



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:48 PM UTC

PDB ID : 8FFV / pdb_00008ffv
EMDB ID : EMD-29068
Title : Cryo-EM structure of the GR-Hsp90-FKBP52 complex
Authors : Noddings, C.M.; Agard, D.A.
Deposited on : 2022-12-10
Resolution : 3.01 Å(reported)
Based on initial models : 1M2Z, 5FWK, 1EJF

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:

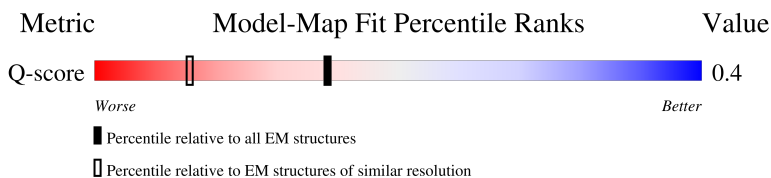
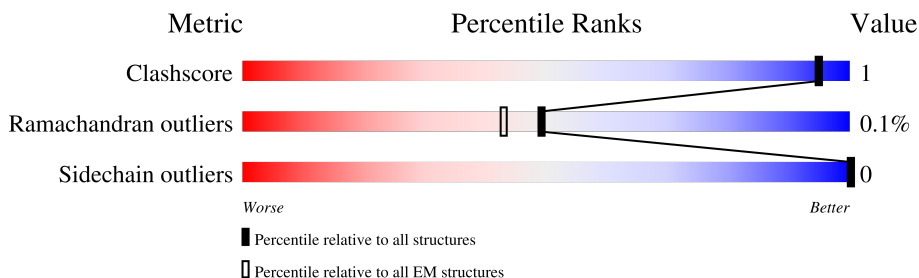
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.01 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	13882 (2.51 - 3.51)

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	459	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31656 atoms, of which 15829 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	644	Total	C	H	N	O	S	0	0
			10478	3308	5248	876	1022	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 FKBP4, N-terminally processed.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	409	Total	C	H	N	O	S	0	0
			6547	2085	3266	559	624	13		

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

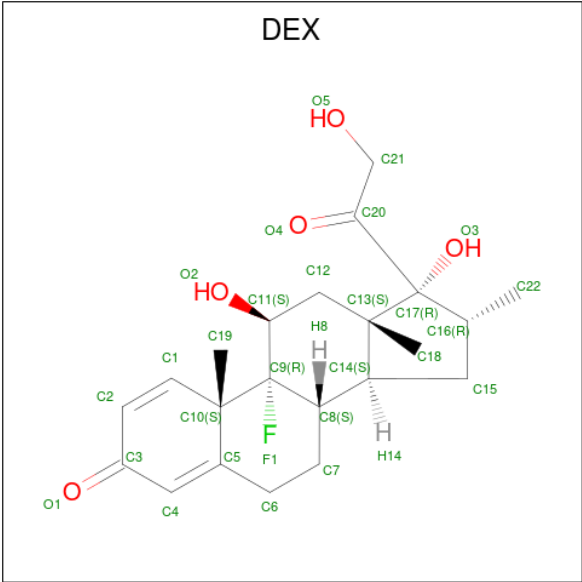


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- 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).

