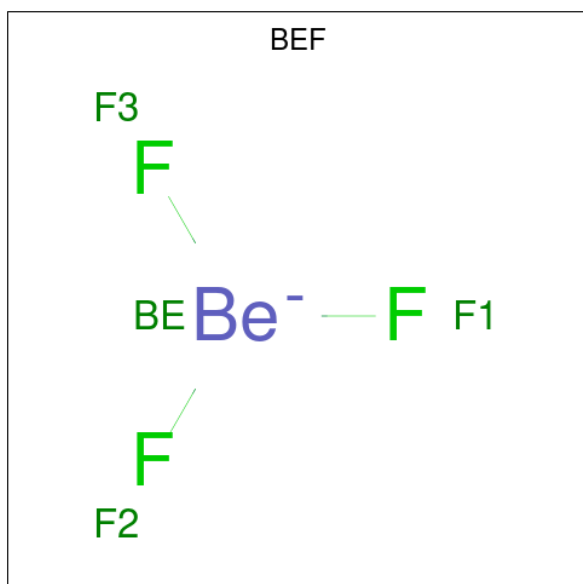
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Mg	0
			1	1	
22	b	1	Total	Mg	0
			1	1	

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
23	b	1	39	10	12	5	10	2	0

- Molecule 24 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $BeF_3$ ).

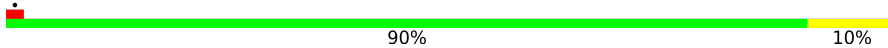


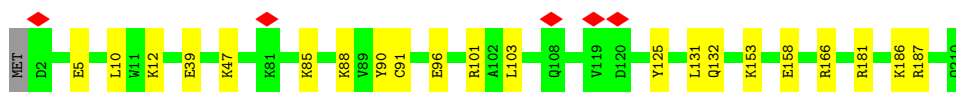
Mol	Chain	Residues	Atoms		AltConf
			Total	Be F	
24	b	1	4	1 3	0





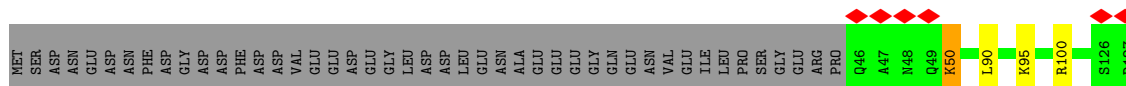


Chain E:  90% 10%




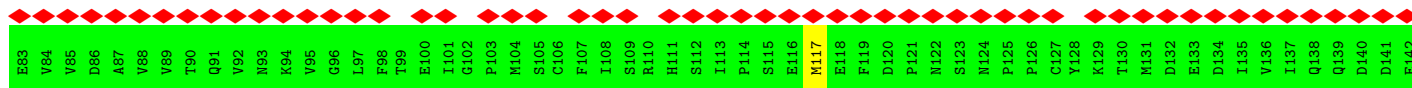
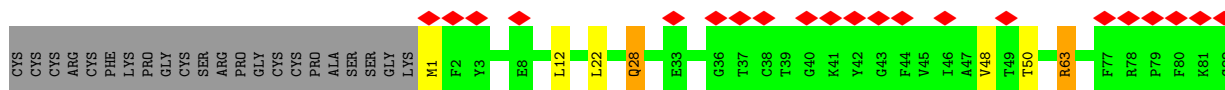
- Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F:  5% 61% 35%



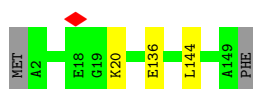
- Molecule 7: RPB7

Chain G:  41% 64% 33%




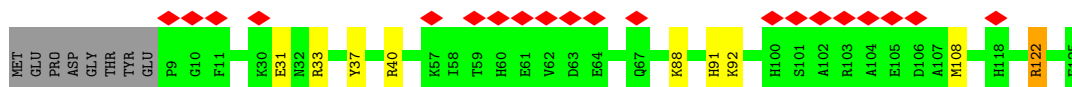
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  97%



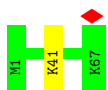
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  16% 86% 6% 6%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  99%



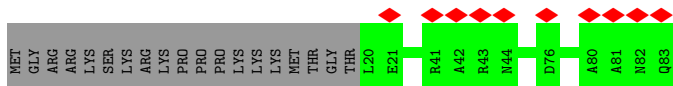
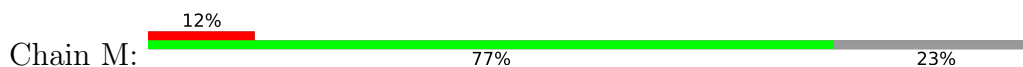
- Molecule 11: RNA\_pol\_L\_2 domain-containing protein



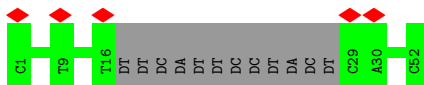
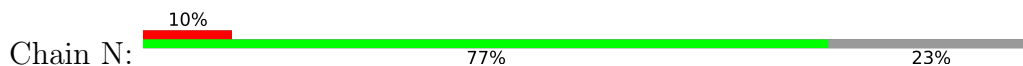
- Molecule 12: RNA polymerase II subunit K



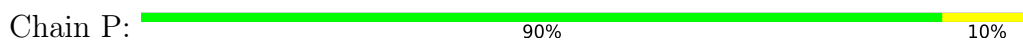
- Molecule 13: Transcription elongation factor 1 homolog



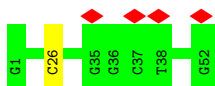
- Molecule 14: NTS



- Molecule 15: RNA



- Molecule 16: TS



- Molecule 17: DNA excision repair protein ERCC-8







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	544306	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	144	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.120	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00912	Depositor
Map size ( $\text{\AA}$ )	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.05, 1.05, 1.05	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: ADP, BEF, MG, ZN

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	0.57	21/11364 (0.2%)	1.08	127/15342 (0.8%)
2	B	0.59	17/9229 (0.2%)	0.90	70/12458 (0.6%)
3	C	0.60	4/2132 (0.2%)	0.99	19/2896 (0.7%)
4	D	0.62	0/1027	1.45	19/1384 (1.4%)
5	E	0.76	9/1751 (0.5%)	1.18	27/2366 (1.1%)
6	F	0.51	0/667	1.00	8/901 (0.9%)
7	G	0.57	1/1365 (0.1%)	1.26	18/1853 (1.0%)
8	H	0.48	1/1207 (0.1%)	0.81	6/1628 (0.4%)
9	I	0.63	3/972 (0.3%)	1.03	12/1316 (0.9%)
10	J	0.47	0/542	0.96	3/730 (0.4%)
11	K	0.61	2/939 (0.2%)	1.03	11/1271 (0.9%)
12	L	0.91	3/394 (0.8%)	1.54	14/524 (2.7%)
13	M	0.30	0/515	0.46	0/700
14	N	0.54	0/932	0.85	0/1435
15	P	0.80	0/247	0.92	0/384
16	T	0.65	0/1102	0.97	1/1682 (0.1%)
17	a	0.29	0/2908	0.56	1/3939 (0.0%)
18	b	0.28	0/4362	0.53	1/5890 (0.0%)
19	c	0.30	0/2034	0.56	0/2715
20	d	0.29	0/6268	0.54	0/8466
All	All	0.52	61/49957 (0.1%)	0.91	337/67880 (0.5%)

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	A	0	9
2	B	0	6
3	C	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
6	F	0	1
7	G	0	2
9	I	0	2
12	L	0	1
17	a	0	1
All	All	0	28

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	91	CYS	CB-SG	-9.71	1.65	1.82
1	A	771	VAL	CB-CG1	-8.80	1.34	1.52
2	B	301	VAL	CB-CG2	-8.74	1.34	1.52
5	E	39	GLU	CB-CG	-7.52	1.37	1.52
7	G	1	MET	CB-CG	-7.35	1.27	1.51
1	A	1341	VAL	CB-CG1	-7.25	1.37	1.52
2	B	1135	TYR	CE1-CZ	-7.17	1.29	1.38
2	B	357	CYS	CB-SG	-7.13	1.70	1.82
1	A	1014	LYS	CE-NZ	-6.75	1.32	1.49
1	A	114	CYS	CB-SG	-6.66	1.71	1.82
11	K	26	LYS	CD-CE	-6.63	1.34	1.51
2	B	572	CYS	CB-SG	-6.63	1.71	1.82
1	A	1478	GLU	CG-CD	-6.60	1.42	1.51
5	E	187	ARG	CB-CG	-6.43	1.35	1.52
12	L	35	ARG	CZ-NH1	-6.43	1.24	1.33
3	C	63	PHE	CE2-CZ	-6.29	1.25	1.37
1	A	968	VAL	CB-CG1	-6.23	1.39	1.52
5	E	90	TYR	CE1-CZ	-6.13	1.30	1.38
1	A	928	ARG	CB-CG	-6.03	1.36	1.52
2	B	814	TYR	CE2-CZ	-5.98	1.30	1.38
3	C	111	GLN	CG-CD	-5.85	1.37	1.51
1	A	404	GLU	CB-CG	-5.81	1.41	1.52
2	B	632	LYS	CE-NZ	-5.78	1.34	1.49
12	L	25	GLU	CG-CD	-5.75	1.43	1.51
9	I	37	TYR	CE1-CZ	-5.68	1.31	1.38
2	B	92	TYR	CE1-CZ	-5.68	1.31	1.38
2	B	814	TYR	CE1-CZ	-5.67	1.31	1.38
5	E	125	TYR	CE1-CZ	-5.67	1.31	1.38
2	B	814	TYR	CG-CD2	-5.65	1.31	1.39
2	B	1150	ARG	CZ-NH1	-5.65	1.25	1.33
1	A	227	ARG	CZ-NH1	-5.64	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1286	ARG	CG-CD	-5.63	1.37	1.51
1	A	110	VAL	CB-CG1	-5.63	1.41	1.52
8	H	20	LYS	CE-NZ	-5.62	1.34	1.49
2	B	92	TYR	CE2-CZ	-5.48	1.31	1.38
12	L	42	ARG	CZ-NH1	-5.47	1.25	1.33
1	A	255	VAL	CB-CG1	-5.47	1.41	1.52
2	B	92	TYR	CG-CD1	-5.42	1.32	1.39
2	B	57	ARG	CZ-NH1	-5.41	1.26	1.33
5	E	90	TYR	CE2-CZ	-5.38	1.31	1.38
5	E	125	TYR	CG-CD2	-5.37	1.32	1.39
2	B	549	SER	CB-OG	-5.37	1.35	1.42
1	A	1153	ARG	CZ-NH2	-5.37	1.26	1.33
9	I	37	TYR	CE2-CZ	-5.34	1.31	1.38
1	A	954	ARG	CZ-NH1	-5.30	1.26	1.33
2	B	589	LYS	CB-CG	-5.28	1.38	1.52
11	K	26	LYS	CG-CD	-5.27	1.34	1.52
1	A	1075	LYS	CE-NZ	-5.27	1.35	1.49
2	B	1135	TYR	CG-CD1	-5.26	1.32	1.39
5	E	90	TYR	CG-CD2	-5.24	1.32	1.39
1	A	70	ARG	CB-CG	-5.23	1.38	1.52
1	A	914	LYS	CE-NZ	-5.21	1.36	1.49
3	C	63	PHE	CG-CD1	-5.18	1.30	1.38
1	A	1286	ARG	CB-CG	-5.17	1.38	1.52
1	A	708	LYS	CE-NZ	-5.16	1.36	1.49
1	A	928	ARG	CZ-NH1	-5.11	1.26	1.33
5	E	186	LYS	CE-NZ	-5.05	1.36	1.49
2	B	1109	GLU	CG-CD	-5.03	1.44	1.51
3	C	254	LYS	CB-CG	-5.02	1.39	1.52
9	I	37	TYR	CG-CD1	-5.01	1.32	1.39
1	A	954	ARG	CB-CG	-5.01	1.39	1.52

