



Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 08:40 AM EDT

PDB ID : 7KRJ
EMDB ID : EMD-23004
Title : The GR-Maturation Complex: Glucocorticoid Receptor in complex with Hsp90 and co-chaperone p23
Authors : Noddings, C.M.; Wang, Y.-R.; Agard, D.A.
Deposited on : 2020-11-20
Resolution : 2.56 Å (reported)
Based on initial models : 5FWK, 1EJF, 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.dev92
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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

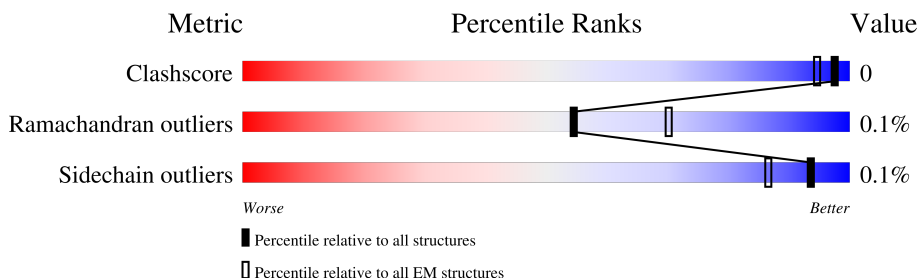
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.56 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 $\leq 5\%$. 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	
1	B	732	
2	C	160	
3	D	258	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26891 atoms, of which 13432 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	627	Total	C	H	N	O	S	0	0
			10240	3234	5144	856	983	23		
1	B	627	Total	C	H	N	O	S	0	0
			10240	3234	5144	856	983	23		

- Molecule 2 is a protein called Prostaglandin E synthase 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	133	Total	C	H	N	O	S	0	0
			2122	683	1021	192	216	10		

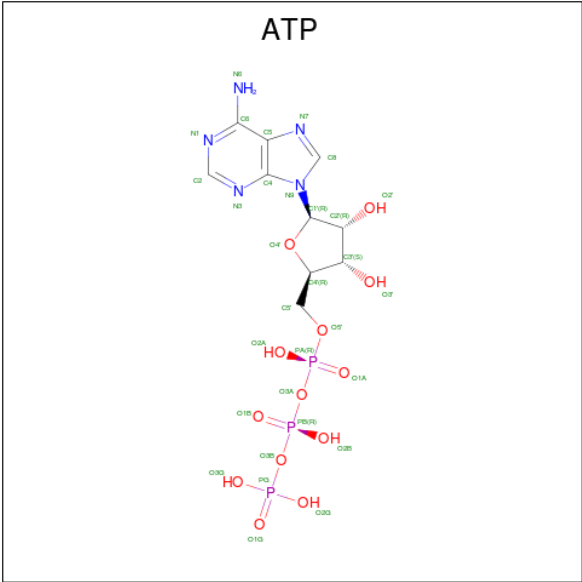
- Molecule 3 is a protein called Glucocorticoid receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	255	Total	C	H	N	O	S	0	0
			4172	1335	2098	341	380	18		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

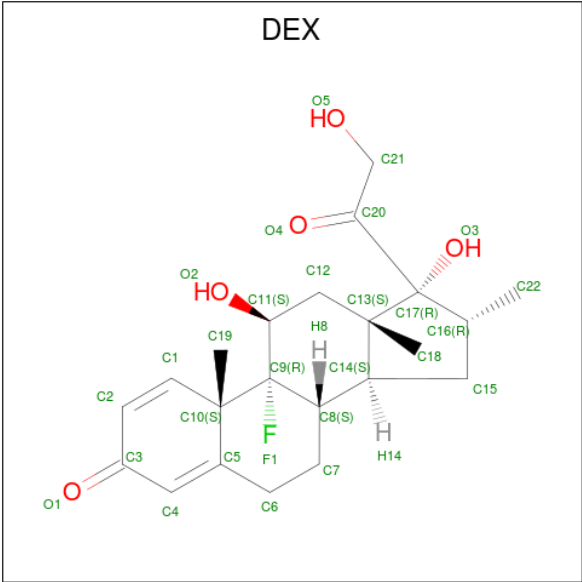


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: DEX) (formula: C₂₂H₂₉FO₅).

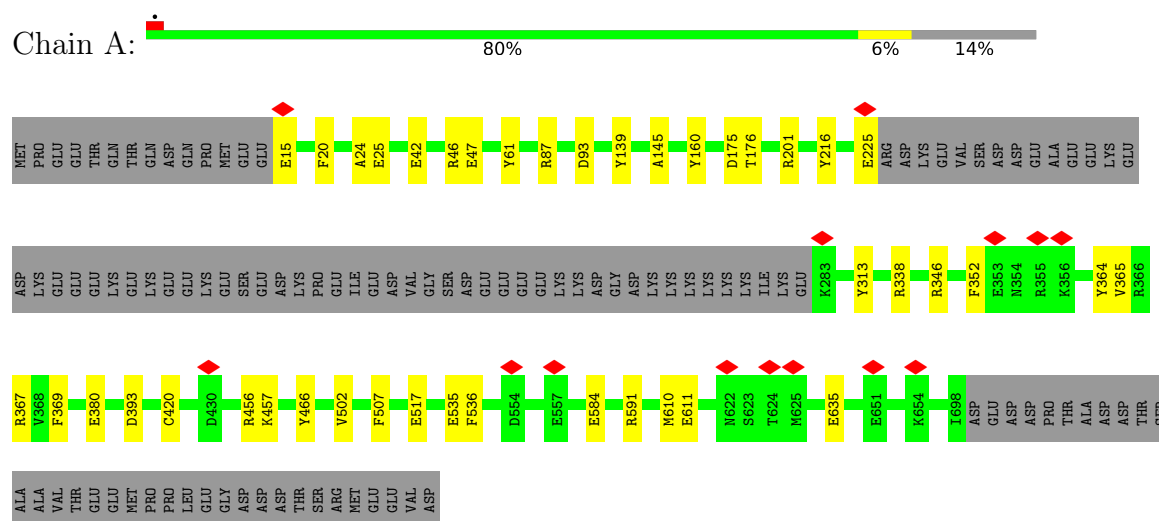


Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	F	H	O	0
			29	22	1	1	5	

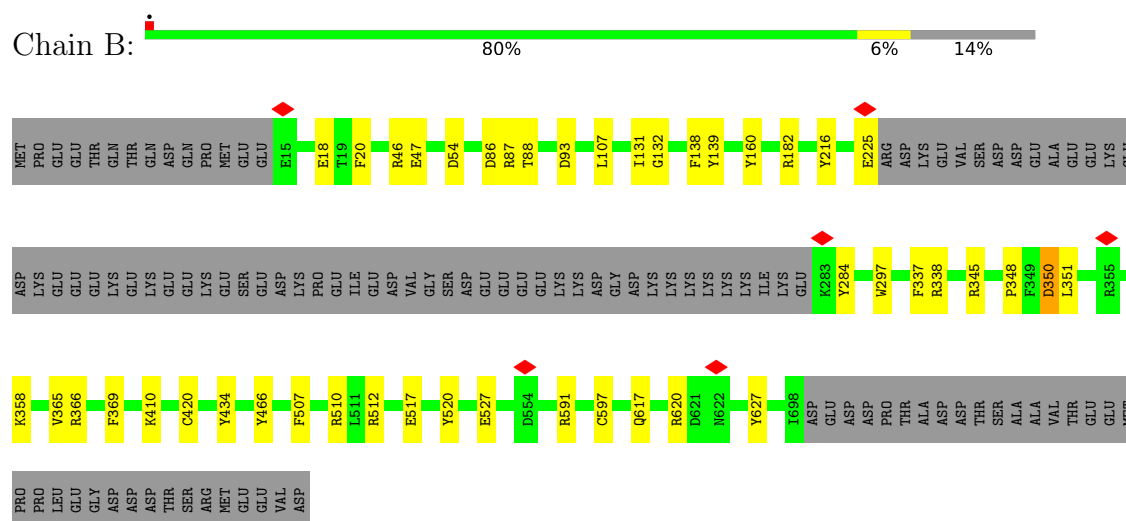
3 Residue-property plots

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.

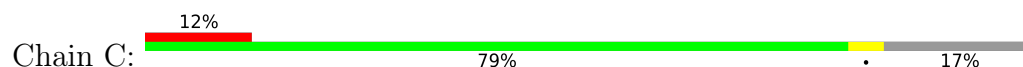
• Molecule 1: Heat shock protein HSP 90-alpha

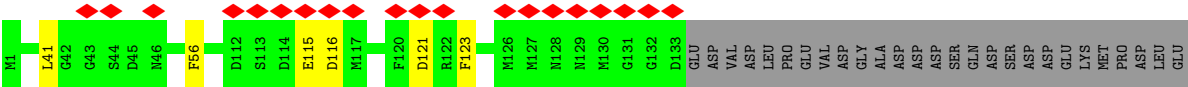


• Molecule 1: Heat shock protein HSP 90-alpha

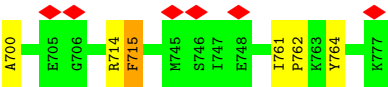
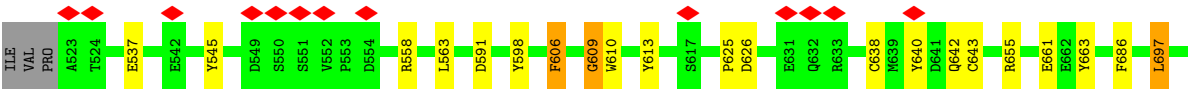
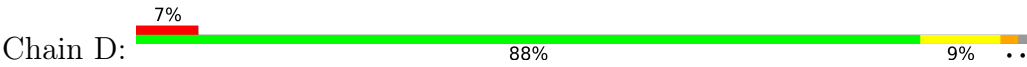


