



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:11 PM UTC

PDB ID : 7KW7 / pdb_00007kw7
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:

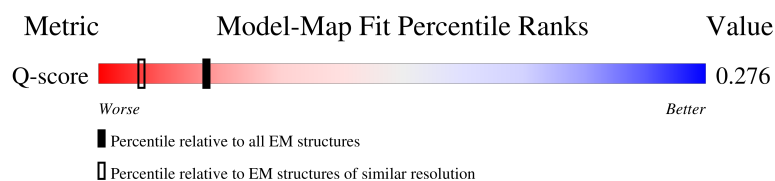
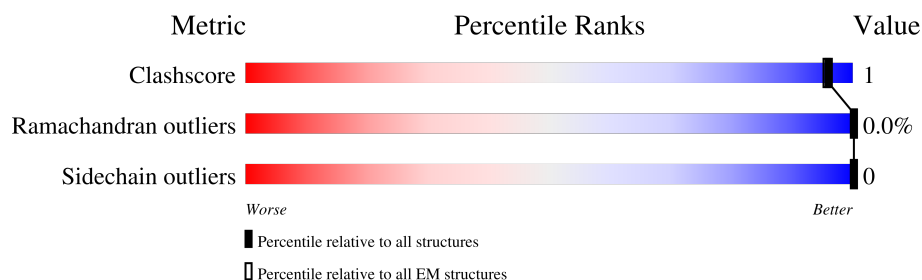
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.57 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12682 (3.07 - 4.07)

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

Mol	Chain	Length	Quality of chain
1	A	732	 81% 15%
1	B	732	 80% 6% 14%
2	C	641	 9% 75% 5% 20%
2	D	641	 55% 41%

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Mol	Chain	Length	Quality of chain
3	E	543	
4	F	777	

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		

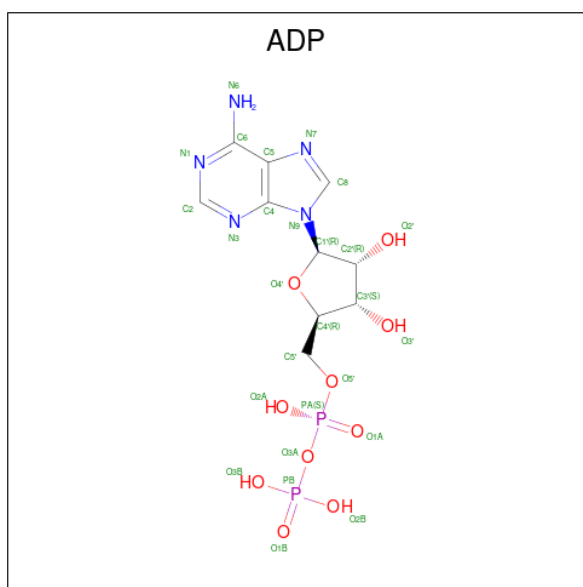
- Molecule 4 is a protein called Glucocorticoid receptor.

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

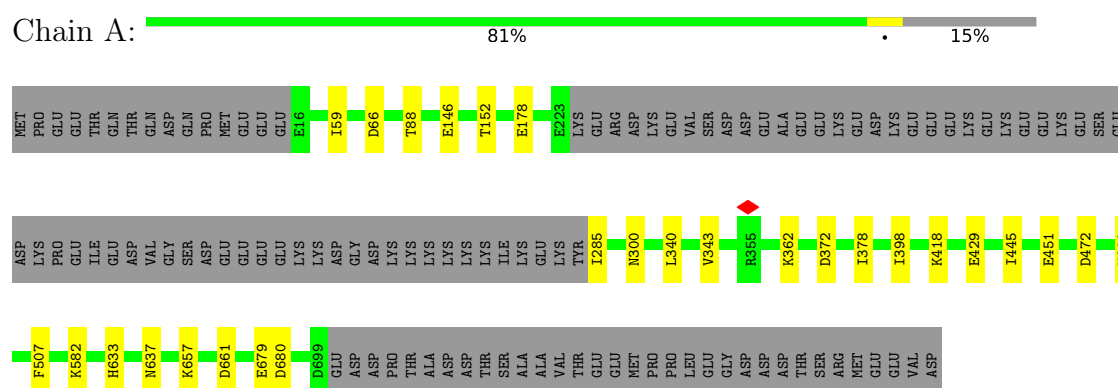
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

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

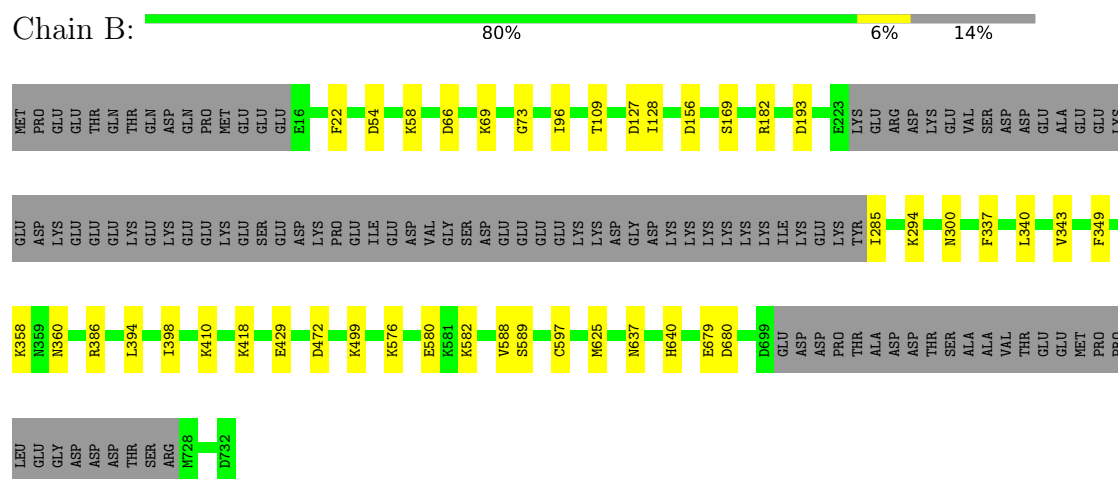
3 Residue-property plots

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.

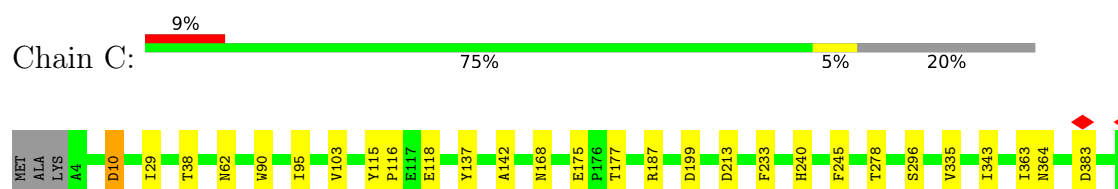
• Molecule 1: Heat shock protein HSP 90-alpha



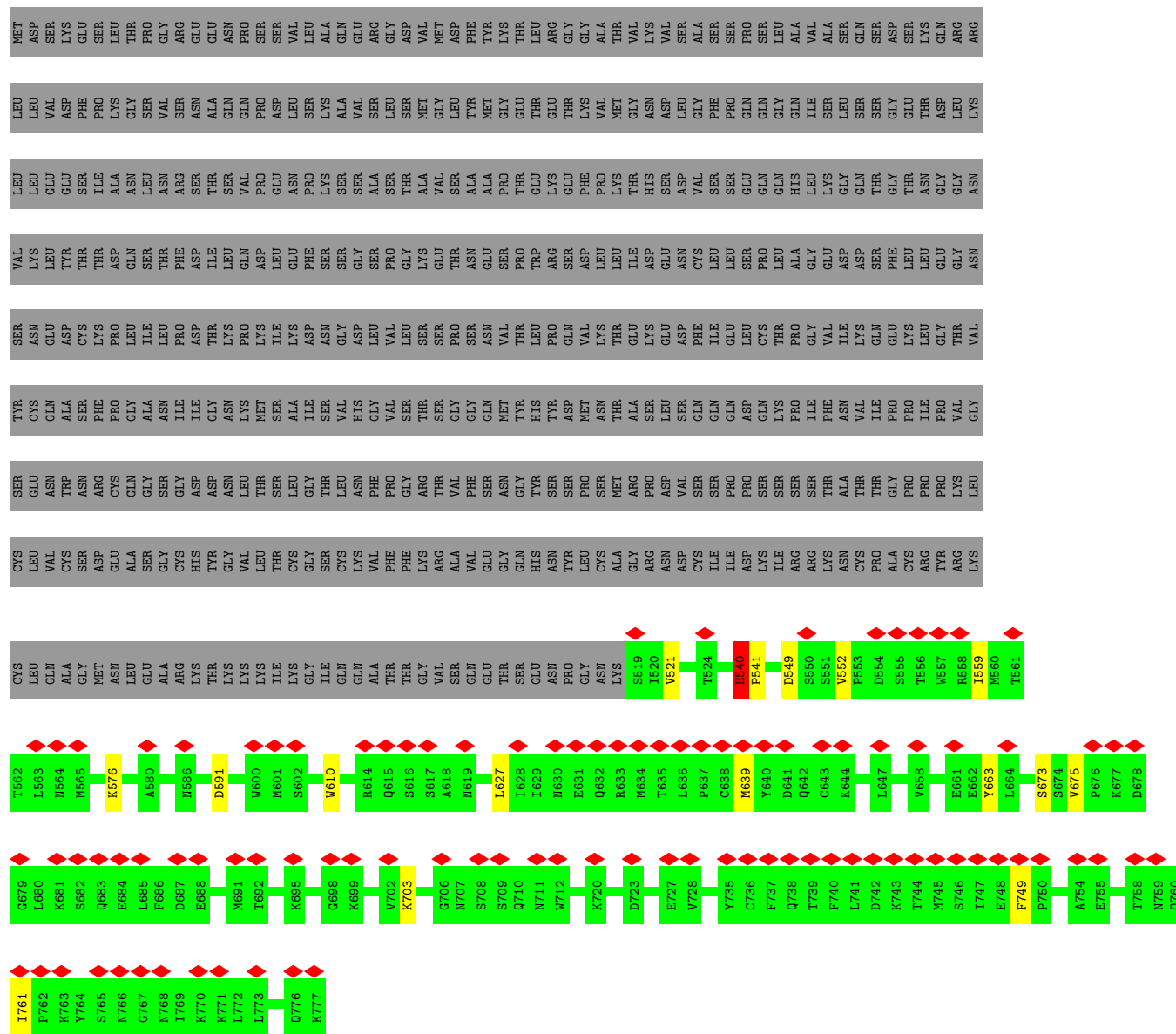
• Molecule 1: Heat shock protein HSP 90-alpha



