



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:29 AM UTC

PDB ID : 8FFW / pdb_00008ffw
EMDB ID : EMD-29069
Title : Cryo-EM structure of the GR-Hsp90-FKBP51 complex
Authors : Noddings, C.M.; Agard, D.A.
Deposited on : 2022-12-10
Resolution : 3.23 Å (reported)
Based on initial models : 1EJF, 5FWK, 1M2Z

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

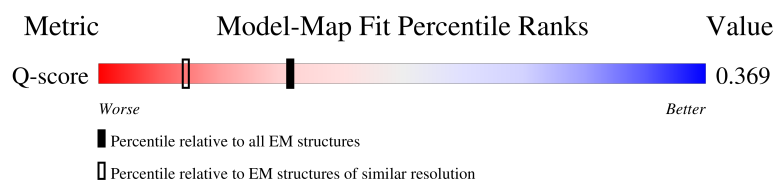
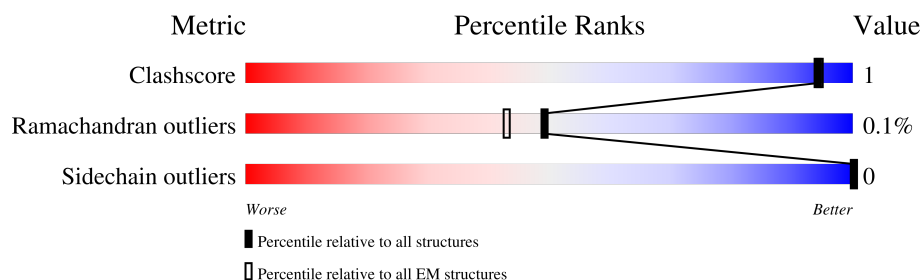
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 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	14612 (2.73 - 3.73)

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	731	
1	B	731	
2	C	360	
3	D	456	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31522 atoms, of which 15767 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	630	Total	C	H	N	O	S	0	0
			10279	3247	5158	859	992	23		
1	B	641	Total	C	H	N	O	S	0	0
			10442	3297	5232	873	1016	24		

- Molecule 2 is a protein called Glucocorticoid receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	259	Total	C	H	N	O	S	0	0
			4235	1355	2132	345	385	18		

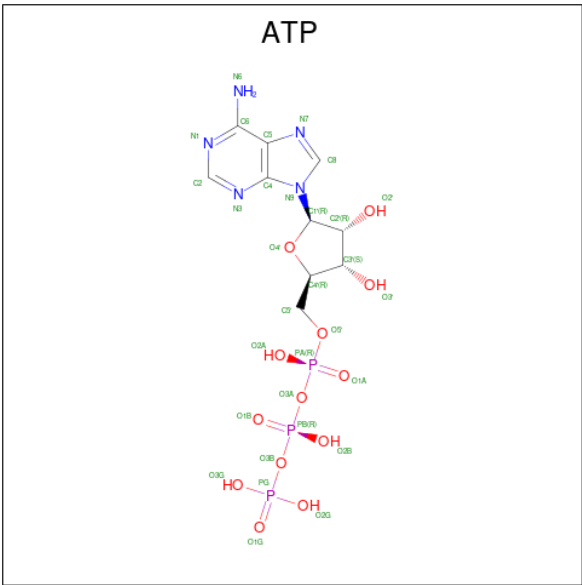
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	602	SER	PHE	engineered mutation	UNP P04150

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP5.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	409	Total	C	H	N	O	S	0	0
			6449	2043	3220	550	616	20		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

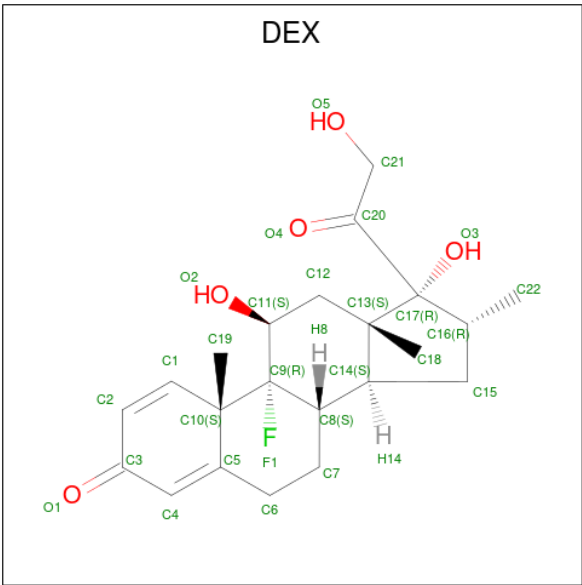


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	

- Molecule 6 is DEXAMETHASONE (CCD ID: DEX) (formula: C₂₂H₂₉FO₅) (labeled as "Ligand of Interest" by depositor).

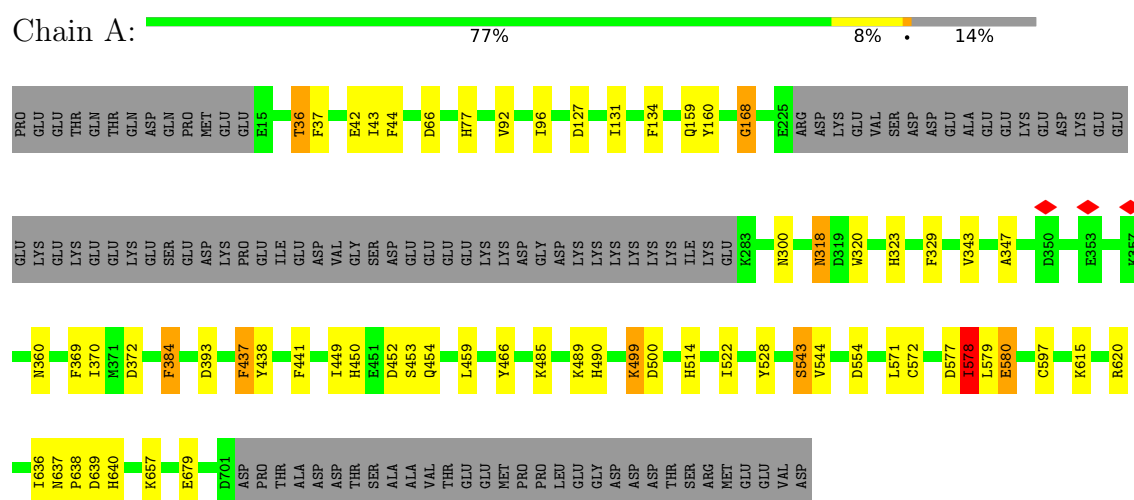


Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	H	O	
6	C	1	29	22	1	1	5	0

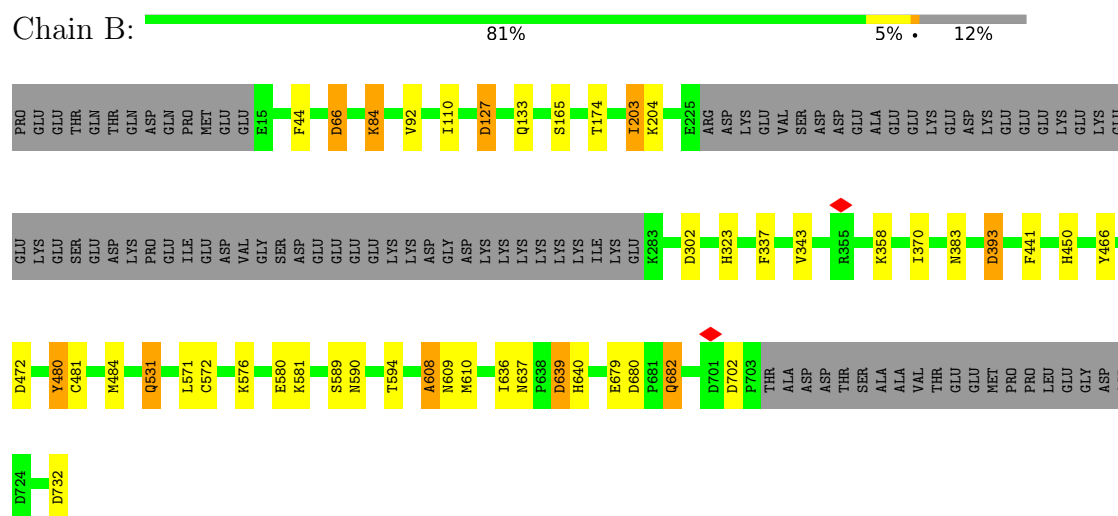
3 Residue-property plots

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

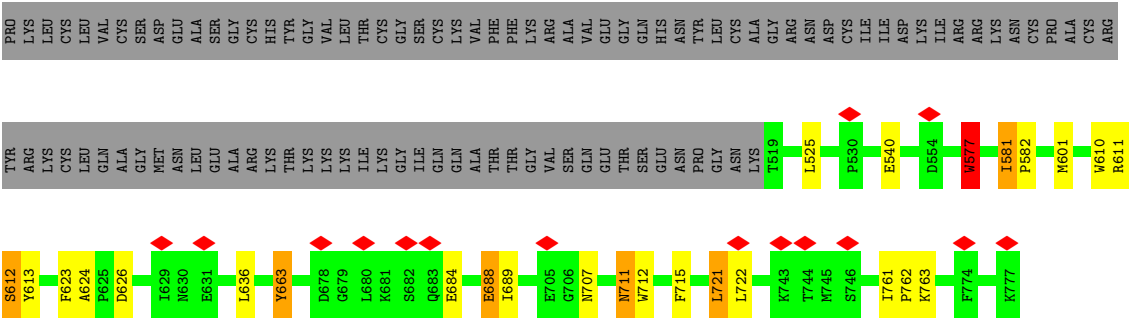


• Molecule 1: Heat shock protein HSP 90-alpha

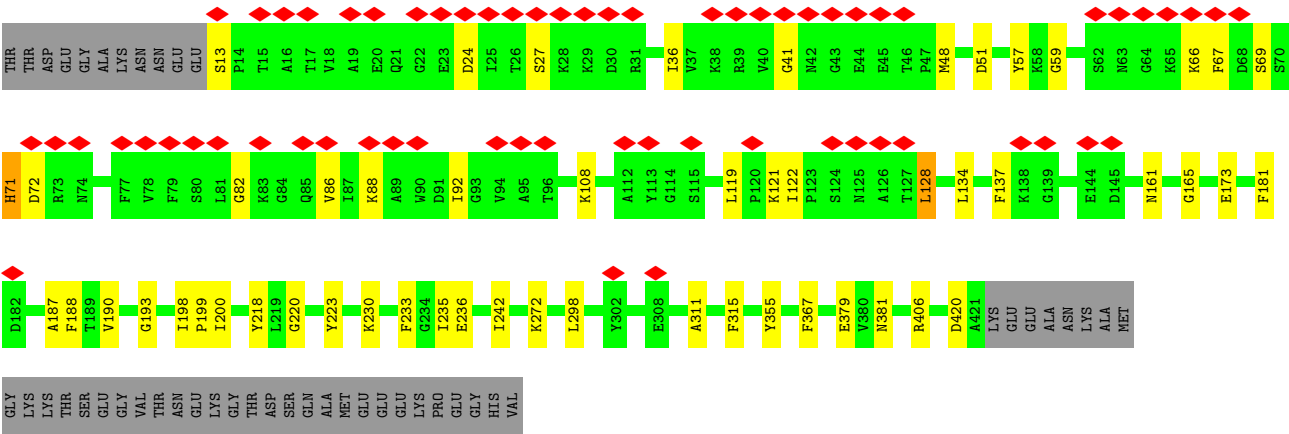
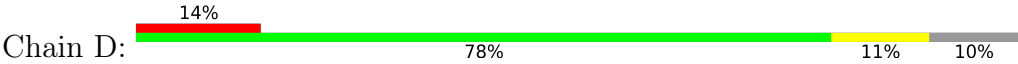