• Molecule 2: Prostaglandin E synthase 3





• Molecule 3: Glucocorticoid receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140217	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	250.5, 250.5, 250.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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: ATP, DEX, 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	1.45	24/5179 (0.5%)	0.95	12/6962 (0.2%)
1	B	1.44	22/5179 (0.4%)	1.01	22/6962 (0.3%)
2	C	1.42	2/1127 (0.2%)	0.91	1/1514 (0.1%)
3	D	1.39	9/2119 (0.4%)	0.99	11/2866 (0.4%)
All	All	1.43	57/13604 (0.4%)	0.97	46/18304 (0.3%)

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	2
1	B	0	3
3	D	0	4
All	All	0	9

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	123	PHE	CB-CG	-9.44	1.35	1.51
3	D	643	CYS	CB-SG	-8.62	1.67	1.82
1	A	369	PHE	CB-CG	-8.26	1.37	1.51
1	B	466	TYR	CB-CG	-7.99	1.39	1.51
1	A	93	ASP	CB-CG	-7.91	1.35	1.51
1	B	369	PHE	CB-CG	-7.65	1.38	1.51
1	A	466	TYR	CB-CG	-6.85	1.41	1.51
3	D	663	TYR	CB-CG	-6.78	1.41	1.51
1	B	20	PHE	CB-CG	-6.73	1.40	1.51
1	A	160	TYR	CB-CG	-6.53	1.41	1.51
1	B	93	ASP	CB-CG	-6.51	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	TYR	CB-CG	-6.50	1.42	1.51
3	D	715	PHE	CB-CG	-6.46	1.40	1.51
3	D	764	TYR	CB-CG	-6.41	1.42	1.51
3	D	537	GLU	CG-CD	6.37	1.61	1.51
1	A	160	TYR	CG-CD1	-6.21	1.31	1.39
1	B	597	CYS	CB-SG	-6.20	1.71	1.82
3	D	545	TYR	CB-CG	-6.12	1.42	1.51
1	B	627	TYR	CB-CG	-6.11	1.42	1.51
1	A	584	GLU	CB-CG	-6.04	1.40	1.52
1	B	160	TYR	CB-CG	-5.97	1.42	1.51
3	D	640	TYR	CB-CG	-5.92	1.42	1.51
2	C	56	PHE	CB-CG	-5.89	1.41	1.51
1	A	502	VAL	CB-CG1	-5.88	1.40	1.52
1	A	225	GLU	CB-CG	5.83	1.63	1.52
1	B	138	PHE	CB-CG	-5.79	1.41	1.51
1	A	507	PHE	CB-CG	-5.70	1.41	1.51
1	A	420	CYS	CB-SG	-5.69	1.72	1.81
1	A	47	GLU	CG-CD	-5.67	1.43	1.51
1	A	20	PHE	CB-CG	-5.63	1.41	1.51
1	B	225	GLU	CB-CG	5.56	1.62	1.52
1	B	18	GLU	CD-OE1	-5.49	1.19	1.25
1	B	527	GLU	CD-OE2	-5.45	1.19	1.25
1	B	160	TYR	CG-CD1	-5.43	1.32	1.39
1	A	15	GLU	CB-CG	5.34	1.62	1.52
1	A	611	GLU	CD-OE1	-5.34	1.19	1.25
1	A	25	GLU	CD-OE1	-5.33	1.19	1.25
1	A	313	TYR	CB-CG	-5.32	1.43	1.51
3	D	686	PHE	CB-CG	-5.25	1.42	1.51
1	B	507	PHE	CB-CG	-5.25	1.42	1.51
1	A	61	TYR	CB-CG	-5.23	1.43	1.51
1	B	520	TYR	CG-CD2	-5.16	1.32	1.39
1	B	517	GLU	CD-OE1	-5.14	1.20	1.25
1	A	364	TYR	CB-CG	-5.12	1.44	1.51
3	D	661	GLU	CD-OE1	-5.12	1.20	1.25
1	B	337	PHE	CB-CG	-5.10	1.42	1.51
1	B	297	TRP	CB-CG	-5.09	1.41	1.50
1	A	536	PHE	CB-CG	-5.07	1.42	1.51
1	A	635	GLU	CD-OE2	-5.06	1.20	1.25
1	B	216	TYR	CB-CG	-5.05	1.44	1.51
1	B	47	GLU	CD-OE2	-5.04	1.20	1.25
1	B	420	CYS	CB-SG	-5.04	1.73	1.81
1	A	364	TYR	CG-CD2	-5.03	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	TRP	CD2-CE2	-5.02	1.35	1.41
1	B	527	GLU	CD-OE1	-5.02	1.20	1.25
1	A	517	GLU	CD-OE1	-5.01	1.20	1.25
1	A	42	GLU	CD-OE1	-5.01	1.20	1.25

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	LEU	C-N-CA	13.49	150.63	122.30
1	B	366	ARG	C-N-CA	13.26	154.85	121.70
1	B	358	LYS	C-N-CA	12.09	151.93	121.70
1	B	617	GLN	C-N-CA	11.02	149.25	121.70
1	B	365	VAL	C-N-CA	10.56	148.10	121.70
1	A	365	VAL	C-N-CA	10.46	147.84	121.70
1	A	46	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	B	510	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	338	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	B	366	ARG	NE-CZ-NH2	-8.18	116.21	120.30
3	D	613	TYR	CB-CG-CD2	-7.88	116.27	121.00
3	D	606	PHE	CB-CG-CD2	-7.60	115.48	120.80
1	B	627	TYR	CB-CG-CD1	-7.52	116.49	121.00
1	A	87	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	591	ARG	NE-CZ-NH1	7.43	124.02	120.30
3	D	606	PHE	CB-CG-CD1	7.00	125.70	120.80
1	B	338	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	B	182	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	456	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	345	ARG	NE-CZ-NH2	-6.76	116.92	120.30
3	D	714	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	24	ALA	C-N-CA	6.49	137.92	121.70
3	D	655	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	434	TYR	CB-CG-CD1	-6.08	117.35	121.00
3	D	591	ASP	CB-CG-OD1	6.05	123.74	118.30
3	D	640	TYR	CB-CG-CD1	-6.03	117.38	121.00
3	D	558	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	610	MET	CG-SD-CE	5.87	109.58	100.20
1	A	346	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	D	598	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	A	591	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	46	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	54	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	366	ARG	NE-CZ-NH1	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	139	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	145	ALA	C-N-CA	5.38	135.14	121.70
1	B	284	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	B	620	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	512	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	D	613	TYR	CB-CG-CD1	5.16	124.09	121.00
1	B	131	ILE	C-N-CA	-5.11	111.57	122.30
1	A	139	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	D	609	GLY	CA-C-O	-5.08	111.46	120.60
1	A	201	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	C	41	LEU	C-N-CA	-5.04	111.72	122.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	PHE	Mainchain
1	A	380	GLU	Mainchain
1	B	348	PRO	Mainchain
1	B	350	ASP	Mainchain
1	B	351	LEU	Mainchain
3	D	609	GLY	Mainchain
3	D	610	TRP	Mainchain
3	D	697	LEU	Mainchain
3	D	715	PHE	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	5096	5144	5141	3	0
1	B	5096	5144	5137	3	0
2	C	1101	1021	1021	3	0
3	D	2074	2098	2097	5	0
4	A	31	12	12	0	0
4	B	31	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	D	28	1	29	1	0
All	All	13459	13432	13449	13	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 0.

All (13) 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)
1:A:457:LYS:NZ	1:A:535:GLU:OE2	2.42	0.52
1:B:86:ASP:O	1:B:88:THR:N	2.46	0.49
1:B:350:ASP:OD1	1:B:350:ASP:N	2.45	0.47
1:A:393:ASP:OD1	1:A:393:ASP:N	2.42	0.47
2:C:121:ASP:OD1	2:C:121:ASP:N	2.45	0.47
2:C:115:GLU:O	2:C:116:ASP:C	2.52	0.47
3:D:625:PRO:O	3:D:626:ASP:HB2	2.15	0.46
1:B:410:LYS:NZ	2:C:115:GLU:OE2	2.49	0.46
3:D:761:ILE:N	3:D:762:PRO:HD2	2.33	0.43
3:D:563:LEU:HB3	6:D:801:DEX:H11	1.99	0.43
3:D:697:LEU:O	3:D:700:ALA:N	2.53	0.42
1:A:175:ASP:OD1	1:A:176:THR:N	2.53	0.41
3:D:638:CYS:O	3:D:642:GLN:N	2.52	0.41

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	623/732 (85%)	609 (98%)	14 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	623/732 (85%)	608 (98%)	13 (2%)	2 (0%)	41	50
2	C	131/160 (82%)	131 (100%)	0	0	100	100
3	D	253/258 (98%)	249 (98%)	4 (2%)	0	100	100
All	All	1630/1882 (87%)	1597 (98%)	31 (2%)	2 (0%)	54	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	ARG
1	B	132	GLY

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	568/666 (85%)	567 (100%)	1 (0%)	93	97
1	B	568/666 (85%)	568 (100%)	0	100	100
2	C	124/149 (83%)	124 (100%)	0	100	100
3	D	234/237 (99%)	233 (100%)	1 (0%)	91	95
All	All	1494/1718 (87%)	1492 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ARG
3	D	606	PHE