All (337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1286	ARG	CG-CD-NE	23.32	160.77	111.80
4	D	41	LEU	CB-CG-CD1	22.83	149.81	111.00
1	A	958	ARG	CG-CD-NE	22.55	159.16	111.80
4	D	65	LEU	CB-CG-CD2	-19.11	78.51	111.00
1	A	266	MET	CA-CB-CG	18.51	144.77	113.30
4	D	41	LEU	CB-CG-CD2	-17.93	80.52	111.00
3	C	240	ARG	CG-CD-NE	17.63	148.82	111.80
7	G	28	GLN	CA-CB-CG	17.08	150.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	GLN	CA-CB-CG	16.87	150.52	113.40
1	A	105	LYS	CA-CB-CG	16.09	148.80	113.40
1	A	1031	ARG	CG-CD-NE	15.73	144.84	111.80
7	G	63	ARG	CG-CD-NE	14.88	143.05	111.80
1	A	70	ARG	CG-CD-NE	14.13	141.47	111.80
10	J	41	LYS	CA-CB-CG	14.07	144.36	113.40
7	G	117	MET	CB-CG-SD	13.94	154.22	112.40
2	B	169	ARG	CG-CD-NE	13.56	140.28	111.80
4	D	65	LEU	CB-CG-CD1	13.55	134.03	111.00
1	A	708	LYS	CB-CG-CD	13.04	145.50	111.60
11	K	26	LYS	CB-CG-CD	13.01	145.43	111.60
1	A	928	ARG	CG-CD-NE	-13.00	84.50	111.80
1	A	407	ARG	CG-CD-NE	12.74	138.55	111.80
1	A	1153	ARG	CG-CD-NE	12.56	138.19	111.80
4	D	88	LEU	CB-CG-CD1	-12.31	90.07	111.00
1	A	407	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	A	958	ARG	CA-CB-CG	12.22	140.28	113.40
3	C	111	GLN	CA-CB-CG	12.21	140.27	113.40
1	A	266	MET	CB-CG-SD	12.21	149.02	112.40
1	A	407	ARG	CA-CB-CG	12.15	140.14	113.40
1	A	105	LYS	CB-CG-CD	12.05	142.92	111.60
1	A	241	ARG	CA-CB-CG	11.99	139.78	113.40
5	E	101	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	A	938	LEU	CB-CG-CD1	11.90	131.23	111.00
1	A	1341	VAL	CG1-CB-CG2	-11.71	92.16	110.90
6	F	50	LYS	CA-CB-CG	11.64	139.02	113.40
3	C	225	LYS	CA-CB-CG	11.59	138.90	113.40
2	B	388	TYR	CB-CG-CD2	-11.58	114.05	121.00
8	H	144	LEU	CB-CG-CD1	11.57	130.68	111.00
1	A	1031	ARG	CB-CG-CD	11.57	141.67	111.60
4	D	92	LEU	CA-CB-CG	11.55	141.87	115.30
7	G	12	LEU	CB-CG-CD1	11.23	130.10	111.00
2	B	1138	ARG	CG-CD-NE	11.19	135.30	111.80
7	G	12	LEU	CA-CB-CG	11.10	140.83	115.30
1	A	938	LEU	CB-CG-CD2	-11.05	92.21	111.00
2	B	780	VAL	CG1-CB-CG2	-10.92	93.43	110.90
1	A	241	ARG	CG-CD-NE	10.79	134.47	111.80
1	A	108	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	255	VAL	CG1-CB-CG2	-10.65	93.85	110.90
7	G	12	LEU	CB-CG-CD2	-10.63	92.93	111.00
5	E	47	LYS	CD-CE-NZ	10.59	136.05	111.70
5	E	166	ARG	CB-CG-CD	10.42	138.70	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	48	VAL	CG1-CB-CG2	-10.42	94.23	110.90
7	G	28	GLN	N-CA-CB	10.38	129.28	110.60
12	L	37	ARG	CA-CB-CG	10.33	136.12	113.40
5	E	153	LYS	CD-CE-NZ	10.32	135.45	111.70
1	A	707	LYS	CG-CD-CE	10.30	142.79	111.90
1	A	958	ARG	N-CA-CB	10.26	129.07	110.60
5	E	103	LEU	CB-CG-CD2	-10.25	93.58	111.00
11	K	23	LYS	CA-CB-CG	10.25	135.94	113.40
10	J	41	LYS	CB-CG-CD	10.13	137.94	111.60
8	H	144	LEU	CB-CG-CD2	-10.06	93.89	111.00
1	A	914	LYS	CB-CG-CD	9.89	137.32	111.60
2	B	296	GLU	CA-CB-CG	9.62	134.55	113.40
1	A	407	ARG	CB-CG-CD	-9.58	86.69	111.60
5	E	101	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	A	743	ARG	CG-CD-NE	-9.46	91.93	111.80
2	B	57	ARG	NE-CZ-NH2	9.44	125.02	120.30
12	L	51	ARG	NE-CZ-NH1	9.41	125.00	120.30
3	C	240	ARG	CB-CG-CD	9.40	136.04	111.60
1	A	771	VAL	CG1-CB-CG2	-9.39	95.88	110.90
2	B	255	ARG	NE-CZ-NH2	9.32	124.96	120.30
2	B	917	LYS	CD-CE-NZ	9.28	133.04	111.70
5	E	132	GLN	CA-CB-CG	9.26	133.77	113.40
1	A	1260	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	A	914	LYS	CD-CE-NZ	9.14	132.73	111.70
1	A	1155	LYS	CD-CE-NZ	9.14	132.72	111.70
6	F	50	LYS	CB-CG-CD	9.09	135.24	111.60
11	K	26	LYS	CD-CE-NZ	-9.07	90.84	111.70
9	I	88	LYS	CB-CG-CD	8.99	134.98	111.60
1	A	112	PHE	CB-CG-CD2	-8.97	114.52	120.80
5	E	12	LYS	CA-CB-CG	8.95	133.10	113.40
5	E	103	LEU	CB-CG-CD1	8.90	126.13	111.00
2	B	95	LYS	CG-CD-CE	8.86	138.47	111.90
5	E	88	LYS	CA-CB-CG	8.80	132.76	113.40
1	A	1479	LYS	CA-CB-CG	8.79	132.73	113.40
2	B	1121	LEU	CB-CG-CD2	8.76	125.89	111.00
1	A	928	ARG	CB-CG-CD	8.67	134.15	111.60
2	B	393	LEU	CB-CG-CD2	8.67	125.73	111.00
4	D	41	LEU	CD1-CG-CD2	-8.66	84.52	110.50
9	I	40	ARG	CB-CG-CD	8.63	134.04	111.60
4	D	41	LEU	CA-CB-CG	-8.57	95.60	115.30
12	L	37	ARG	CG-CD-NE	-8.56	93.82	111.80
2	B	613	ARG	NE-CZ-NH2	8.54	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	MET	CG-SD-CE	8.49	113.78	100.20
1	A	382	ARG	NE-CZ-NH2	8.47	124.54	120.30
4	D	88	LEU	CB-CG-CD2	8.44	125.34	111.00
9	I	40	ARG	CG-CD-NE	-8.43	94.09	111.80
1	A	928	ARG	CA-CB-CG	8.42	131.92	113.40
1	A	708	LYS	CD-CE-NZ	8.41	131.05	111.70
2	B	109	MET	CB-CG-SD	8.38	137.53	112.40
1	A	707	LYS	CD-CE-NZ	-8.36	92.47	111.70
3	C	109	GLU	CA-CB-CG	8.35	131.77	113.40
3	C	228	ARG	CD-NE-CZ	8.29	135.21	123.60
1	A	108	ARG	NE-CZ-NH1	8.28	124.44	120.30
9	I	33	ARG	CB-CG-CD	8.26	133.08	111.60
2	B	53	MET	CA-CB-CG	8.25	127.33	113.30
1	A	1459	MET	CB-CG-SD	-8.21	87.76	112.40
6	F	90	LEU	CB-CG-CD1	8.18	124.90	111.00
2	B	159	THR	OG1-CB-CG2	-8.17	91.22	110.00
2	B	169	ARG	CB-CG-CD	8.17	132.83	111.60
1	A	116	LYS	CD-CE-NZ	-8.15	92.95	111.70
2	B	87	LYS	CG-CD-CE	8.11	136.22	111.90
7	G	28	GLN	CB-CA-C	-8.10	94.21	110.40
10	J	41	LYS	CB-CA-C	-8.09	94.22	110.40
1	A	1478	GLU	N-CA-CB	-8.08	96.05	110.60
2	B	393	LEU	CB-CG-CD1	8.01	124.62	111.00
2	B	632	LYS	CD-CE-NZ	8.01	130.12	111.70
1	A	751	LYS	CD-CE-NZ	8.00	130.10	111.70
2	B	173	GLU	CA-CB-CG	8.00	130.99	113.40
5	E	101	ARG	CD-NE-CZ	7.98	134.78	123.60
2	B	24	GLU	CA-CB-CG	7.97	130.93	113.40
1	A	938	LEU	CD1-CG-CD2	-7.95	86.64	110.50
7	G	1	MET	CG-SD-CE	-7.85	87.64	100.20
1	A	266	MET	CB-CA-C	7.82	126.04	110.40
1	A	573	LYS	CD-CE-NZ	-7.82	93.71	111.70
1	A	914	LYS	CA-CB-CG	7.82	130.60	113.40
1	A	1460	LEU	CB-CG-CD2	7.78	124.22	111.00
6	F	95	LYS	CD-CE-NZ	7.77	129.57	111.70
2	B	578	LYS	CD-CE-NZ	7.75	129.54	111.70
2	B	770	ARG	NE-CZ-NH2	7.74	124.17	120.30
4	D	44	ARG	CB-CG-CD	7.74	131.71	111.60
1	A	397	PHE	CB-CG-CD1	-7.72	115.39	120.80
1	A	1085	GLU	CA-CB-CG	7.60	130.12	113.40
7	G	63	ARG	CB-CG-CD	7.58	131.30	111.60
1	A	1102	MET	CG-SD-CE	7.58	112.32	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	92	LEU	CB-CG-CD1	7.53	123.79	111.00
1	A	241	ARG	CB-CG-CD	-7.51	92.07	111.60
1	A	1155	LYS	CA-CB-CG	7.43	129.76	113.40
1	A	583	ARG	CB-CG-CD	7.42	130.90	111.60
1	A	1478	GLU	CB-CA-C	7.41	125.22	110.40
1	A	407	ARG	CD-NE-CZ	7.39	133.95	123.60
1	A	1478	GLU	CA-CB-CG	7.38	129.65	113.40
11	K	17	LYS	CD-CE-NZ	7.38	128.66	111.70
2	B	1163	MET	CA-CB-CG	7.36	125.81	113.30
2	B	109	MET	CG-SD-CE	7.30	111.88	100.20
2	B	301	VAL	CA-CB-CG2	7.29	121.83	110.90
1	A	108	ARG	CD-NE-CZ	7.28	133.78	123.60
12	L	37	ARG	NE-CZ-NH1	-7.27	116.66	120.30
2	B	770	ARG	CG-CD-NE	7.26	127.05	111.80
5	E	10	LEU	CB-CG-CD1	-7.25	98.68	111.00
1	A	266	MET	N-CA-CB	-7.24	97.57	110.60
2	B	995	GLU	CA-CB-CG	7.21	129.26	113.40
1	A	697	LYS	CD-CE-NZ	7.18	128.22	111.70
9	I	108	MET	CG-SD-CE	7.16	111.66	100.20
1	A	711	GLN	N-CA-CB	-7.14	97.74	110.60
7	G	63	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	B	301	VAL	CB-CA-C	-7.13	97.85	111.40
7	G	12	LEU	CD1-CG-CD2	-7.13	89.12	110.50
1	A	1054	MET	CG-SD-CE	7.11	111.57	100.20
4	D	20	LEU	CB-CG-CD2	-7.08	98.97	111.00
11	K	17	LYS	CG-CD-CE	7.06	133.08	111.90
12	L	37	ARG	CB-CG-CD	7.01	129.83	111.60
2	B	380	ARG	CB-CG-CD	7.00	129.81	111.60
1	A	1059	ARG	CB-CG-CD	7.00	129.81	111.60
2	B	95	LYS	CD-CE-NZ	6.99	127.77	111.70
3	C	111	GLN	CB-CA-C	6.94	124.28	110.40
12	L	51	ARG	CG-CD-NE	6.90	126.29	111.80
1	A	110	VAL	CA-CB-CG2	6.90	121.25	110.90
12	L	42	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	A	266	MET	CG-SD-CE	-6.88	89.19	100.20
5	E	12	LYS	N-CA-CB	6.83	122.90	110.60
2	B	255	ARG	CG-CD-NE	6.80	126.08	111.80
2	B	95	LYS	CB-CG-CD	-6.79	93.94	111.60
1	A	382	ARG	NE-CZ-NH1	-6.79	116.91	120.30
5	E	5	GLU	CA-CB-CG	6.77	128.30	113.40
1	A	1199	MET	CB-CG-SD	6.77	132.71	112.40
3	C	111	GLN	N-CA-CB	-6.76	98.44	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	548	TRP	N-CA-C	-6.75	92.76	111.00
1	A	743	ARG	CB-CA-C	6.75	123.89	110.40
2	B	1010	LYS	CG-CD-CE	6.73	132.09	111.90
3	C	268	GLN	CA-CB-CG	6.69	128.12	113.40
1	A	1405	MET	N-CA-CB	-6.68	98.58	110.60
1	A	573	LYS	CG-CD-CE	6.62	131.76	111.90
1	A	711	GLN	CB-CA-C	6.60	123.60	110.40
1	A	1286	ARG	CD-NE-CZ	-6.57	114.40	123.60
5	E	96	GLU	CA-CB-CG	6.56	127.82	113.40
2	B	815	LYS	CD-CE-NZ	6.54	126.75	111.70
1	A	619	LYS	CD-CE-NZ	6.52	126.69	111.70
1	A	743	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	301	VAL	CA-CB-CG1	6.50	120.65	110.90
1	A	1212	LEU	CB-CG-CD1	6.47	121.99	111.00
5	E	88	LYS	CD-CE-NZ	6.44	126.51	111.70
2	B	548	TRP	CB-CG-CD2	-6.43	118.23	126.60