• Molecule 2: Heat shock 70 kDa protein 1A



Chain F: 13% 31% 67%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	338.88, 338.88, 338.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ADP, K, MG

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	1.17	5/5138 (0.1%)	1.21	21/6909 (0.3%)
1	B	1.14	3/5179 (0.1%)	1.21	31/6961 (0.4%)
2	C	1.08	4/3998 (0.1%)	1.30	29/5410 (0.5%)
2	D	1.17	4/2986 (0.1%)	1.24	23/4035 (0.6%)
3	E	1.06	4/2706 (0.1%)	1.26	27/3625 (0.7%)
4	F	0.99	2/2148 (0.1%)	1.26	16/2907 (0.6%)
All	All	1.12	22/22155 (0.1%)	1.24	147/29847 (0.5%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	175	GLU	CD-OE1	-9.98	1.06	1.25
2	C	175	GLU	CD-OE2	-9.62	1.07	1.25
2	C	199	ASP	CG-OD1	-9.11	1.08	1.25
2	D	10	ASP	CG-OD2	-9.08	1.08	1.25
2	C	175	GLU	CD-OE1	-8.30	1.09	1.25
2	D	175	GLU	CD-OE2	-8.18	1.09	1.25
4	F	627	LEU	CB-CG	6.89	1.67	1.53
1	B	285	ILE	CB-CG1	6.82	1.67	1.53
3	E	543	ARG	NE-CZ	6.58	1.40	1.33
3	E	268	VAL	CB-CG2	-5.87	1.33	1.52
1	A	285	ILE	CB-CG1	5.65	1.64	1.53
1	A	59	ILE	CB-CG1	-5.58	1.42	1.53
3	E	521	HIS	CB-CG	-5.51	1.42	1.50
2	C	10	ASP	CG-OD2	-5.48	1.15	1.25
4	F	639	MET	CG-SD	-5.47	1.67	1.80
1	B	640	HIS	CB-CG	-5.34	1.42	1.50
1	A	507	PHE	CB-CG	-5.31	1.38	1.50
1	B	340	LEU	CB-CG	-5.31	1.42	1.53
3	E	404	TYR	CG-CD1	-5.28	1.28	1.39
1	A	340	LEU	CB-CG	-5.26	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	633	HIS	CB-CG	-5.15	1.43	1.50
2	D	175	GLU	C-N	5.04	1.40	1.33