• Molecule 2: Glucocorticoid receptor





● Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171778	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 ($e^-/\text{\AA}^2$)	69, 45.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.315	Depositor
Minimum map value	-0.437	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	267.19998, 267.19998, 267.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8349999, 0.8349999, 0.8349999	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: MG, DEX, ATP

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	1.44	14/5204 (0.3%)	1.37	52/6996 (0.7%)
1	B	1.38	5/5293 (0.1%)	1.39	40/7114 (0.6%)
2	C	1.14	2/2149 (0.1%)	1.33	24/2909 (0.8%)
3	D	1.17	4/3287 (0.1%)	1.57	52/4398 (1.2%)
All	All	1.33	25/15933 (0.2%)	1.41	168/21417 (0.8%)

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
1	B	0	8
2	C	0	5
All	All	0	22

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	71	HIS	CB-CG	-10.41	1.35	1.50
2	C	663	TYR	CB-CG	-7.73	1.34	1.51
1	A	323	HIS	CB-CG	-7.44	1.39	1.50
1	B	337	PHE	CB-CG	-7.24	1.33	1.50
3	D	128	LEU	CB-CG	-7.12	1.39	1.53
1	A	450	HIS	CB-CG	-6.40	1.41	1.50
1	A	369	PHE	CB-CG	-6.21	1.36	1.50
1	A	43	ILE	N-CA	-6.13	1.38	1.46
1	A	329	PHE	CB-CG	-6.04	1.36	1.50
1	A	640	HIS	CB-CG	-5.89	1.42	1.50
1	B	640	HIS	CB-CG	-5.86	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TYR	CB-CG	-5.79	1.39	1.51
1	A	77	HIS	CB-CG	-5.62	1.42	1.50
1	A	437	PHE	CB-CG	-5.55	1.37	1.50
1	A	459	LEU	CB-CG	-5.55	1.42	1.53
1	A	490	HIS	CB-CG	-5.48	1.42	1.50
1	B	450	HIS	CB-CG	-5.37	1.42	1.50
1	B	323	HIS	CB-CG	-5.29	1.42	1.50
3	D	298	LEU	CG-CD1	-5.26	1.35	1.52
1	A	159	GLN	CB-CG	-5.18	1.36	1.52
1	A	466	TYR	CB-CG	-5.14	1.40	1.51
1	A	37	PHE	CB-CG	-5.10	1.39	1.50
3	D	137	PHE	CB-CG	-5.07	1.39	1.50
1	B	466	TYR	CB-CG	-5.06	1.40	1.51
2	C	623	PHE	CB-CG	-5.04	1.39	1.50

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	TYR	CA-C-N	25.22	154.74	120.44
1	A	528	TYR	C-N-CA	25.22	154.74	120.44
3	D	48	MET	CA-C-N	23.62	153.13	122.90
3	D	48	MET	C-N-CA	23.62	153.13	122.90
1	B	484	MET	CA-C-N	20.65	153.36	120.94
1	B	484	MET	C-N-CA	20.65	153.36	120.94
1	B	594	THR	CA-C-N	20.41	149.48	120.49
1	B	594	THR	C-N-CA	20.41	149.48	120.49
3	D	41	GLY	CA-C-N	18.05	154.09	122.32
3	D	41	GLY	C-N-CA	18.05	154.09	122.32
3	D	92	ILE	CA-C-N	17.03	154.78	121.41
3	D	92	ILE	C-N-CA	17.03	154.78	121.41
1	B	302	ASP	CA-C-N	15.44	150.78	122.06
1	B	302	ASP	C-N-CA	15.44	150.78	122.06
2	C	689	ILE	N-CA-C	-12.25	98.59	111.58
3	D	223	TYR	N-CA-C	-8.94	102.95	114.04
2	C	612	SER	CA-C-O	-8.76	111.27	120.55
1	A	578	ILE	CA-C-N	-8.67	110.26	122.74
1	A	578	ILE	C-N-CA	-8.67	110.26	122.74
1	B	680	ASP	CA-C-N	8.65	128.38	119.56
1	B	680	ASP	C-N-CA	8.65	128.38	119.56
1	A	134	PHE	N-CA-C	-8.19	97.80	110.17
1	A	43	ILE	N-CA-C	-8.10	103.25	113.22
2	C	722	LEU	N-CA-C	-7.97	102.45	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	VAL	N-CA-C	-7.96	104.61	112.17
1	A	578	ILE	CA-C-O	-7.80	111.83	121.11
3	D	230	LYS	CA-C-N	7.79	127.43	119.56
3	D	230	LYS	C-N-CA	7.79	127.43	119.56
1	B	343	VAL	CA-C-N	7.72	127.67	120.03
1	B	343	VAL	C-N-CA	7.72	127.67	120.03
2	C	577	TRP	CA-C-O	-7.58	112.86	120.82
1	A	578	ILE	N-CA-C	-7.41	99.13	109.21
1	A	343	VAL	CA-C-N	7.33	127.76	119.92
1	A	343	VAL	C-N-CA	7.33	127.76	119.92
3	D	24	ASP	N-CA-C	7.25	119.90	108.67
1	B	203	ILE	CA-C-O	-7.07	113.60	120.95
3	D	233	PHE	N-CA-C	-7.06	102.78	111.40
1	B	84	LYS	CA-C-O	-7.06	112.94	120.42
1	A	438	TYR	N-CA-C	-7.05	103.35	112.23
2	C	612	SER	CA-C-N	-7.03	109.29	121.66
2	C	612	SER	C-N-CA	-7.03	109.29	121.66
2	C	613	TYR	N-CA-C	-7.00	104.56	113.23
1	A	36	THR	CA-C-N	-6.96	109.89	121.92
1	A	36	THR	C-N-CA	-6.96	109.89	121.92
1	A	437	PHE	CA-C-O	-6.92	113.56	120.82
1	B	370	ILE	CB-CA-C	-6.89	105.86	111.71
1	B	204	LYS	N-CA-C	-6.86	103.25	111.69
1	A	36	THR	CA-C-O	-6.86	111.82	119.78
1	A	320	TRP	N-CA-C	-6.84	105.88	114.56
3	D	119	LEU	N-CA-C	-6.79	101.21	109.83
3	D	381	ASN	CA-C-N	6.74	126.44	119.56
3	D	381	ASN	C-N-CA	6.74	126.44	119.56
1	B	127	ASP	CA-C-N	-6.74	113.28	122.91
1	B	127	ASP	C-N-CA	-6.74	113.28	122.91
3	D	200	ILE	N-CA-C	6.66	119.37	111.05
3	D	59	GLY	N-CA-C	6.65	120.33	110.42
3	D	181	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	637	ASN	CA-C-N	6.49	126.11	119.56
1	B	637	ASN	C-N-CA	6.49	126.11	119.56
3	D	108	LYS	CA-C-N	6.47	126.98	119.47
3	D	108	LYS	C-N-CA	6.47	126.98	119.47
3	D	367	PHE	CA-CB-CG	-6.47	107.33	113.80
1	B	165	SER	N-CA-C	-6.47	100.89	110.46
1	B	639	ASP	CA-C-O	-6.47	112.73	120.55
1	A	441	PHE	N-CA-C	6.45	121.19	112.88
3	D	242	ILE	N-CA-C	6.42	117.10	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	581	ILE	N-CA-C	6.35	114.09	108.63
1	A	639	ASP	N-CA-C	-6.33	105.19	113.17
2	C	540	GLU	CA-C-N	6.33	126.30	120.03
2	C	540	GLU	C-N-CA	6.33	126.30	120.03
1	A	522	ILE	N-CA-C	6.27	117.39	112.12
1	A	92	VAL	N-CA-C	6.21	116.80	108.11
1	A	636	ILE	N-CA-C	6.20	116.86	108.17
1	A	347	ALA	CA-C-N	6.16	126.13	120.03
1	A	347	ALA	C-N-CA	6.16	126.13	120.03
1	B	679	GLU	N-CA-C	6.09	117.92	111.28
1	B	110	ILE	N-CA-C	6.07	116.82	110.62
2	C	688	GLU	CA-C-O	-6.03	112.68	119.79
3	D	86	VAL	N-CA-C	6.02	119.55	113.47
1	A	489	LYS	N-CA-C	-6.00	105.79	114.12
1	A	543	SER	CA-C-O	-5.97	114.41	121.16
1	B	337	PHE	CA-CB-CG	5.95	119.75	113.80
3	D	134	LEU	N-CA-C	5.91	119.89	109.96
2	C	721	LEU	CA-C-O	-5.91	112.82	119.79
3	D	161	ASN	CA-C-N	5.90	125.81	119.85
3	D	161	ASN	C-N-CA	5.90	125.81	119.85
1	A	500	ASP	N-CA-C	-5.87	105.20	112.90
3	D	165	GLY	N-CA-C	-5.87	107.49	114.48
1	B	480	TYR	CA-C-O	-5.86	114.34	120.55
3	D	122	ILE	CA-C-N	5.84	125.80	119.78
3	D	122	ILE	C-N-CA	5.84	125.80	119.78
3	D	128	LEU	N-CA-C	5.84	118.06	109.24
3	D	188	PHE	N-CA-C	5.83	118.91	110.28
3	D	315	PHE	CA-CB-CG	5.82	119.62	113.80
3	D	13	SER	CA-C-N	5.79	126.19	119.47
3	D	13	SER	C-N-CA	5.79	126.19	119.47
1	B	639	ASP	CA-C-N	-5.78	113.56	122.87
1	B	639	ASP	C-N-CA	-5.78	113.56	122.87
3	D	220	GLY	CA-C-N	5.78	125.91	119.32
3	D	220	GLY	C-N-CA	5.78	125.91	119.32
1	B	127	ASP	CA-C-O	-5.75	112.83	119.56
1	A	578	ILE	O-C-N	-5.74	115.94	122.72
1	A	554	ASP	CA-CB-CG	-5.71	106.89	112.60
1	B	92	VAL	N-CA-C	5.71	116.10	108.11
1	A	499	LYS	CA-C-O	-5.65	113.48	119.97
2	C	715	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	682	GLN	CA-C-O	-5.61	112.69	119.59
1	B	337	PHE	CB-CA-C	-5.59	97.69	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ILE	CB-CA-C	-5.58	106.97	111.71
1	B	481	CYS	N-CA-C	-5.57	106.49	113.28
2	C	711	ASN	N-CA-C	-5.55	104.87	111.69
1	A	360	ASN	N-CA-C	5.50	119.78	112.30
3	D	190	VAL	N-CA-C	5.45	116.17	110.62
3	D	173	GLU	N-CA-C	5.43	117.96	111.71
1	B	531	GLN	CA-C-O	-5.43	114.22	120.24
1	B	358	LYS	N-CA-C	5.42	119.96	113.23
1	A	580	GLU	N-CA-C	5.42	117.89	111.33
3	D	27	SER	N-CA-C	-5.42	99.27	110.80
1	A	597	CYS	N-CA-C	5.41	116.36	108.14
3	D	121	LYS	CA-C-N	-5.40	118.15	122.85
3	D	121	LYS	C-N-CA	-5.40	118.15	122.85
1	B	608	ALA	N-CA-C	-5.39	103.01	110.35
1	A	168	GLY	CA-C-O	-5.39	113.02	119.01
1	A	66	ASP	CA-C-N	5.38	125.47	119.87
1	A	66	ASP	C-N-CA	5.38	125.47	119.87
1	A	127	ASP	CA-C-N	-5.36	115.78	122.48
1	A	127	ASP	C-N-CA	-5.36	115.78	122.48
1	A	96	ILE	CB-CA-C	-5.33	104.94	112.14
2	C	525	LEU	CA-C-N	5.33	125.27	119.78
2	C	525	LEU	C-N-CA	5.33	125.27	119.78
3	D	218	TYR	CA-C-N	-5.32	115.92	122.84
3	D	218	TYR	C-N-CA	-5.32	115.92	122.84
3	D	379	GLU	N-CA-C	-5.32	105.15	111.69
1	A	37	PHE	N-CA-C	5.31	120.03	113.50
3	D	311	ALA	N-CA-C	-5.29	105.59	111.36
1	A	393	ASP	N-CA-C	5.28	118.87	111.74
1	B	66	ASP	CA-C-N	5.28	125.36	119.87
1	B	66	ASP	C-N-CA	5.28	125.36	119.87
1	B	393	ASP	N-CA-C	5.27	119.46	112.30
3	D	137	PHE	CA-C-N	-5.25	115.22	122.30
3	D	137	PHE	C-N-CA	-5.25	115.22	122.30
3	D	69	SER	CA-C-N	5.23	128.97	120.60
3	D	69	SER	C-N-CA	5.23	128.97	120.60
1	B	441	PHE	N-CA-C	5.23	119.20	112.41
1	A	449	ILE	N-CA-C	-5.22	106.05	111.58
1	B	636	ILE	N-CA-C	5.20	115.46	108.17
2	C	581	ILE	CA-C-N	5.19	125.19	119.90
2	C	581	ILE	C-N-CA	5.19	125.19	119.90
1	A	300	ASN	CA-C-N	5.16	125.45	119.47
1	A	300	ASN	C-N-CA	5.16	125.45	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	763	LYS	N-CA-C	-5.12	105.39	111.69
2	C	636	LEU	CA-C-N	5.11	125.15	119.32
2	C	636	LEU	C-N-CA	5.11	125.15	119.32
1	A	318	ASN	CA-CB-CG	5.11	117.71	112.60
2	C	624	ALA	CA-C-N	5.09	125.13	119.32
2	C	624	ALA	C-N-CA	5.09	125.13	119.32
1	A	453	SER	N-CA-C	5.09	117.56	111.71
3	D	187	ALA	CA-C-N	5.08	128.08	120.87
3	D	187	ALA	C-N-CA	5.08	128.08	120.87
2	C	611	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	B	174	THR	N-CA-C	-5.07	102.78	110.28
3	D	36	ILE	N-CA-C	-5.06	106.52	111.88
3	D	193	GLY	N-CA-C	-5.06	106.61	113.24
1	A	131	ILE	N-CA-C	-5.03	103.01	109.30
1	A	384	PHE	CA-C-O	-5.01	113.44	119.15
1	A	637	ASN	CA-C-N	5.01	124.62	119.56
1	A	637	ASN	C-N-CA	5.01	124.62	119.56
1	A	679	GLU	N-CA-C	5.01	119.10	112.89