2	B	357	CYS	CA-CB-SG	6.41	125.55	114.00
8	H	20	LYS	CD-CE-NZ	6.41	126.45	111.70
3	C	254	LYS	CB-CG-CD	6.41	128.26	111.60
3	C	240	ARG	CD-NE-CZ	-6.40	114.64	123.60
1	A	743	ARG	CD-NE-CZ	6.40	132.55	123.60
5	E	85	LYS	CA-CB-CG	6.38	127.44	113.40
1	A	430	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	430	ARG	CB-CG-CD	-6.36	95.06	111.60
2	B	555	GLU	CA-CB-CG	6.34	127.35	113.40
1	A	762	GLU	CA-CB-CG	6.33	127.33	113.40
2	B	1091	ARG	NE-CZ-NH2	-6.31	117.14	120.30
6	F	100	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	743	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	B	200	MET	CA-CB-CG	6.23	123.89	113.30
9	I	40	ARG	CA-CB-CG	6.22	127.08	113.40
1	A	1075	LYS	CD-CE-NZ	6.18	125.92	111.70
4	D	44	ARG	NE-CZ-NH1	-6.17	117.21	120.30
9	I	88	LYS	CA-CB-CG	6.17	126.97	113.40
12	L	51	ARG	NH1-CZ-NH2	-6.16	112.62	119.40
1	A	1459	MET	CA-CB-CG	6.15	123.75	113.30
3	C	228	ARG	CG-CD-NE	6.15	124.71	111.80
1	A	19	LYS	CG-CD-CE	6.14	130.33	111.90
2	B	613	ARG	CG-CD-NE	6.14	124.70	111.80
11	K	110	LYS	CG-CD-CE	6.10	130.20	111.90
2	B	520	VAL	CA-CB-CG1	6.09	120.04	110.90
11	K	114	GLU	CA-CB-CG	6.09	126.80	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	VAL	CA-CB-CG1	6.08	120.02	110.90
6	F	100	ARG	CG-CD-NE	6.05	124.50	111.80
4	D	88	LEU	CA-CB-CG	6.04	129.20	115.30
2	B	380	ARG	CG-CD-NE	6.03	124.47	111.80
1	A	1376	LYS	CG-CD-CE	6.02	129.96	111.90
5	E	103	LEU	CD1-CG-CD2	-6.02	92.44	110.50
5	E	101	ARG	CG-CD-NE	6.01	124.43	111.80
12	L	29	LYS	CB-CG-CD	5.99	127.16	111.60
1	A	1376	LYS	CD-CE-NZ	5.98	125.46	111.70
5	E	186	LYS	CD-CE-NZ	5.98	125.46	111.70
1	A	1102	MET	CB-CG-SD	5.97	130.30	112.40
9	I	31	GLU	CA-CB-CG	5.97	126.53	113.40
9	I	92	LYS	CA-CB-CG	5.92	126.43	113.40
1	A	105	LYS	CD-CE-NZ	-5.92	98.08	111.70
2	B	548	TRP	CB-CG-CD1	5.92	134.70	127.00
1	A	1279	MET	CG-SD-CE	5.91	109.66	100.20
5	E	39	GLU	N-CA-CB	5.89	121.20	110.60
1	A	899	GLU	CA-CB-CG	5.89	126.35	113.40
2	B	173	GLU	CB-CA-C	5.88	122.16	110.40
9	I	122	ARG	CG-CD-NE	5.88	124.14	111.80
5	E	101	ARG	CB-CG-CD	5.87	126.87	111.60
2	B	296	GLU	N-CA-CB	-5.87	100.03	110.60
1	A	1329	LYS	CD-CE-NZ	5.87	125.19	111.70
2	B	840	MET	CB-CG-SD	5.87	130.00	112.40
3	C	228	ARG	NE-CZ-NH1	-5.87	117.37	120.30
2	B	1150	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	818	GLU	CA-CB-CG	5.83	126.24	113.40
1	A	241	ARG	N-CA-CB	5.83	121.09	110.60
16	T	26	DC	O4'-C4'-C3'	-5.81	102.18	104.50
7	G	117	MET	CG-SD-CE	5.81	109.50	100.20
5	E	39	GLU	CA-CB-CG	5.80	126.16	113.40
1	A	573	LYS	CB-CG-CD	5.79	126.66	111.60
1	A	1260	ARG	CA-CB-CG	5.79	126.14	113.40
1	A	1479	LYS	CD-CE-NZ	-5.79	98.39	111.70
7	G	22	LEU	CA-CB-CG	5.79	128.61	115.30
9	I	122	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	105	LYS	N-CA-CB	-5.77	100.21	110.60
1	A	1054	MET	CB-CG-SD	5.76	129.67	112.40
2	B	255	ARG	NH1-CZ-NH2	-5.76	113.07	119.40
9	I	33	ARG	CA-CB-CG	-5.75	100.75	113.40
1	A	700	GLN	CA-CB-CG	5.74	126.03	113.40
1	A	856	GLU	CA-CB-CG	5.74	126.02	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	29	LYS	CD-CE-NZ	-5.73	98.53	111.70
1	A	407	ARG	CB-CA-C	-5.72	98.97	110.40
1	A	1160	ARG	NE-CZ-NH1	-5.71	117.44	120.30
2	B	266	GLU	CA-CB-CG	5.71	125.97	113.40
4	D	65	LEU	CD1-CG-CD2	-5.71	93.38	110.50
2	B	403	LEU	CB-CG-CD2	-5.68	101.35	111.00
1	A	226	LYS	CG-CD-CE	5.67	128.93	111.90
12	L	35	ARG	NE-CZ-NH1	-5.67	117.46	120.30
8	H	144	LEU	CD1-CG-CD2	-5.67	93.51	110.50
11	K	110	LYS	CD-CE-NZ	5.64	124.67	111.70
2	B	385	ARG	NE-CZ-NH1	-5.62	117.49	120.30
2	B	613	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
2	B	325	GLY	N-CA-C	5.58	127.05	113.10
1	A	1153	ARG	CB-CG-CD	-5.55	97.16	111.60
4	D	92	LEU	CB-CG-CD2	-5.55	101.57	111.00
2	B	1010	LYS	CD-CE-NZ	-5.54	98.95	111.70
17	a	121	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	968	VAL	CA-CB-CG2	5.54	119.20	110.90
7	G	63	ARG	CD-NE-CZ	5.53	131.34	123.60
1	A	227	ARG	NE-CZ-NH2	5.53	123.06	120.30
2	B	917	LYS	CG-CD-CE	5.50	128.39	111.90
1	A	248	MET	CG-SD-CE	5.49	108.99	100.20
3	C	253	LYS	C-N-CA	-5.49	107.98	121.70
1	A	914	LYS	CG-CD-CE	-5.48	95.47	111.90
1	A	1090	LEU	CB-CG-CD2	5.47	120.30	111.00
1	A	954	ARG	CG-CD-NE	-5.46	100.34	111.80
3	C	111	GLN	CB-CG-CD	5.45	125.77	111.60
5	E	181	ARG	NE-CZ-NH1	5.43	123.02	120.30
4	D	47	GLN	CA-CB-CG	5.42	125.33	113.40
4	D	20	LEU	CD1-CG-CD2	-5.42	94.23	110.50
3	C	254	LYS	CA-CB-CG	-5.42	101.48	113.40
11	K	23	LYS	CD-CE-NZ	-5.42	99.23	111.70
11	K	110	LYS	CB-CG-CD	-5.41	97.53	111.60
4	D	44	ARG	CA-CB-CG	5.38	125.23	113.40
2	B	173	GLU	N-CA-CB	-5.36	100.95	110.60
2	B	1121	LEU	CB-CG-CD1	5.35	120.10	111.00
1	A	226	LYS	CB-CG-CD	5.35	125.51	111.60
1	A	1303	GLN	CA-CB-CG	5.34	125.16	113.40
3	C	108	ASN	CB-CA-C	-5.33	99.74	110.40
12	L	15	MET	CG-SD-CE	5.33	108.73	100.20
7	G	50	THR	CA-CB-CG2	5.32	119.84	112.40
12	L	35	ARG	CD-NE-CZ	5.31	131.04	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	379	ARG	NE-CZ-NH1	5.31	122.95	120.30
6	F	100	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	116	LYS	CB-CG-CD	5.28	125.32	111.60
8	H	136	GLU	N-CA-CB	5.25	120.06	110.60
2	B	520	VAL	CG1-CB-CG2	5.25	119.30	110.90
7	G	1	MET	CB-CA-C	-5.24	99.93	110.40
1	A	580	LEU	CB-CG-CD1	5.23	119.89	111.00
1	A	241	ARG	CB-CA-C	-5.21	99.97	110.40
1	A	1260	ARG	NH1-CZ-NH2	-5.21	113.66	119.40
5	E	12	LYS	CG-CD-CE	5.21	127.54	111.90
12	L	29	LYS	CG-CD-CE	5.21	127.53	111.90
2	B	908	MET	CG-SD-CE	5.21	108.53	100.20
1	A	1262	MET	CG-SD-CE	5.18	108.49	100.20
5	E	12	LYS	CB-CA-C	-5.17	100.05	110.40
1	A	231	GLU	CA-CB-CG	5.16	124.75	113.40
8	H	144	LEU	CA-CB-CG	-5.16	103.44	115.30
3	C	109	GLU	N-CA-CB	5.15	119.88	110.60
1	A	112	PHE	CB-CG-CD1	5.15	124.41	120.80
11	K	26	LYS	CA-CB-CG	5.15	124.73	113.40
3	C	67	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	1286	ARG	CB-CG-CD	5.14	124.97	111.60
1	A	743	ARG	CA-CB-CG	5.13	124.70	113.40
2	B	1145	GLN	CA-CB-CG	5.13	124.68	113.40
1	A	719	LYS	CB-CG-CD	-5.11	98.31	111.60
1	A	1260	ARG	CG-CD-NE	5.10	122.50	111.80
1	A	1059	ARG	CG-CD-NE	5.09	122.48	111.80
2	B	358	GLU	CA-CB-CG	5.07	124.56	113.40
2	B	610	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	A	707	LYS	CB-CA-C	5.07	120.53	110.40
6	F	50	LYS	CD-CE-NZ	5.06	123.34	111.70
2	B	380	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	B	780	VAL	CA-CB-CG2	-5.04	103.33	110.90
2	B	995	GLU	CB-CA-C	-5.03	100.35	110.40
5	E	158	GLU	CA-CB-CG	5.02	124.44	113.40
18	b	634	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PHE	Sidechain
1	A	1478	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	397	PHE	Sidechain
1	A	407	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	538	VAL	Peptide
1	A	707	LYS	Peptide
1	A	711	GLN	Sidechain
1	A	935	GLN	Peptide
2	B	1135	TYR	Sidechain
2	B	1138	ARG	Sidechain
2	B	169	ARG	Sidechain
2	B	388	TYR	Sidechain
2	B	547	GLU	Peptide
2	B	995	GLU	Peptide
3	C	110	ASP	Peptide
3	C	111	GLN	Sidechain,Peptide
3	C	228	ARG	Sidechain
3	C	253	LYS	Peptide
5	E	131	LEU	Peptide
6	F	50	LYS	Peptide
7	G	28	GLN	Sidechain
7	G	63	ARG	Sidechain
9	I	122	ARG	Sidechain
9	I	91	HIS	Peptide
12	L	37	ARG	Peptide
17	a	174	LYS	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	A	1399/1970 (71%)	1348 (96%)	51 (4%)	0	100	100
2	B	1122/1167 (96%)	1072 (96%)	50 (4%)	0	100	100
3	C	256/275 (93%)	248 (97%)	8 (3%)	0	100	100
4	D	126/142 (89%)	117 (93%)	9 (7%)	0	100	100
5	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/254 (66%)	159 (94%)	10 (6%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	115/125 (92%)	106 (92%)	9 (8%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	M	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
17	a	363/396 (92%)	343 (94%)	20 (6%)	0	100	100
18	b	512/1493 (34%)	486 (95%)	26 (5%)	0	100	100
19	c	258/709 (36%)	247 (96%)	11 (4%)	0	100	100
20	d	765/1140 (67%)	730 (95%)	35 (5%)	0	100	100
All	All	5802/8483 (68%)	5542 (96%)	260 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1241/1749 (71%)	1239 (100%)	2 (0%)	93	98
2	B	992/1021 (97%)	988 (100%)	4 (0%)	91	97
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	108/126 (86%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/217 (68%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	103 (99%)	1 (1%)	76	90
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	59/76 (78%)	59 (100%)	0	100	100
17	a	320/348 (92%)	320 (100%)	0	100	100
18	b	466/1297 (36%)	465 (100%)	1 (0%)	93	98
19	c	196/608 (32%)	194 (99%)	2 (1%)	76	90
20	d	685/999 (69%)	684 (100%)	1 (0%)	93	98
All	All	5150/7456 (69%)	5139 (100%)	11 (0%)	93	98