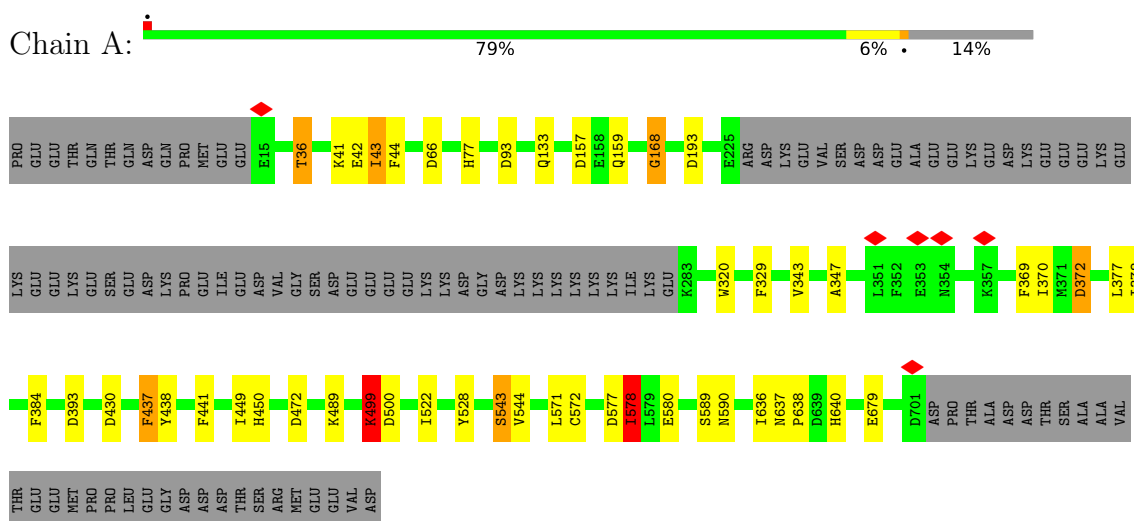


Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	H	O	
6	C	1	29	22	1	1	5	0

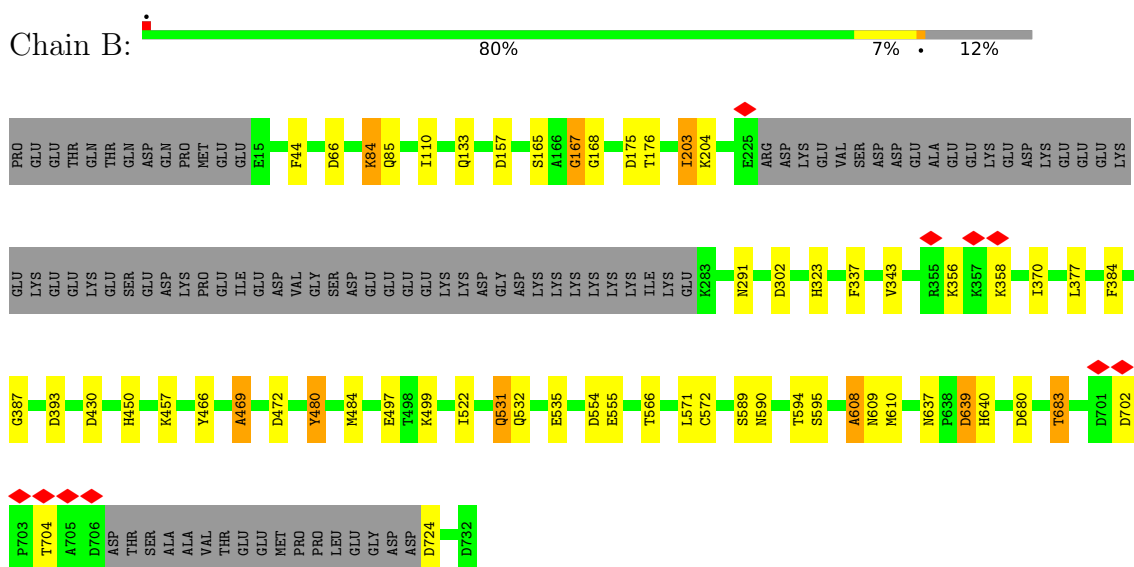
3 Residue-property plots

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

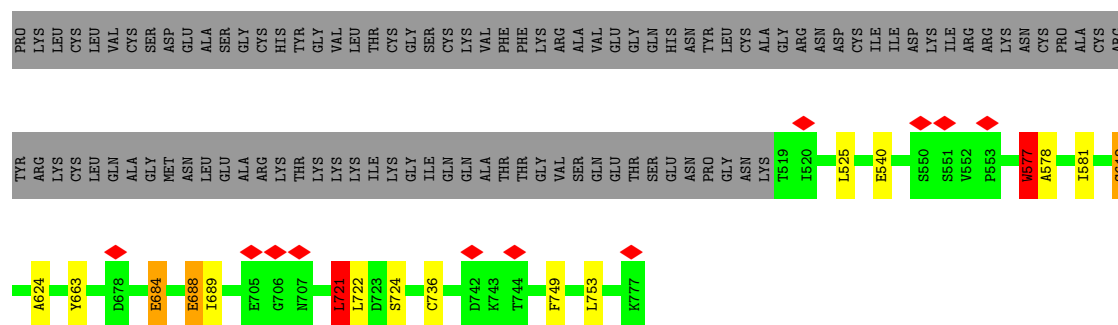


• Molecule 1: Heat shock protein HSP 90-alpha



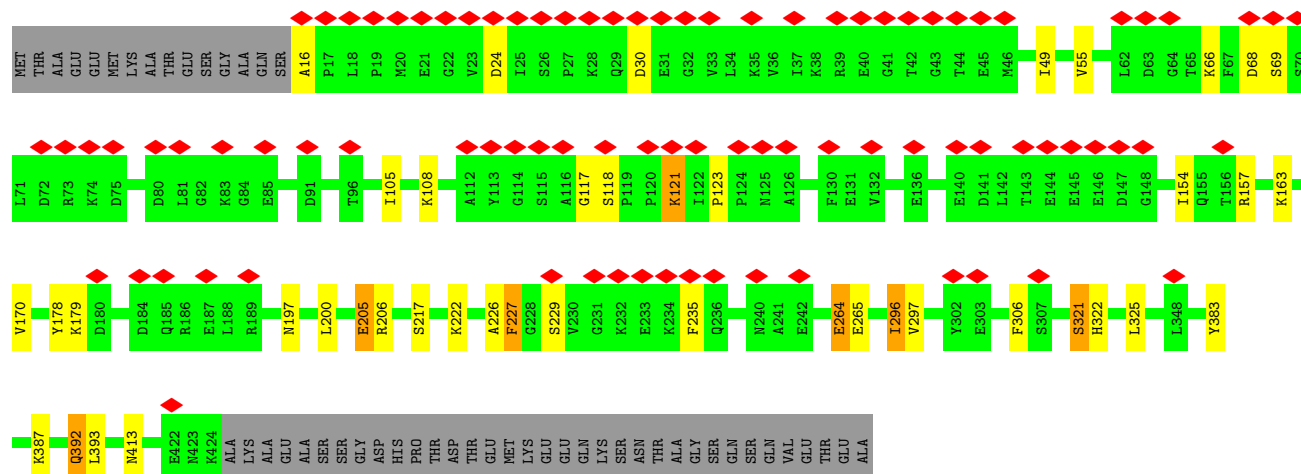
• Molecule 2: Glucocorticoid receptor

Chain C:  67% 28%



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP4, N-terminally processed

Chain D:  19% 80% 8% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	307109	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 ($e^-/\text{\AA}^2$)	67	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	2.197	Depositor
Minimum map value	-0.492	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	267.19998, 267.19998, 267.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: DEX, ATP, 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	1.29	7/5204 (0.1%)	1.32	38/6996 (0.5%)