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	GLY	Mainchain
1	A	36	THR	Mainchain
1	A	384	PHE	Mainchain
1	A	42	GLU	Mainchain
1	A	437	PHE	Mainchain
1	A	499	LYS	Mainchain
1	A	543	SER	Mainchain
1	A	578	ILE	Mainchain
1	A	638	PRO	Mainchain
1	B	127	ASP	Mainchain
1	B	203	ILE	Mainchain
1	B	472	ASP	Mainchain
1	B	480	TYR	Mainchain
1	B	531	GLN	Mainchain
1	B	639	ASP	Mainchain
1	B	682	GLN	Mainchain
1	B	84	LYS	Mainchain
2	C	577	TRP	Mainchain
2	C	612	SER	Mainchain

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Mol	Chain	Res	Type	Group
2	C	684	GLU	Mainchain
2	C	688	GLU	Mainchain
2	C	721	LEU	Mainchain

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	5121	5158	5156	11	0
1	B	5210	5232	5229	12	0
2	C	2103	2132	2131	8	0
3	D	3229	3220	3219	11	0
4	A	31	12	12	0	0
4	B	31	12	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	C	28	1	29	2	0
All	All	15755	15767	15788	38	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 (38) 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:C:577:TRP:O	2:C:577:TRP:CG	2.59	0.56
3:D:51:ASP:OD1	3:D:82:GLY:N	2.41	0.53
1:A:615:LYS:O	1:A:620:ARG:NH2	2.43	0.52
1:A:318:ASN:HB3	2:C:712:TRP:CZ2	2.48	0.48
1:A:44:PHE:CD1	1:A:44:PHE:C	2.89	0.47
3:D:198:ILE:O	3:D:199:PRO:C	2.54	0.47
3:D:235:ILE:O	3:D:236:GLU:C	2.57	0.47
1:A:578:ILE:O	1:A:579:LEU:C	2.58	0.46
1:B:589:SER:OG	1:B:590:ASN:N	2.47	0.46
3:D:66:LYS:NZ	3:D:72:ASP:OD2	2.48	0.46
2:C:626:ASP:OD2	3:D:88:LYS:NZ	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:O	1:A:572:CYS:C	2.57	0.45
1:B:576:LYS:O	1:B:580:GLU:N	2.50	0.45
1:A:372:ASP:OD1	1:A:372:ASP:N	2.45	0.45
2:C:601:MET:HE1	6:C:801:DEX:H521	1.98	0.45
1:B:44:PHE:CD1	1:B:44:PHE:C	2.94	0.44
1:B:702:ASP:O	3:D:406:ARG:NH2	2.50	0.44
1:A:577:ASP:C	1:A:578:ILE:O	2.59	0.44
6:C:801:DEX:H112	6:C:801:DEX:H211	1.99	0.44
1:B:393:ASP:OD1	1:B:393:ASP:N	2.41	0.44
1:A:452:ASP:OD1	1:A:454:GLN:NE2	2.51	0.44
1:B:609:ASN:O	1:B:610:MET:C	2.57	0.43
1:B:732:ASP:OD1	3:D:272:LYS:NZ	2.52	0.43
1:B:383:ASN:N	1:B:383:ASN:OD1	2.50	0.42
1:A:485:LYS:NZ	1:A:514:HIS:O	2.52	0.42
3:D:67:PHE:CG	3:D:128:LEU:HD21	2.54	0.42
3:D:355:TYR:CD2	3:D:355:TYR:C	2.97	0.42
1:B:66:ASP:OD1	1:B:66:ASP:C	2.62	0.42
1:A:578:ILE:O	1:A:580:GLU:N	2.53	0.41
3:D:57:TYR:CE1	3:D:71:HIS:HB3	2.55	0.41
2:C:707:ASN:O	2:C:711:ASN:ND2	2.54	0.41
1:B:608:ALA:O	1:B:609:ASN:HB2	2.20	0.41
1:B:571:LEU:O	1:B:572:CYS:C	2.62	0.41
1:A:657:LYS:NZ	3:D:420:ASP:O	2.53	0.41
1:B:581:LYS:H	1:B:581:LYS:HD3	1.85	0.41
2:C:761:ILE:N	2:C:762:PRO:HD2	2.35	0.41
2:C:610:TRP:HB2	2:C:663:TYR:CE1	2.56	0.41
2:C:581:ILE:HA	2:C:582:PRO:HD3	1.96	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	626/731 (86%)	619 (99%)	7 (1%)	0	100	100
1	B	635/731 (87%)	624 (98%)	10 (2%)	1 (0%)	43	72
2	C	257/360 (71%)	255 (99%)	2 (1%)	0	100	100
3	D	407/456 (89%)	399 (98%)	8 (2%)	0	100	100
All	All	1925/2278 (84%)	1897 (98%)	27 (1%)	1 (0%)	49	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	GLN

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	571/665 (86%)	571 (100%)	0	100	100
1	B	582/665 (88%)	582 (100%)	0	100	100
2	C	238/323 (74%)	238 (100%)	0	100	100
3	D	339/377 (90%)	339 (100%)	0	100	100
All	All	1730/2030 (85%)	1730 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	ASN
2	C	630	ASN
2	C	642	GLN
3	D	21	GLN
3	D	161	ASN
3	D	210	GLN
3	D	322	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DEX	C	801	-	31,31,31	1.98	9 (29%)	53,53,53	2.86	28 (52%)
4	ATP	B	801	5	32,33,33	1.88	9 (28%)	48,52,52	1.68	8 (16%)
4	ATP	A	801	5	32,33,33	1.93	8 (25%)	48,52,52	1.81	10 (20%)