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	ARG
1	A	1059	ARG
2	B	331	THR
2	B	393	LEU
2	B	1072	ARG
2	B	1080	ARG
11	K	47	LYS
18	b	670	ARG
19	c	41	ARG
19	c	71	ARG
20	d	938	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	350	HIS
17	a	33	ASN
18	b	1397	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	10	A

There are no RNA pucker outliers to report.

### 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 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\# Z  > 2$
23	ADP	b	1501	22	24,29,29	0.93	1 (4%)	29,45,45	1.38	4 (13%)
24	BEF	b	1502	-	0,3,3	-	-	-	-	-

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
23	ADP	b	1501	22	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	1501	ADP	C5-C4	2.28	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	1501	ADP	N3-C2-N1	-3.73	122.84	128.68
23	b	1501	ADP	PA-O3A-PB	-2.93	122.78	132.83
23	b	1501	ADP	C4-C5-N7	-2.47	106.82	109.40
23	b	1501	ADP	C3'-C2'-C1'	2.35	104.51	100.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

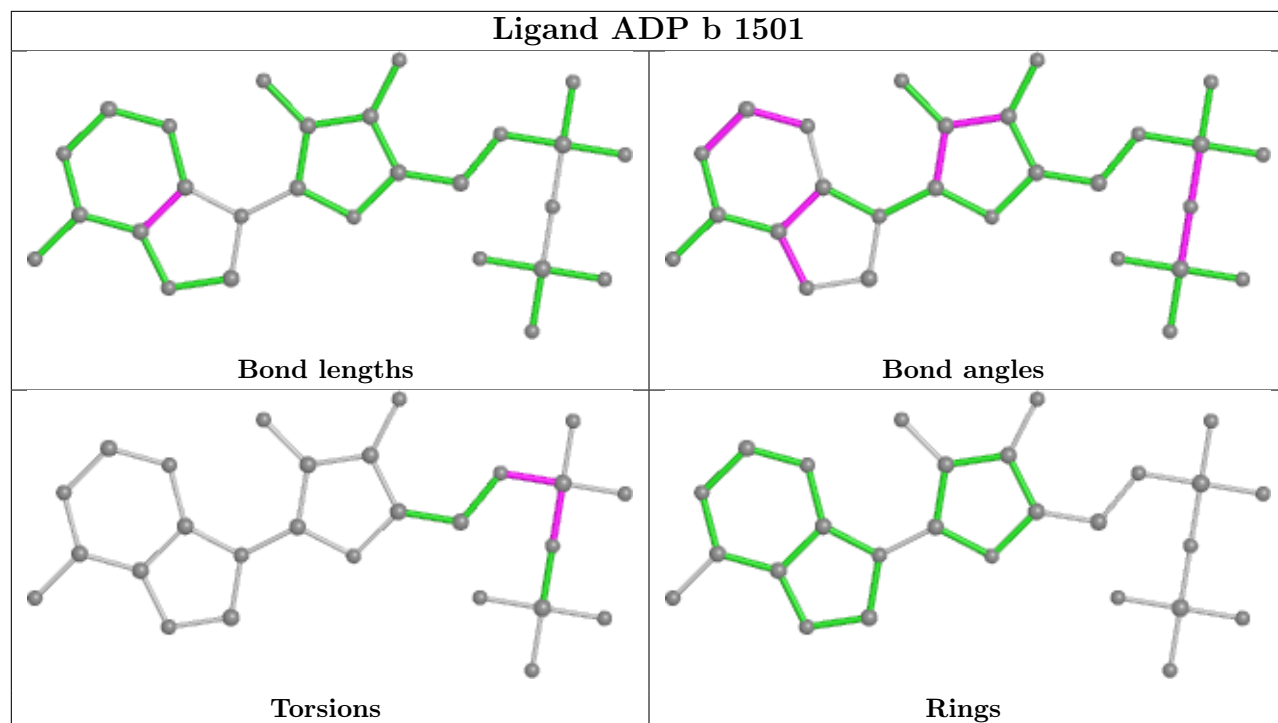
Mol	Chain	Res	Type	Atoms
23	b	1501	ADP	PB-O3A-PA-O2A
23	b	1501	ADP	PB-O3A-PA-O1A
23	b	1501	ADP	C5'-O5'-PA-O1A

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.