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

Mol	Chain	Res	Type
3	D	775	HIS

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 monosaccharides 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$
4	ATP	B	801	5	26,33,33	1.57	6 (23%)	31,52,52	1.26	4 (12%)
6	DEX	D	801	-	31,31,31	1.59	6 (19%)	52,53,53	2.73	25 (48%)
4	ATP	A	801	5	26,33,33	1.52	4 (15%)	31,52,52	1.26	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
4	ATP	B	801	5	-	3/18/38/38	0/3/3/3
6	DEX	D	801	-	-	0/8/84/84	0/4/4/4
4	ATP	A	801	5	-	3/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	ATP	C2-N3	3.82	1.38	1.32
6	D	801	DEX	C10-C1	3.80	1.54	1.50
4	A	801	ATP	C2-N3	3.69	1.38	1.32
6	D	801	DEX	C2-C3	3.35	1.53	1.45
6	D	801	DEX	C4-C3	3.15	1.53	1.45
4	A	801	ATP	C5-C4	3.09	1.49	1.40
4	B	801	ATP	C5-C4	3.06	1.49	1.40
4	B	801	ATP	C4-N3	2.96	1.39	1.35
4	A	801	ATP	C4-N3	2.89	1.39	1.35
6	D	801	DEX	C9-C8	2.87	1.58	1.54
4	B	801	ATP	C2-N1	2.73	1.39	1.33
6	D	801	DEX	C10-C5	2.67	1.56	1.52
4	A	801	ATP	C2-N1	2.55	1.38	1.33
6	D	801	DEX	F1-C9	-2.31	1.38	1.42
4	B	801	ATP	PG-O2G	-2.15	1.46	1.54
4	B	801	ATP	C6-C5	2.01	1.50	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	801	DEX	C12-C11-C9	7.10	117.90	112.93
6	D	801	DEX	C9-C8-C14	6.42	114.25	109.26
6	D	801	DEX	C7-C8-C9	6.32	116.78	110.94
6	D	801	DEX	C6-C5-C10	5.41	118.94	115.61
6	D	801	DEX	F1-C9-C11	-4.63	98.70	102.72
6	D	801	DEX	C15-C14-C8	4.45	123.20	119.07
4	A	801	ATP	N3-C2-N1	-4.33	121.91	128.68
4	B	801	ATP	N3-C2-N1	-4.19	122.12	128.68
6	D	801	DEX	C19-C10-C1	-3.97	102.48	106.63
6	D	801	DEX	C1-C2-C3	-3.94	118.11	121.47
6	D	801	DEX	C5-C4-C3	-3.81	119.39	122.72
6	D	801	DEX	C10-C9-C11	3.30	117.93	115.52
6	D	801	DEX	C18-C13-C12	-3.08	106.85	111.11
6	D	801	DEX	C13-C17-C20	3.00	116.08	112.89
6	D	801	DEX	C10-C5-C4	2.94	124.26	122.12
6	D	801	DEX	C15-C16-C17	2.53	106.89	105.07
6	D	801	DEX	C2-C3-C4	2.51	119.69	117.13
6	D	801	DEX	C6-C5-C4	-2.44	116.79	120.87
6	D	801	DEX	O4-C20-C17	-2.43	119.79	122.68
6	D	801	DEX	C6-C7-C8	2.38	116.46	111.74
6	D	801	DEX	C12-C13-C14	2.31	110.08	108.03
4	B	801	ATP	C4-C5-N7	-2.27	107.03	109.40
4	A	801	ATP	C4-C5-N7	-2.22	107.08	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	801	DEX	F1-C9-C8	-2.22	103.95	105.95
6	D	801	DEX	C13-C17-C16	2.22	104.96	102.86
6	D	801	DEX	C9-C10-C5	2.17	108.98	106.69
6	D	801	DEX	C9-C10-C1	2.17	112.33	109.86
6	D	801	DEX	C7-C8-C14	2.14	116.29	111.47
4	B	801	ATP	N6-C6-N1	2.09	122.91	118.57
6	D	801	DEX	C10-C1-C2	2.09	125.90	124.38
4	B	801	ATP	PB-O3B-PG	-2.04	125.83	132.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

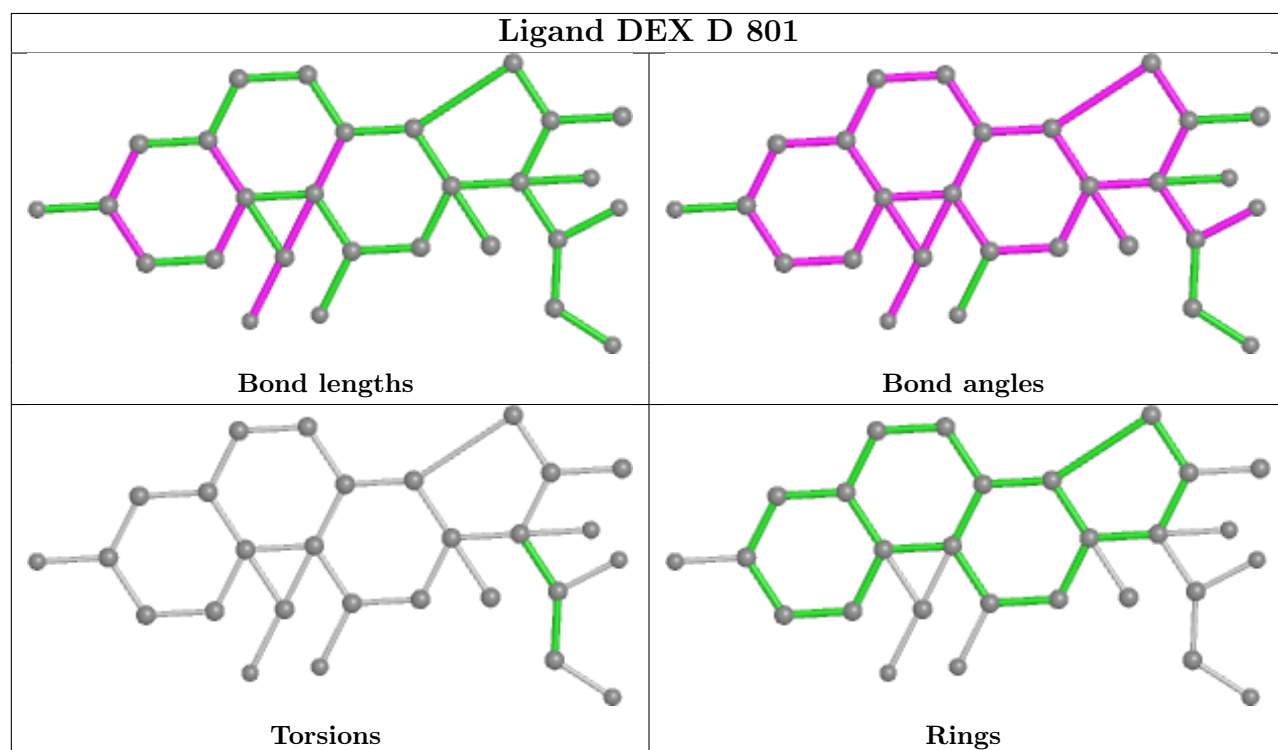
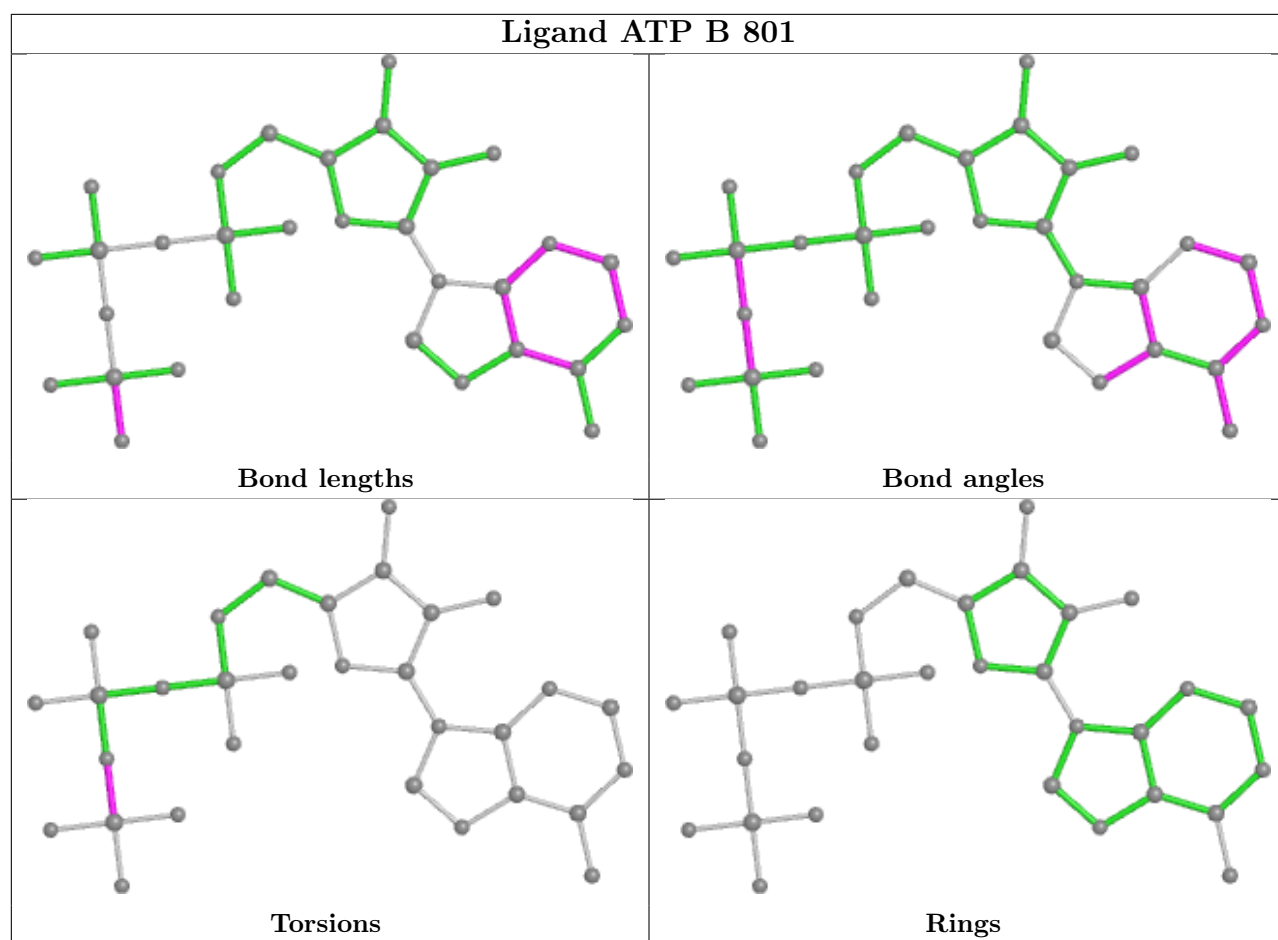
Mol	Chain	Res	Type	Atoms
4	A	801	ATP	PB-O3B-PG-O1G
4	B	801	ATP	PB-O3B-PG-O1G
4	A	801	ATP	PB-O3B-PG-O2G
4	A	801	ATP	PB-O3B-PG-O3G
4	B	801	ATP	PB-O3B-PG-O2G
4	B	801	ATP	PB-O3B-PG-O3G