1	B	1.29	6/5313 (0.1%)	1.37	49/7142 (0.7%)
2	C	1.11	1/2149 (0.0%)	1.29	23/2909 (0.8%)
3	D	1.03	0/3345	1.35	39/4493 (0.9%)
All	All	1.22	14/16011 (0.1%)	1.34	149/21540 (0.7%)

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	9
2	C	0	5
3	D	0	7
All	All	0	30

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	450	HIS	CB-CG	-8.44	1.38	1.50
1	B	450	HIS	CB-CG	-7.56	1.39	1.50
1	A	329	PHE	CB-CG	-6.42	1.35	1.50
1	A	640	HIS	CB-CG	-6.00	1.41	1.50
1	B	337	PHE	CB-CG	-5.64	1.37	1.50
1	A	369	PHE	CB-CG	-5.60	1.37	1.50
1	B	291	ASN	CB-CG	-5.47	1.38	1.52
1	A	77	HIS	CB-CG	-5.44	1.42	1.50
1	B	323	HIS	CB-CG	-5.37	1.42	1.50
1	B	640	HIS	CB-CG	-5.29	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	TYR	CB-CG	-5.29	1.40	1.51
1	A	43	ILE	N-CA	-5.24	1.39	1.46
1	A	159	GLN	CB-CG	-5.21	1.36	1.52
2	C	663	TYR	CB-CG	-5.10	1.40	1.51