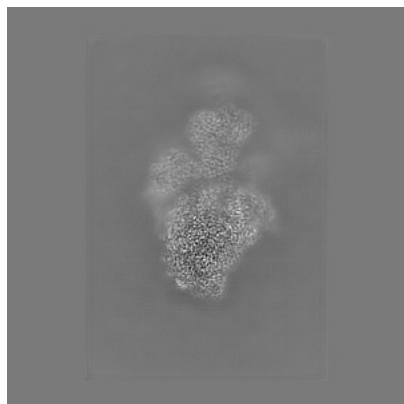
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15825. These allow visual inspection of the internal detail of the map and identification of artifacts.

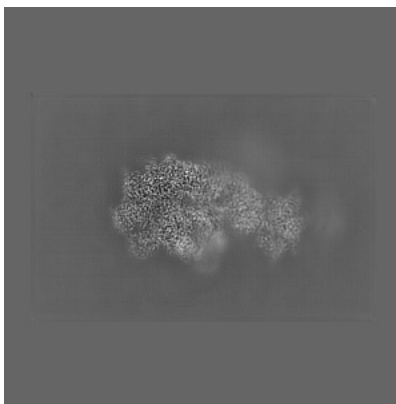
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

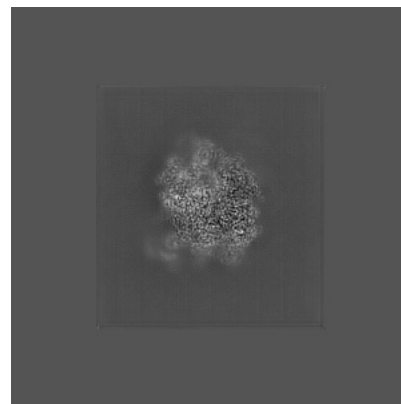
#### 6.1.1 Primary map



X

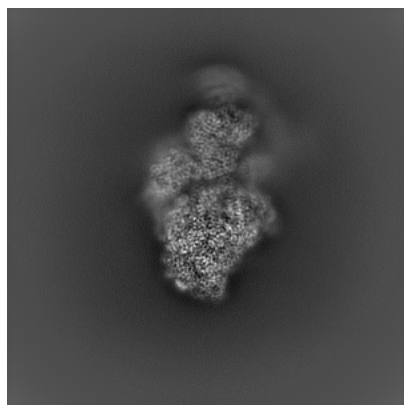


Y

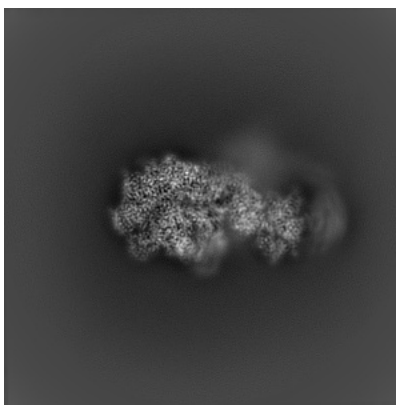


Z

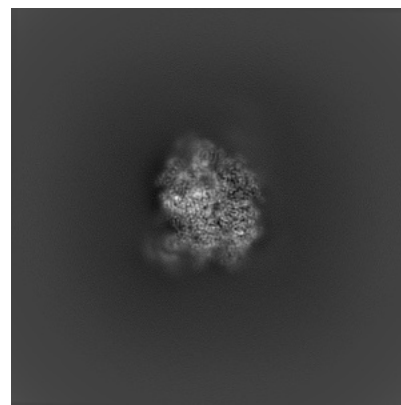
#### 6.1.2 Raw map



X



Y

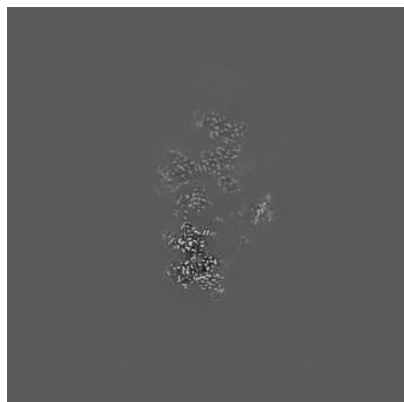


Z

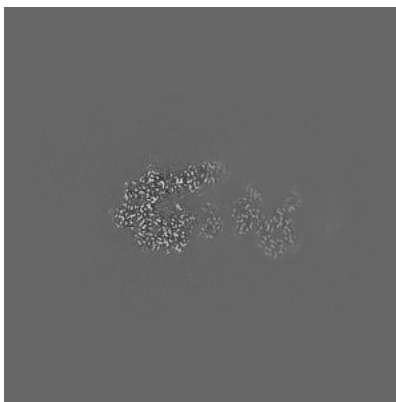
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

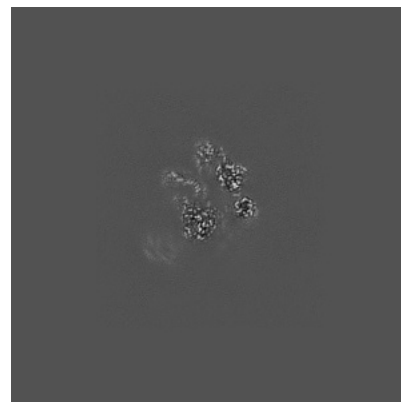
### 6.2.1 Primary map



X Index: 210

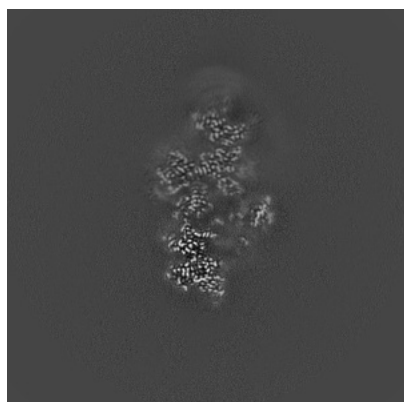


Y Index: 210

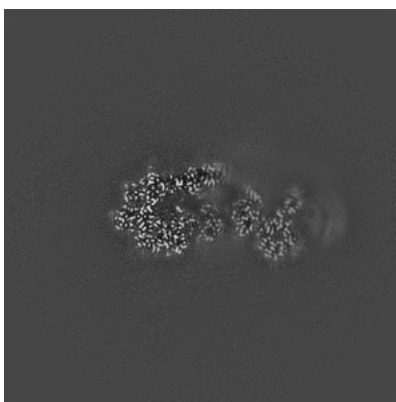


Z Index: 210

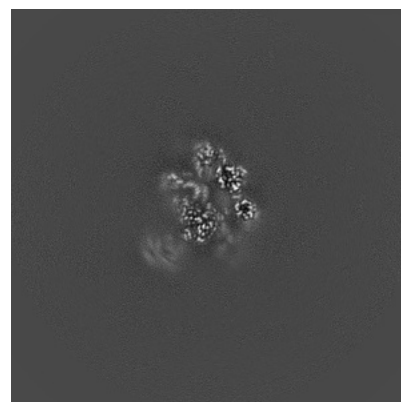
### 6.2.2 Raw map



X Index: 210



Y Index: 210

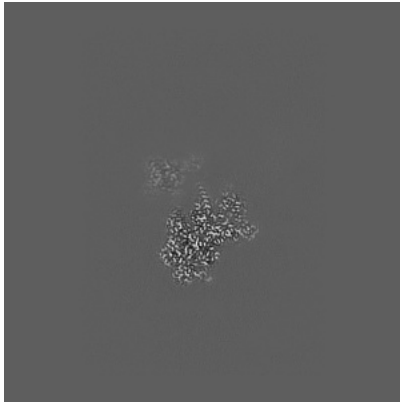


Z Index: 210

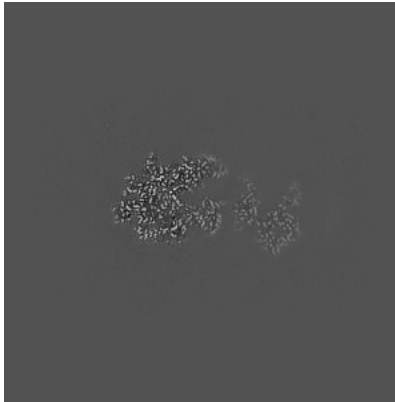
The images above show central slices of the map in three orthogonal directions.