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	390	ASN	CA-C-N	9.81	129.56	119.56
3	E	390	ASN	C-N-CA	9.81	129.56	119.56
3	E	424	GLU	CA-C-N	7.81	127.52	119.56
3	E	424	GLU	C-N-CA	7.81	127.52	119.56
1	B	343	VAL	CA-C-N	7.75	127.70	120.03
1	B	343	VAL	C-N-CA	7.75	127.70	120.03
1	A	59	ILE	CB-CA-C	-7.65	102.00	112.02
2	C	29	ILE	N-CA-C	7.55	118.75	108.17
1	A	300	ASN	CA-C-N	7.49	127.20	119.56
1	A	300	ASN	C-N-CA	7.49	127.20	119.56
1	B	66	ASP	CA-C-N	7.42	127.09	119.82
1	B	66	ASP	C-N-CA	7.42	127.09	119.82
2	C	240	HIS	CA-CB-CG	7.40	121.20	113.80
1	A	66	ASP	CA-C-N	7.37	127.08	119.56
1	A	66	ASP	C-N-CA	7.37	127.08	119.56
3	E	524	ASN	CA-C-N	7.30	127.94	119.47
3	E	524	ASN	C-N-CA	7.30	127.94	119.47
2	C	233	PHE	N-CA-C	-7.25	103.09	112.23
1	B	360	ASN	N-CA-C	7.13	120.59	110.68
4	F	552	VAL	CA-C-N	7.11	127.27	120.31
4	F	552	VAL	C-N-CA	7.11	127.27	120.31
4	F	761	ILE	CB-CA-C	-7.08	106.98	113.70
4	F	749	PHE	CA-C-N	6.96	126.92	120.03
4	F	749	PHE	C-N-CA	6.96	126.92	120.03
1	B	680	ASP	CA-C-N	6.92	126.61	119.56
1	B	680	ASP	C-N-CA	6.92	126.61	119.56
1	B	169	SER	N-CA-C	6.90	119.82	108.99
1	B	109	THR	CA-C-N	-6.83	115.23	121.65
1	B	109	THR	C-N-CA	-6.83	115.23	121.65
1	A	680	ASP	CA-CB-CG	-6.81	105.79	112.60
2	C	95	ILE	N-CA-C	6.78	117.66	108.17
4	F	521	VAL	CA-C-N	6.70	126.64	120.21
4	F	521	VAL	C-N-CA	6.70	126.64	120.21
2	C	278	THR	N-CA-C	-6.55	105.02	114.12
3	E	530	LYS	N-CA-C	-6.54	103.64	111.69
1	A	343	VAL	CA-C-N	6.53	126.50	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	VAL	C-N-CA	6.53	126.50	120.03
2	D	90	TRP	CA-C-N	6.42	126.04	119.56
2	D	90	TRP	C-N-CA	6.42	126.04	119.56
2	C	335	VAL	N-CA-C	6.09	116.64	108.11
2	D	137	TYR	CA-C-N	6.00	125.94	119.76
2	D	137	TYR	C-N-CA	6.00	125.94	119.76
3	E	218	LEU	CA-C-N	5.98	125.94	119.78
3	E	218	LEU	C-N-CA	5.98	125.94	119.78
2	C	500	LYS	N-CA-C	5.96	117.30	108.60
2	C	435	GLN	CA-C-N	5.96	127.06	120.45
2	C	435	GLN	C-N-CA	5.96	127.06	120.45
1	B	349	PHE	CA-C-N	5.94	130.20	120.63
1	B	349	PHE	C-N-CA	5.94	130.20	120.63
3	E	255	ASP	CA-C-N	5.91	125.53	119.56
3	E	255	ASP	C-N-CA	5.91	125.53	119.56
1	B	300	ASN	CA-C-N	5.90	127.22	119.84
1	B	300	ASN	C-N-CA	5.90	127.22	119.84
2	C	187	ARG	CA-C-N	5.90	132.80	121.54
2	C	187	ARG	C-N-CA	5.90	132.80	121.54
1	B	398	ILE	N-CA-C	5.89	116.78	108.36
4	F	639	MET	CA-C-N	5.88	128.75	120.28
4	F	639	MET	C-N-CA	5.88	128.75	120.28
1	A	398	ILE	N-CA-C	5.86	116.75	108.36
3	E	514	ASP	CA-C-N	5.84	125.52	119.56
3	E	514	ASP	C-N-CA	5.84	125.52	119.56
2	D	233	PHE	N-CA-C	-5.82	104.53	111.69
2	D	177	THR	N-CA-C	-5.82	105.01	111.36
2	C	296	SER	N-CA-C	5.79	117.87	109.07
2	C	142	ALA	N-CA-C	5.78	117.86	109.07
4	F	540	GLU	CA-C-N	5.77	125.73	119.78
4	F	540	GLU	C-N-CA	5.77	125.73	119.78
4	F	675	VAL	CA-C-N	5.77	125.72	119.78
4	F	675	VAL	C-N-CA	5.77	125.72	119.78
2	C	38	THR	CA-C-N	5.77	125.70	119.76
2	C	38	THR	C-N-CA	5.77	125.70	119.76
1	B	394	LEU	CA-C-N	5.74	125.69	119.78
1	B	394	LEU	C-N-CA	5.74	125.69	119.78
4	F	591	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	637	ASN	CA-C-N	5.68	125.30	119.56
1	B	637	ASN	C-N-CA	5.68	125.30	119.56
1	A	152	THR	N-CA-C	5.67	118.70	109.06
3	E	359	LEU	N-CA-C	-5.67	105.09	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	GLU	N-CA-C	-5.66	104.73	111.69
2	C	199	ASP	OD1-CG-OD2	-5.65	109.34	122.90
2	C	90	TRP	CA-C-N	5.63	125.72	119.87
2	C	90	TRP	C-N-CA	5.63	125.72	119.87
1	B	358	LYS	CA-C-N	5.61	131.81	121.70
1	B	358	LYS	C-N-CA	5.61	131.81	121.70
2	C	168	ASN	CA-C-N	-5.58	114.08	122.01
2	C	168	ASN	C-N-CA	-5.58	114.08	122.01
2	C	199	ASP	CA-CB-CG	5.58	118.18	112.60
2	D	198	PHE	CA-CB-CG	5.58	119.38	113.80
2	C	343	ILE	CA-C-N	5.57	125.94	119.47
2	C	343	ILE	C-N-CA	5.57	125.94	119.47
1	B	589	SER	N-CA-C	5.57	118.52	110.28
1	B	625	MET	N-CA-C	5.56	117.97	108.90
1	A	378	ILE	CA-C-N	5.56	125.53	120.03
1	A	378	ILE	C-N-CA	5.56	125.53	120.03
3	E	322	PHE	CA-CB-CG	-5.54	108.26	113.80
1	B	386	ARG	CA-C-N	-5.54	113.27	120.91
1	B	386	ARG	C-N-CA	-5.54	113.27	120.91
1	B	96	ILE	N-CA-C	5.52	117.95	111.05
1	A	178	GLU	CA-C-N	5.48	125.95	120.14
1	A	178	GLU	C-N-CA	5.48	125.95	120.14
2	D	343	ILE	CA-C-N	5.46	125.81	119.47
2	D	343	ILE	C-N-CA	5.46	125.81	119.47
1	A	637	ASN	CA-C-N	5.45	125.06	119.56
1	A	637	ASN	C-N-CA	5.45	125.06	119.56
2	C	137	TYR	CA-C-N	5.42	125.68	119.83
2	C	137	TYR	C-N-CA	5.42	125.68	119.83
2	C	177	THR	N-CA-C	-5.41	105.46	111.36
3	E	481	SER	CA-C-N	5.40	125.06	119.56
3	E	481	SER	C-N-CA	5.40	125.06	119.56
2	D	364	ASN	CA-C-N	5.38	125.04	119.56
2	D	364	ASN	C-N-CA	5.38	125.04	119.56
1	A	429	GLU	N-CA-C	-5.37	103.45	110.53
3	E	356	ASN	CA-C-N	5.36	126.54	119.84
3	E	356	ASN	C-N-CA	5.36	126.54	119.84
4	F	673	SER	N-CA-C	5.36	119.54	112.89
2	D	192	GLU	N-CA-C	-5.36	103.32	110.55
1	B	337	PHE	CA-CB-CG	5.34	119.14	113.80
2	D	80	ASP	CA-C-N	5.31	125.63	119.47
2	D	80	ASP	C-N-CA	5.31	125.63	119.47
2	D	142	ALA	N-CA-C	5.31	117.46	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	233	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	445	ILE	N-CA-C	-5.27	105.58	110.53
1	B	588	VAL	CA-C-N	5.26	128.34	120.87
1	B	588	VAL	C-N-CA	5.26	128.34	120.87
4	F	559	ILE	N-CA-C	-5.25	104.33	111.89
3	E	268	VAL	CB-CA-C	-5.24	105.16	112.02
2	C	62	ASN	CA-CB-CG	5.24	117.84	112.60
3	E	299	ILE	N-CA-C	-5.22	105.44	110.72
2	D	284	ILE	N-CA-C	5.19	115.32	107.75
3	E	484	ASP	N-CA-C	-5.15	105.74	111.36
1	A	451	GLU	N-CA-C	5.14	119.54	113.12
2	D	103	VAL	N-CA-C	5.11	115.21	107.80
3	E	492	ASP	CA-C-N	5.11	126.22	119.84
3	E	492	ASP	C-N-CA	5.11	126.22	119.84
1	A	88	THR	N-CA-C	5.11	116.95	109.24
2	D	115	TYR	CA-C-N	5.10	125.38	119.47
2	D	115	TYR	C-N-CA	5.10	125.38	119.47
3	E	462	LYS	N-CA-C	5.09	116.52	111.07
2	D	168	ASN	CA-C-N	-5.09	114.67	121.80
2	D	168	ASN	C-N-CA	-5.09	114.67	121.80
3	E	517	ALA	N-CA-C	-5.08	105.74	111.28
1	B	22	PHE	N-CA-C	5.06	118.31	110.17
2	C	383	ASP	N-CA-C	5.04	117.41	109.39
2	C	103	VAL	N-CA-C	5.03	115.09	107.80
2	D	20	VAL	CA-C-N	-5.02	116.31	122.84
2	D	20	VAL	C-N-CA	-5.02	116.31	122.84
1	B	597	CYS	N-CA-C	5.01	115.76	108.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5056	5101	5099	5	0
1	B	5098	5135	5132	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3938	3959	3958	8	0
2	D	2938	2944	2943	12	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	41	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 (41) 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:CG	7:D:703:K:K	1.82	1.15
2:D:10:ASP:OD2	7:D:703:K:K	1.56	1.14
2:C:10:ASP:CG	7:C:703:K:K	1.99	0.99
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:363:ILE:O	2:C:364:ASN:C	2.59	0.45
2:C:245:PHE:CD2	2:C:245:PHE:C	2.95	0.44
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
2:D:151:ASN:OD1	2:D:151:ASN:C	2.61	0.43
4:F:610:TRP:HB2	4:F:663:TYR:CE1	2.53	0.43
4:F:549:ASP:OD2	4:F:576:LYS:NZ	2.52	0.43
2:D:96:ASN:OD1	2:D:96:ASN:C	2.62	0.42
2:D:363:ILE:O	2:D:364:ASN:C	2.61	0.42
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
1:B:127:ASP:CG	1:B:128:ILE:N	2.79	0.40
2:D:327:ASP:C	2:D:327:ASP:OD1	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
3	E	325/543 (60%)	323 (99%)	2 (1%)	0	100	100
4	F	257/777 (33%)	252 (98%)	4 (2%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	564 (100%)	0	100	100
1	B	569/666 (85%)	569 (100%)	0	100	100
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%)	238 (100%)	0	100	100
All	All	2393/3550 (67%)	2393 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	ASN
1	A	106	ASN
1	A	194	GLN
1	A	501	GLN
1	A	655	ASN
1	A	682	GLN
1	B	79	ASN
1	B	123	GLN

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Mol	Chain	Res	Type
1	B	194	GLN
1	B	360	ASN
1	B	450	HIS
1	B	454	GLN
2	C	227	HIS
2	C	434	ASN
3	E	368	ASN
3	E	372	GLN
3	E	378	GLN
3	E	452	GLN
3	E	475	GLN
4	F	775	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	701	-	28,29,29	1.98	7 (25%)	43,45,45	1.68	8 (18%)
5	ADP	D	701	6	28,29,29	2.07	8 (28%)	43,45,45	1.74	8 (18%)

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	C	701	-	-	7/16/32/32	0/3/3/3
5	ADP	D	701	6	-	3/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	701	ADP	C5-C4	5.79	1.49	1.39
5	D	701	ADP	C5-C4	5.64	1.49	1.39
5	D	701	ADP	C4-N3	4.06	1.42	1.34
5	D	701	ADP	C2-N3	3.87	1.40	1.33
5	C	701	ADP	C4-N3	3.81	1.41	1.34
5	C	701	ADP	C2-N3	3.58	1.40	1.33
5	C	701	ADP	C5-C6	3.50	1.50	1.41
5	D	701	ADP	C2-N1	3.31	1.39	1.33
5	D	701	ADP	C5-C6	3.20	1.49	1.41
5	C	701	ADP	C2-N1	2.62	1.38	1.33
5	D	701	ADP	C5-N7	-2.56	1.34	1.39
5	D	701	ADP	C8-N7	2.33	1.36	1.31
5	C	701	ADP	C8-N7	2.33	1.36	1.31
5	C	701	ADP	C5-N7	-2.24	1.35	1.39
5	D	701	ADP	PA-O3A	2.12	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	ADP	C5-C4-N3	-4.85	120.04	126.72
5	D	701	ADP	N3-C4-N9	4.62	135.02	127.17
5	C	701	ADP	C5-C4-N3	-4.50	120.53	126.72
5	C	701	ADP	N3-C4-N9	4.25	134.39	127.17
5	D	701	ADP	N3-C2-N1	-4.09	122.39	128.58
5	C	701	ADP	N3-C2-N1	-3.66	123.05	128.58
5	D	701	ADP	C2-N3-C4	3.19	119.63	111.83
5	C	701	ADP	C2-N3-C4	3.05	119.27	111.83
5	C	701	ADP	C4-N9-C8	2.46	108.32	105.74
5	D	701	ADP	C5-C6-N6	-2.45	117.23	123.29
5	D	701	ADP	C5-N7-C8	2.44	107.29	103.45
5	D	701	ADP	N6-C6-N1	2.21	123.30	118.38
5	D	701	ADP	C4-N9-C8	2.20	108.05	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	701	ADP	C5-N7-C8	2.18	106.88	103.45
5	C	701	ADP	O3A-PA-O1A	-2.11	104.36	110.70
5	C	701	ADP	O2A-PA-O1A	2.09	122.18	112.44

There are no chirality outliers.

