Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 08:37 PM EST

PDB ID	:	7KW7
EMDB ID	:	EMD-23050
Title	:	Atomic cryoEM structure of Hsp90-Hsp70-Hop-GR
Authors	:	Wang, R.Y.; Noddings, C.M.; Kirschke, E.; Myasnikov, A.; Johnson, J.L.; Agard, D.A.
Deposited on	:	2020-11-30
Resolution	:	3.57 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

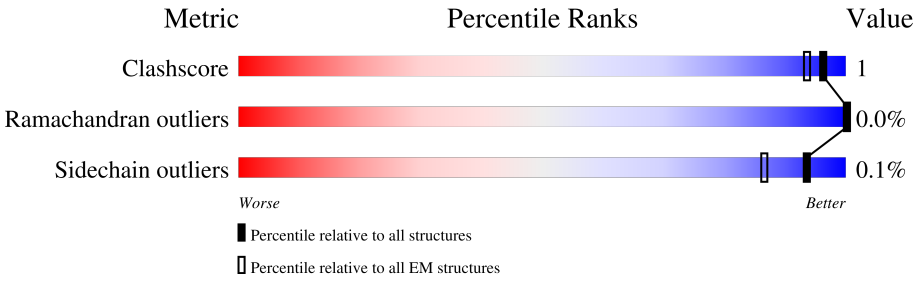
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.57 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)
Clashscore	158937	4297
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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	732	80% 5% 15%
1	B	732	79% 7% 14%
2	C	641	9% 77% · 20%
2	D	641	57% · 41%
3	E	543	56% · 40%
4	F	777	13% 31% · 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	K	C	703	-	-	X	-
7	K	D	703	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43804 atoms, of which 21952 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	623	Total	C	H	N	O	S	0	0
			10157	3207	5101	850	976	23		
1	B	628	Total	C	H	N	O	S	0	0
			10233	3231	5135	855	988	24		

- Molecule 2 is a protein called Heat shock 70 kDa protein 1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	511	Total	C	H	N	O	S	0	0
			7897	2474	3959	683	772	9		
2	D	379	Total	C	H	N	O	S	0	0
			5882	1850	2944	516	565	7		

- Molecule 3 is a protein called Stress-induced-phosphoprotein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	327	Total	C	H	N	O	S	0	0
			5321	1667	2659	464	511	20		

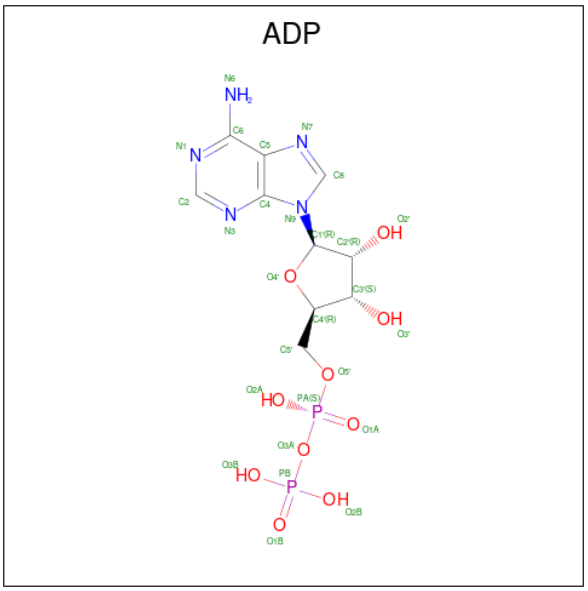
- Molecule 4 is a protein called Glucocorticoid receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	259	Total	C	H	N	O	S	0	0
			4232	1354	2130	345	385	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	519	SER	THR	conflict	UNP P04150
F	602	SER	PHE	engineered mutation	UNP P04150

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

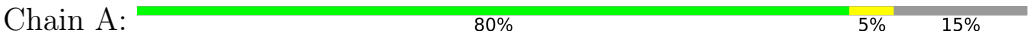
Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	K	0
			1	1	
7	D	1	Total	K	0
			1	1	

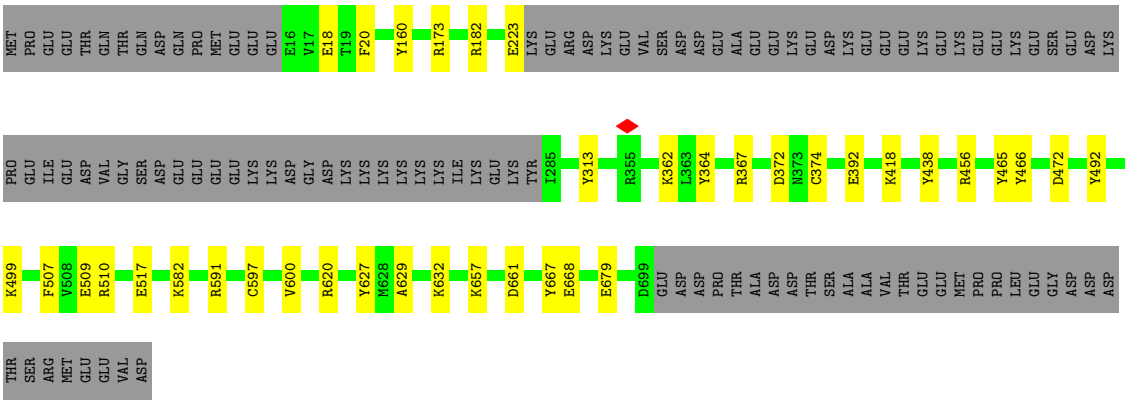
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Heat shock protein HSP 90-alpha

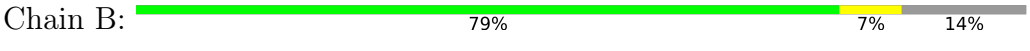
Chain A:

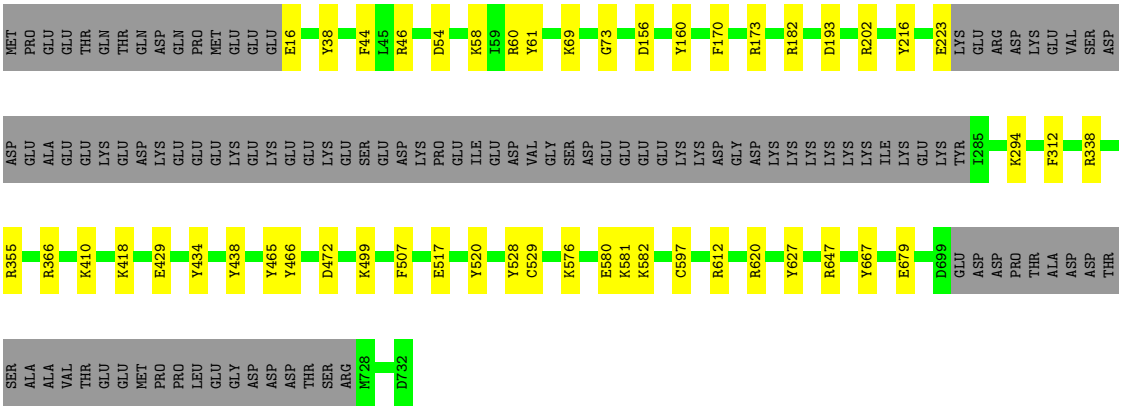




• Molecule 1: Heat shock protein HSP 90-alpha

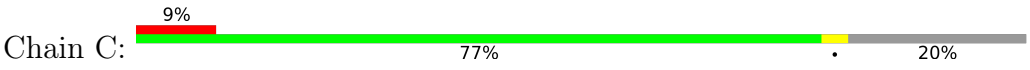
Chain B:

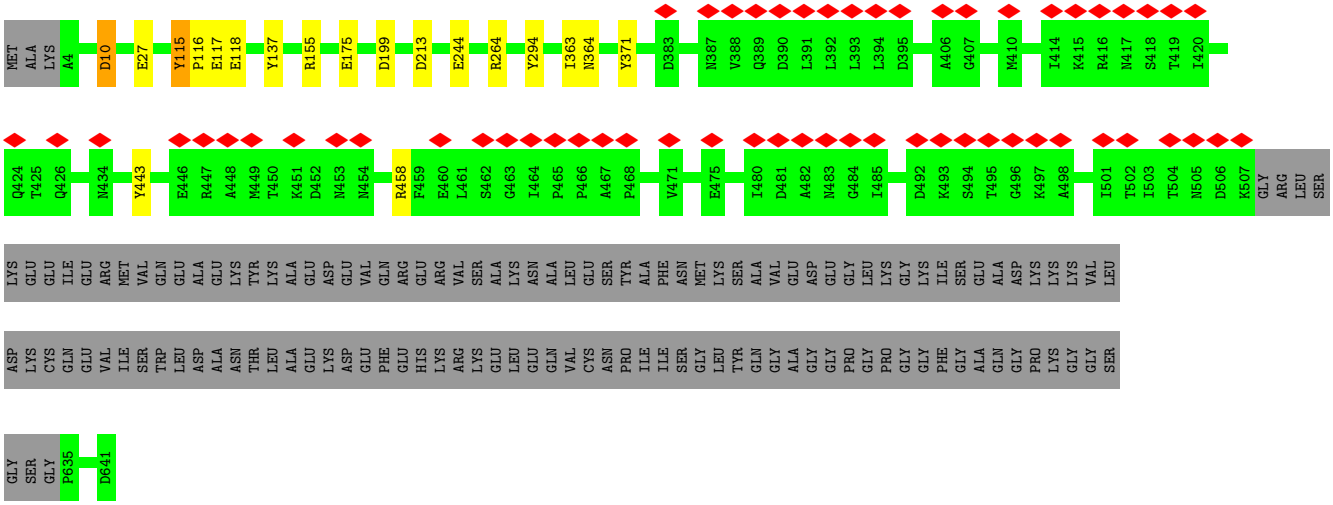




• Molecule 2: Heat shock 70 kDa protein 1A

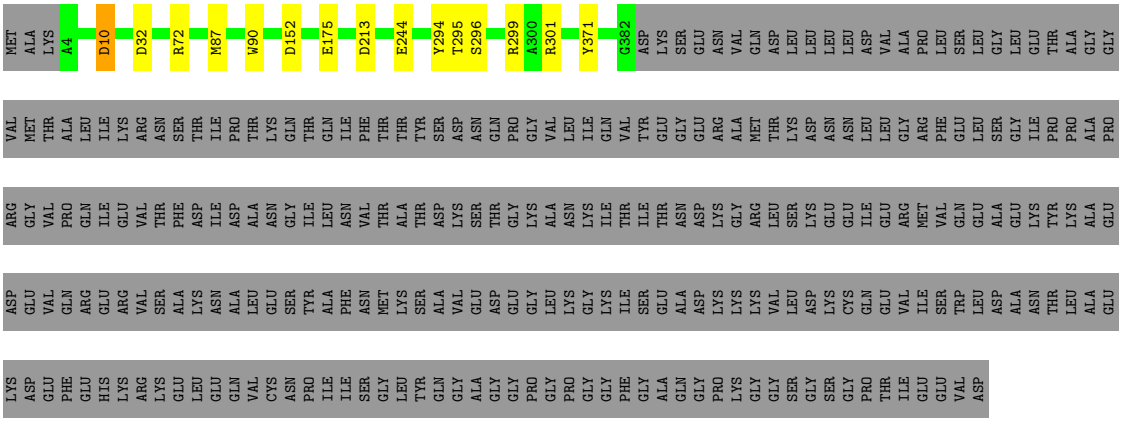
Chain C:





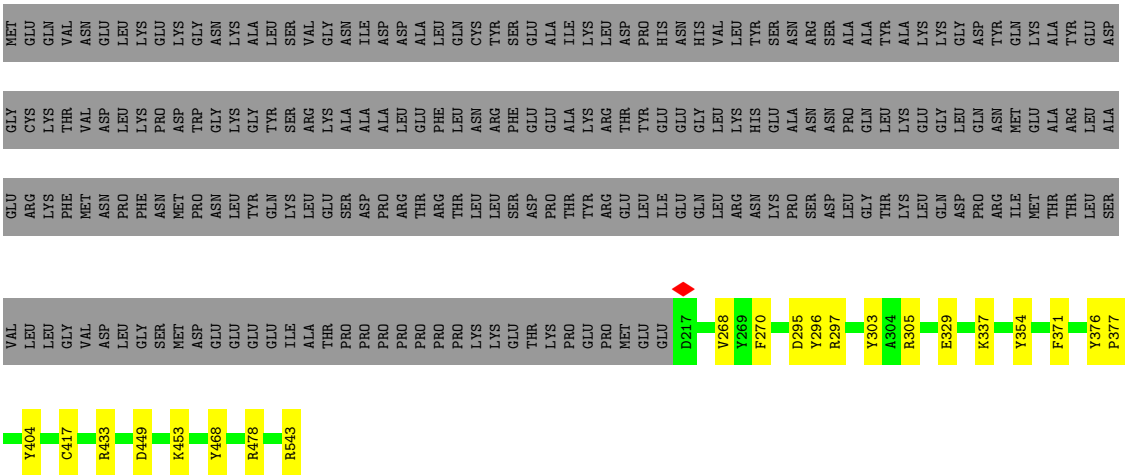
• Molecule 2: Heat shock 70 kDa protein 1A

Chain D:



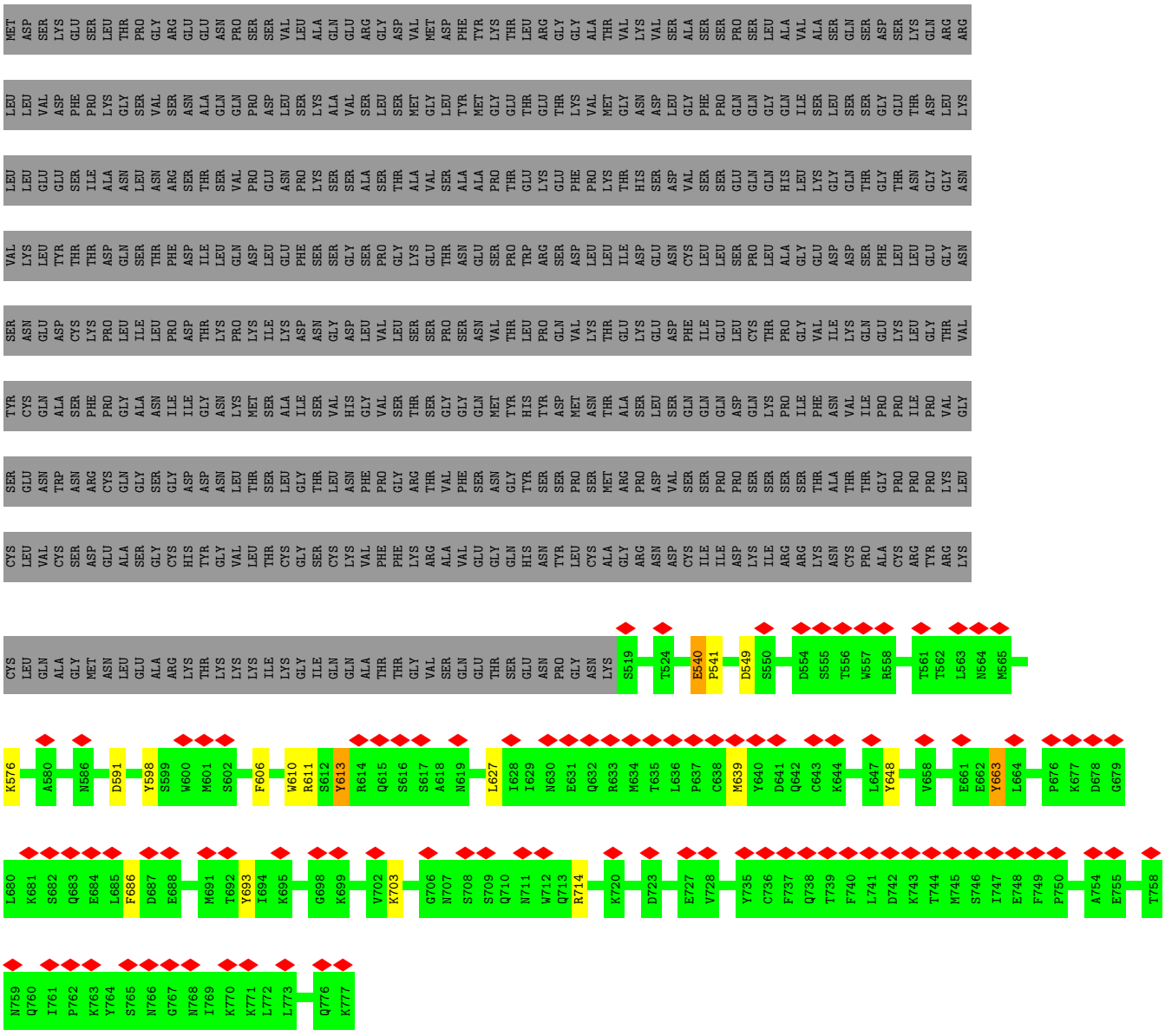
• Molecule 3: Stress-induced-phosphoprotein 1

Chain E:



• Molecule 4: Glucocorticoid receptor

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85619	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	338.88, 338.88, 338.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, ADP

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	1.23	20/5138 (0.4%)	0.94	12/6909 (0.2%)
1	B	1.21	19/5179 (0.4%)	0.95	15/6961 (0.2%)
2	C	1.09	12/3998 (0.3%)	0.97	13/5410 (0.2%)
2	D	1.18	6/2986 (0.2%)	0.94	7/4035 (0.2%)
3	E	1.16	9/2706 (0.3%)	0.98	8/3625 (0.2%)
4	F	0.98	5/2148 (0.2%)	0.98	9/2907 (0.3%)
All	All	1.16	71/22155 (0.3%)	0.96	64/29847 (0.2%)