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	TYR	CA-C-N	24.64	153.95	120.44
1	A	528	TYR	C-N-CA	24.64	153.95	120.44
1	B	594	THR	CA-C-N	22.95	153.08	120.49
1	B	594	THR	C-N-CA	22.95	153.08	120.49
1	B	484	MET	CA-C-N	17.55	152.91	120.97
1	B	484	MET	C-N-CA	17.55	152.91	120.97
1	B	302	ASP	CA-C-N	16.34	152.45	122.06
1	B	302	ASP	C-N-CA	16.34	152.45	122.06
2	C	689	ILE	N-CA-C	-9.04	101.14	111.00
3	D	206	ARG	N-CA-C	-8.72	101.24	112.23
1	A	578	ILE	N-CA-C	-8.70	97.38	109.21
1	B	337	PHE	CA-CB-CG	8.29	122.09	113.80
2	C	612	SER	CA-C-O	-8.09	111.98	120.55
3	D	393	LEU	N-CA-C	-8.00	101.86	111.69
1	B	203	ILE	CA-C-O	-7.97	112.66	120.95
1	B	165	SER	N-CA-C	-7.77	97.51	109.24
3	D	264	GLU	CA-C-O	-7.75	112.34	120.55
2	C	577	TRP	CA-C-O	-7.75	112.69	120.82
1	A	343	VAL	CA-C-N	7.66	127.61	120.03
1	A	343	VAL	C-N-CA	7.66	127.61	120.03
1	A	578	ILE	CA-C-O	-7.65	112.01	121.11
2	C	722	LEU	N-CA-C	-7.61	102.64	112.23
1	A	36	THR	CA-C-O	-7.61	111.05	119.34
1	B	358	LYS	N-CA-C	7.55	120.40	111.71
1	B	680	ASP	CA-C-N	7.53	127.24	119.56
1	B	680	ASP	C-N-CA	7.53	127.24	119.56
3	D	235	PHE	CA-CB-CG	7.46	121.25	113.80
1	B	532	GLN	N-CA-C	-7.42	104.36	113.41
1	B	66	ASP	CA-C-N	7.36	127.06	119.56
1	B	66	ASP	C-N-CA	7.36	127.06	119.56
2	C	613	TYR	N-CA-C	-7.24	104.26	113.23
2	C	540	GLU	CA-C-N	7.19	127.15	120.03
2	C	540	GLU	C-N-CA	7.19	127.15	120.03
1	A	489	LYS	N-CA-C	-7.04	104.18	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	VAL	CA-C-N	7.04	127.00	120.03
1	B	343	VAL	C-N-CA	7.04	127.00	120.03
3	D	322	HIS	N-CA-C	-7.00	103.73	112.90
3	D	321	SER	CA-C-O	-6.91	112.03	119.97
1	A	66	ASP	CA-C-N	6.90	126.60	119.56
1	A	66	ASP	C-N-CA	6.90	126.60	119.56
3	D	222	LYS	CA-C-N	6.88	127.45	119.47
3	D	222	LYS	C-N-CA	6.88	127.45	119.47
2	C	688	GLU	CA-C-O	-6.88	113.13	120.42
1	A	578	ILE	CA-C-N	-6.83	112.66	124.82
1	A	578	ILE	C-N-CA	-6.83	112.66	124.82
1	B	370	ILE	CB-CA-C	-6.80	105.93	111.71
1	A	544	VAL	N-CA-C	-6.68	105.82	112.17
1	A	437	PHE	CA-C-O	-6.67	113.81	120.82
3	D	383	TYR	CA-C-N	6.65	126.34	119.56