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
6	DEX	C	801	-	-	6/8/84/84	0/4/4/4
4	ATP	B	801	5	-	2/22/38/38	0/3/3/3
4	ATP	A	801	5	-	3/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	ATP	C5-C4	6.07	1.49	1.39
4	B	801	ATP	C5-C4	6.01	1.49	1.39
6	C	801	DEX	C10-C1	4.14	1.55	1.50
4	B	801	ATP	C5-C6	3.95	1.52	1.41
6	C	801	DEX	C10-C5	3.94	1.57	1.52
4	A	801	ATP	C5-C6	3.93	1.51	1.41
6	C	801	DEX	C17-C20	3.59	1.57	1.53
6	C	801	DEX	C9-C8	3.35	1.58	1.54
6	C	801	DEX	C4-C3	3.30	1.53	1.45
6	C	801	DEX	C2-C3	3.24	1.54	1.46
4	A	801	ATP	C5-N7	-3.22	1.33	1.39
4	B	801	ATP	C5-N7	-3.13	1.33	1.39
4	B	801	ATP	C4-N3	2.82	1.39	1.34
4	B	801	ATP	C2-N1	2.69	1.38	1.33
6	C	801	DEX	O4-C20	2.63	1.25	1.21
4	A	801	ATP	C2-N1	2.53	1.38	1.33
4	A	801	ATP	C4-N3	2.53	1.39	1.34
4	B	801	ATP	PB-O3B	2.41	1.62	1.59
4	B	801	ATP	C2-N3	2.33	1.38	1.33
4	A	801	ATP	C4-N9	-2.32	1.32	1.37
4	B	801	ATP	C8-N7	2.28	1.36	1.31
6	C	801	DEX	C9-C11	2.25	1.56	1.54
4	A	801	ATP	C2-N3	2.24	1.37	1.33
4	A	801	ATP	C8-N7	2.22	1.35	1.31
4	B	801	ATP	C4-N9	-2.08	1.33	1.37
6	C	801	DEX	C13-C14	2.03	1.58	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	801	DEX	C9-C8-C14	7.44	115.87	109.34
6	C	801	DEX	C12-C11-C9	7.07	118.40	112.96
6	C	801	DEX	C21-C20-C17	6.84	123.40	117.63
6	C	801	DEX	C6-C5-C10	5.80	119.52	115.70
4	A	801	ATP	C5-C4-N3	-5.45	119.21	126.72
4	B	801	ATP	C5-C4-N3	-5.35	119.35	126.72
6	C	801	DEX	C7-C8-C9	5.05	116.69	110.98
6	C	801	DEX	C13-C17-C20	4.86	119.22	112.86
4	B	801	ATP	N3-C2-N1	-4.31	122.05	128.58
4	A	801	ATP	N3-C2-N1	-4.27	122.12	128.58
4	A	801	ATP	N3-C4-N9	4.24	134.38	127.17
4	B	801	ATP	N3-C4-N9	4.21	134.32	127.17
6	C	801	DEX	C15-C14-C8	4.04	122.88	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	ATP	C2-N3-C4	4.01	121.61	111.83
4	B	801	ATP	C2-N3-C4	3.95	121.47	111.83
6	C	801	DEX	C19-C10-C1	-3.79	102.09	106.64
4	A	801	ATP	C4-C5-N7	-3.75	106.30	110.58
6	C	801	DEX	C10-C9-C11	3.68	118.11	115.49
4	B	801	ATP	C4-C5-N7	-3.48	106.60	110.58
6	C	801	DEX	C1-C2-C3	-3.42	118.61	121.49
6	C	801	DEX	C5-C4-C3	-3.37	119.66	122.72
6	C	801	DEX	C9-C10-C5	3.17	110.16	106.80
6	C	801	DEX	C6-C5-C4	-2.87	116.28	120.86
6	C	801	DEX	C10-C5-C4	2.86	124.20	122.15
6	C	801	DEX	C18-C13-C12	-2.75	107.28	111.08
6	C	801	DEX	F1-C9-C10	2.75	106.56	104.16
6	C	801	DEX	C9-C10-C1	2.67	113.27	109.98
6	C	801	DEX	C7-C8-C14	2.66	117.47	111.50
6	C	801	DEX	F1-C9-C11	-2.65	98.94	102.58
4	A	801	ATP	C5-N7-C8	2.60	107.54	103.45
4	A	801	ATP	O2A-PA-O1A	2.60	124.53	112.44
4	A	801	ATP	C6-C5-N7	2.57	137.04	132.09
6	C	801	DEX	O4-C20-C17	-2.56	119.75	122.78
4	B	801	ATP	C5-N7-C8	2.51	107.40	103.45
6	C	801	DEX	C22-C16-C17	2.47	119.95	114.96
4	B	801	ATP	C6-C5-N7	2.41	136.73	132.09
4	B	801	ATP	C2-N1-C6	2.34	122.57	118.73
4	A	801	ATP	C2-N1-C6	2.30	122.51	118.73
6	C	801	DEX	C6-C7-C8	2.27	116.11	111.70
6	C	801	DEX	C15-C16-C17	2.23	106.59	105.10
6	C	801	DEX	C17-C13-C14	-2.23	97.34	99.35
6	C	801	DEX	C2-C3-C4	2.22	119.38	117.12
6	C	801	DEX	C22-C16-C15	-2.22	109.69	113.39
6	C	801	DEX	C10-C1-C2	2.10	125.97	124.37
6	C	801	DEX	O2-C11-C12	-2.04	105.43	110.11
4	A	801	ATP	O2B-PB-O3A	-2.01	101.83	107.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	ATP	C5'-O5'-PA-O2A
4	A	801	ATP	O4'-C4'-C5'-O5'
6	C	801	DEX	C13-C17-C20-C21
6	C	801	DEX	C13-C17-C20-O4

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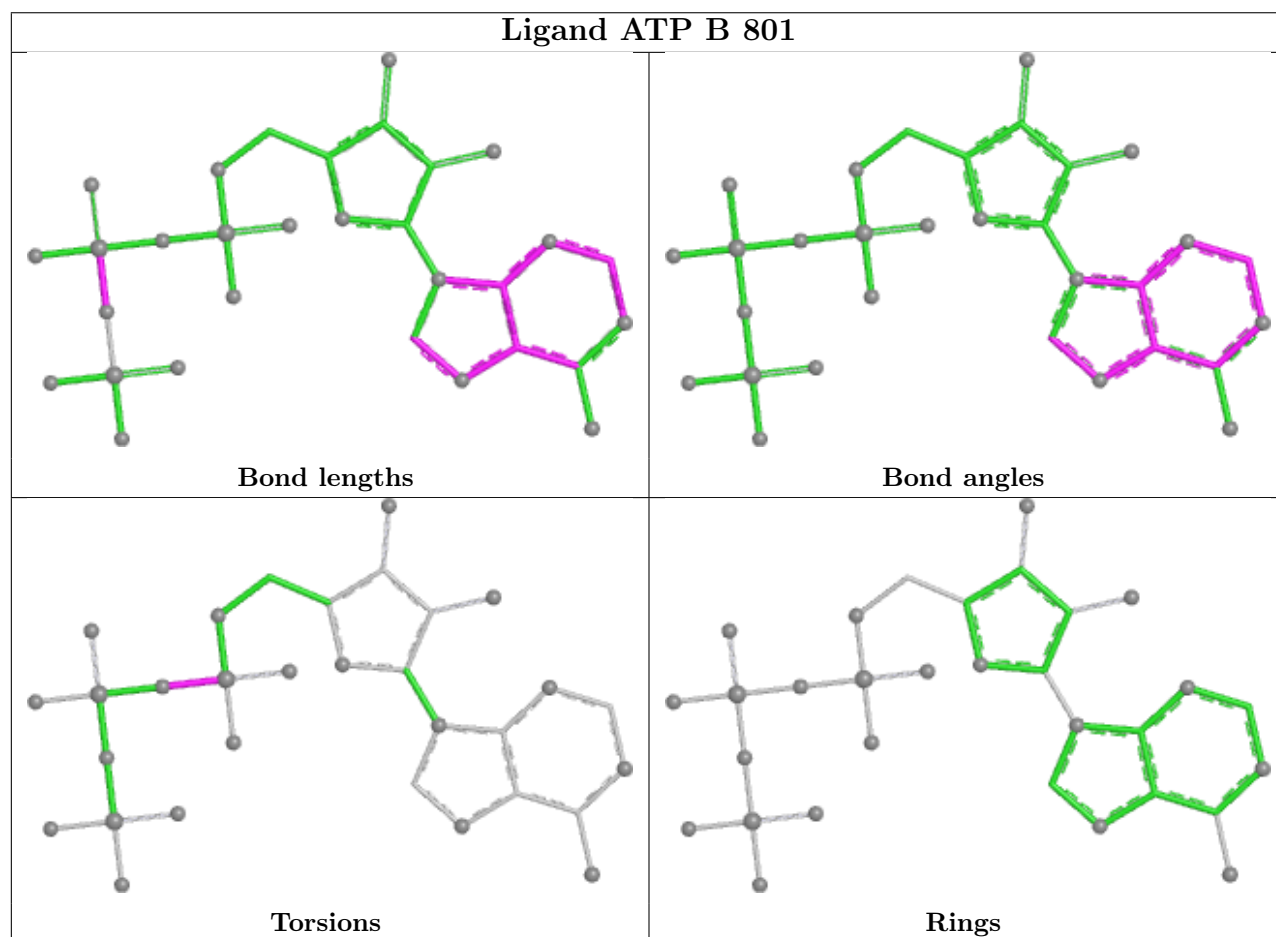
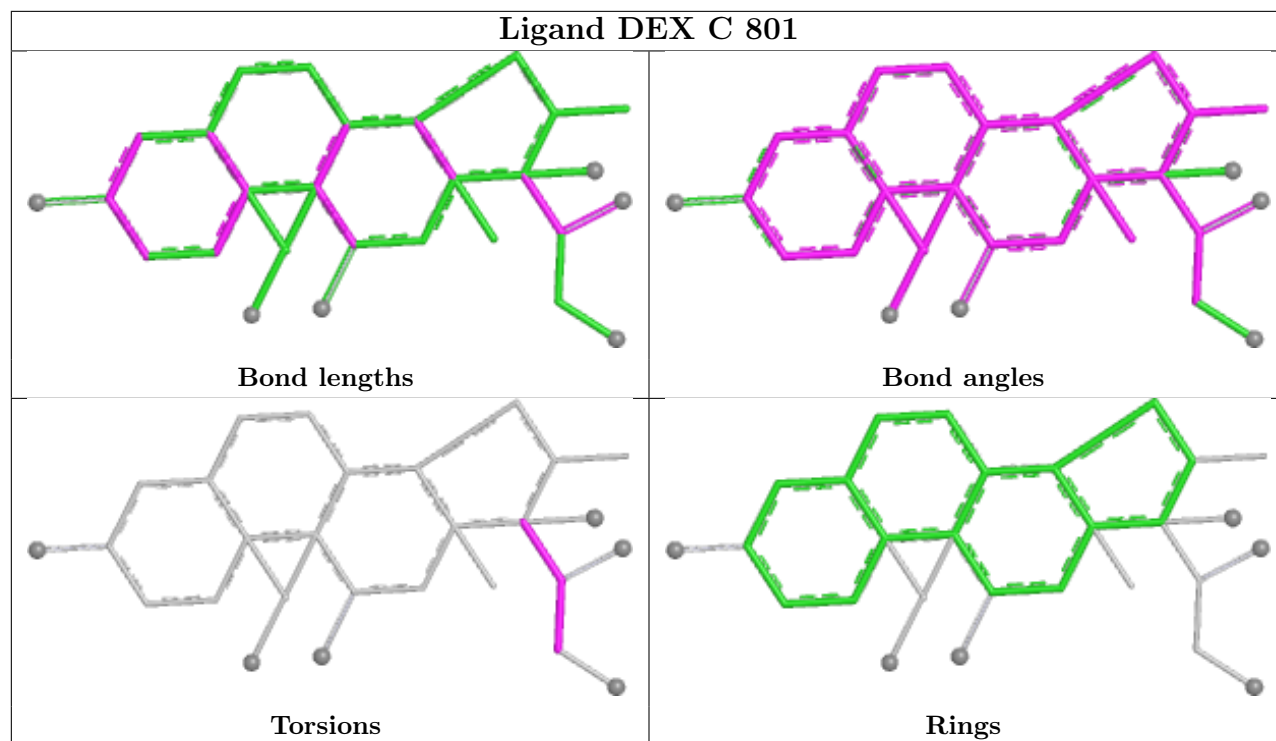
Mol	Chain	Res	Type	Atoms
6	C	801	DEX	O3-C17-C20-C21
6	C	801	DEX	O3-C17-C20-O4
6	C	801	DEX	C17-C20-C21-O5
6	C	801	DEX	O4-C20-C21-O5
4	A	801	ATP	C3'-C4'-C5'-O5'
4	B	801	ATP	PB-O3A-PA-O2A
4	B	801	ATP	PB-O3A-PA-O1A