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	175	GLU	CD-OE1	-17.52	1.06	1.25
2	C	175	GLU	CD-OE2	-16.89	1.07	1.25
2	C	175	GLU	CD-OE1	-14.60	1.09	1.25
2	D	175	GLU	CD-OE2	-14.40	1.09	1.25
3	E	268	VAL	CB-CG2	-9.37	1.33	1.52
3	E	404	TYR	CG-CD1	-8.38	1.28	1.39
1	A	507	PHE	CB-CG	-7.60	1.38	1.51
2	C	199	ASP	CG-OD1	-7.53	1.08	1.25
2	D	10	ASP	CG-OD2	-7.50	1.08	1.25
2	D	244	GLU	CG-CD	-7.29	1.41	1.51
1	B	597	CYS	CB-SG	-7.22	1.70	1.82
1	A	597	CYS	CB-SG	-7.10	1.70	1.82
1	B	466	TYR	CB-CG	-7.09	1.41	1.51
1	A	509	GLU	CD-OE1	-6.98	1.18	1.25
3	E	371	PHE	CB-CG	-6.92	1.39	1.51
2	D	244	GLU	CD-OE1	-6.85	1.18	1.25
2	D	371	TYR	CB-CG	-6.72	1.41	1.51
1	B	216	TYR	CB-CG	-6.56	1.41	1.51
1	B	507	PHE	CB-CG	-6.53	1.40	1.51
1	A	160	TYR	CB-CG	-6.44	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	244	GLU	CG-CD	-6.32	1.42	1.51
1	B	465	TYR	CB-CG	-6.04	1.42	1.51
3	E	404	TYR	CD1-CE1	-6.00	1.30	1.39
4	F	663	TYR	CB-CG	-6.00	1.42	1.51
1	A	466	TYR	CB-CG	-5.98	1.42	1.51
1	B	438	TYR	CB-CG	-5.97	1.42	1.51
1	A	223	GLU	CB-CG	5.96	1.63	1.52
1	A	374	CYS	CB-SG	-5.96	1.72	1.81
1	B	529	CYS	CB-SG	-5.93	1.72	1.81
1	B	160	TYR	CB-CG	-5.89	1.42	1.51
1	A	20	PHE	CB-CG	-5.86	1.41	1.51
1	B	44	PHE	CB-CG	-5.85	1.41	1.51
1	A	160	TYR	CG-CD1	-5.83	1.31	1.39
1	B	528	TYR	CB-CG	-5.82	1.43	1.51
1	B	312	PHE	CB-CG	-5.81	1.41	1.51
2	C	244	GLU	CD-OE2	-5.80	1.19	1.25
2	C	115	TYR	CG-CD2	-5.80	1.31	1.39
2	C	115	TYR	CB-CG	-5.78	1.43	1.51
3	E	303	TYR	CB-CG	-5.76	1.43	1.51
1	A	667	TYR	CB-CG	-5.70	1.43	1.51
1	B	16	GLU	CB-CG	5.63	1.62	1.52
3	E	417	CYS	CB-SG	-5.61	1.72	1.81
1	B	517	GLU	CD-OE1	-5.58	1.19	1.25
3	E	543	ARG	NE-CZ	5.57	1.40	1.33
1	B	667	TYR	CB-CG	-5.50	1.43	1.51
1	B	38	TYR	CB-CG	-5.50	1.43	1.51
1	A	517	GLU	CD-OE1	-5.48	1.19	1.25
1	A	600	VAL	CB-CG1	-5.43	1.41	1.52
2	C	115	TYR	CD2-CE2	-5.41	1.31	1.39
4	F	639	MET	CG-SD	-5.41	1.67	1.81
4	F	686	PHE	CB-CG	-5.39	1.42	1.51
1	A	465	TYR	CB-CG	-5.34	1.43	1.51
1	A	517	GLU	CD-OE2	-5.33	1.19	1.25
2	C	27	GLU	CD-OE1	-5.33	1.19	1.25
1	A	668	GLU	CD-OE1	-5.29	1.19	1.25
3	E	468	TYR	CB-CG	-5.28	1.43	1.51
1	B	517	GLU	CD-OE2	-5.27	1.19	1.25
1	A	438	TYR	CB-CG	-5.25	1.43	1.51
1	B	223	GLU	CB-CG	5.18	1.61	1.52
1	A	492	TYR	CG-CD2	-5.17	1.32	1.39
1	B	44	PHE	CG-CD1	-5.16	1.31	1.38
2	C	117	GLU	CD-OE1	-5.16	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	606	PHE	CB-CG	-5.15	1.42	1.51
1	A	627	TYR	CB-CG	-5.11	1.44	1.51
2	C	137	TYR	CB-CG	-5.10	1.44	1.51
1	A	392	GLU	CD-OE2	-5.08	1.20	1.25
4	F	627	LEU	CB-CG	5.06	1.67	1.52
1	A	18	GLU	CD-OE1	-5.05	1.20	1.25
1	B	170	PHE	CB-CG	-5.04	1.42	1.51
2	C	244	GLU	CD-OE1	-5.01	1.20	1.25
3	E	329	GLU	CD-OE1	-5.01	1.20	1.25

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	404	TYR	CB-CG-CD1	-10.93	114.44	121.00
2	C	199	ASP	CB-CG-OD1	10.31	127.58	118.30
2	D	301	ARG	NE-CZ-NH2	-10.29	115.15	120.30
4	F	613	TYR	CB-CG-CD2	-9.21	115.48	121.00
1	B	612	ARG	NE-CZ-NH2	-9.04	115.78	120.30
2	D	299	ARG	NE-CZ-NH2	-8.97	115.81	120.30
4	F	693	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	B	173	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	A	456	ARG	NE-CZ-NH2	-8.26	116.17	120.30
2	D	175	GLU	OE1-CD-OE2	-8.22	113.44	123.30
1	B	46	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	366	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	338	ARG	NE-CZ-NH2	-7.70	116.45	120.30
3	E	404	TYR	CB-CG-CD2	7.64	125.59	121.00
2	C	294	TYR	CB-CG-CD2	-7.49	116.51	121.00
3	E	297	ARG	NE-CZ-NH2	-7.35	116.62	120.30
2	C	199	ASP	OD1-CG-OD2	-7.34	109.34	123.30
2	C	155	ARG	NE-CZ-NH1	7.13	123.87	120.30
2	C	443	TYR	CB-CG-CD2	-7.10	116.74	121.00
2	D	294	TYR	CB-CG-CD2	-6.94	116.83	121.00
1	A	510	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	C	115	TYR	CB-CG-CD2	-6.81	116.92	121.00
1	A	364	TYR	CB-CG-CD2	-6.72	116.97	121.00
4	F	611	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	647	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	C	264	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	355	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	173	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	60	ARG	NE-CZ-NH2	-6.50	117.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	543	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	510	ARG	NE-CZ-NH1	6.30	123.45	120.30
3	E	433	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	173	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	202	ARG	NE-CZ-NH2	-6.10	117.25	120.30
4	F	714	ARG	NE-CZ-NH2	-6.04	117.28	120.30
4	F	613	TYR	CB-CG-CD1	5.94	124.57	121.00
1	A	313	TYR	CB-CG-CD2	-5.94	117.44	121.00
2	C	155	ARG	NE-CZ-NH2	-5.90	117.35	120.30
3	E	478	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	C	10	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	434	TYR	CB-CG-CD1	-5.80	117.52	121.00
4	F	648	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	B	173	ARG	NE-CZ-NH1	5.73	123.17	120.30
4	F	598	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	B	620	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	520	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	367	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	438	TYR	CB-CG-CD1	-5.50	117.70	121.00
2	C	458	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	D	10	ASP	CB-CG-OD1	5.46	123.21	118.30
2	D	72	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	160	TYR	CB-CG-CD1	-5.44	117.73	121.00
1	A	182	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	61	TYR	CB-CG-CD1	-5.39	117.77	121.00
2	C	199	ASP	CB-CG-OD2	5.30	123.07	118.30
2	C	371	TYR	CB-CG-CD1	-5.30	117.82	121.00
4	F	591	ASP	CB-CG-OD1	5.29	123.06	118.30
4	F	606	PHE	CB-CG-CD1	-5.25	117.13	120.80
2	D	32	ASP	CB-CG-OD2	5.22	123.00	118.30
3	E	303	TYR	CB-CG-CD2	-5.21	117.87	121.00
3	E	354	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	A	591	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	627	TYR	CB-CG-CD1	-5.15	117.91	121.00
2	C	294	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5056	5101	5099	6	0
1	B	5098	5135	5132	11	0
2	C	3938	3959	3958	7	0
2	D	2938	2944	2943	8	0
3	E	2662	2659	2658	5	0
4	F	2102	2130	2129	4	0
5	C	27	12	12	0	0
5	D	27	12	12	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	C	1	0	0	3	0
7	D	1	0	0	3	0
All	All	21852	21952	21943	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:ASP:OD1	7:D:703:K:K	1.52	1.21
2:C:10:ASP:OD1	7:C:703:K:K	1.52	1.19
2:D:10:ASP:OD2	7:D:703:K:K	1.56	1.14
2:D:10:ASP:CG	7:D:703:K:K	1.82	1.10
2:C:10:ASP:CG	7:C:703:K:K	1.99	0.94
2:C:10:ASP:OD2	7:C:703:K:K	1.81	0.91
1:A:418:LYS:NZ	2:C:213:ASP:OD2	2.34	0.60
1:B:418:LYS:NZ	2:D:213:ASP:OD2	2.36	0.57
1:B:294:LYS:NZ	2:D:152:ASP:OD2	2.41	0.54
1:B:54:ASP:OD2	1:B:58:LYS:NZ	2.40	0.53
1:A:472:ASP:OD1	1:A:499:LYS:NZ	2.42	0.52
3:E:270:PHE:CZ	3:E:305:ARG:HB3	2.44	0.52
1:A:657:LYS:NZ	1:A:661:ASP:OD2	2.43	0.51
2:D:152:ASP:N	2:D:152:ASP:OD1	2.43	0.51
1:A:582:LYS:NZ	1:A:679:GLU:OE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:449:ASP:OD2	3:E:453:LYS:NZ	2.45	0.49
4:F:540:GLU:H	4:F:541:PRO:CD	2.27	0.47
2:C:115:TYR:O	2:C:118:GLU:HG2	2.15	0.47
3:E:295:ASP:OD1	3:E:296:TYR:N	2.48	0.47
1:B:410:LYS:NZ	4:F:703:LYS:O	2.47	0.46
1:B:582:LYS:NZ	1:B:679:GLU:OE2	2.45	0.46
1:A:362:LYS:NZ	1:A:372:ASP:OD1	2.47	0.46
1:B:576:LYS:O	1:B:580:GLU:N	2.48	0.46
1:B:73:GLY:O	1:B:182:ARG:NH1	2.50	0.45
1:B:69:LYS:NZ	1:B:156:ASP:OD2	2.49	0.45
1:B:429:GLU:O	3:E:337:LYS:NZ	2.50	0.45
2:D:87:MET:HA	2:D:90:TRP:CE3	2.53	0.44
1:B:472:ASP:OD1	1:B:499:LYS:NZ	2.51	0.44
4:F:610:TRP:HB2	4:F:663:TYR:CE1	2.53	0.43
1:A:629:ALA:O	1:A:632:LYS:NZ	2.47	0.43
4:F:549:ASP:OD2	4:F:576:LYS:NZ	2.52	0.43
3:E:376:TYR:N	3:E:377:PRO:CD	2.82	0.42
2:C:115:TYR:CD1	2:C:116:PRO:HD2	2.54	0.41
1:B:193:ASP:OD1	1:B:193:ASP:N	2.53	0.41
2:D:295:THR:OG1	2:D:296:SER:N	2.52	0.41
2:C:363:ILE:O	2:C:364:ASN:C	2.59	0.40