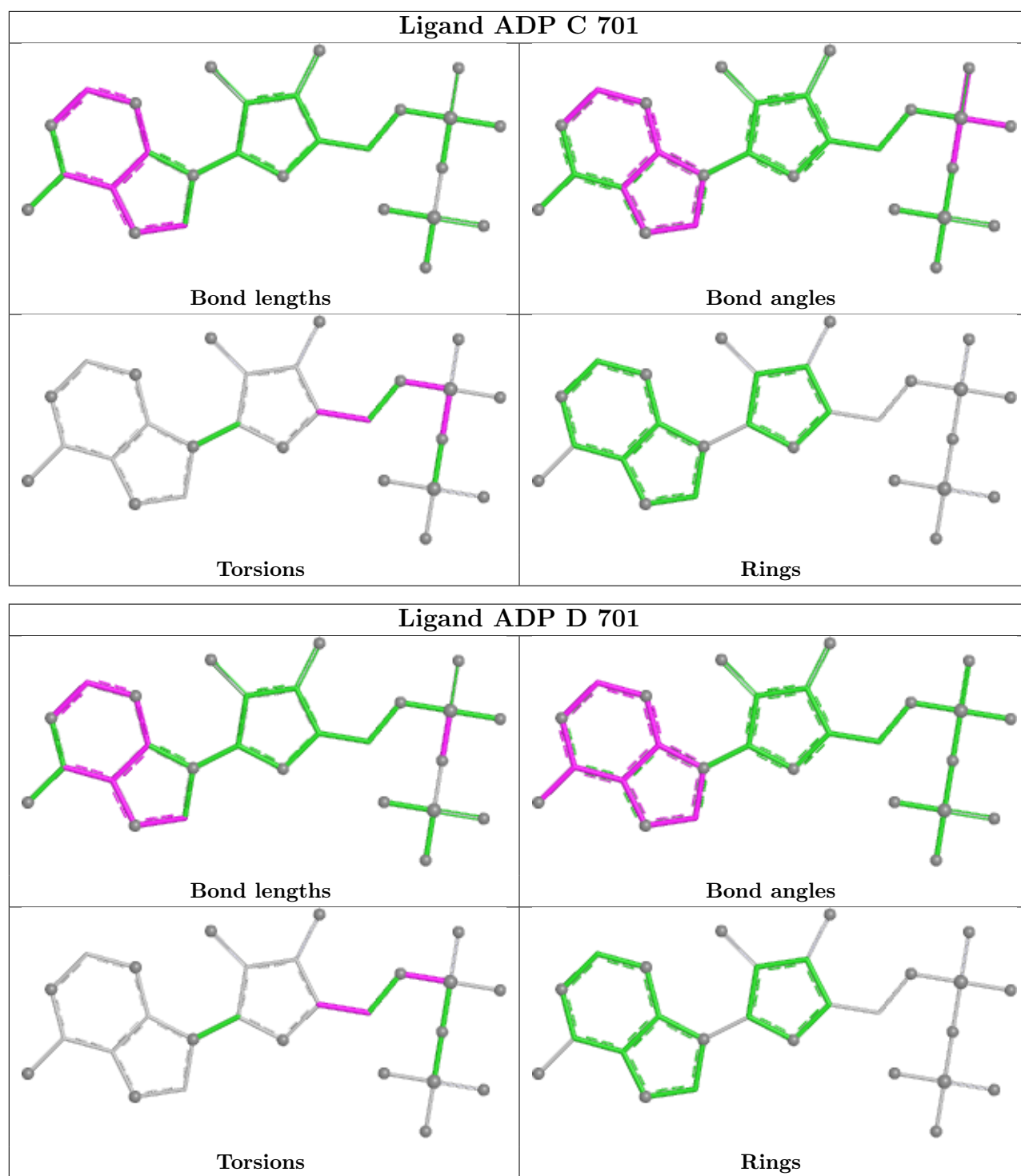
All (10) torsion outliers are listed below:

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	C5'-O5'-PA-O3A
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	D	701	ADP	C5'-O5'-PA-O1A
5	C	701	ADP	PB-O3A-PA-O1A
5	C	701	ADP	PB-O3A-PA-O2A

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

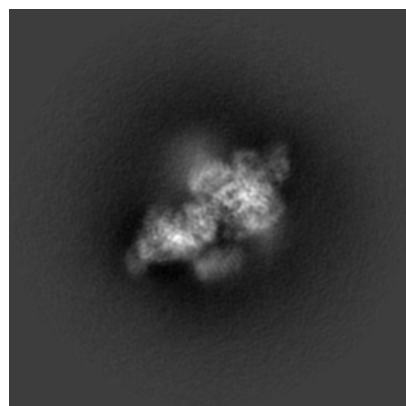
6 Map visualisation [i](#)

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.

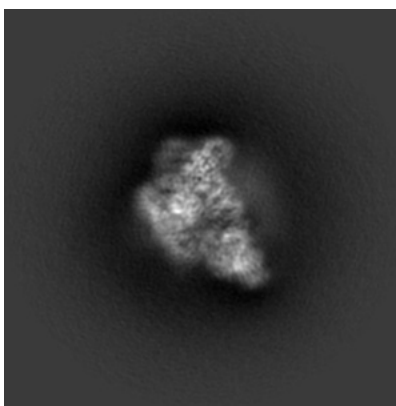
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

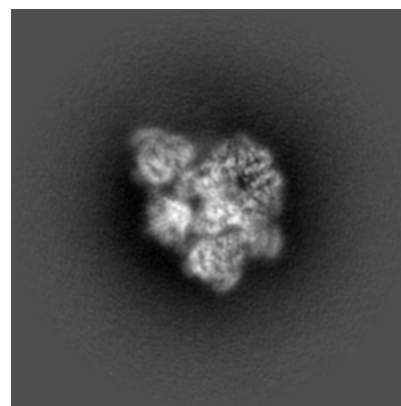
6.1.1 Primary map



X

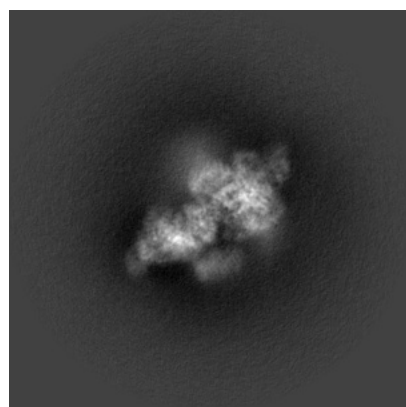


Y

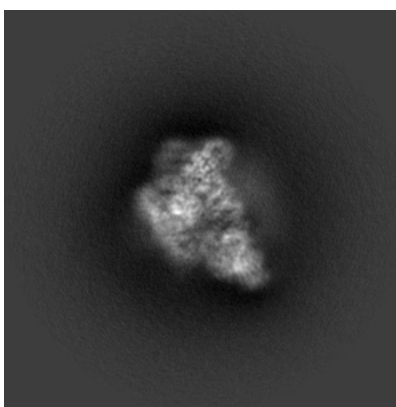


Z

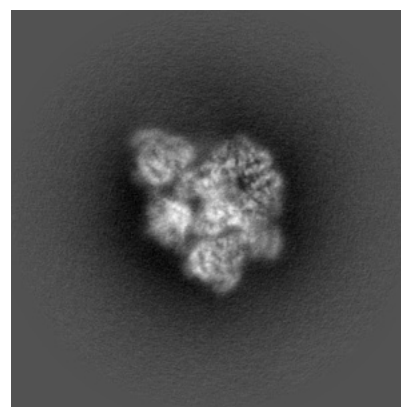
6.1.2 Raw map



X



Y

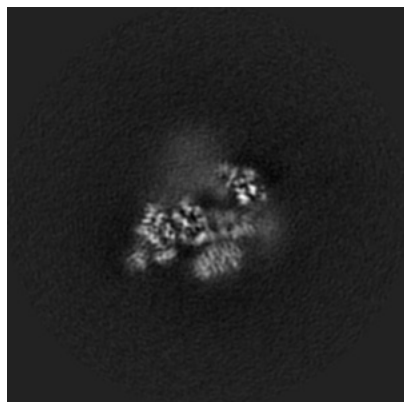


Z

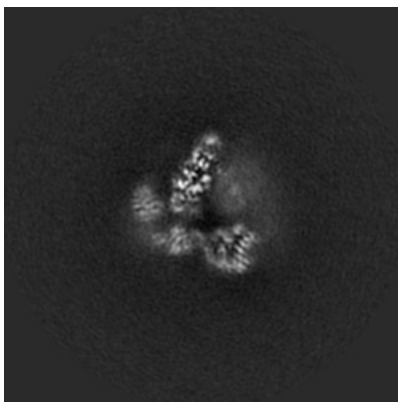
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