3	D	383	TYR	C-N-CA	6.65	126.34	119.56
3	D	227	PHE	CA-CB-CG	6.65	120.45	113.80
1	B	637	ASN	CA-C-N	6.62	126.75	119.87
1	B	637	ASN	C-N-CA	6.62	126.75	119.87
1	A	347	ALA	CA-C-N	6.58	126.55	120.03
1	A	347	ALA	C-N-CA	6.58	126.55	120.03
1	A	438	TYR	N-CA-C	-6.54	103.99	112.23
1	A	43	ILE	N-CA-C	-6.46	103.24	112.35
1	B	639	ASP	CA-C-O	-6.42	112.78	120.55
1	B	356	LYS	N-CA-C	-6.38	101.93	110.55
1	A	320	TRP	N-CA-C	-6.37	104.95	114.64
2	C	581	ILE	N-CA-C	6.36	114.10	108.63
3	D	392	GLN	CA-C-O	-6.34	112.68	119.97
3	D	200	LEU	CA-C-N	6.30	126.27	119.78
3	D	200	LEU	C-N-CA	6.30	126.27	119.78
1	A	449	ILE	N-CA-C	-6.27	105.62	111.45
1	B	480	TYR	CA-C-O	-6.26	114.20	120.90
3	D	265	GLU	N-CA-C	-6.25	104.35	112.23
3	D	108	LYS	CA-C-N	6.21	126.40	119.32
3	D	108	LYS	C-N-CA	6.21	126.40	119.32
3	D	296	ILE	CA-C-O	-6.21	114.49	120.95
1	A	637	ASN	CA-C-N	6.08	126.19	119.87
1	A	637	ASN	C-N-CA	6.08	126.19	119.87
2	C	749	PHE	CA-C-N	6.01	125.97	119.78
2	C	749	PHE	C-N-CA	6.01	125.97	119.78
1	A	636	ILE	N-CA-C	6.00	116.56	108.17
1	B	531	GLN	CA-C-O	-6.00	114.06	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	170	VAL	N-CA-C	5.99	116.50	108.11
1	B	110	ILE	N-CA-C	5.98	116.72	110.62
3	D	30	ASP	CA-C-N	5.97	133.19	122.38
3	D	30	ASP	C-N-CA	5.97	133.19	122.38
3	D	16	ALA	CA-C-N	5.96	125.90	119.76
3	D	16	ALA	C-N-CA	5.96	125.90	119.76
3	D	24	ASP	CA-CB-CG	5.91	118.51	112.60
2	C	721	LEU	CA-C-O	-5.88	112.85	119.79
1	B	337	PHE	CB-CA-C	-5.88	97.10	109.38
1	A	168	GLY	CA-C-O	-5.83	112.55	119.01
3	D	297	VAL	N-CA-C	-5.78	105.10	110.53
1	B	497	GLU	N-CA-C	5.75	117.55	111.28
1	A	578	ILE	O-C-N	-5.74	115.94	122.72
3	D	123	PRO	N-CA-C	-5.73	104.97	110.47
3	D	325	LEU	N-CA-C	-5.71	105.13	111.36
1	A	500	ASP	N-CA-C	-5.70	105.44	112.90
1	B	702	ASP	CA-C-N	5.69	125.36	119.56
1	B	702	ASP	C-N-CA	5.69	125.36	119.56
1	A	499	LYS	CA-C-O	-5.66	113.46	119.97
2	C	612	SER	CA-C-N	-5.66	111.70	121.66
2	C	612	SER	C-N-CA	-5.66	111.70	121.66
2	C	578	ALA	N-CA-C	5.65	117.43	111.28
1	B	683	THR	CA-C-O	-5.64	112.47	119.18