There are no symmetry-related clashes.

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	619/732 (85%)	611 (99%)	8 (1%)	0	100	100
1	B	622/732 (85%)	614 (99%)	8 (1%)	0	100	100
2	C	507/641 (79%)	498 (98%)	9 (2%)	0	100	100
2	D	377/641 (59%)	374 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	325/543 (60%)	323 (99%)	2 (1%)	0	100 100
4	F	257/777 (33%)	252 (98%)	4 (2%)	1 (0%)	34 71
All	All	2707/4066 (67%)	2672 (99%)	34 (1%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	540	GLU

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	564/666 (85%)	563 (100%)	1 (0%)	93 98
1	B	569/666 (85%)	568 (100%)	1 (0%)	93 98
2	C	427/529 (81%)	427 (100%)	0	100 100
2	D	313/529 (59%)	313 (100%)	0	100 100
3	E	282/472 (60%)	282 (100%)	0	100 100
4	F	238/688 (35%)	237 (100%)	1 (0%)	91 97
All	All	2393/3550 (67%)	2390 (100%)	3 (0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	620	ARG
1	B	581	LYS
4	F	613	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	452	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
5	ADP	D	701	6	24,29,29	1.96	4 (16%)	29,45,45	1.31	3 (10%)
5	ADP	C	701	-	24,29,29	1.83	5 (20%)	29,45,45	1.23	2 (6%)

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
5	ADP	D	701	6	-	3/12/32/32	0/3/3/3
5	ADP	C	701	-	-	7/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	701	ADP	C2-N3	5.40	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	701	ADP	C2-N3	5.08	1.40	1.32
5	D	701	ADP	C4-N3	4.61	1.42	1.35
5	C	701	ADP	C4-N3	4.27	1.41	1.35
5	C	701	ADP	C5-C4	3.21	1.49	1.40
5	D	701	ADP	C2-N1	3.17	1.39	1.33
5	D	701	ADP	C5-C4	3.11	1.49	1.40
5	C	701	ADP	C2-N1	2.52	1.38	1.33
5	C	701	ADP	C6-C5	2.00	1.50	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	701	ADP	N3-C2-N1	-4.02	122.39	128.68
5	C	701	ADP	N3-C2-N1	-3.60	123.05	128.68
5	D	701	ADP	N6-C6-N1	2.28	123.30	118.57
5	D	701	ADP	C5-C6-N6	-2.05	117.23	120.35
5	C	701	ADP	O2A-PA-O1A	2.01	122.18	112.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	701	ADP	C5'-O5'-PA-O1A
5	C	701	ADP	C5'-O5'-PA-O2A
5	C	701	ADP	C3'-C4'-C5'-O5'
5	D	701	ADP	C3'-C4'-C5'-O5'
5	C	701	ADP	O4'-C4'-C5'-O5'
5	D	701	ADP	O4'-C4'-C5'-O5'
5	C	701	ADP	PB-O3A-PA-O1A
5	C	701	ADP	PB-O3A-PA-O2A
5	C	701	ADP	C5'-O5'-PA-O3A
5	D	701	ADP	C5'-O5'-PA-O1A

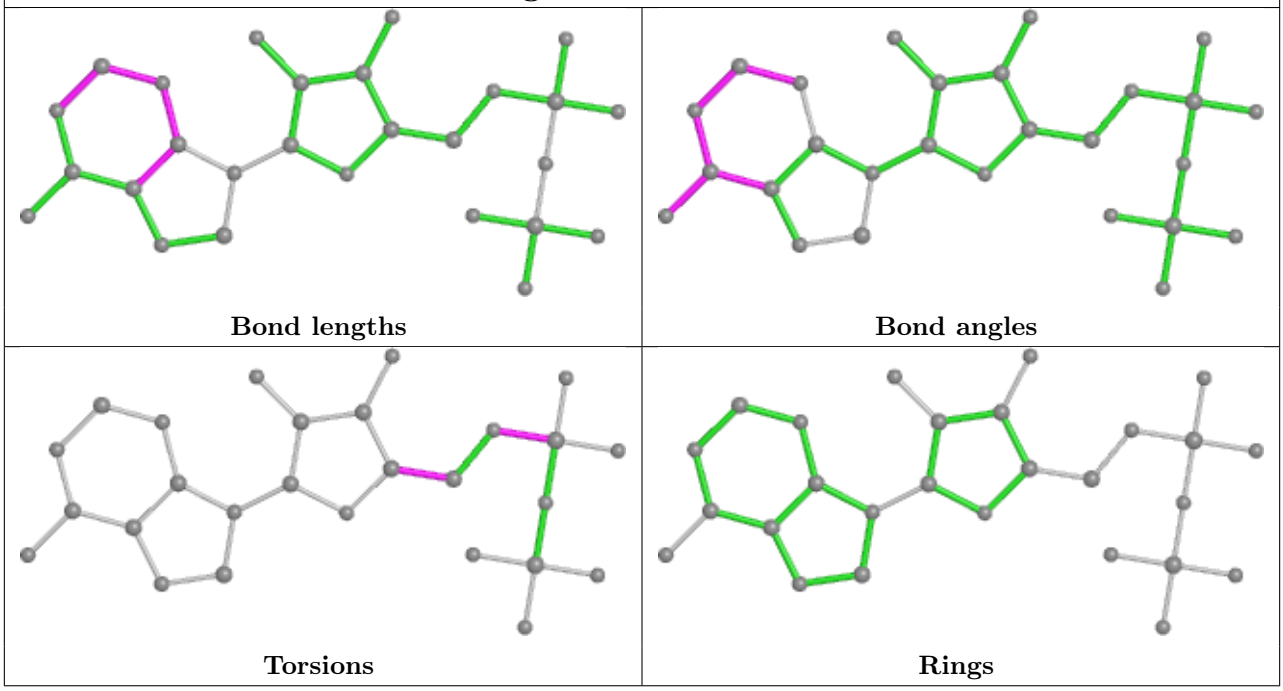
There are no ring outliers.

No monomer is involved in short contacts.

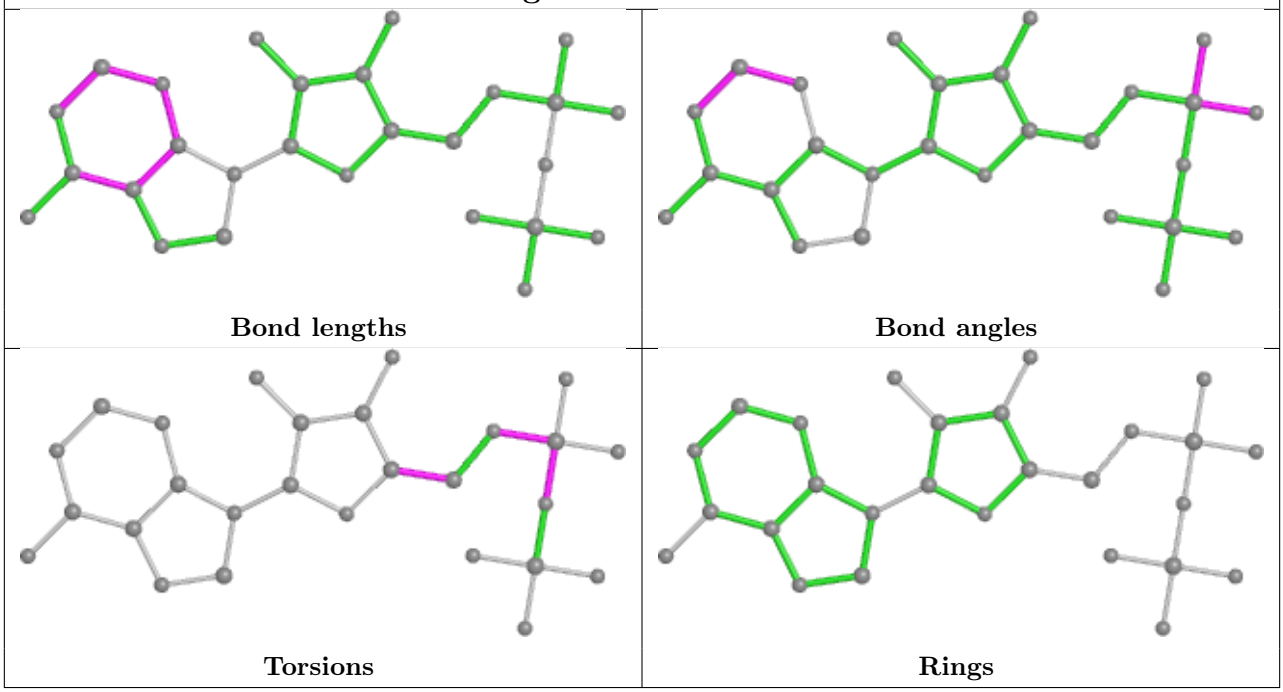
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP D 701



Ligand ADP C 701



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.