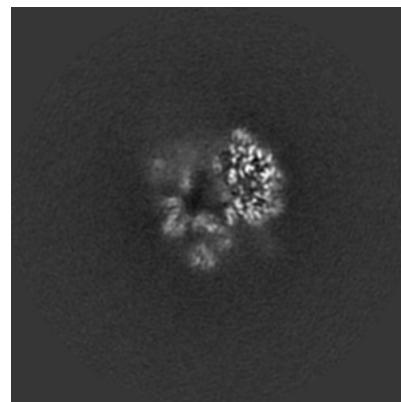
6.2.1 Primary map



X Index: 160

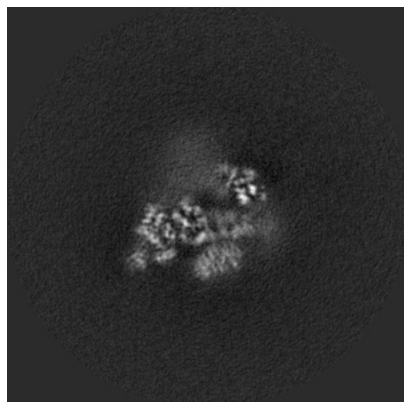


Y Index: 160

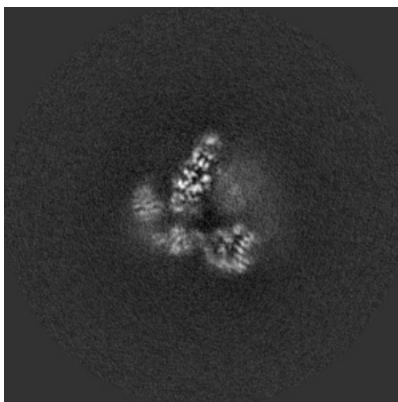


Z Index: 160

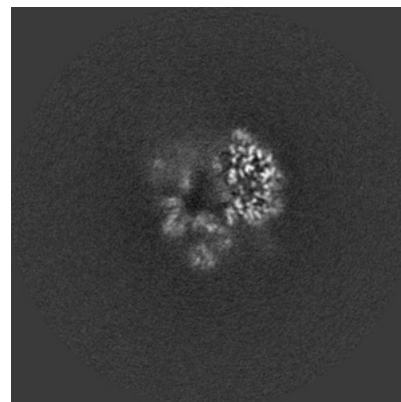
6.2.2 Raw map



X Index: 160



Y Index: 160

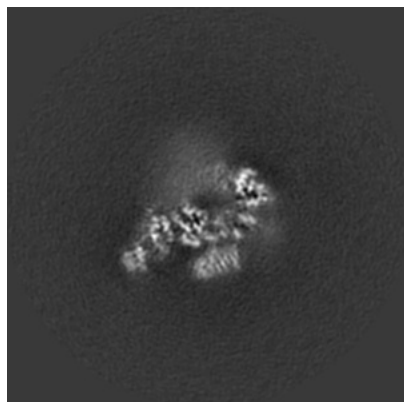


Z Index: 160

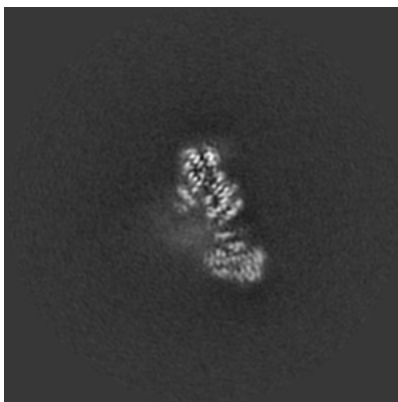
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

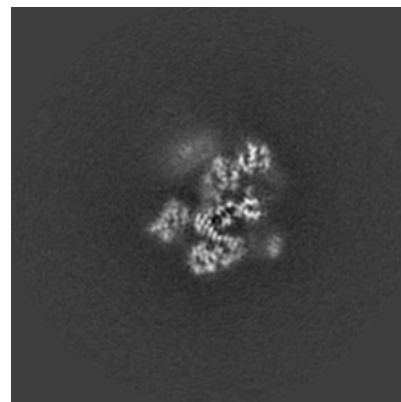
6.3.1 Primary map



X Index: 164

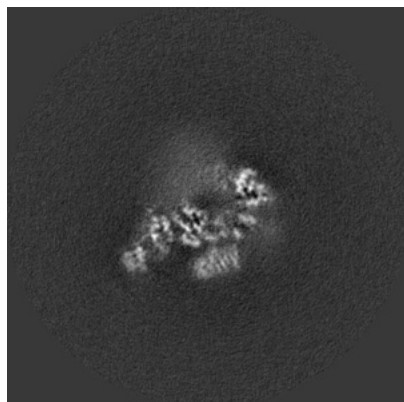


Y Index: 194

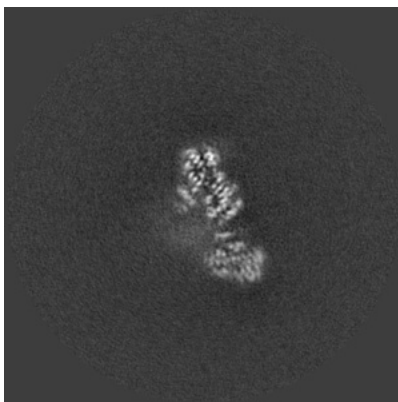


Z Index: 148

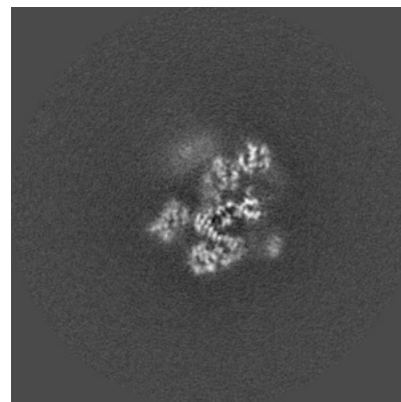
6.3.2 Raw map



X Index: 164



Y Index: 194

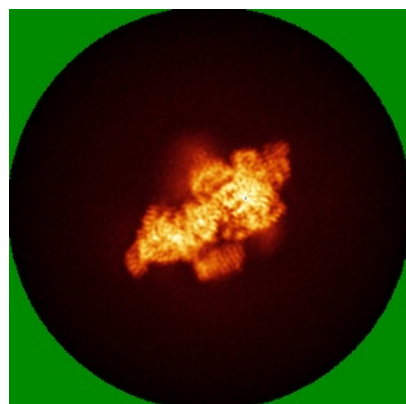


Z Index: 148

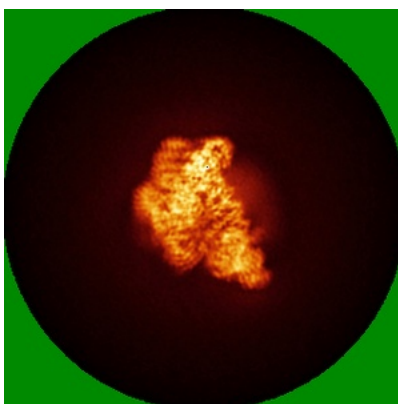
The images above show the largest variance slices of the map in three orthogonal directions.