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

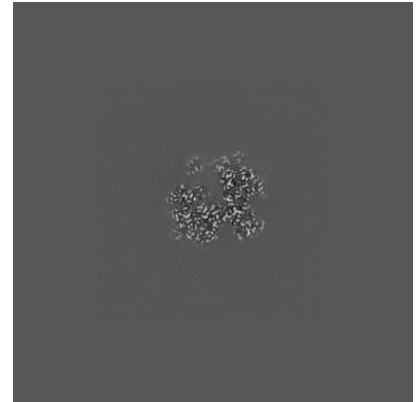
### 6.3.1 Primary map



X Index: 236

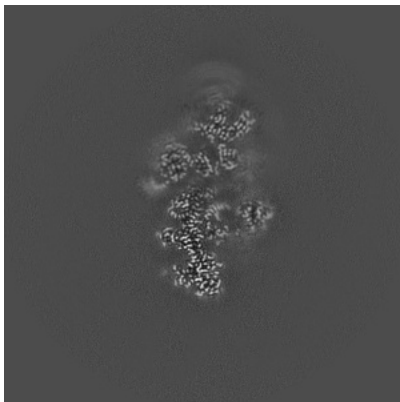


Y Index: 206

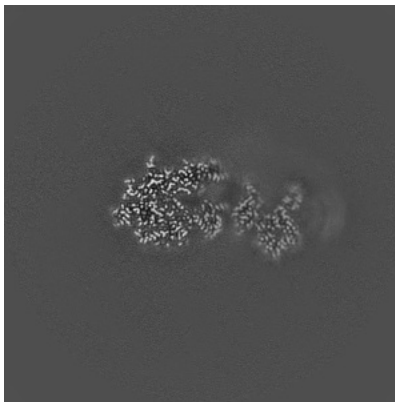


Z Index: 173

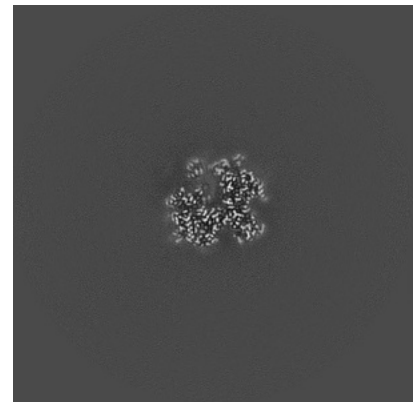
### 6.3.2 Raw map



X Index: 202



Y Index: 207

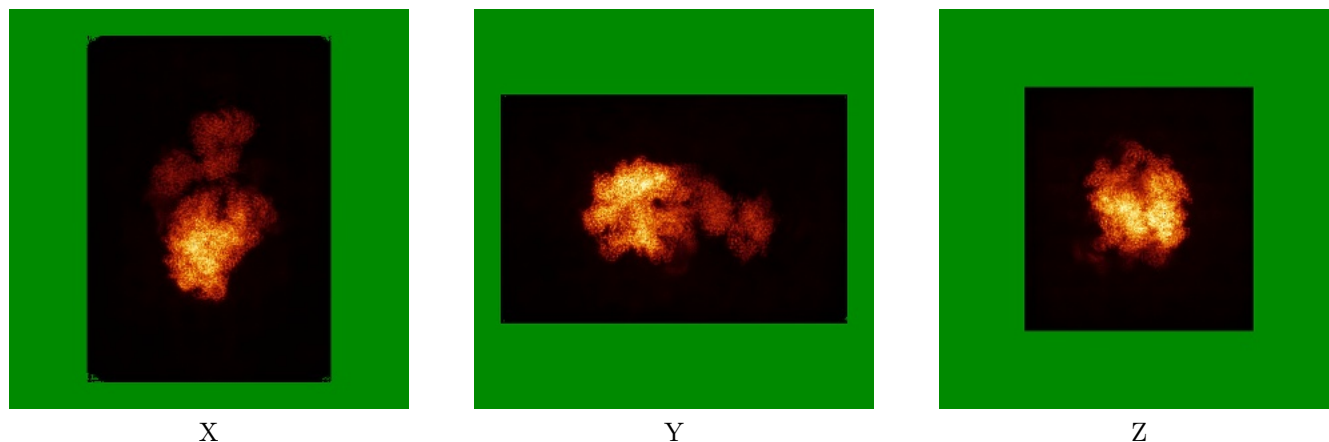


Z Index: 173

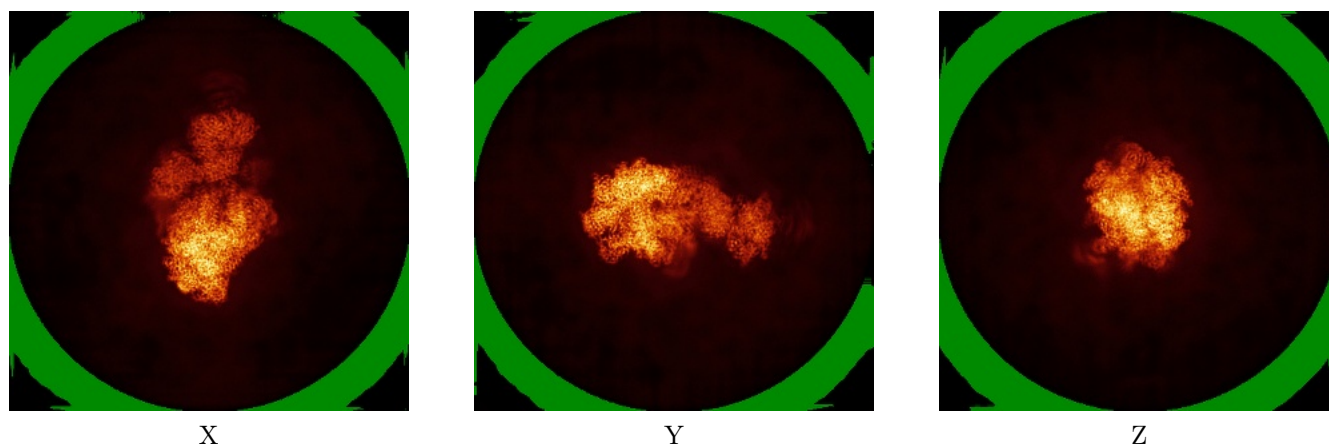
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



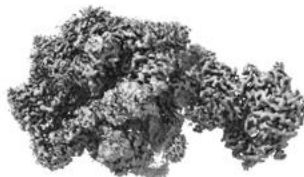
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

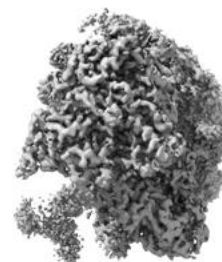
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00912. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

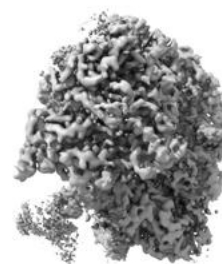
### 6.5.2 Raw map



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.

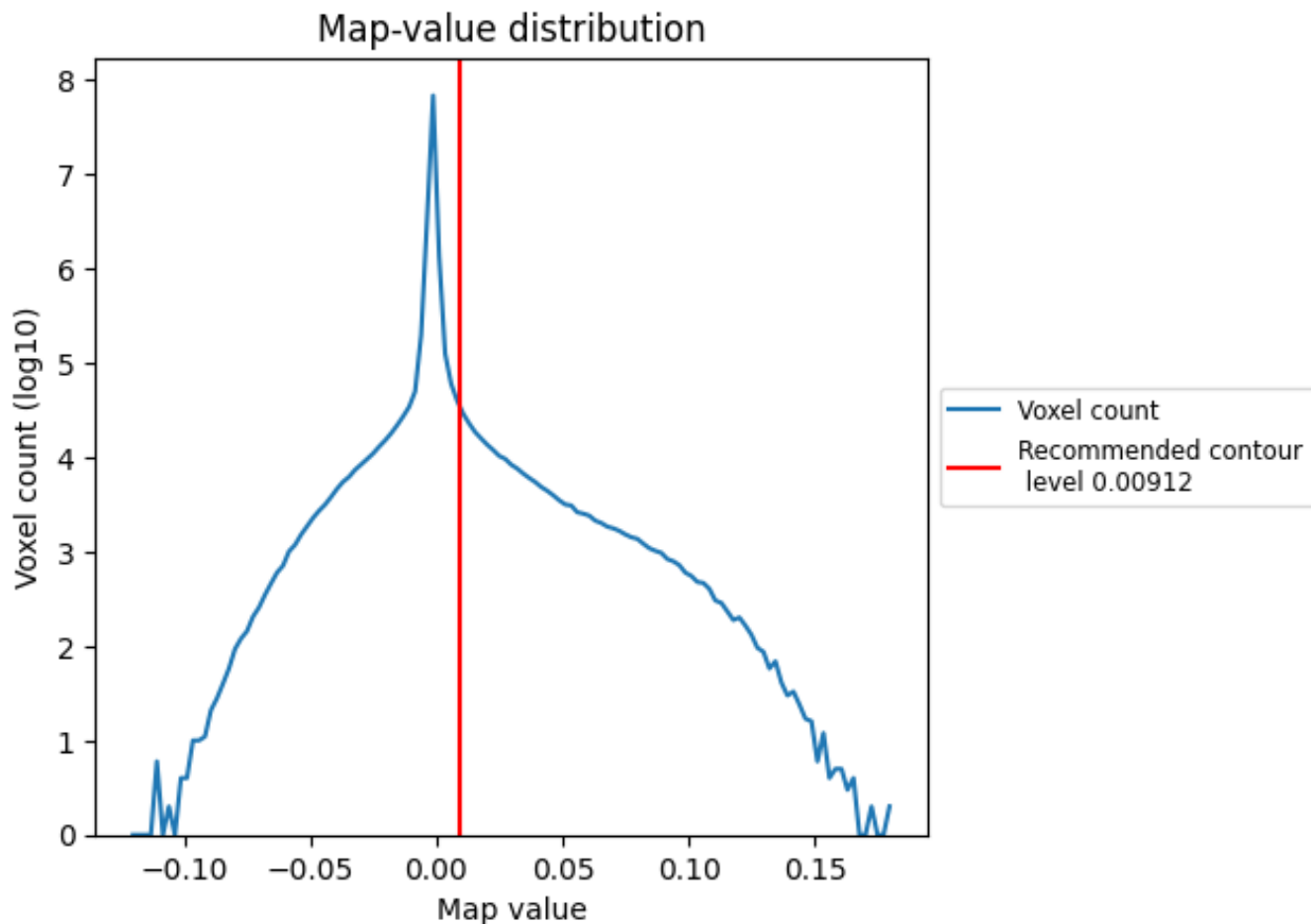
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