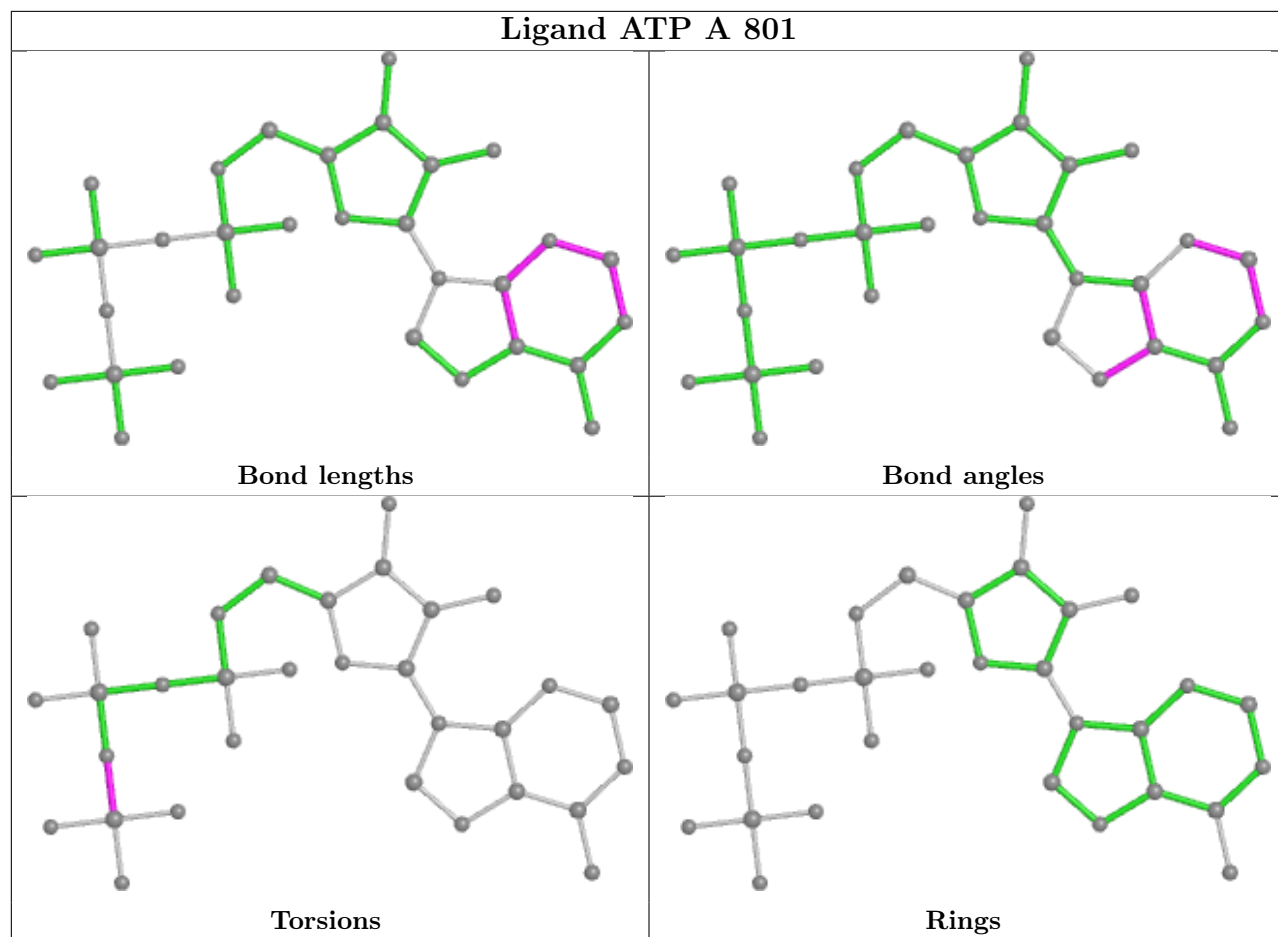
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	801	DEX	1	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.

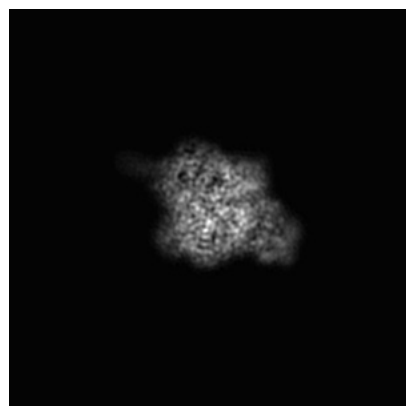
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23004. These allow visual inspection of the internal detail of the map and identification of artifacts.

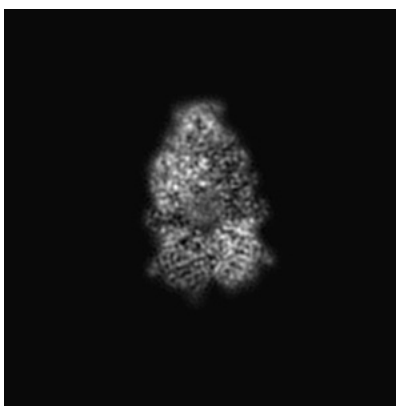
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