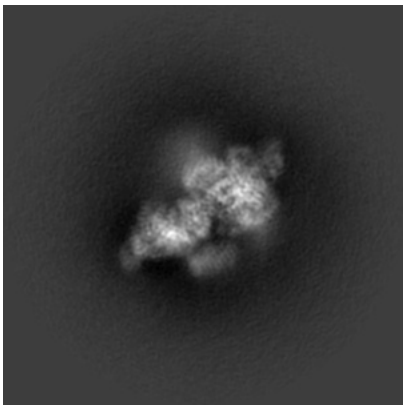
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23050. These allow visual inspection of the internal detail of the map and identification of artifacts.

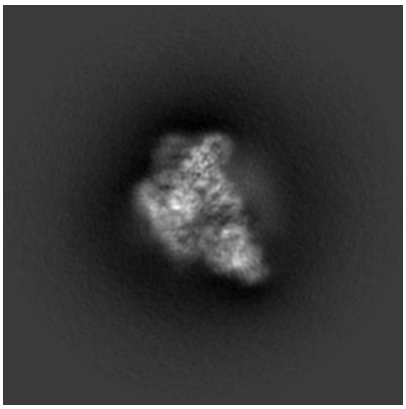
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

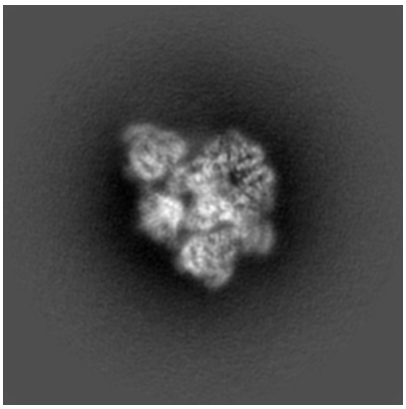
6.1.1 Primary map



X

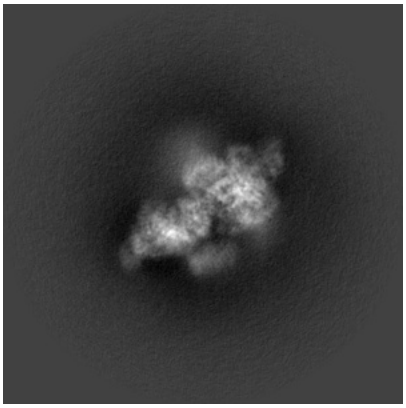


Y

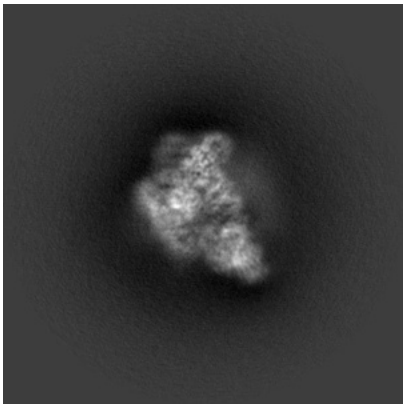


Z

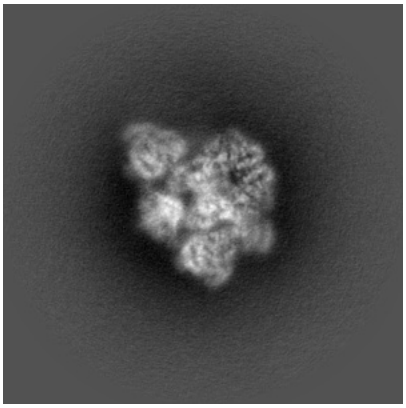
6.1.2 Raw map



X



Y

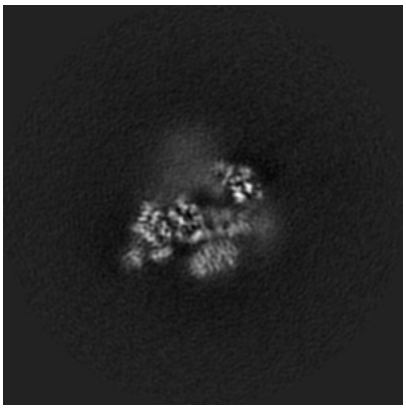


Z

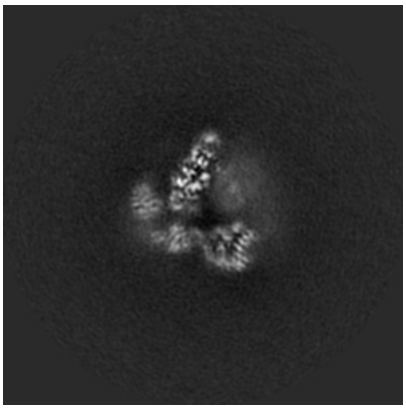
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

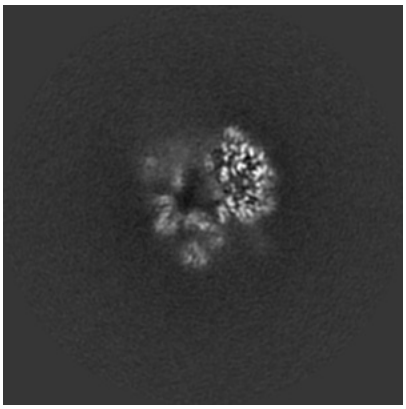
6.2.1 Primary map



X Index: 160

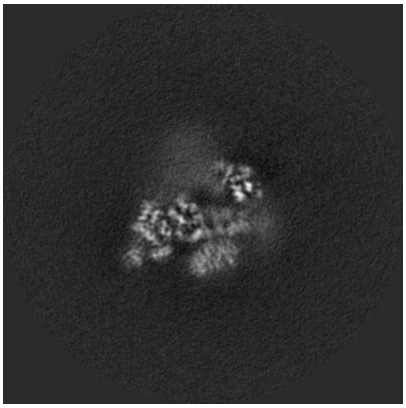


Y Index: 160

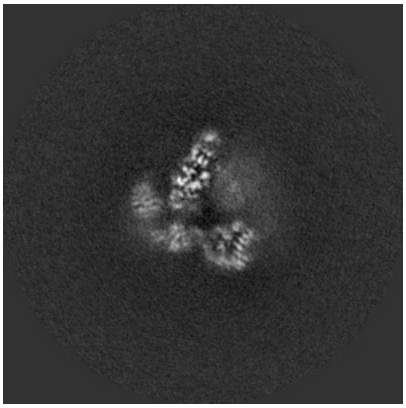


Z Index: 160

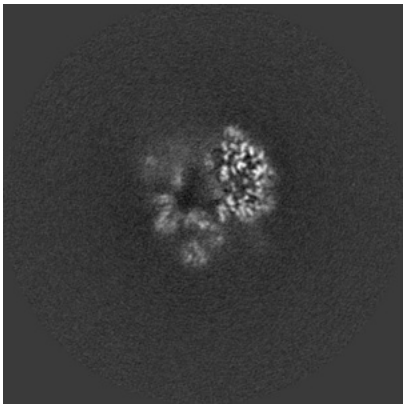
6.2.2 Raw map



X Index: 160



Y Index: 160

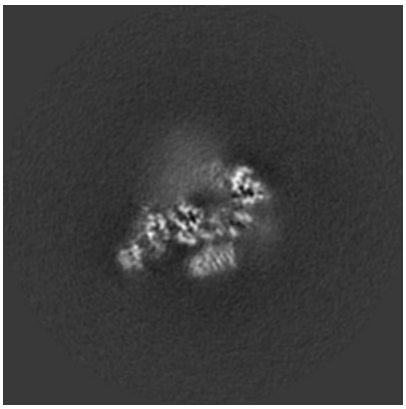


Z Index: 160

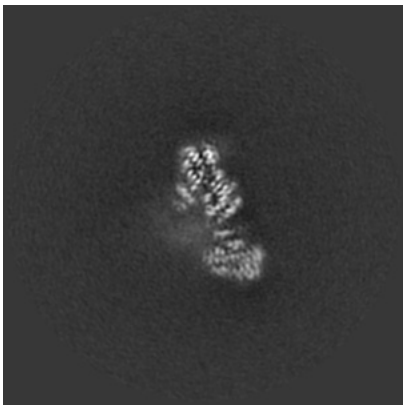
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