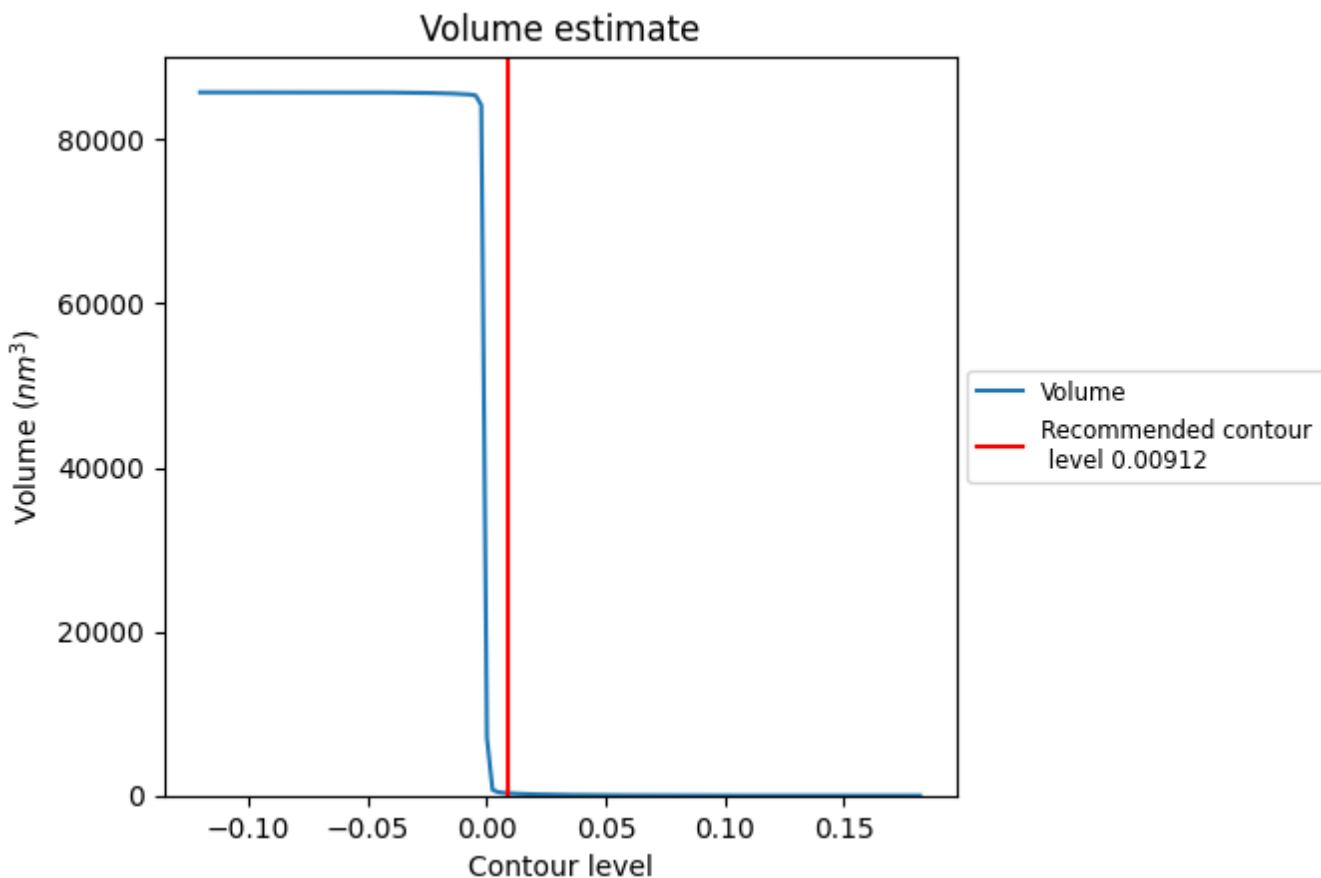
This section contains the results of statistical analysis of the map.

### 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](#)

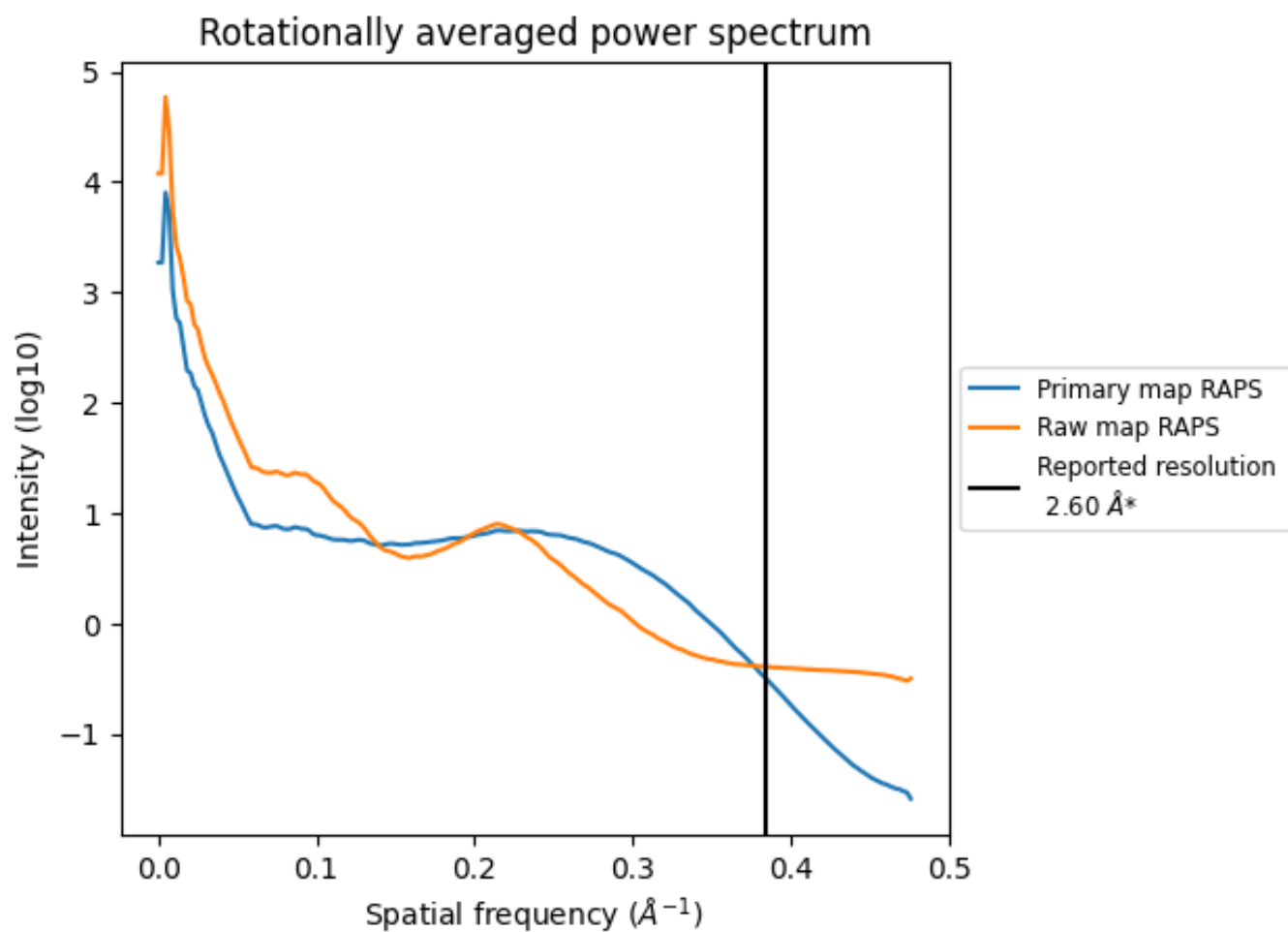


The volume at the recommended contour level is 287 nm<sup>3</sup>; this corresponds to an approximate mass of 259 kDa.

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

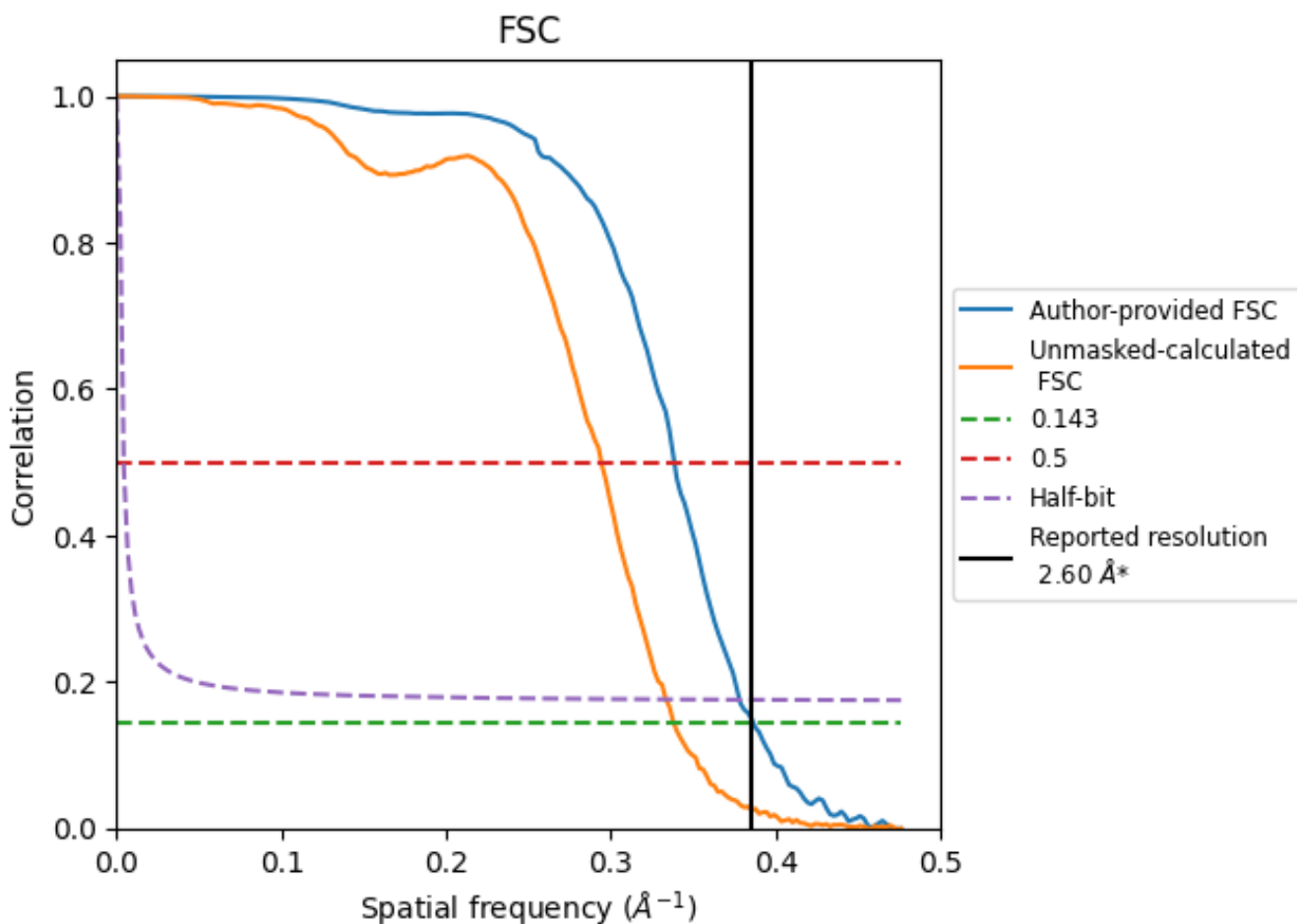


\*Reported resolution corresponds to spatial frequency of  $0.385 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