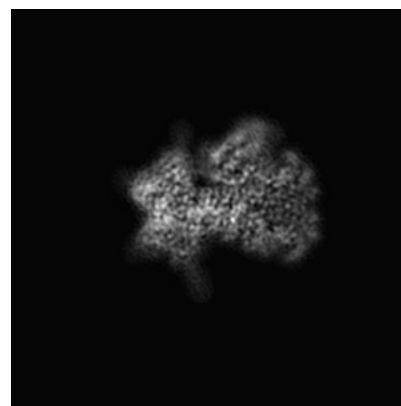
6.1.1 Primary map



X

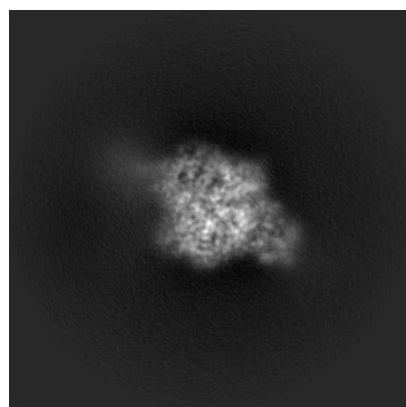


Y

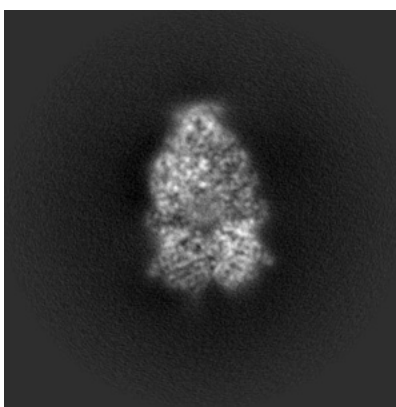


Z

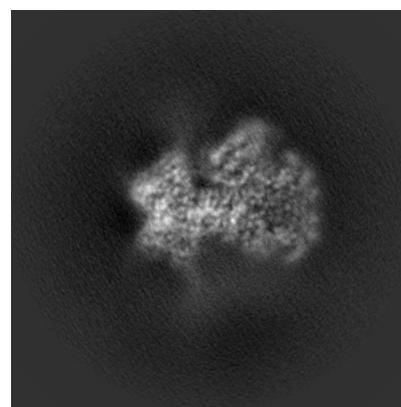
6.1.2 Raw map



X



Y

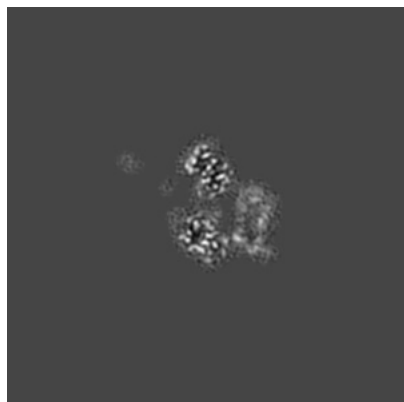


Z

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

6.2 Central slices [i](#)

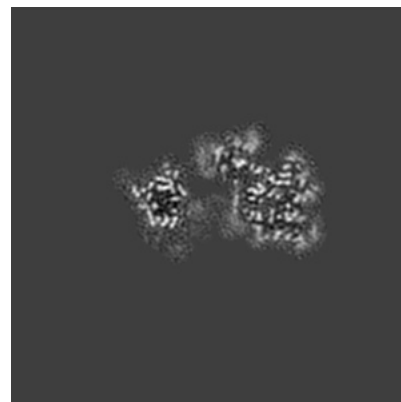
6.2.1 Primary map



X Index: 150

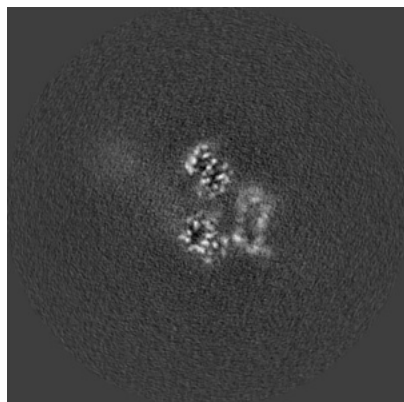


Y Index: 150

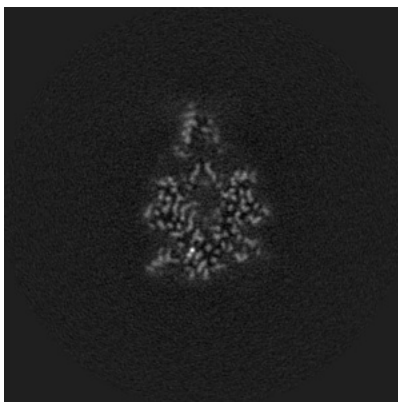


Z Index: 150

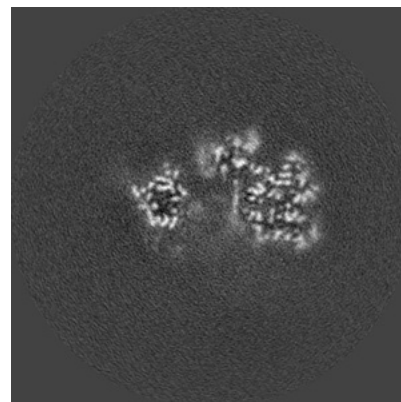
6.2.2 Raw map



X Index: 150



Y Index: 150

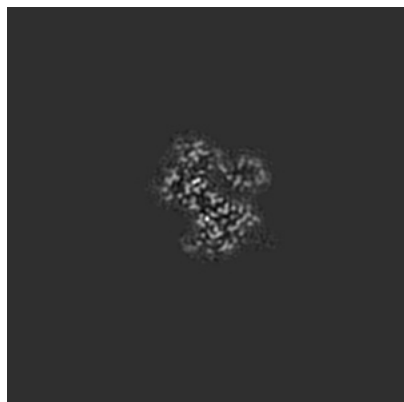


Z Index: 150

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

6.3 Largest variance slices [i](#)

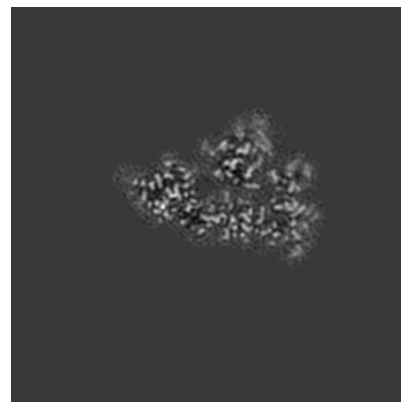
6.3.1 Primary map



X Index: 116

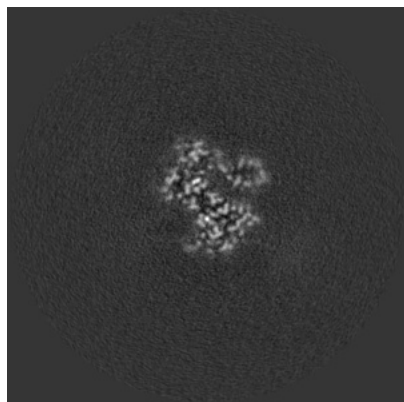


Y Index: 150

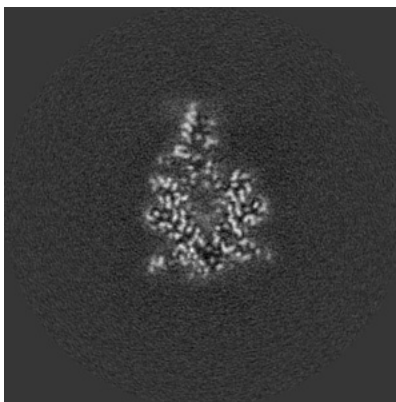


Z Index: 138

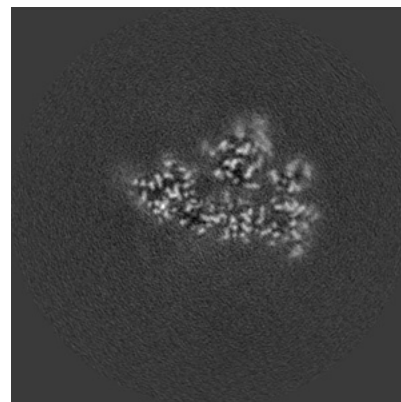
6.3.2 Raw map



X Index: 116



Y Index: 148

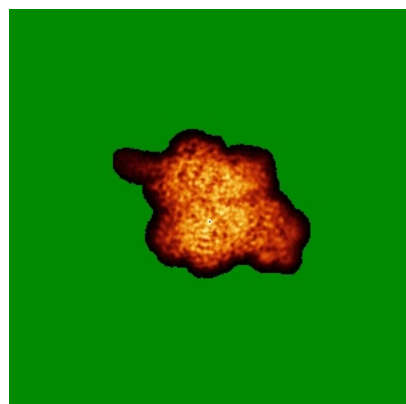


Z Index: 138

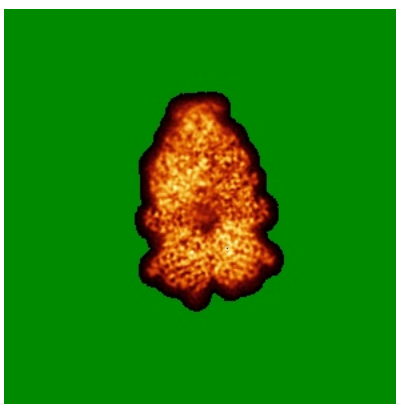
The images above show the largest variance slices of the map in three orthogonal directions.

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

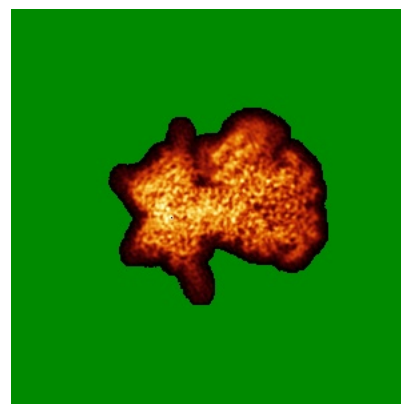
6.4.1 Primary map



X

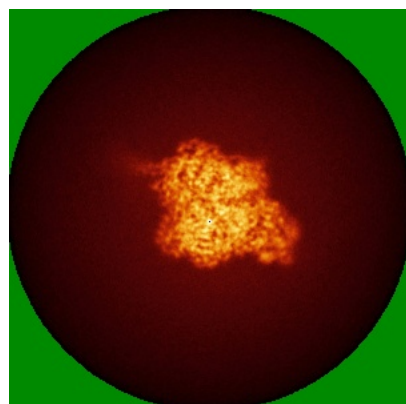


Y

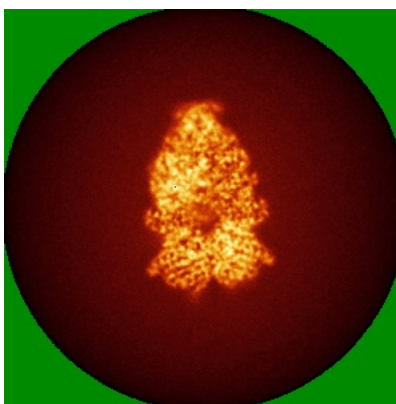


Z

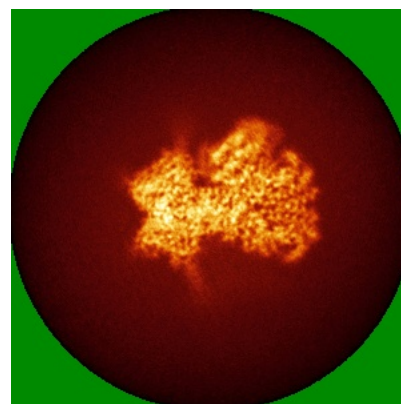
6.4.2 Raw map



X



Y

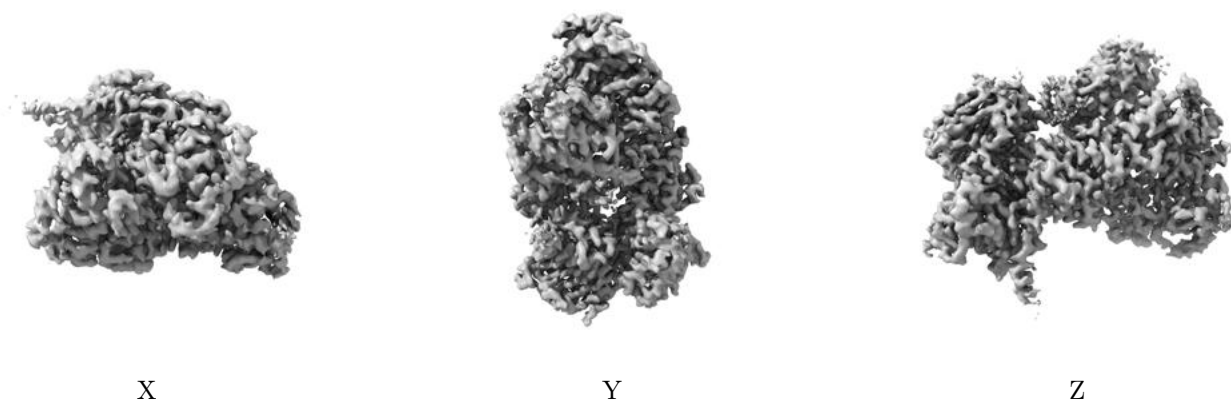


Z

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.