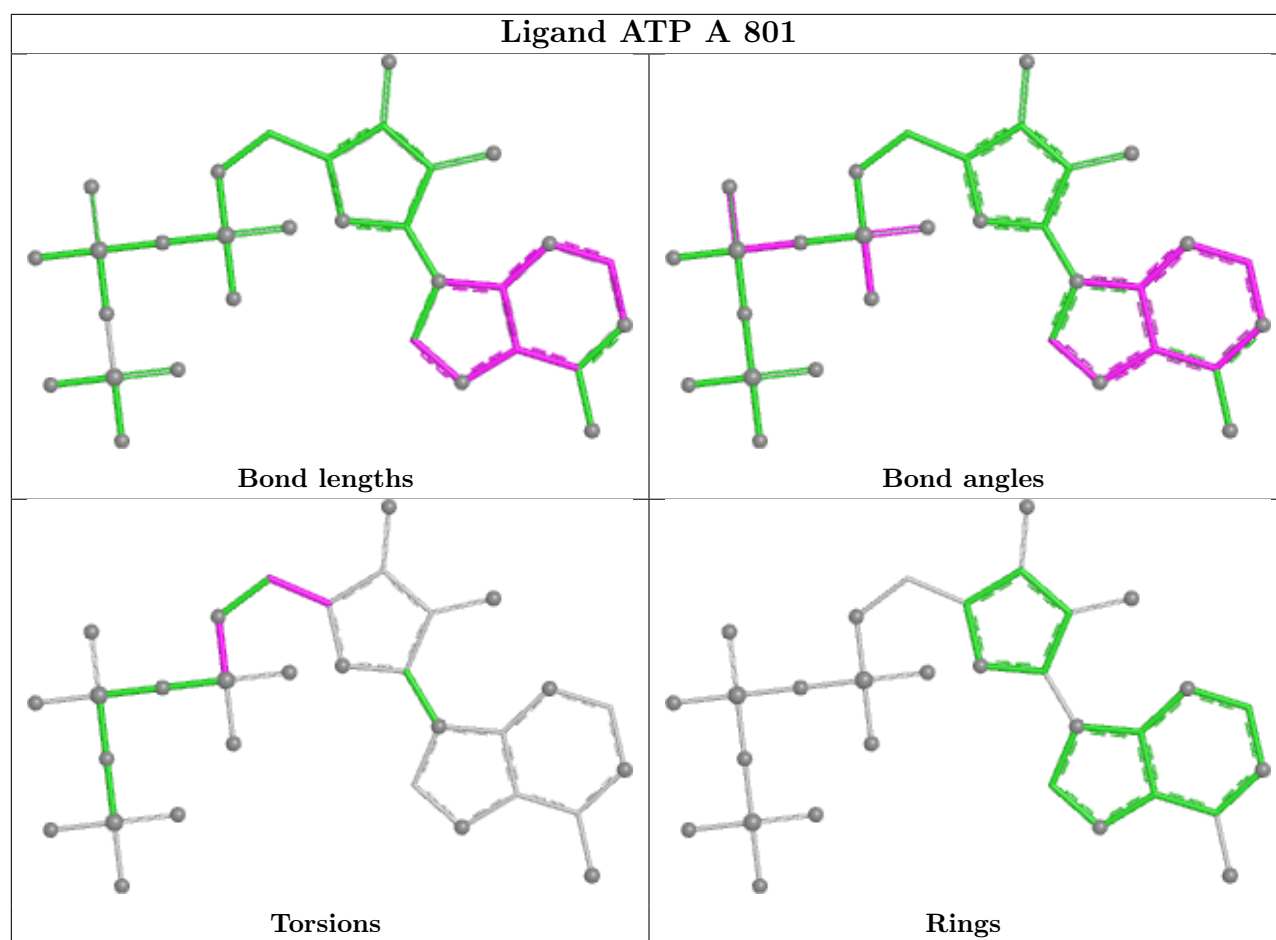
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	801	DEX	2	0

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.

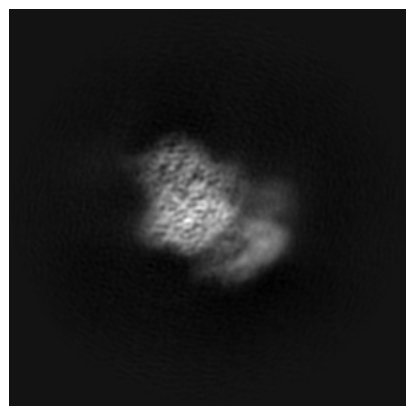
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29069. These allow visual inspection of the internal detail of the map and identification of artifacts.

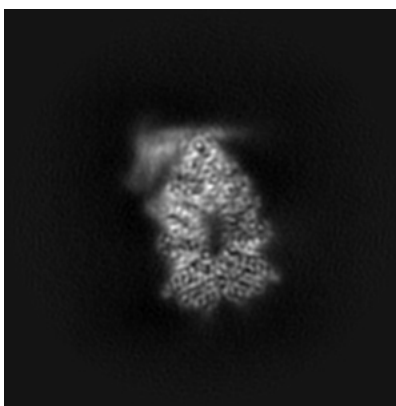
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

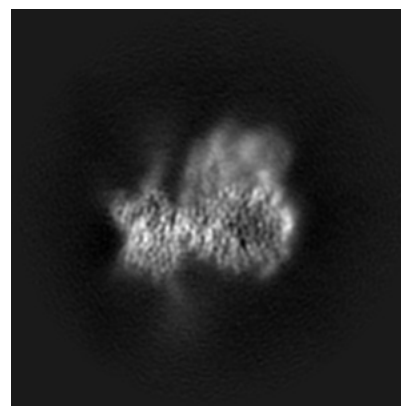
6.1.1 Primary map



X

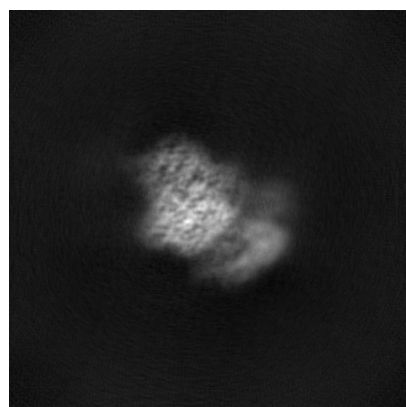


Y

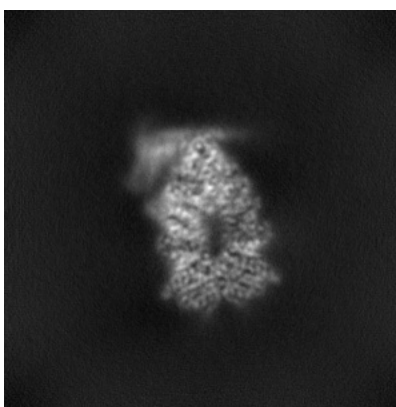


Z

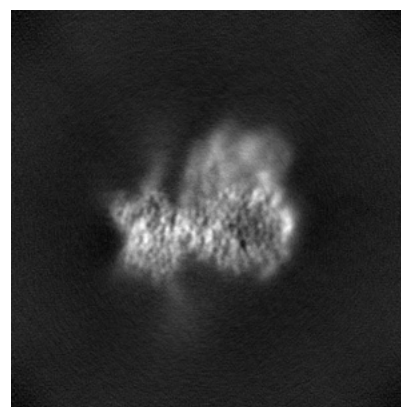
6.1.2 Raw map



X



Y

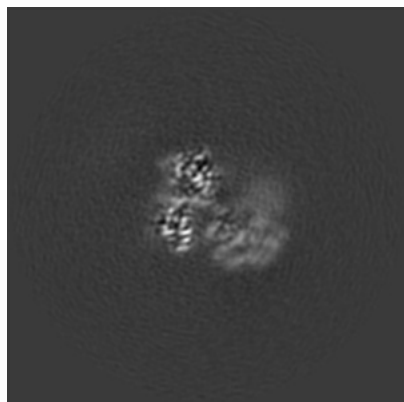


Z

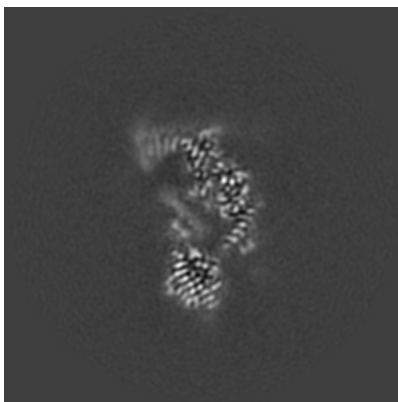
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

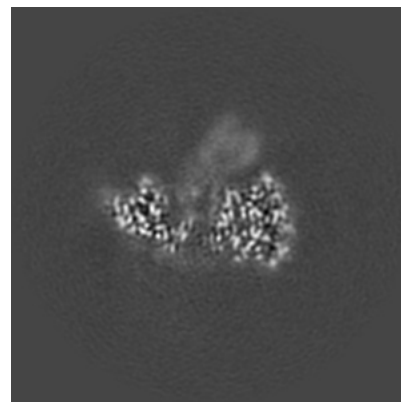
6.2.1 Primary map



X Index: 160

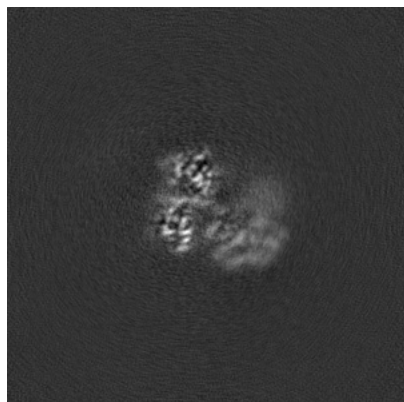


Y Index: 160

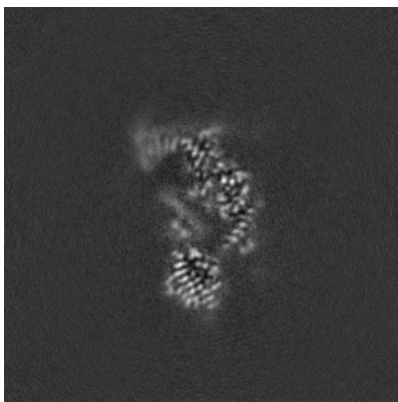


Z Index: 160

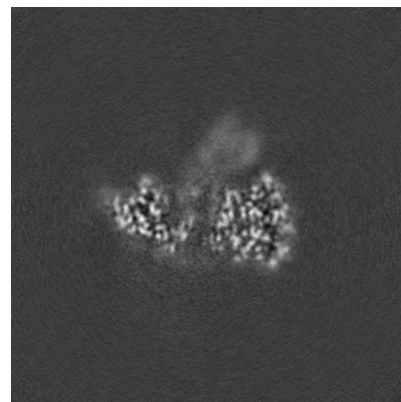
6.2.2 Raw map



X Index: 160



Y Index: 160

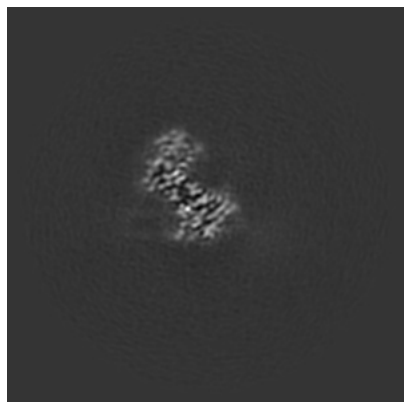


Z Index: 160

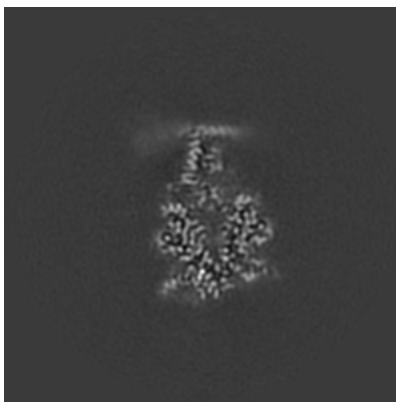
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