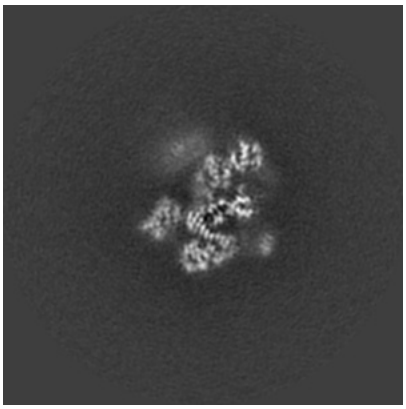
6.3.1 Primary map



X Index: 164

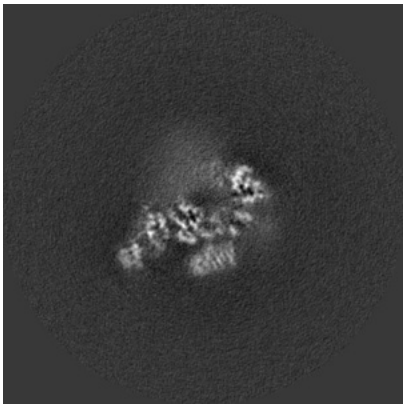


Y Index: 194

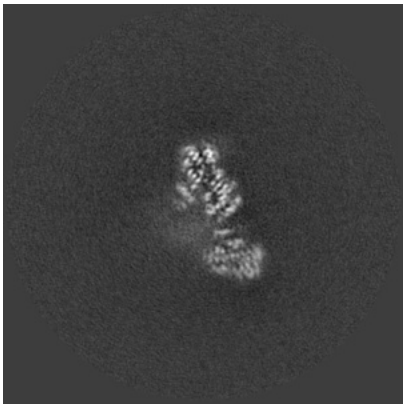


Z Index: 148

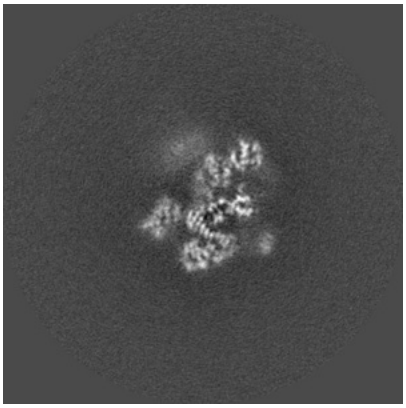
6.3.2 Raw map



X Index: 164



Y Index: 194

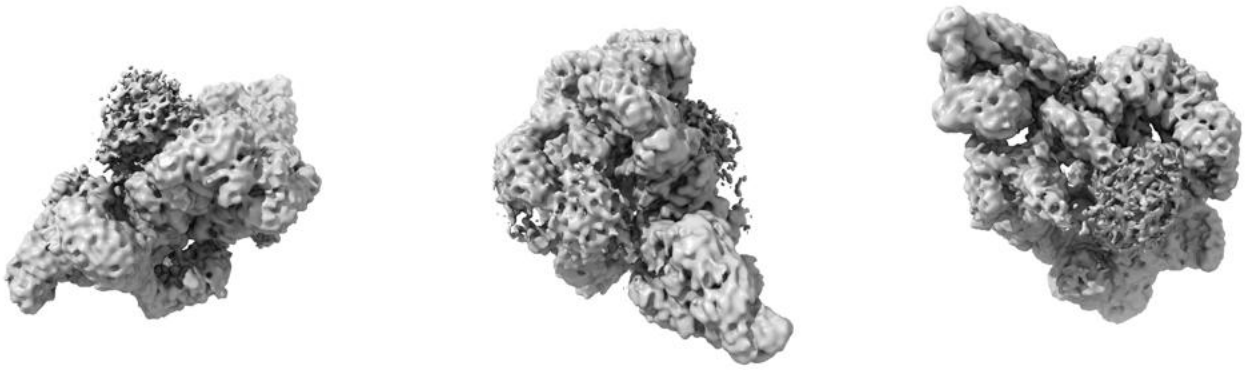


Z Index: 148

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. 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

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.

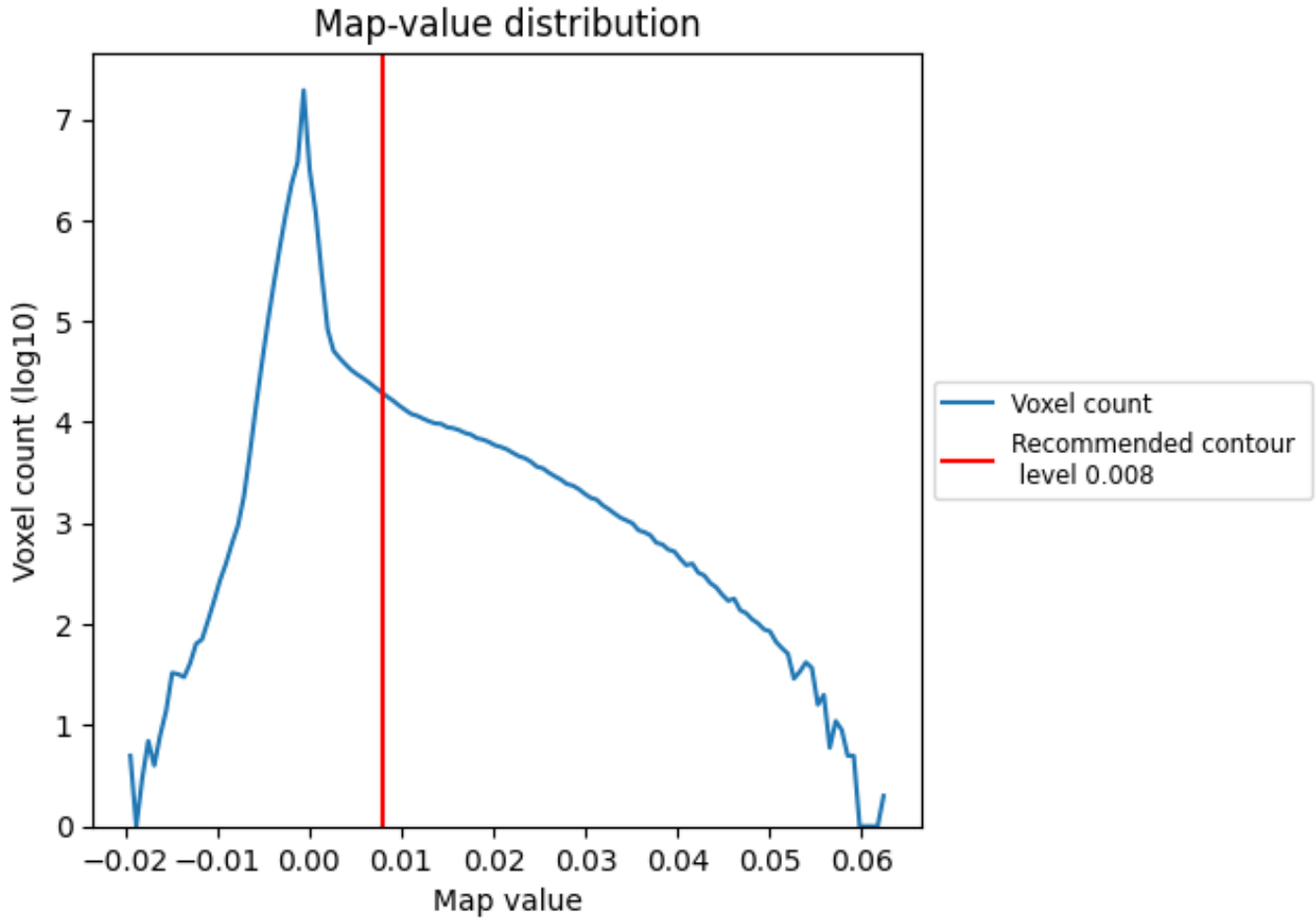
6.5 Mask visualisation (i)

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

7 Map analysis

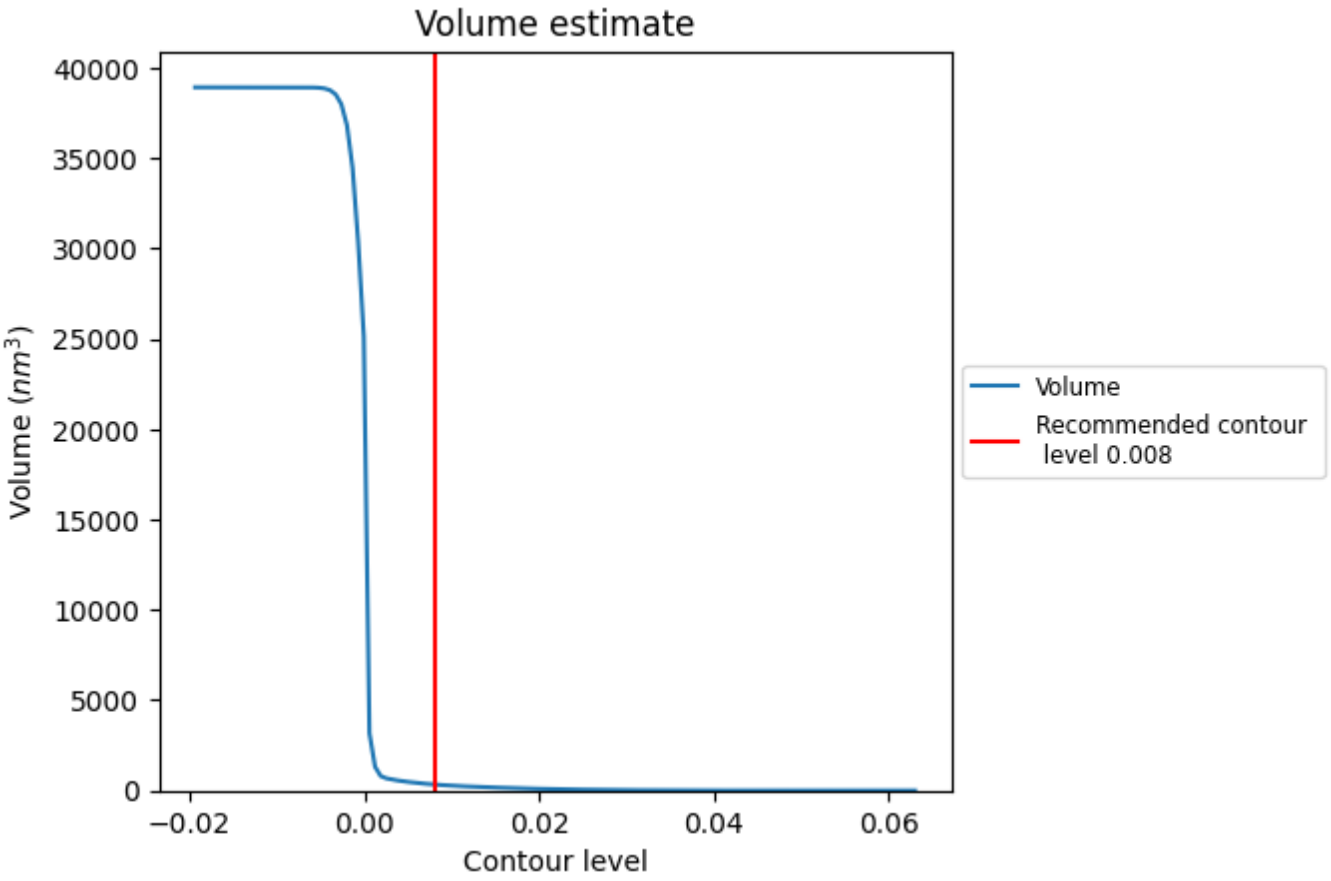
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