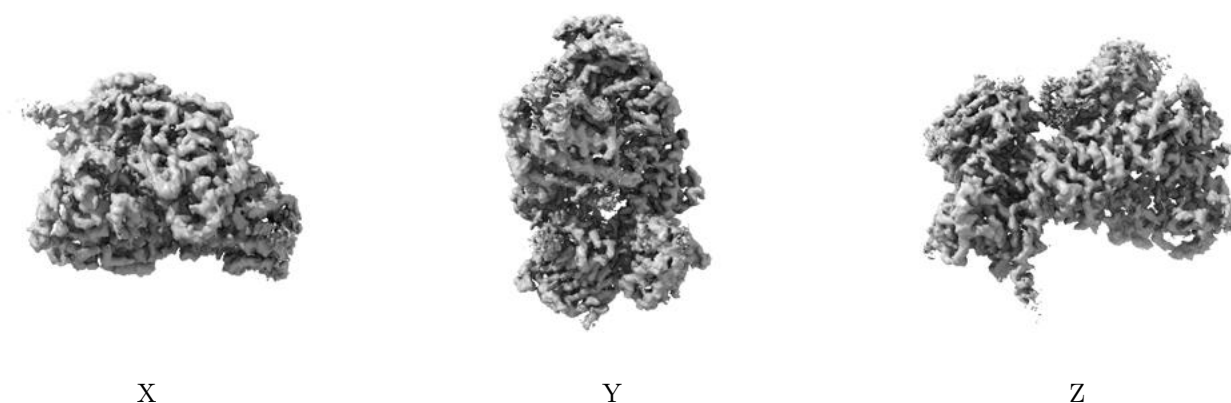
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

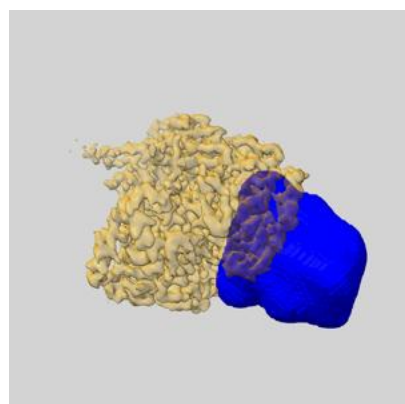
6.6 Mask visualisation [i](#)

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

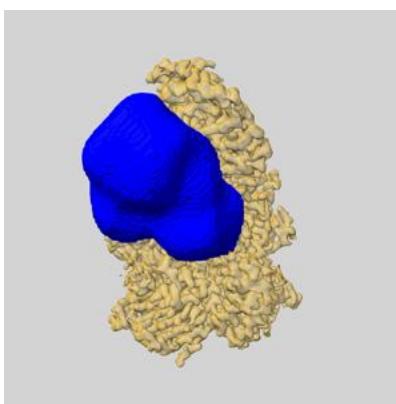
A mask typically either:

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

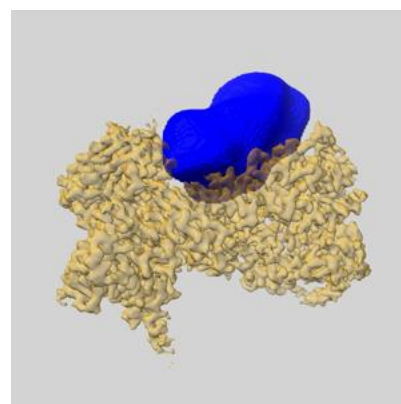
6.6.1 emd_23004_msk_2.map [i](#)



X

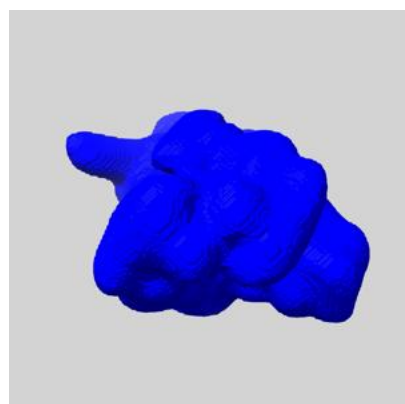


Y

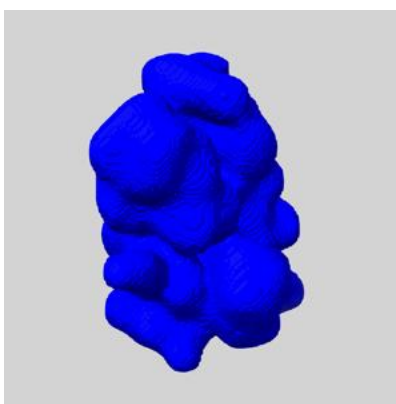


Z

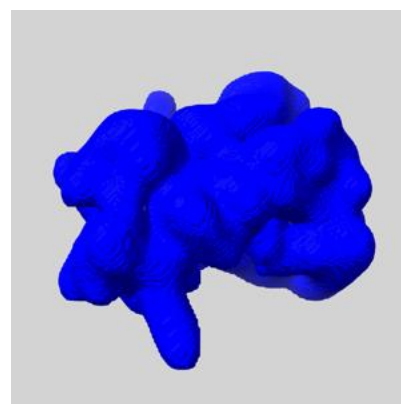
6.6.2 emd_23004_msk_1.map [i](#)