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

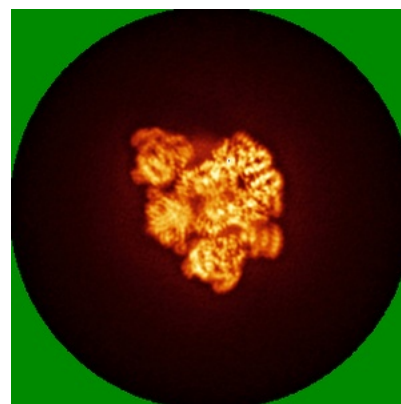
6.4.1 Primary map



X

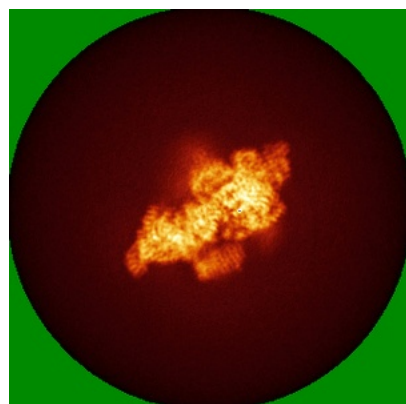


Y

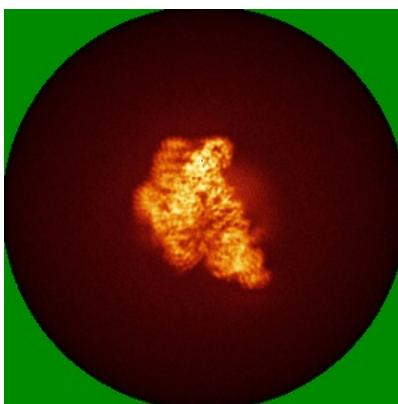


Z

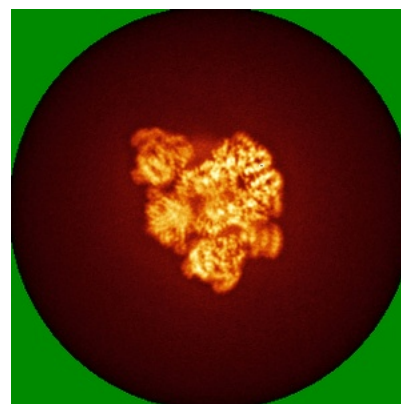
6.4.2 Raw map



X



Y



Z

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

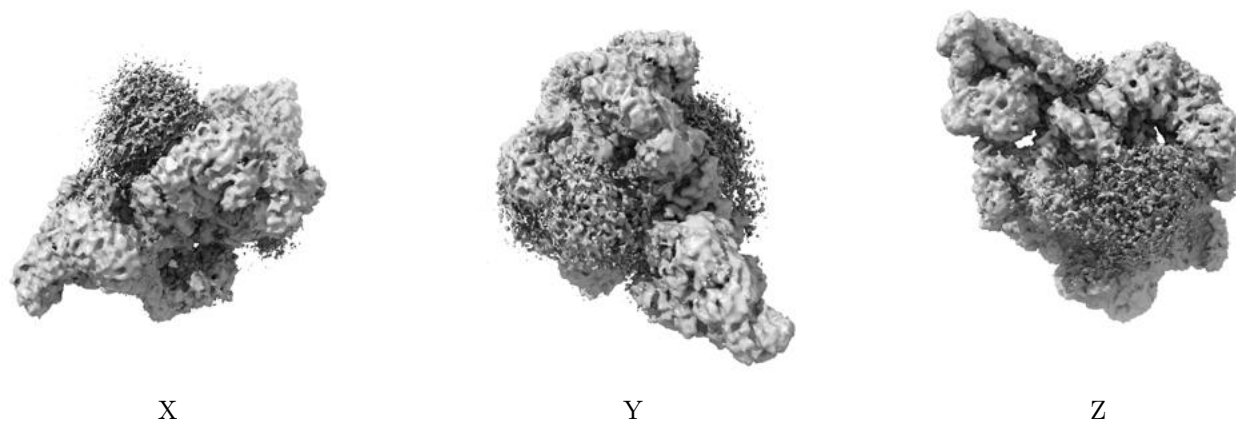
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

6.5.2 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.

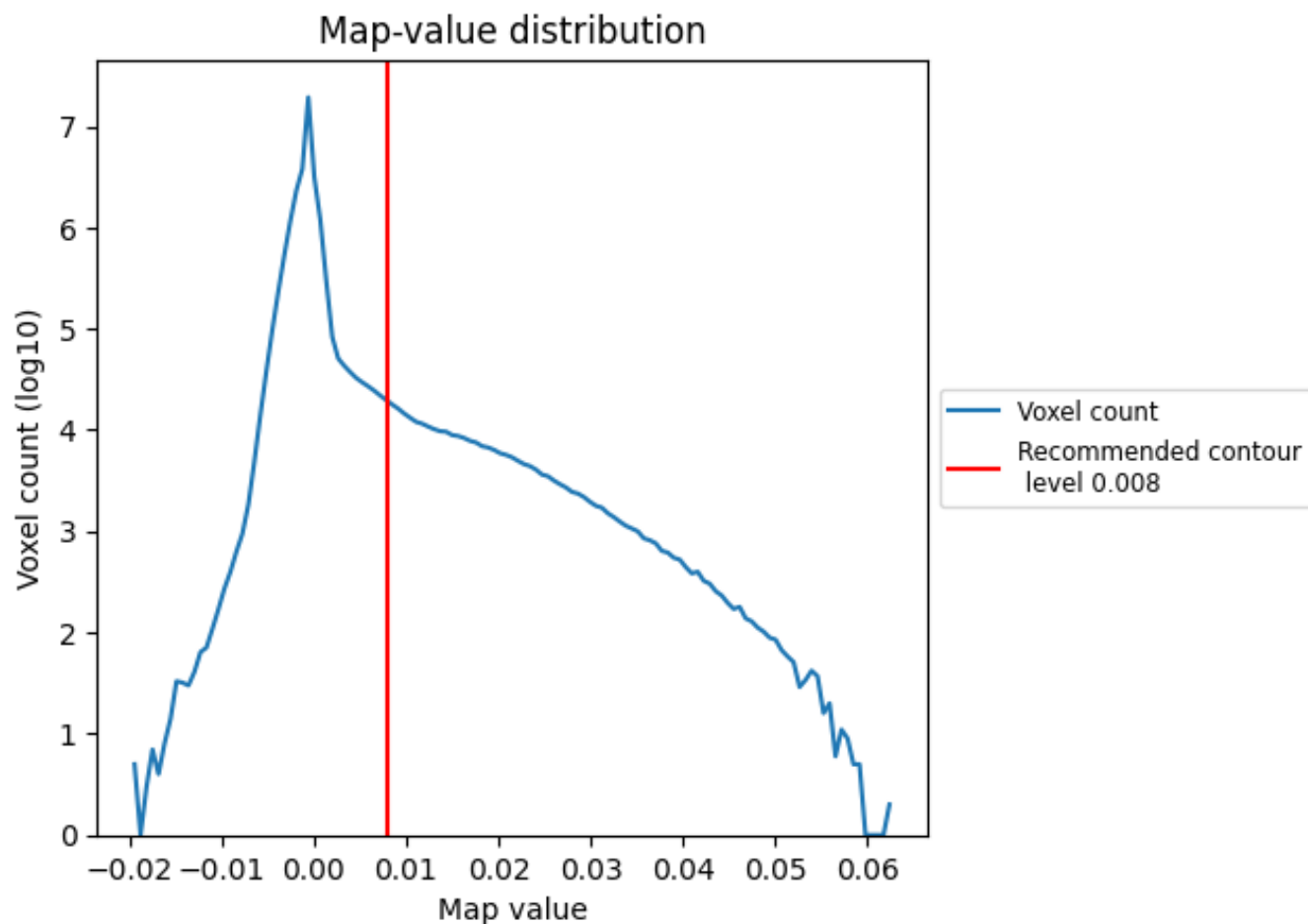
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

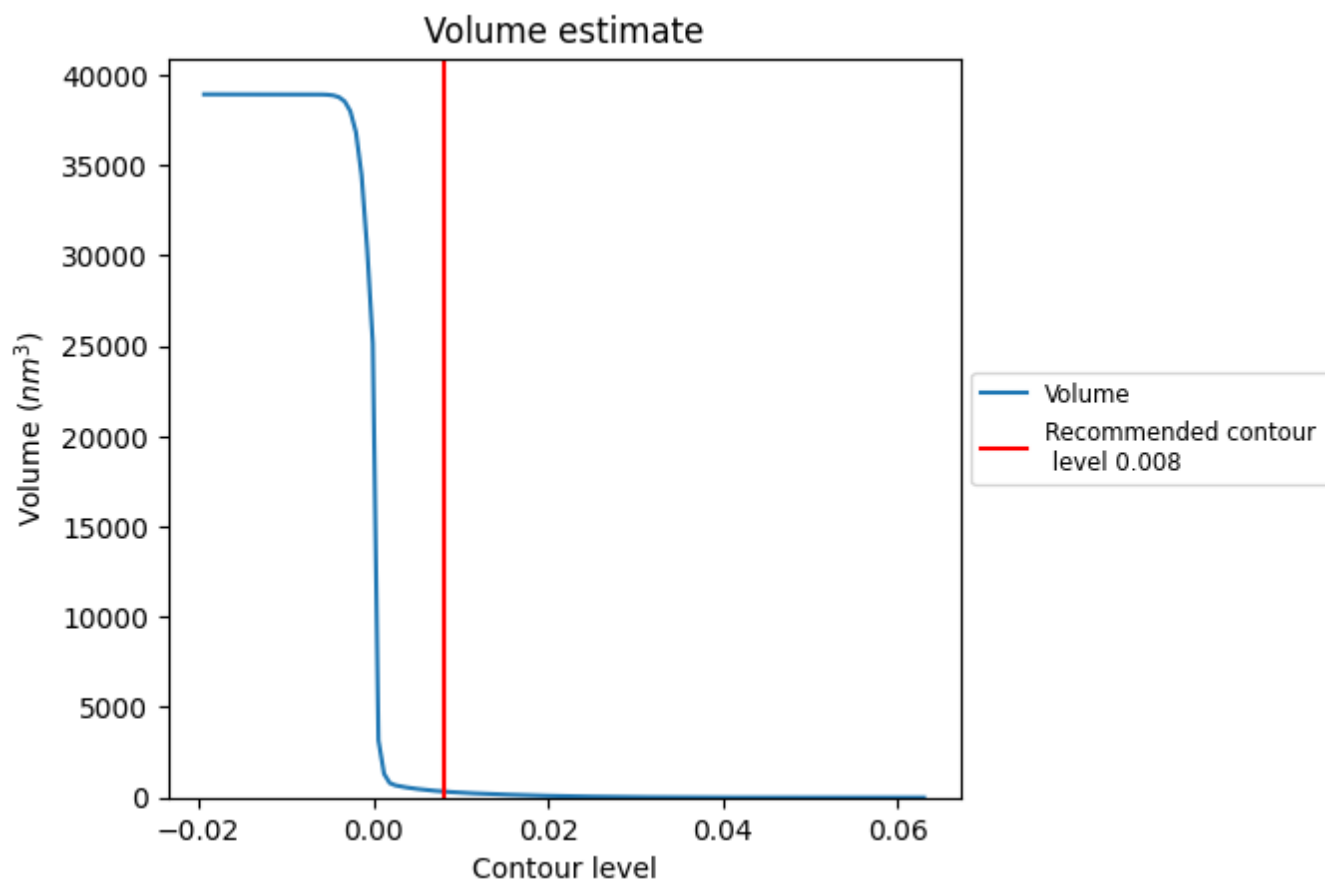
This section contains the results of statistical analysis of the map.