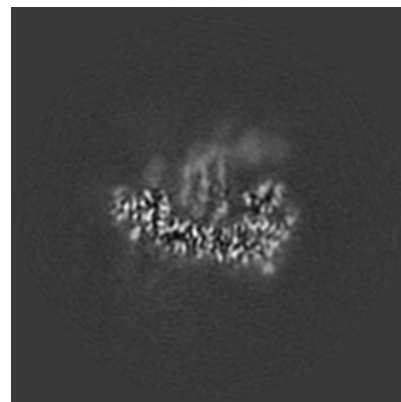
6.3.1 Primary map



X Index: 107

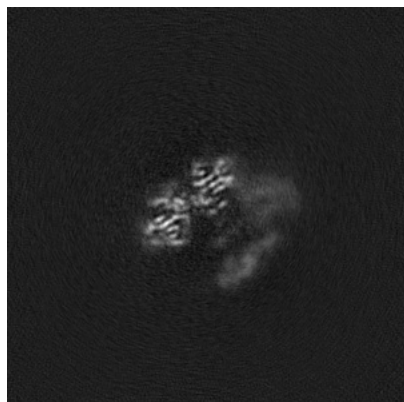


Y Index: 144

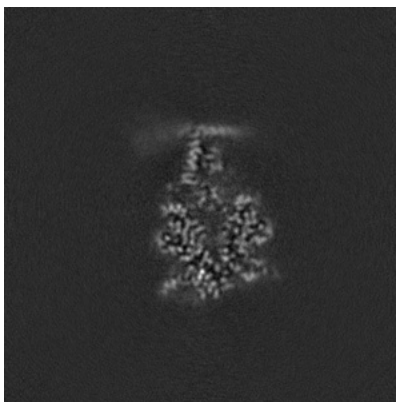


Z Index: 150

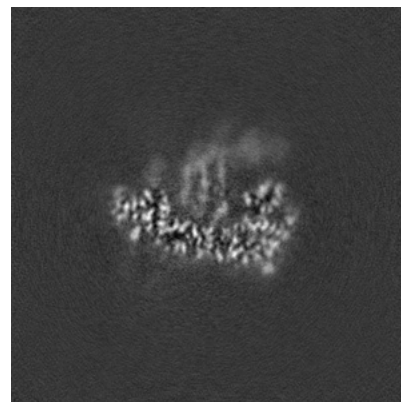
6.3.2 Raw map



X Index: 178



Y Index: 144

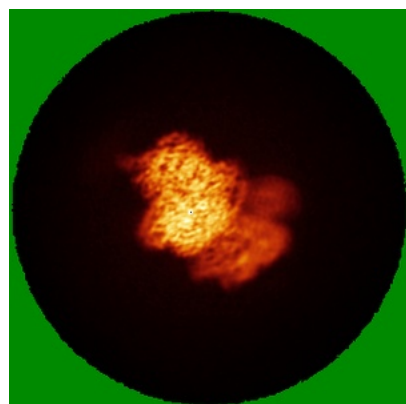


Z Index: 150

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

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

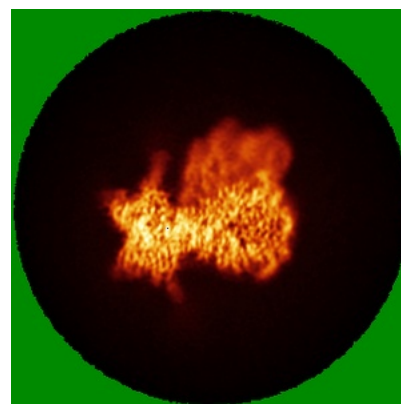
6.4.1 Primary map



X

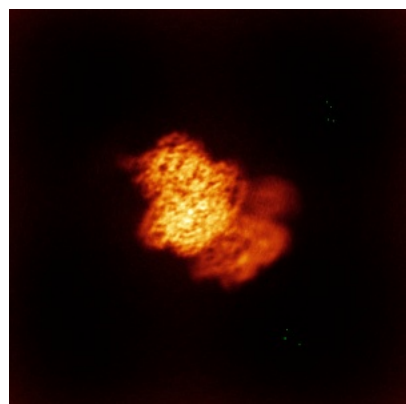


Y

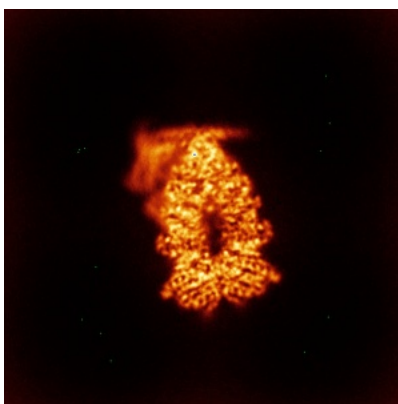


Z

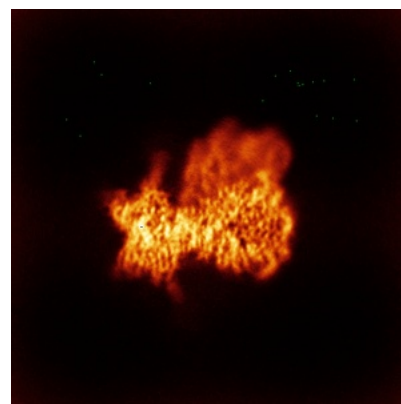
6.4.2 Raw map



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.

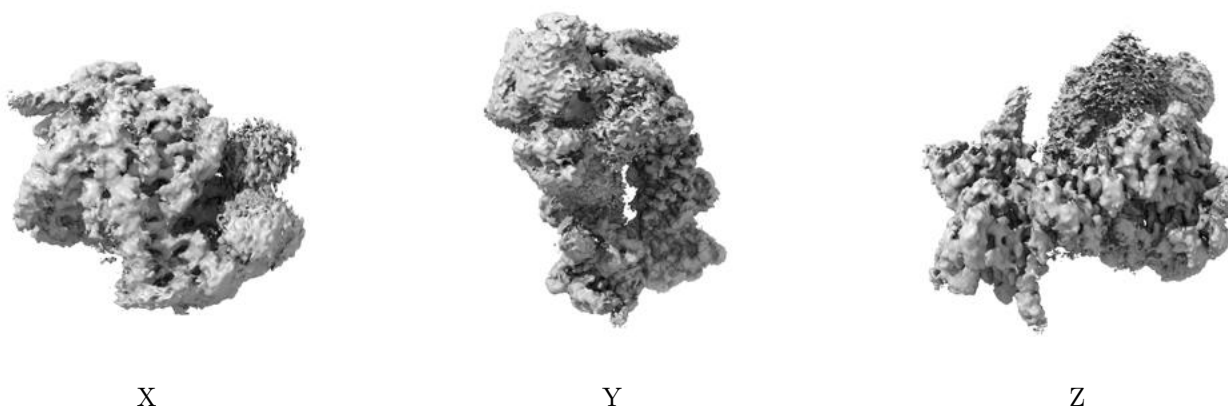
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

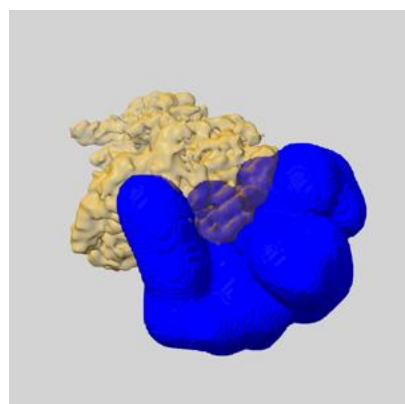
6.6 Mask visualisation [i](#)

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

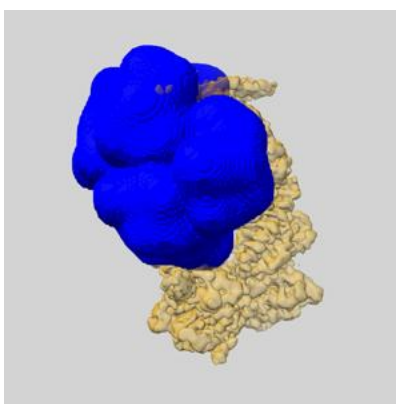
A mask typically either:

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

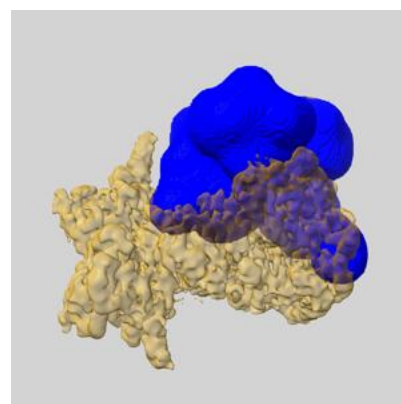
6.6.1 emd_29069_msk_3.map [i](#)



X

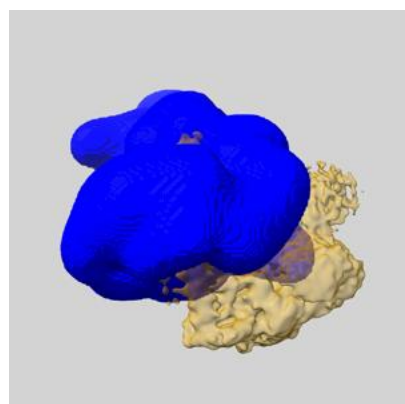


Y

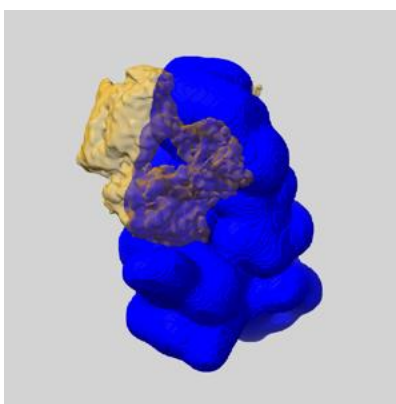


Z

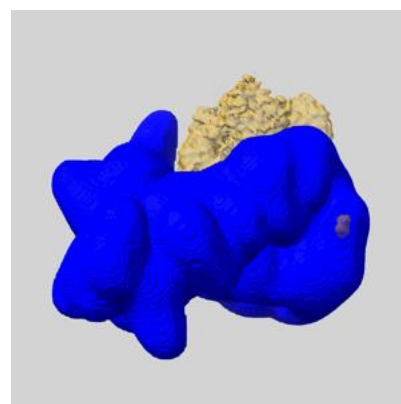
6.6.2 emd_29069_msk_2.map [i](#)



X

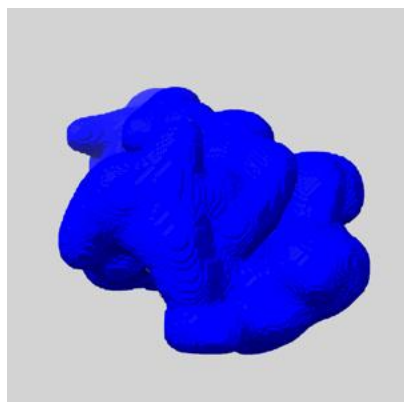


Y

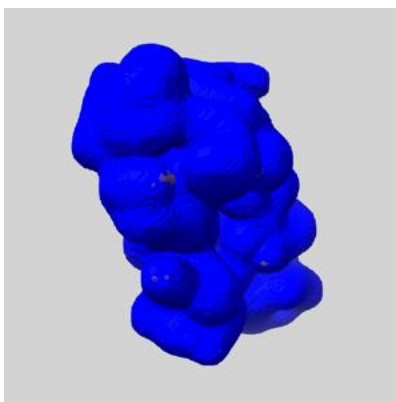


Z

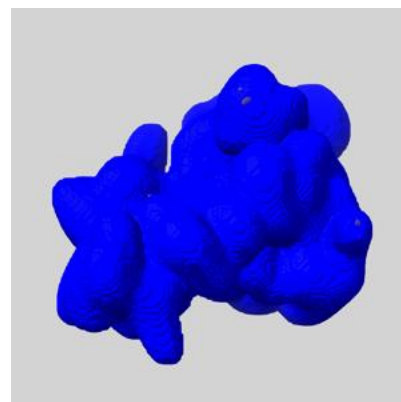
6.6.3 emd_29069_msk_1.map [i](#)