1	A	393	ASP	N-CA-C	5.59	119.29	111.74
1	A	378	ILE	CA-C-N	5.53	125.48	119.78
1	A	378	ILE	C-N-CA	5.53	125.48	119.78
1	B	85	GLN	N-CA-C	-5.53	106.38	113.23
3	D	163	LYS	CA-C-N	5.53	125.50	120.03
3	D	163	LYS	C-N-CA	5.53	125.50	120.03
3	D	205	GLU	N-CA-C	-5.52	104.90	111.69
2	C	624	ALA	CA-C-N	5.50	125.17	119.56
2	C	624	ALA	C-N-CA	5.50	125.17	119.56
1	A	441	PHE	N-CA-C	5.49	119.96	112.88
1	B	639	ASP	CA-C-N	-5.48	114.05	122.87
1	B	639	ASP	C-N-CA	-5.48	114.05	122.87
1	B	204	LYS	N-CA-C	-5.47	105.33	112.23
1	B	566	THR	N-CA-C	-5.47	106.38	113.16
1	A	377	LEU	N-CA-C	5.47	118.16	111.82
2	C	581	ILE	CA-C-N	5.46	125.39	119.76
2	C	581	ILE	C-N-CA	5.46	125.39	119.76
3	D	55	VAL	N-CA-C	5.45	117.94	108.95
1	B	384	PHE	N-CA-C	-5.41	106.15	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	GLY	N-CA-C	-5.37	107.26	115.00
1	B	377	LEU	N-CA-C	5.37	117.21	111.36
1	A	679	GLU	N-CA-C	5.36	119.54	112.89
2	C	525	LEU	CA-C-N	5.36	125.26	119.85
2	C	525	LEU	C-N-CA	5.36	125.26	119.85
3	D	30	ASP	N-CA-C	-5.28	106.81	113.20
1	B	157	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	469	ALA	CA-C-O	-5.25	113.59	120.00
1	B	704	THR	N-CA-C	5.25	117.23	108.99
1	B	167	GLY	CA-C-N	-5.25	113.90	122.40
1	B	167	GLY	C-N-CA	-5.25	113.90	122.40
1	A	543	SER	CA-C-O	-5.24	115.24	121.16
1	A	522	ILE	N-CA-C	5.23	116.51	112.12
2	C	684	GLU	CA-C-O	-5.23	112.83	119.31
3	D	321	SER	O-C-N	-5.22	115.85	122.27
1	A	157	ASP	CA-CB-CG	5.22	117.82	112.60
3	D	306	PHE	CA-CB-CG	5.21	119.01	113.80
2	C	753	LEU	N-CA-C	-5.19	106.10	112.90
3	D	217	SER	N-CA-C	5.19	116.95	109.07
1	B	522	ILE	N-CA-C	5.18	116.02	111.56
1	B	84	LYS	CA-C-O	-5.15	113.04	119.38
3	D	105	ILE	N-CA-C	5.14	116.10	108.23
1	B	387	GLY	N-CA-C	5.13	118.07	110.42
3	D	121	LYS	N-CA-C	5.13	120.18	113.30
1	A	370	ILE	CB-CA-C	-5.12	107.36	111.71
1	A	372	ASP	N-CA-C	5.09	120.60	113.02
1	B	608	ALA	N-CA-C	-5.08	103.45	110.35
3	D	69	SER	N-CA-C	5.06	114.97	108.34
1	B	595	SER	CA-C-N	5.05	124.66	119.56
1	B	595	SER	C-N-CA	5.05	124.66	119.56
3	D	157	ARG	N-CA-C	5.01	116.61	109.14