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.

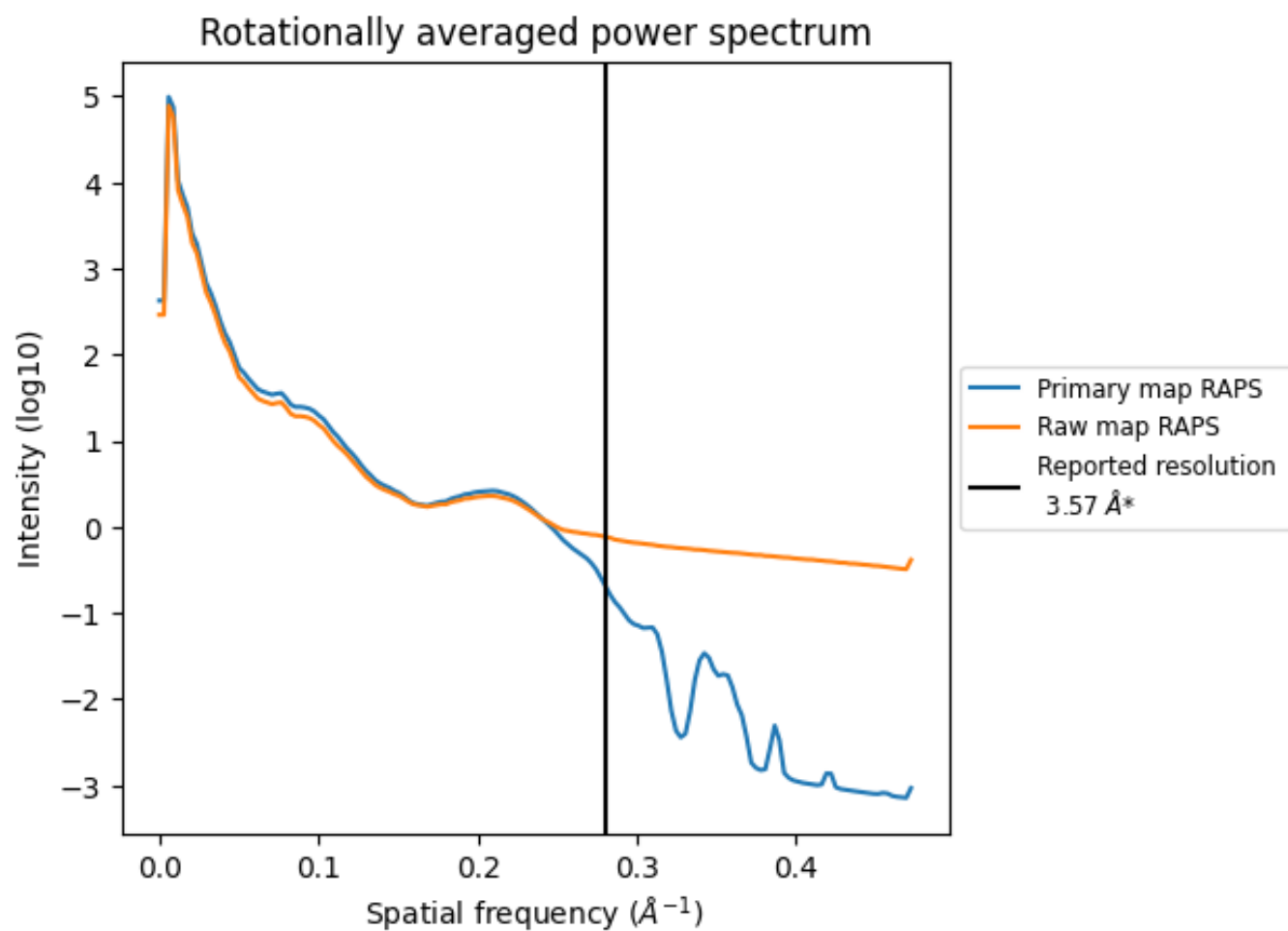
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

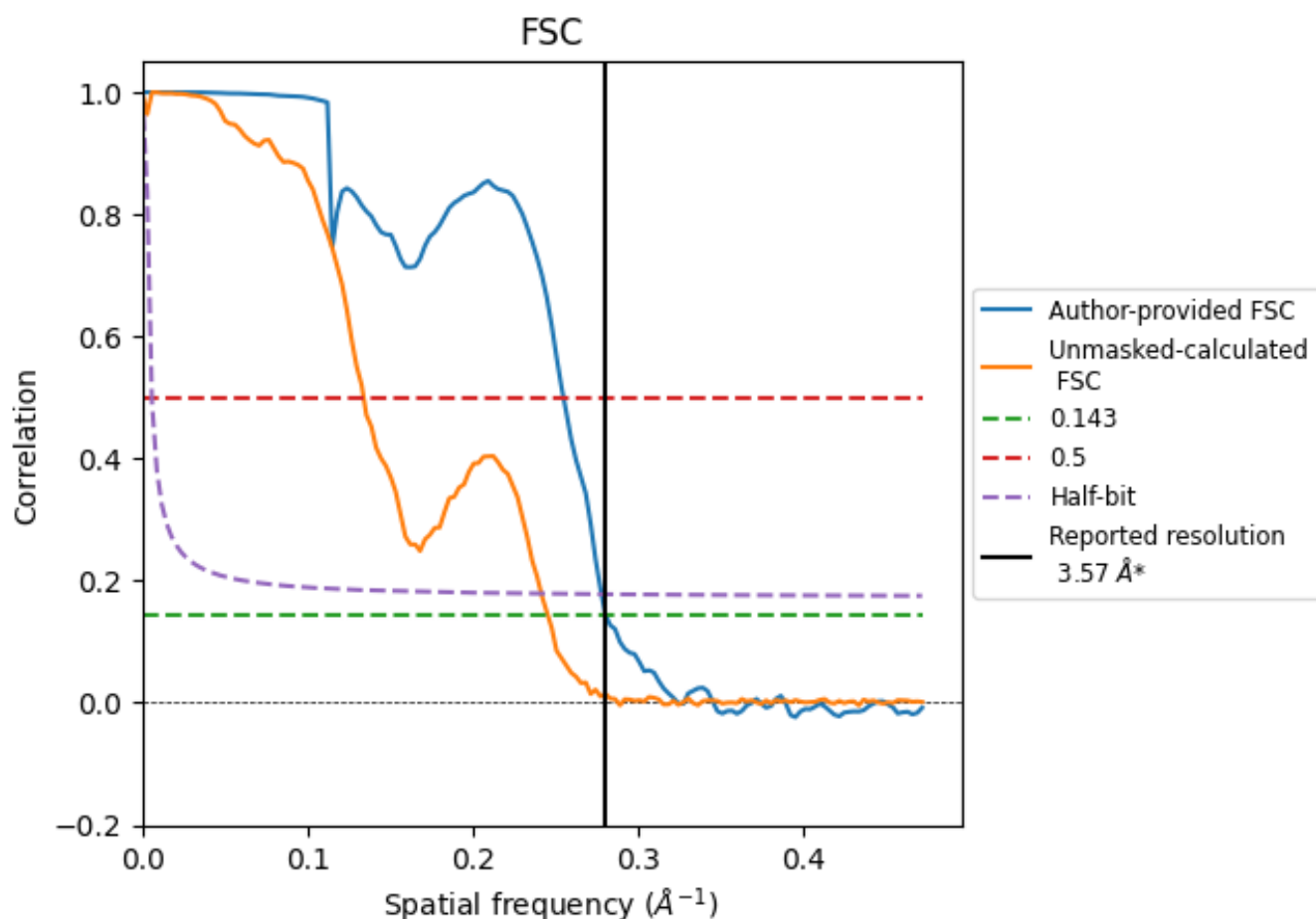


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.280 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