X



Y

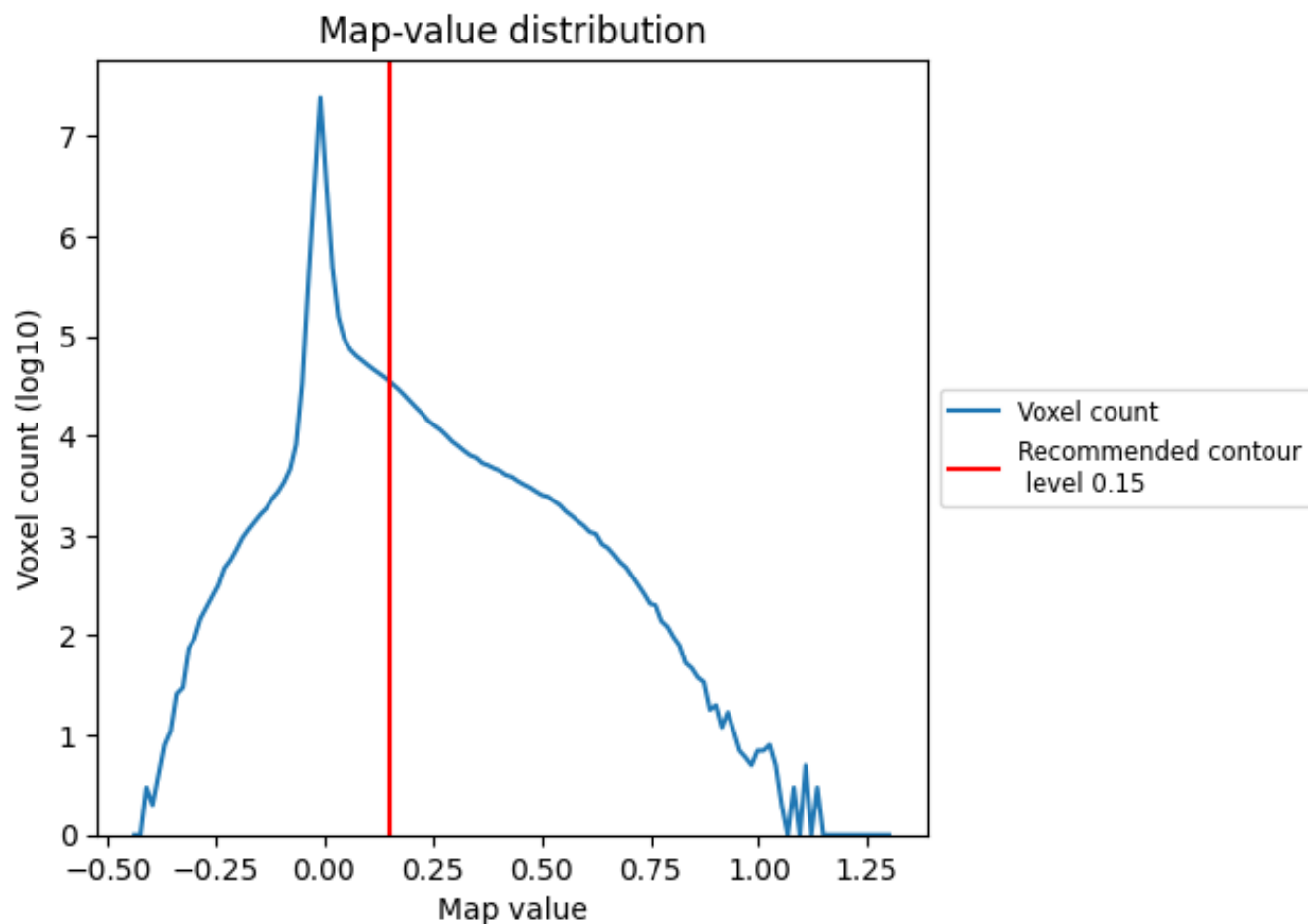


Z

7 Map analysis [i](#)

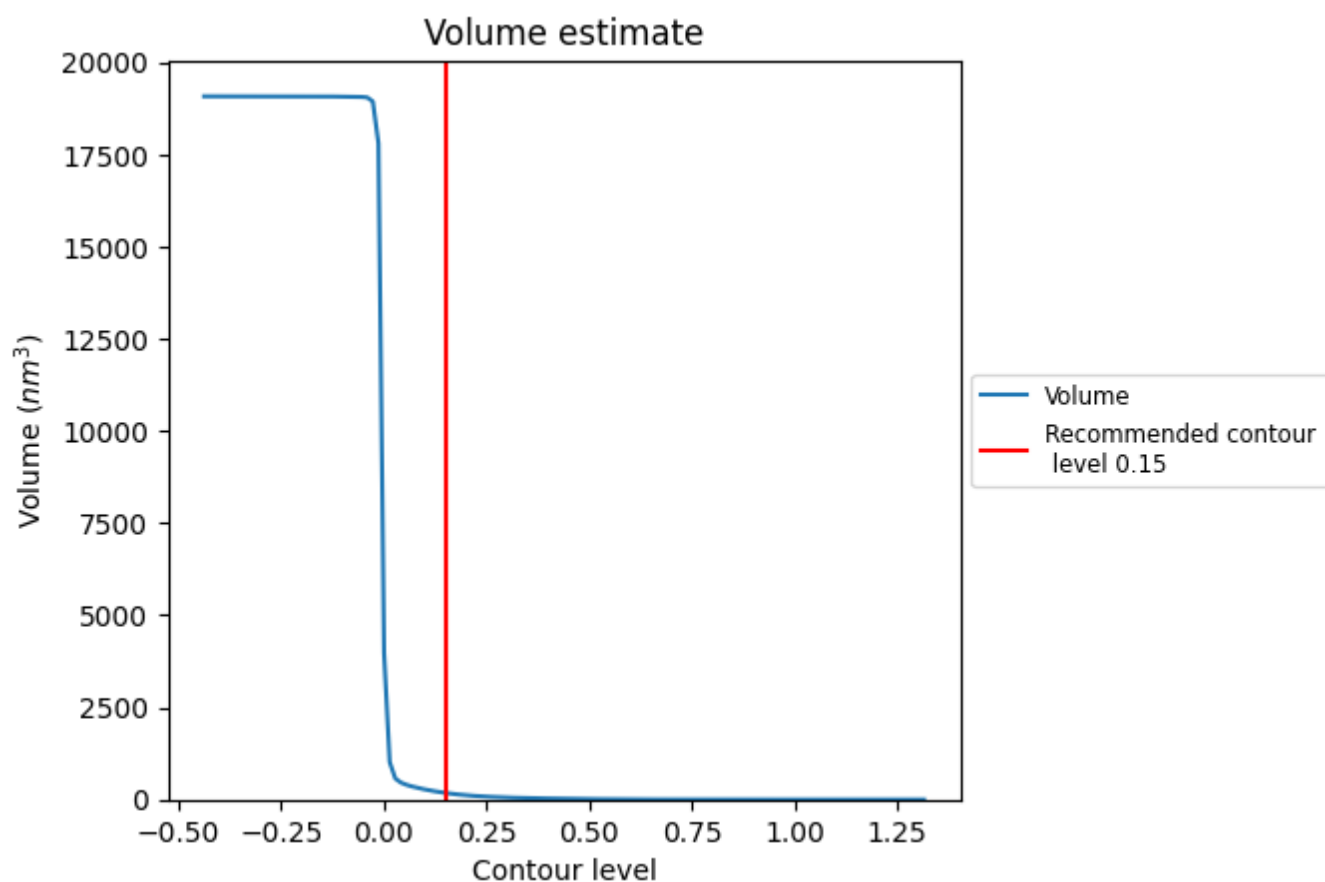
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

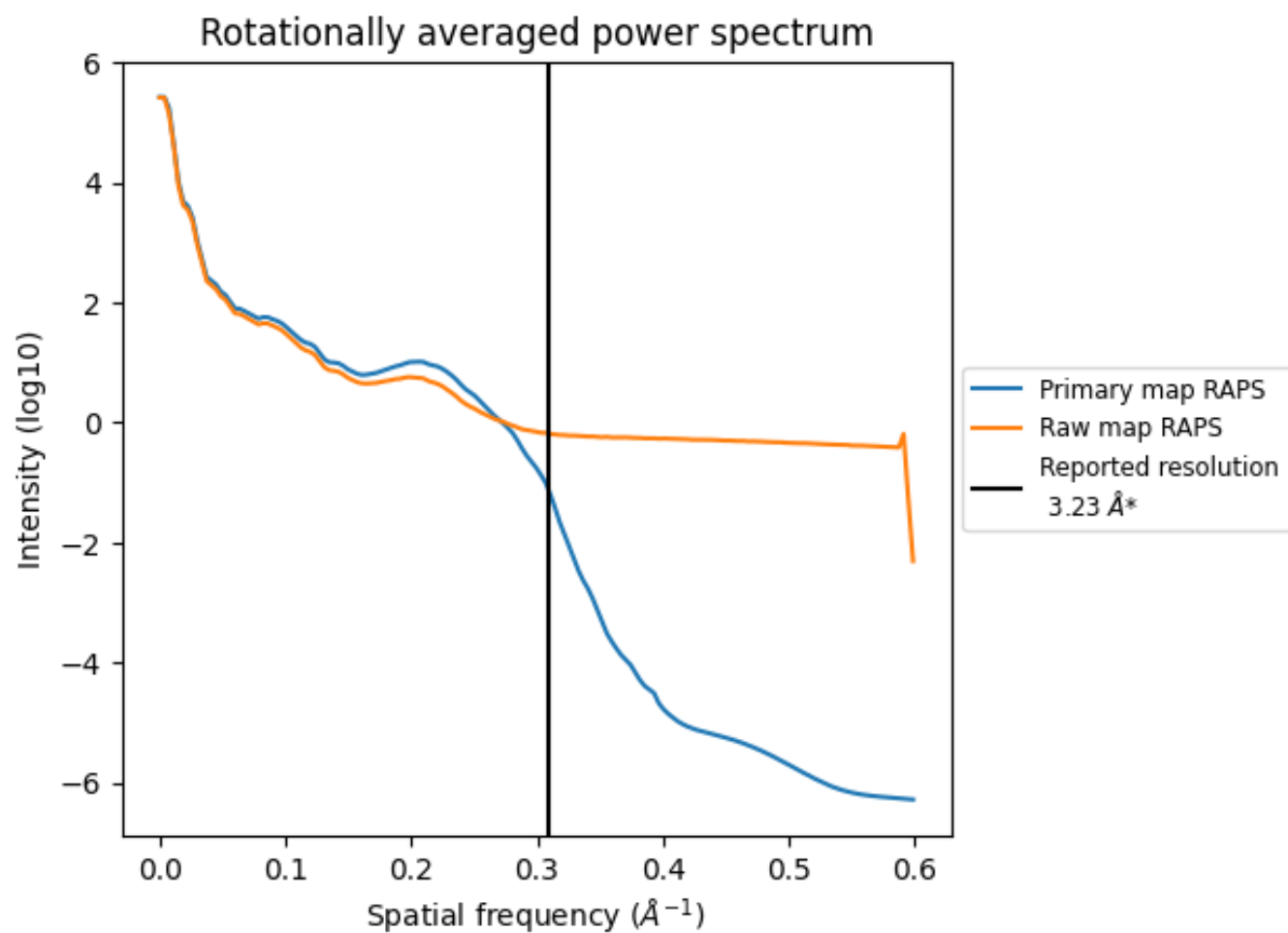
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 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 ⓘ