There are no chirality outliers.

All (30) 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

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Mol	Chain	Res	Type	Group
1	A	543	SER	Mainchain
1	A	578	ILE	Mainchain
1	A	638	PRO	Mainchain
1	B	167	GLY	Mainchain
1	B	203	ILE	Mainchain
1	B	469	ALA	Peptide,Mainchain
1	B	480	TYR	Mainchain
1	B	531	GLN	Mainchain
1	B	639	ASP	Mainchain
1	B	683	THR	Mainchain
1	B	84	LYS	Mainchain
2	C	577	TRP	Mainchain
2	C	612	SER	Mainchain
2	C	684	GLU	Mainchain
2	C	688	GLU	Mainchain
2	C	721	LEU	Mainchain
3	D	197	ASN	Mainchain
3	D	205	GLU	Mainchain
3	D	229	SER	Mainchain
3	D	264	GLU	Mainchain
3	D	296	ILE	Mainchain
3	D	321	SER	Mainchain
3	D	392	GLN	Mainchain

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	5121	5158	5156	11	0
1	B	5230	5248	5245	12	0
2	C	2103	2132	2131	4	0
3	D	3281	3266	3265	8	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	1	0
All	All	15827	15829	15850	34	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 (34) 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
1:A:577:ASP:C	1:A:578:ILE:O	2.46	0.55
3:D:68:ASP:OD2	3:D:121:LYS:NZ	2.42	0.52
1:B:724:ASP:OD2	3:D:387:LYS:NZ	2.42	0.51
2:C:736:CYS:SG	6:C:801:DEX:H811	2.51	0.51
1:A:93:ASP:OD1	1:A:93:ASP:C	2.56	0.49
1:B:457:LYS:NZ	1:B:535:GLU:OE2	2.46	0.49
1:B:554:ASP:OD1	1:B:555:GLU:N	2.46	0.48
3:D:66:LYS:NZ	3:D:68:ASP:OD1	2.43	0.48
2:C:613:TYR:CD1	2:C:613:TYR:C	2.92	0.47
1:A:44:PHE:CD1	1:A:44:PHE:C	2.93	0.46
1:B:472:ASP:OD1	1:B:499:LYS:NZ	2.49	0.45
1:B:589:SER:OG	1:B:590:ASN:N	2.49	0.45
1:A:372:ASP:OD1	1:A:372:ASP:N	2.46	0.45
1:B:393:ASP:OD1	1:B:393:ASP:N	2.40	0.44
1:B:571:LEU:O	1:B:572:CYS:C	2.60	0.44
1:B:44:PHE:CD1	1:B:44:PHE:C	2.96	0.43
3:D:117:GLY:O	3:D:118:SER:C	2.62	0.43
1:A:472:ASP:OD1	1:A:499:LYS:NZ	2.51	0.43
1:A:193:ASP:OD1	1:A:193:ASP:N	2.49	0.43
1:B:609:ASN:O	1:B:610:MET:C	2.61	0.43
3:D:49:ILE:HB	3:D:154:ILE:HB	2.01	0.43
1:A:41:LYS:C	1:A:43:ILE:H	2.23	0.43
3:D:226:ALA:O	3:D:227:PHE:C	2.60	0.42
2:C:721:LEU:O	2:C:724:SER:N	2.53	0.41
1:A:571:LEU:O	1:A:572:CYS:C	2.63	0.41
3:D:178:TYR:O	3:D:179:LYS:C	2.61	0.41
1:B:175:ASP:OD1	1:B:176:THR:N	2.53	0.41
1:A:578:ILE:O	1:A:580:GLU:N	2.54	0.41
1:A:589:SER:OG	1:A:590:ASN:N	2.53	0.41
1:B:430:ASP:C	1:B:430:ASP:OD1	2.64	0.41
1:A:430:ASP:OD1	1:A:430:ASP:C	2.62	0.41
3:D:413:ASN:OD1	3:D:413:ASN:N	2.53	0.40
1:B:608:ALA:O	1:B:609:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	626/731 (86%)	619 (99%)	6 (1%)	1 (0%)	43	75
1	B	638/731 (87%)	627 (98%)	10 (2%)	1 (0%)	43	75
2	C	257/360 (71%)	255 (99%)	2 (1%)	0	100	100
3	D	407/459 (89%)	402 (99%)	5 (1%)	0	100	100
All	All	1928/2281 (84%)	1903 (99%)	23 (1%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	B	133	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/665 (86%)	571 (100%)	0	100	100
1	B	584/665 (88%)	584 (100%)	0	100	100
2	C	238/323 (74%)	238 (100%)	0	100	100
3	D	346/385 (90%)	346 (100%)	0	100	100
All	All	1739/2038 (85%)	1739 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	212	GLN
1	B	194	GLN
1	B	404	GLN
1	B	454	GLN
1	B	455	ASN
1	B	617	GLN
1	B	682	GLN
1	B	686	ASN
3	D	329	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 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	$\# Z > 2$
4	ATP	B	801	5	32,33,33	1.87	8 (25%)	48,52,52	1.74	9 (18%)
4	ATP	A	801	5	32,33,33	1.79	7 (21%)	48,52,52	1.78	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DEX	C	801	-	31,31,31	2.03	12 (38%)	53,53,53	2.85	27 (50%)