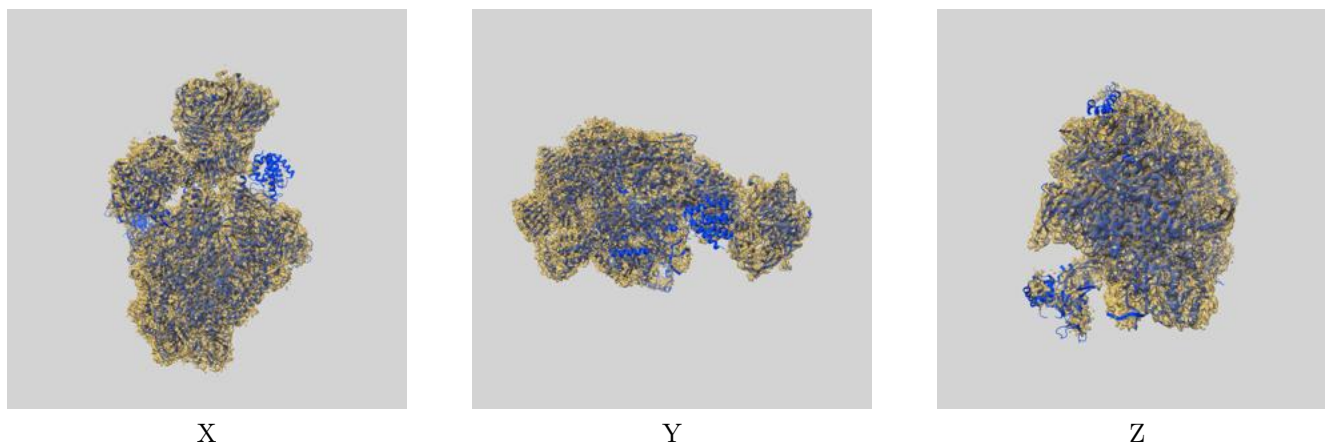
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.95	2.64
Unmasked-calculated*	2.96	3.40	3.00

\*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 2.96 differs from the reported value 2.6 by more than 10 %

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

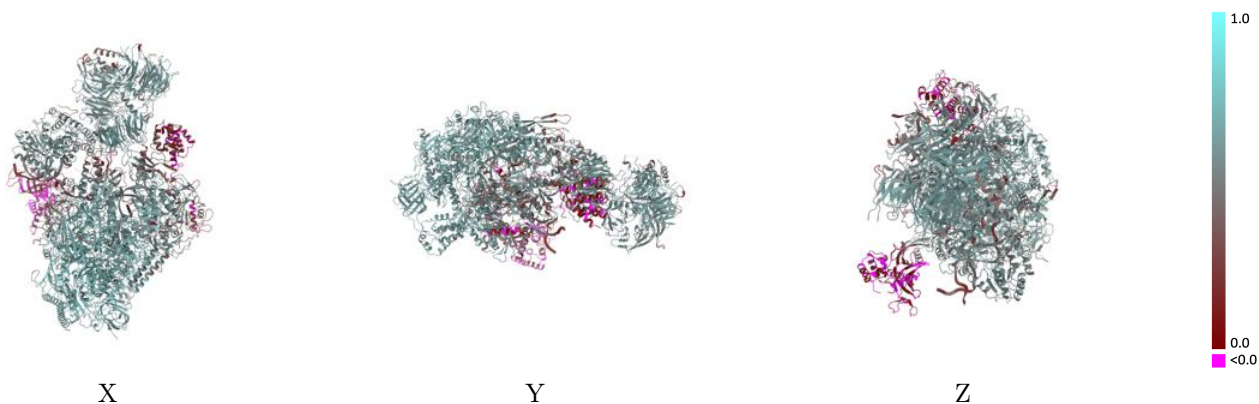
This section contains information regarding the fit between EMDB map EMD-15825 and PDB model 8B3D. Per-residue inclusion information can be found in section 3 on page 9.

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



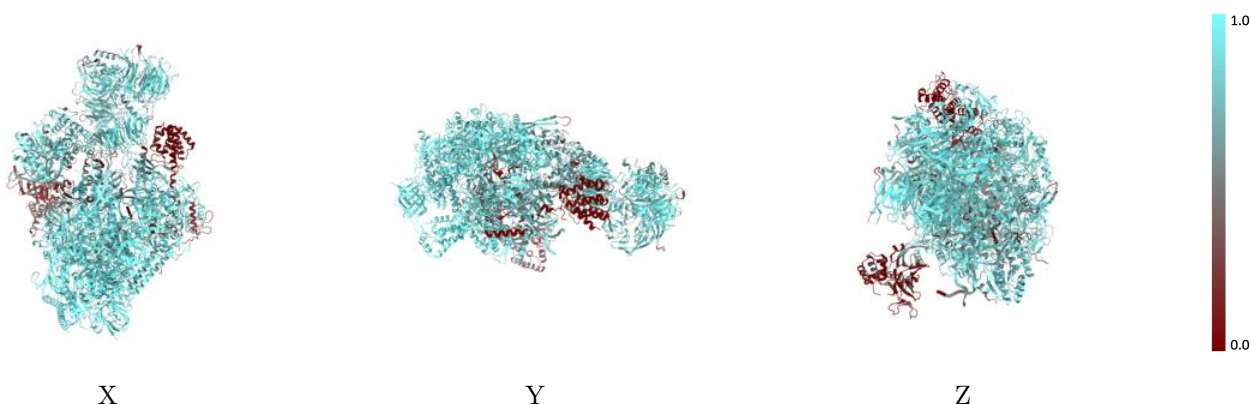
The images above show the 3D surface view of the map at the recommended contour level 0.00912 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



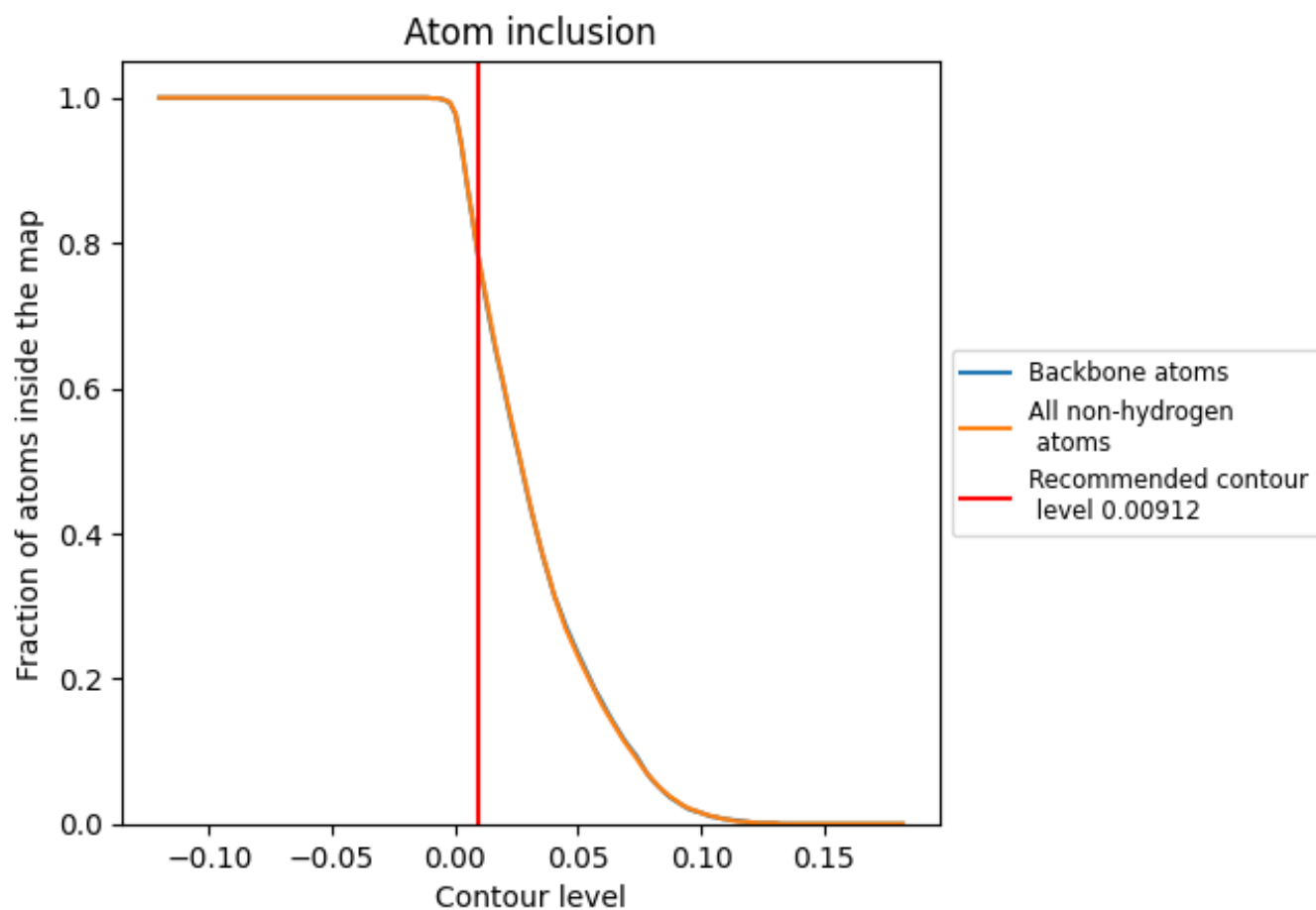
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00912).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.00912) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.5320
A	 0.8690	 0.5780
B	 0.8870	 0.5940
C	 0.9310	 0.6250
D	 0.1550	 0.0350
E	 0.8810	 0.5270
F	 0.8920	 0.6000
G	 0.3650	 0.1960
H	 0.9350	 0.6150
I	 0.7550	 0.4910
J	 0.9410	 0.6430
K	 0.9320	 0.6250
L	 0.8390	 0.5290
M	 0.6490	 0.4530
N	 0.6920	 0.4340
P	 0.9550	 0.6520
T	 0.8170	 0.4740
a	 0.8470	 0.5770
b	 0.7660	 0.5240
c	 0.1030	 0.2010
d	 0.8110	 0.5550