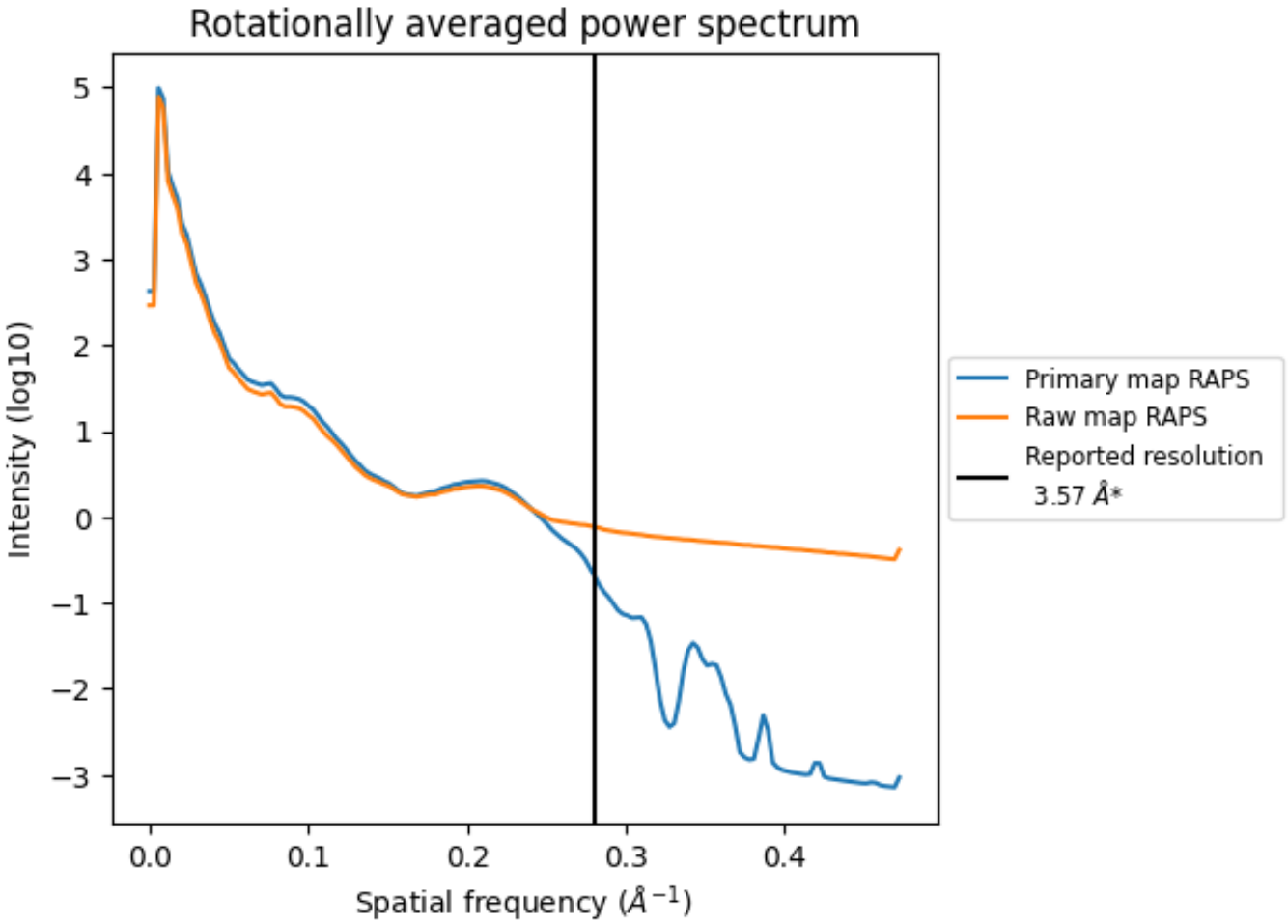
7.2 Volume estimate



The volume at the recommended contour level is 335 nm^3; this corresponds to an approximate mass of 303 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)

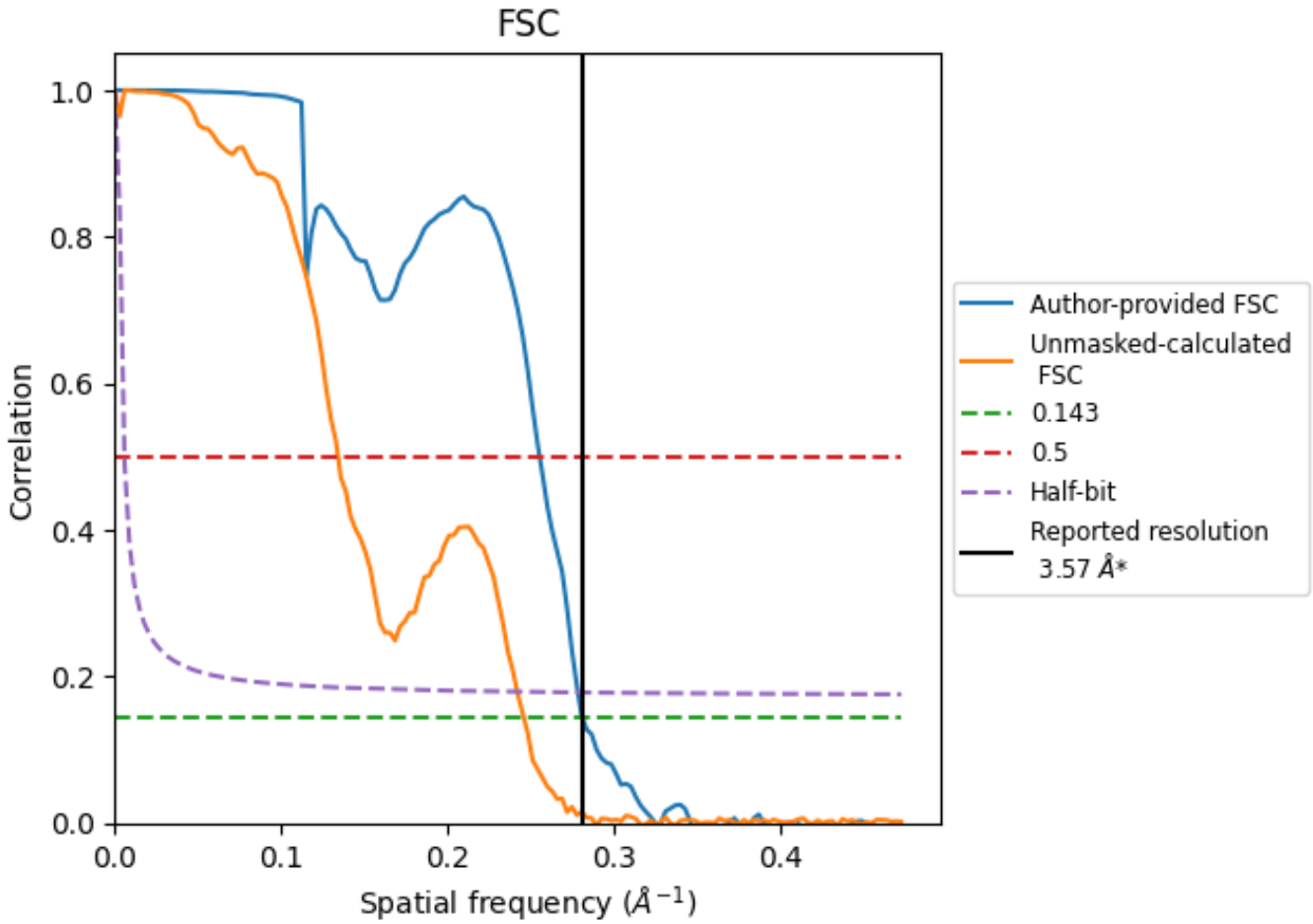


*Reported resolution corresponds to spatial frequency of 0.280 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.280 Å^{-1}