X



Y

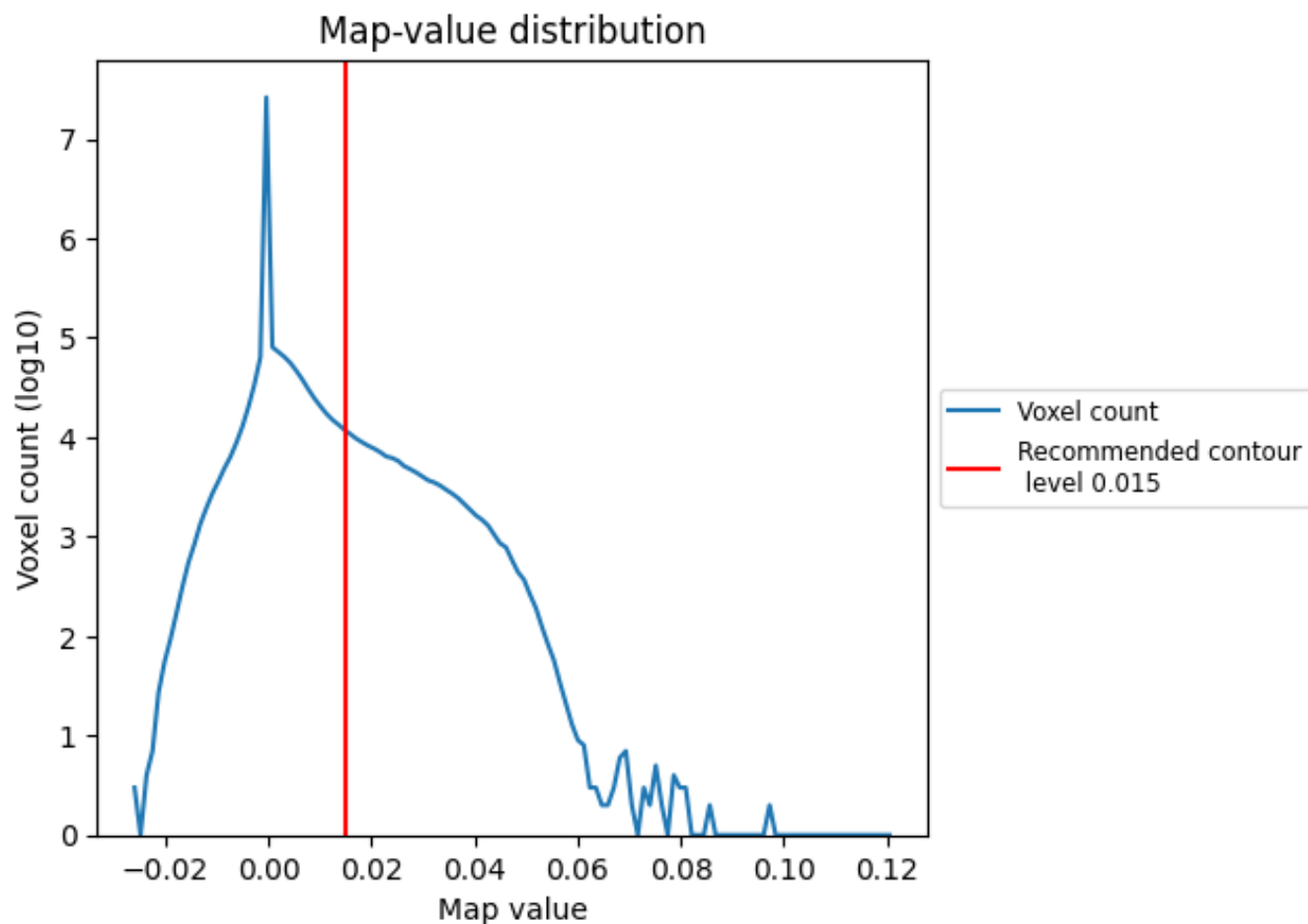


Z

7 Map analysis [i](#)

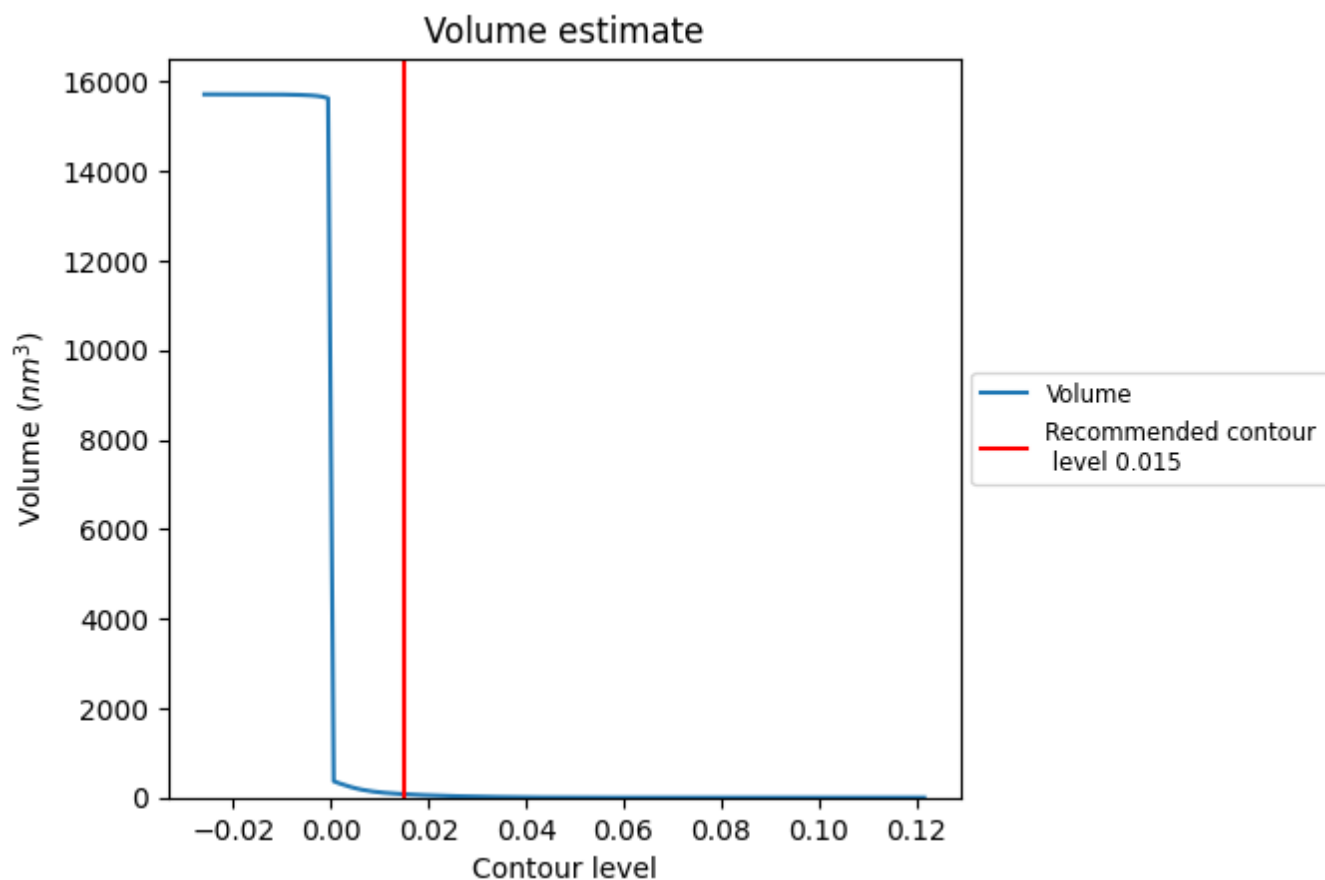
This section contains the results of statistical analysis of the map.

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.

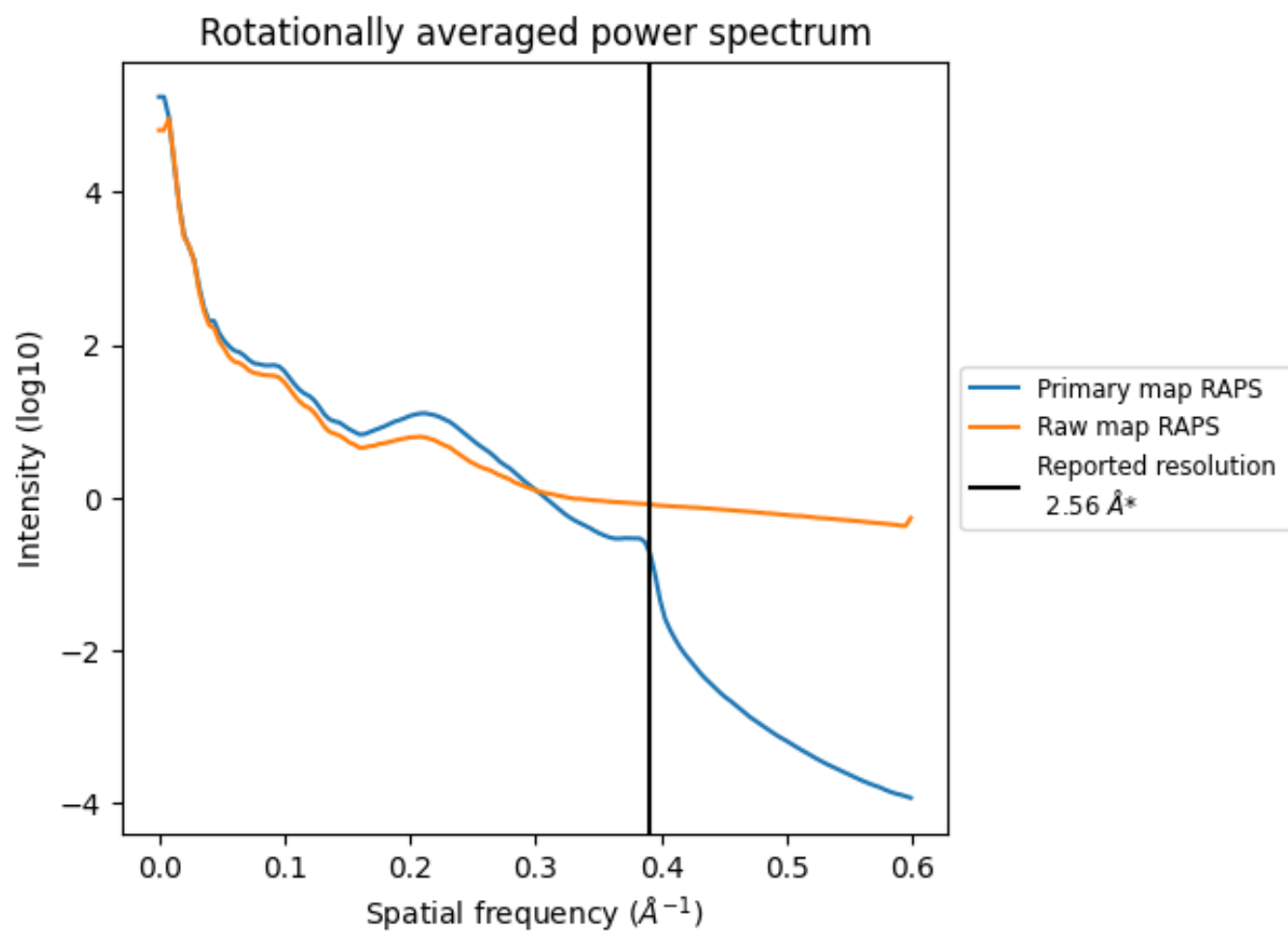
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 76 nm^3 ; this corresponds to an approximate mass of 69 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 ⓘ

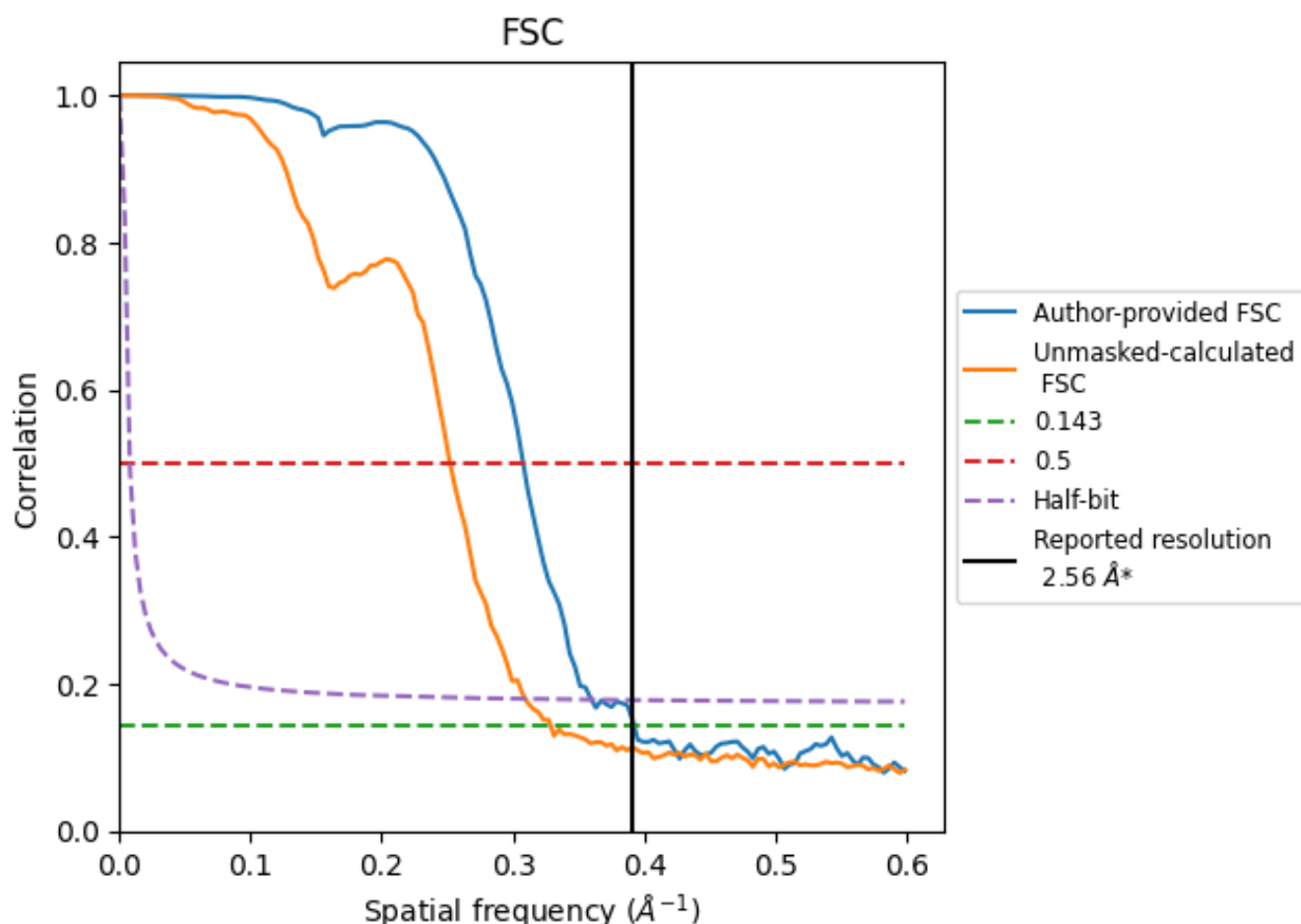


*Reported resolution corresponds to spatial frequency of 0.391 Å⁻¹

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 0.391 \AA^{-1}

8.2 Resolution estimates [i](#)

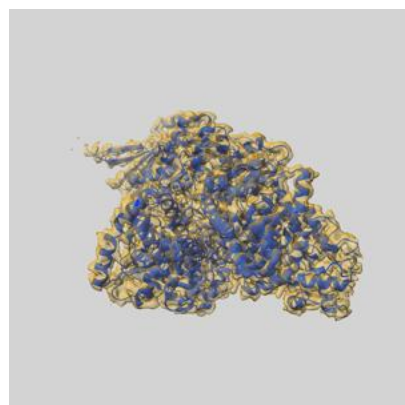
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.55	3.25	2.78
Unmasked-calculated*	3.04	3.97	3.23