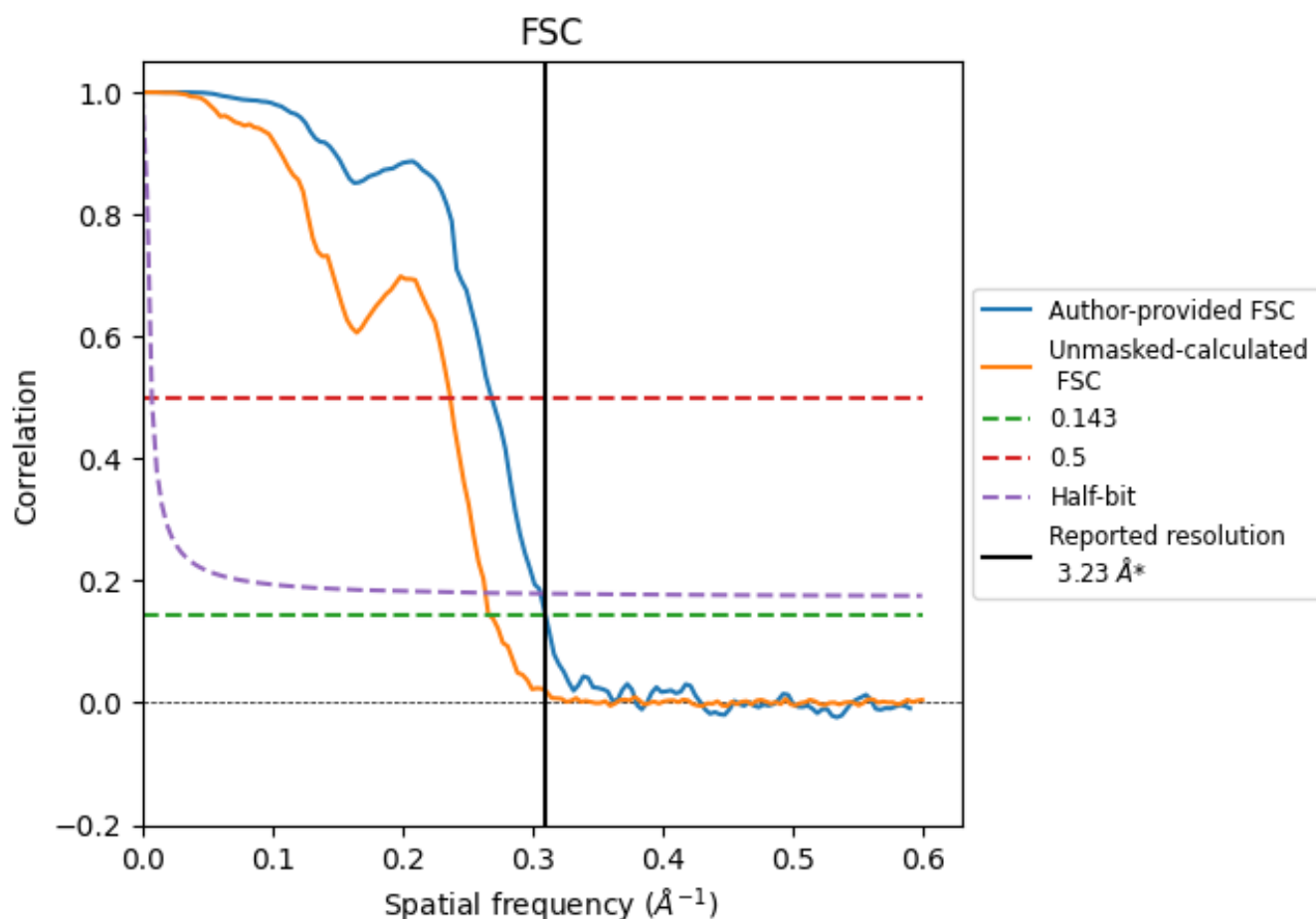


*Reported resolution corresponds to spatial frequency of $0.310 \text{ \AA}^{-1}$

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 $0.310 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

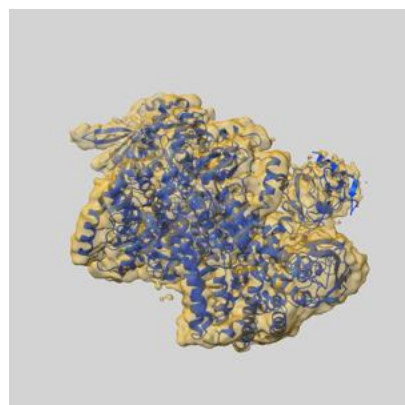
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.73	3.27
Unmasked-calculated*	3.75	4.23	3.80

*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 3.75 differs from the reported value 3.23 by more than 10 %

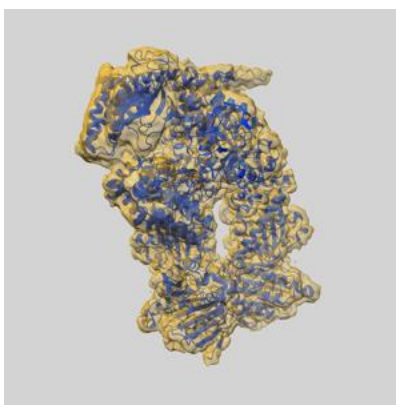
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29069 and PDB model 8FFW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

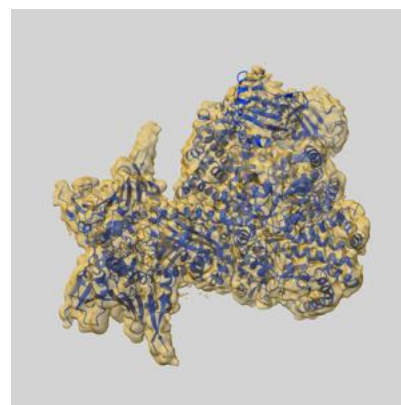
9.1 Map-model overlay [i](#)



X



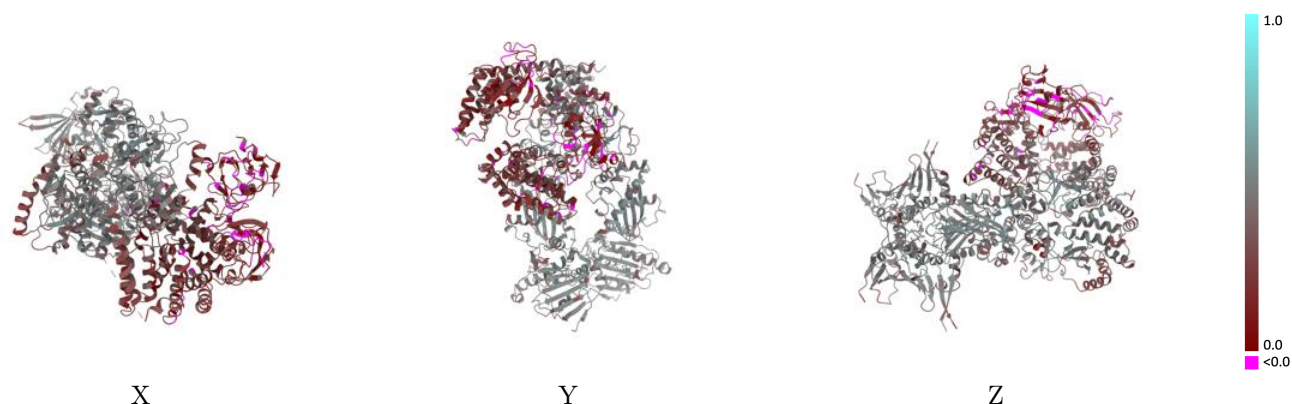
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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](#)



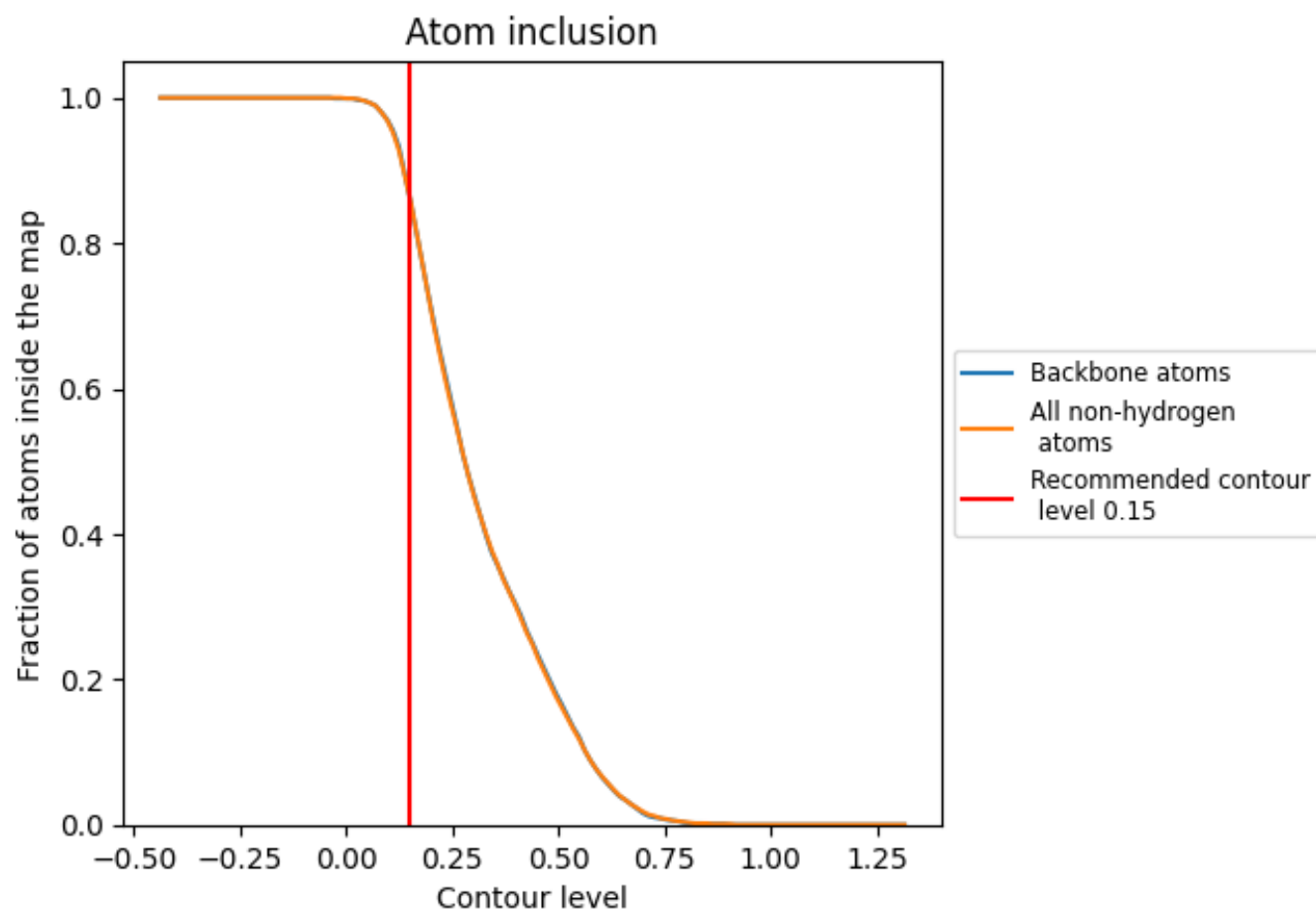
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8640	0.3690
A	0.9230	0.4460
B	0.9150	0.4550
C	0.7870	0.2410
D	0.7390	0.1920