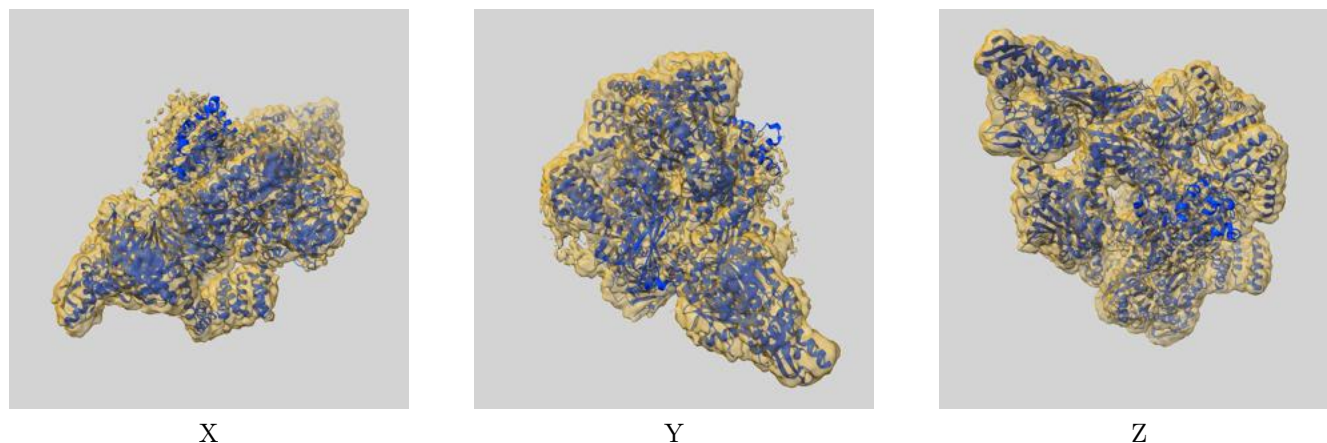
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.56	3.92	3.60
Unmasked-calculated*	4.07	7.46	4.14

*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 [i](#)

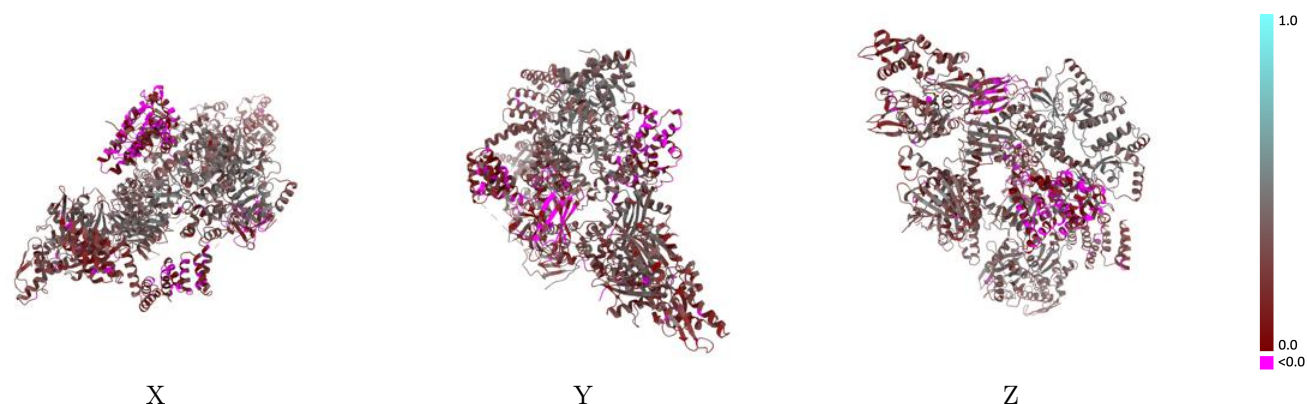
This section contains information regarding the fit between EMDB map EMD-23050 and PDB model 7KW7. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



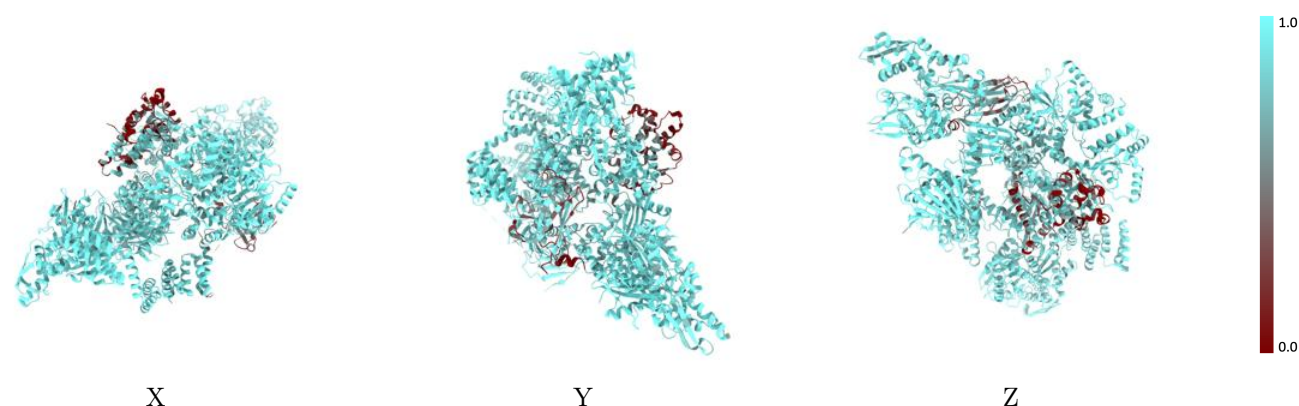
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



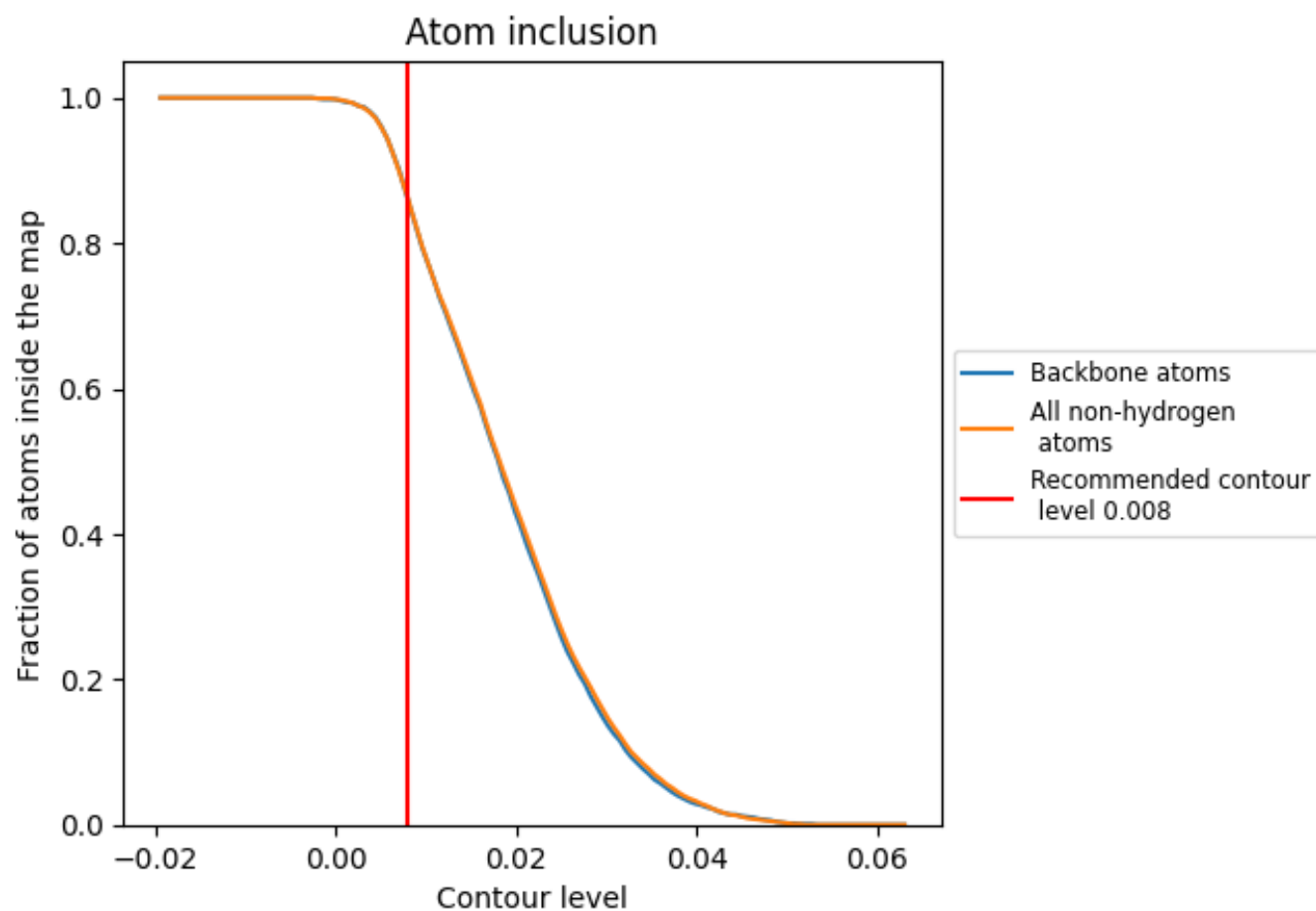
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion ⓘ



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	0.8620	0.2760
A	0.9240	0.3500
B	0.9190	0.3530
C	0.8160	0.2120
D	0.9500	0.3270
E	0.9330	0.1920
F	0.5310	0.0680

1.0

0.0

<0.0