*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 3.04 differs from the reported value 2.56 by more than 10 %

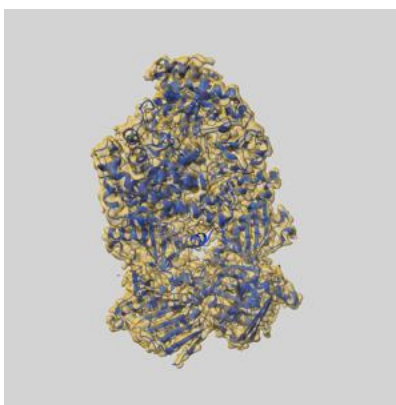
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23004 and PDB model 7KRJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

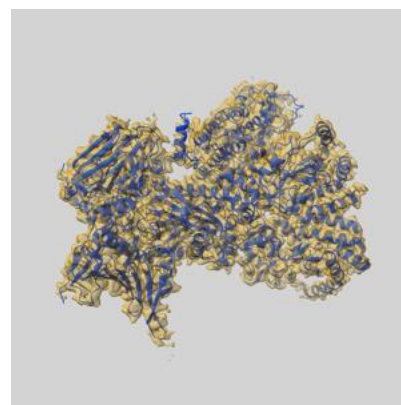
9.1 Map-model overlay [i](#)



X



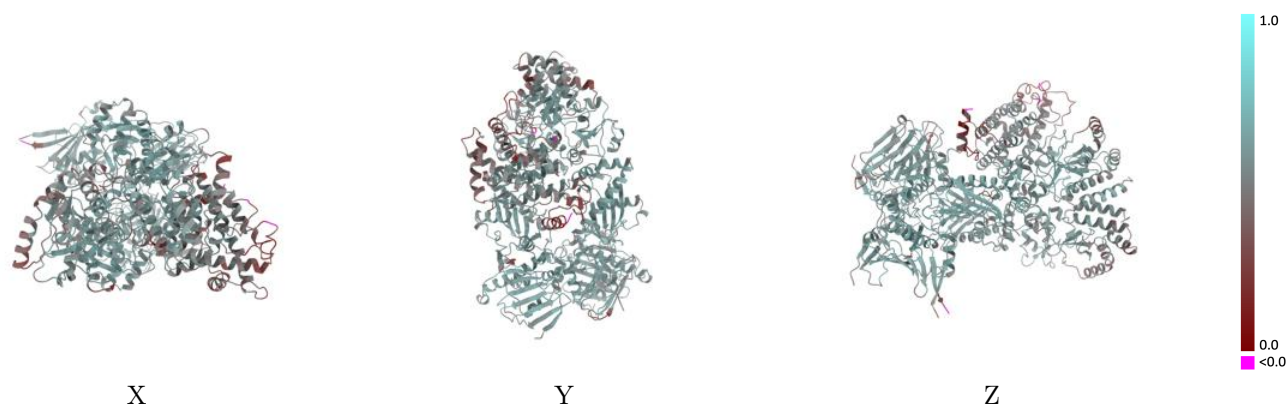
Y



Z

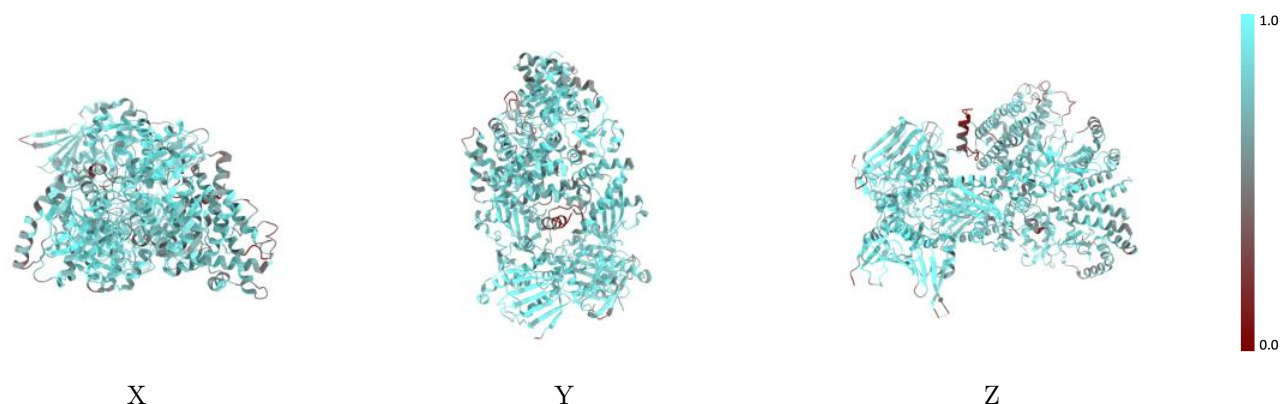
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



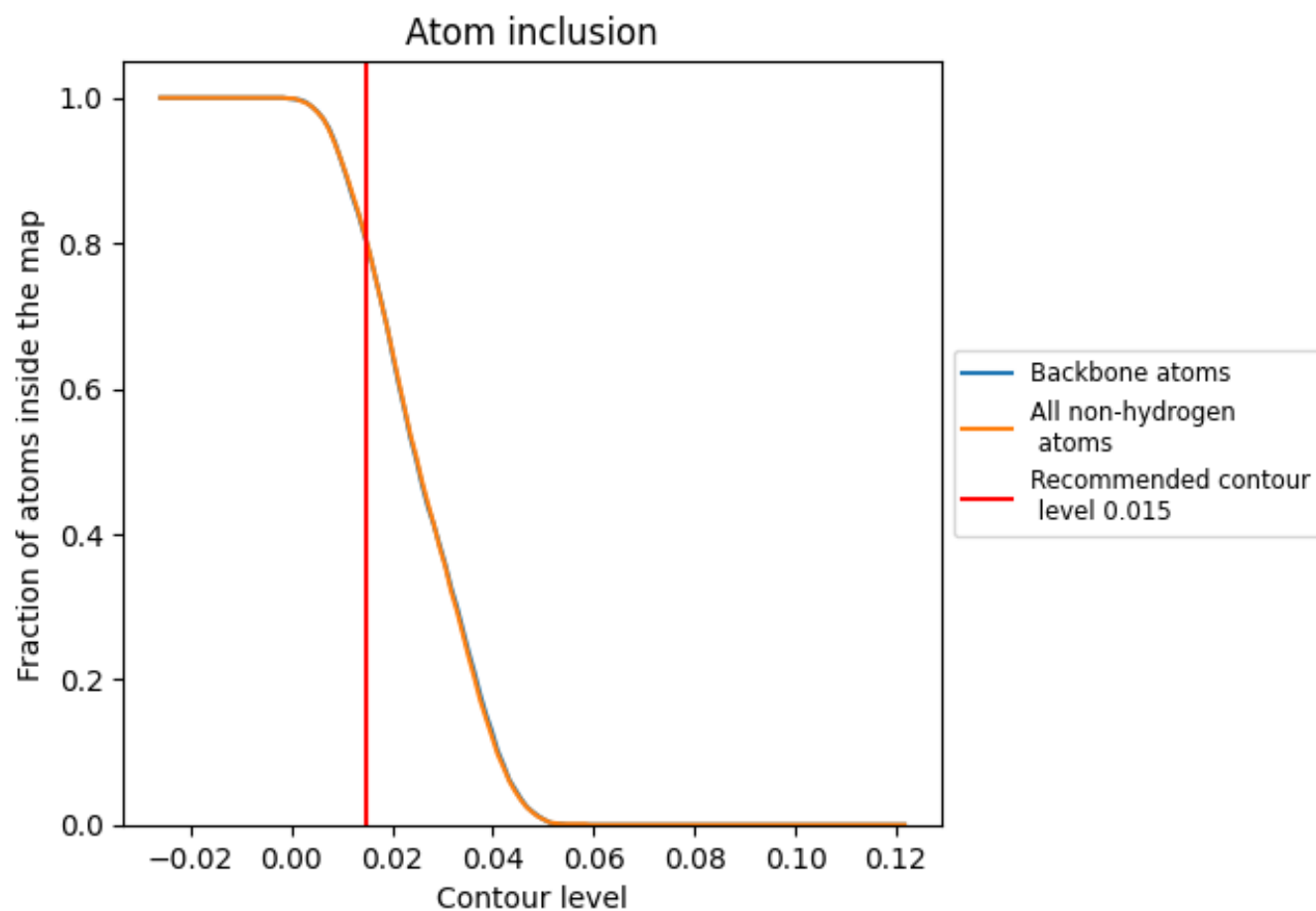
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8020	<div></div> 0.5390
A	<div></div> 0.8290	<div></div> 0.5580
B	<div></div> 0.8450	<div></div> 0.5660
C	<div></div> 0.7120	<div></div> 0.4860
D	<div></div> 0.7380	<div></div> 0.4570