8.2 Resolution estimates (i)

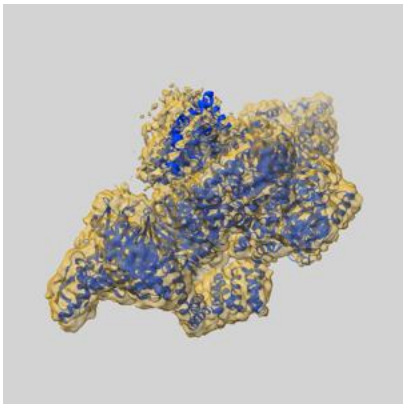
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.56	3.92	3.60
Unmasked-calculated*	4.07	7.46	4.14

*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 4.07 differs from the reported value 3.57 by more than 10 %

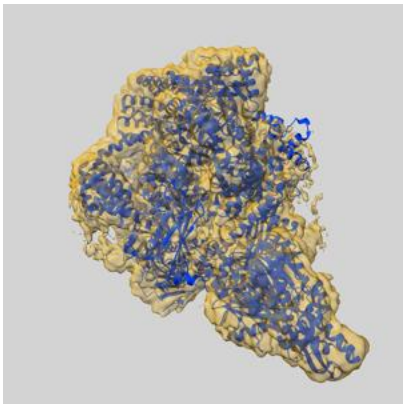
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23050 and PDB model 7KW7. Per-residue inclusion information can be found in section 3 on page 6.

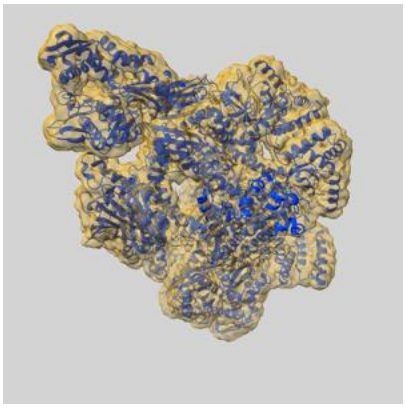
9.1 Map-model overlay



X



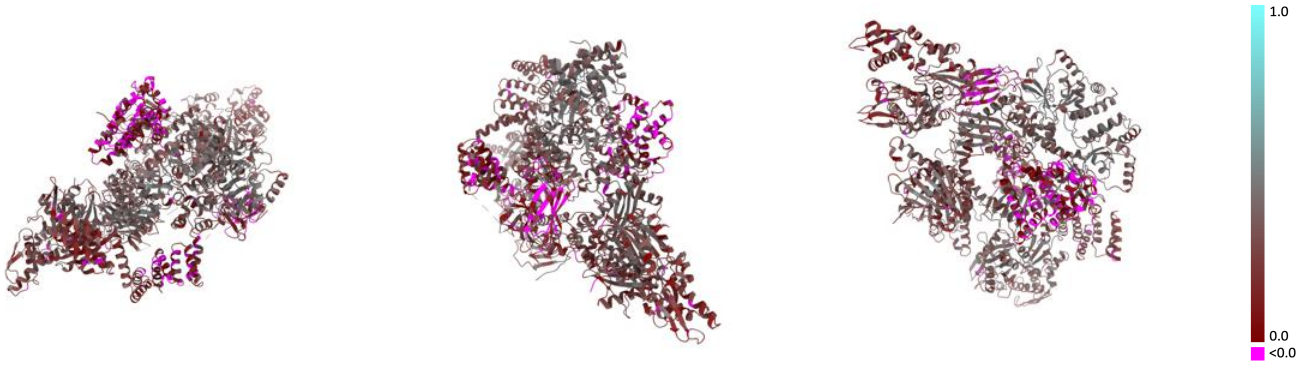
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

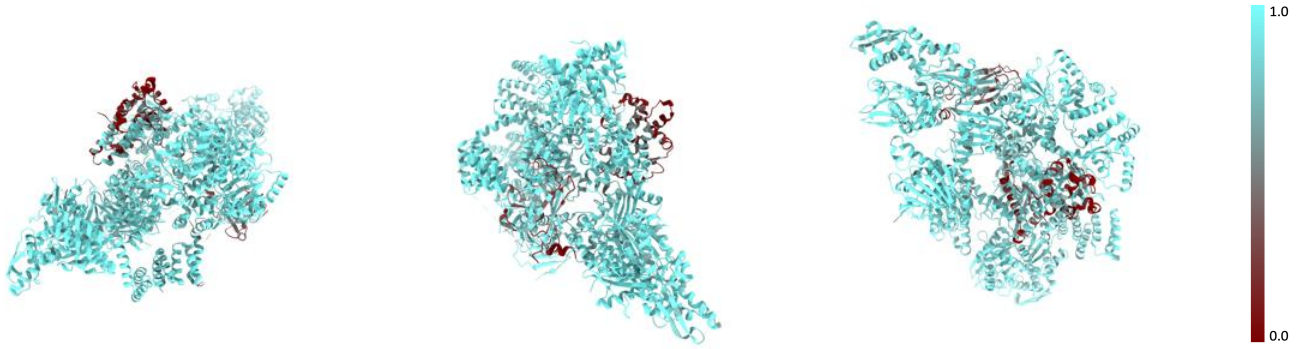
9.2 Q-score mapped to coordinate model



X Y Z

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

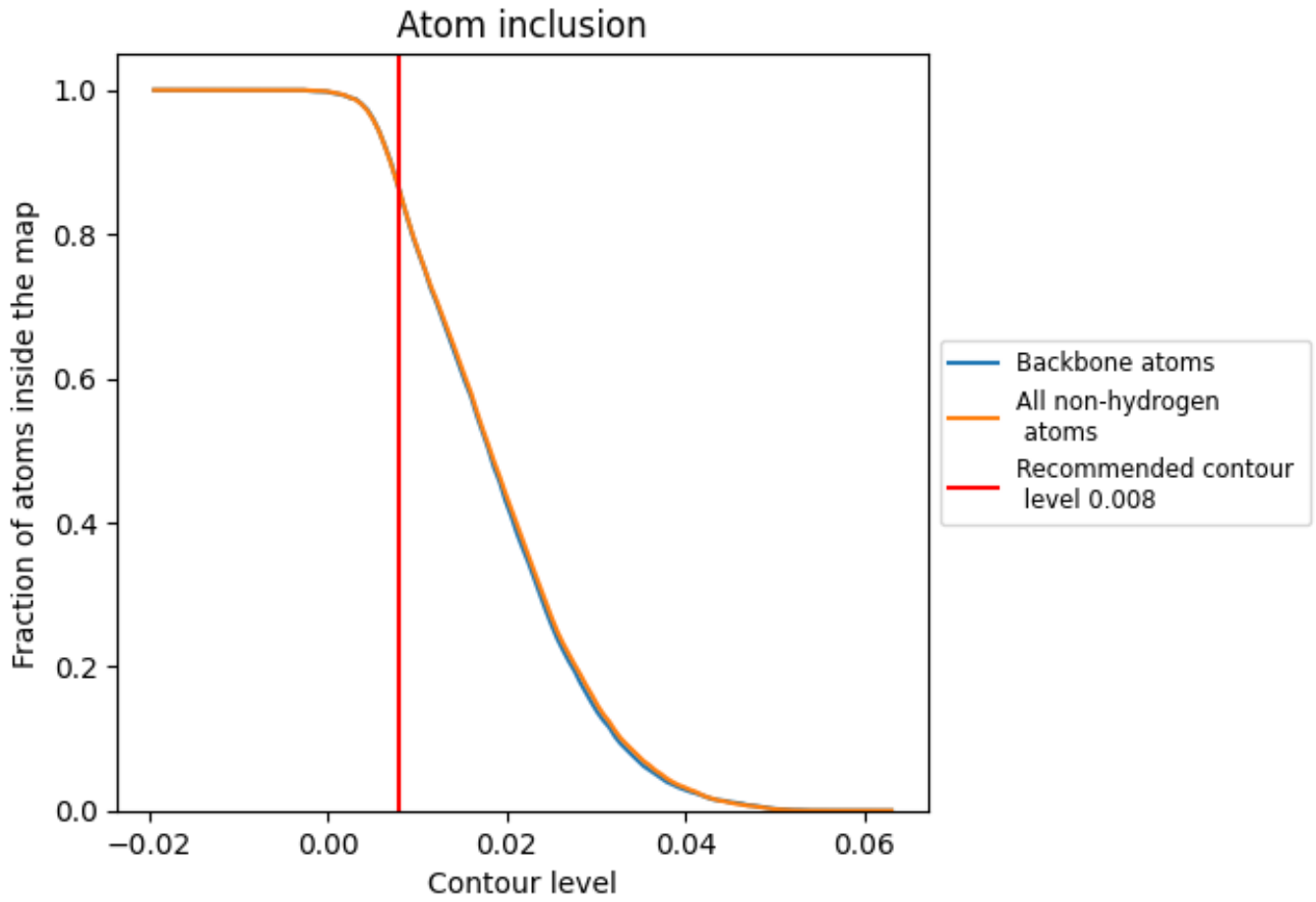
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8616	0.2760
A	0.9242	0.3500
B	0.9186	0.3530
C	0.8160	0.2120
D	0.9495	0.3270
E	0.9330	0.1920
F	0.5308	0.0680