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

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	ATP	C5-C4	5.86	1.49	1.39
4	A	801	ATP	C5-C4	5.80	1.49	1.39
6	C	801	DEX	C10-C1	4.27	1.55	1.50
6	C	801	DEX	C10-C5	3.71	1.57	1.52
4	B	801	ATP	C5-C6	3.60	1.51	1.41
4	A	801	ATP	C5-C6	3.59	1.51	1.41
6	C	801	DEX	C9-C8	3.45	1.58	1.54
6	C	801	DEX	C4-C3	3.45	1.53	1.45
4	B	801	ATP	C5-N7	-3.43	1.32	1.39
6	C	801	DEX	C17-C20	3.26	1.57	1.53
4	A	801	ATP	C5-N7	-3.26	1.33	1.39
6	C	801	DEX	C2-C3	3.24	1.54	1.46
4	A	801	ATP	C4-N3	2.78	1.39	1.34
4	B	801	ATP	C4-N3	2.75	1.39	1.34
4	B	801	ATP	C2-N1	2.74	1.38	1.33
6	C	801	DEX	C9-C11	2.72	1.57	1.54
4	B	801	ATP	PB-O3B	2.68	1.62	1.59
4	A	801	ATP	C2-N1	2.55	1.38	1.33
4	A	801	ATP	C4-N9	-2.50	1.32	1.37
4	B	801	ATP	C2-N3	2.38	1.38	1.33
4	B	801	ATP	C4-N9	-2.20	1.33	1.37
6	C	801	DEX	C10-C9	2.15	1.59	1.57
6	C	801	DEX	C12-C13	2.13	1.57	1.54
6	C	801	DEX	O4-C20	2.13	1.24	1.21
6	C	801	DEX	C13-C14	2.11	1.58	1.54
6	C	801	DEX	C17-C13	2.09	1.59	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	ATP	C2-N3	2.01	1.37	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	801	DEX	C12-C11-C9	6.82	118.20	112.96
6	C	801	DEX	C21-C20-C17	6.36	122.99	117.63
6	C	801	DEX	C9-C8-C14	5.64	114.29	109.34
4	B	801	ATP	C5-C4-N3	-5.44	119.22	126.72
6	C	801	DEX	C13-C17-C20	5.31	119.80	112.86
6	C	801	DEX	C6-C5-C10	5.23	119.15	115.70
4	A	801	ATP	C5-C4-N3	-5.16	119.61	126.72
6	C	801	DEX	C7-C8-C9	5.13	116.78	110.98
4	B	801	ATP	N3-C4-N9	4.51	134.84	127.17
4	A	801	ATP	N3-C2-N1	-4.47	121.81	128.58
6	C	801	DEX	C15-C14-C8	4.43	123.25	119.08
4	B	801	ATP	N3-C2-N1	-4.31	122.06	128.58
4	A	801	ATP	N3-C4-N9	4.20	134.31	127.17
4	A	801	ATP	C2-N3-C4	3.95	121.48	111.83
4	B	801	ATP	C2-N3-C4	3.91	121.38	111.83
6	C	801	DEX	C18-C13-C12	-3.81	105.81	111.08
6	C	801	DEX	C19-C10-C1	-3.77	102.12	106.64
6	C	801	DEX	C10-C9-C11	3.76	118.16	115.49
6	C	801	DEX	C5-C4-C3	-3.68	119.38	122.72
6	C	801	DEX	C1-C2-C3	-3.67	118.39	121.49
6	C	801	DEX	C13-C17-C16	3.45	105.85	102.85
4	A	801	ATP	C4-C5-N7	-3.43	106.66	110.58
6	C	801	DEX	C9-C10-C5	3.28	110.28	106.80
4	B	801	ATP	C4-C5-N7	-3.24	106.88	110.58
6	C	801	DEX	C10-C5-C4	3.13	124.40	122.15
6	C	801	DEX	C15-C16-C17	3.03	107.12	105.10
6	C	801	DEX	C6-C5-C4	-2.76	116.45	120.86
6	C	801	DEX	C6-C7-C8	2.53	116.62	111.70
4	A	801	ATP	C6-C5-N7	2.51	136.93	132.09
4	B	801	ATP	C5-N7-C8	2.46	107.31	103.45
4	A	801	ATP	C5-N7-C8	2.44	107.29	103.45
6	C	801	DEX	C2-C3-C4	2.41	119.56	117.12
4	A	801	ATP	O2B-PB-O1B	2.41	123.64	112.44
6	C	801	DEX	C7-C8-C14	2.37	116.82	111.50
4	A	801	ATP	C2-N1-C6	2.33	122.56	118.73
6	C	801	DEX	C10-C1-C2	2.26	126.08	124.37
6	C	801	DEX	C17-C13-C14	-2.22	97.35	99.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	ATP	C4-N9-C8	2.22	108.06	105.74
6	C	801	DEX	C13-C12-C11	2.17	116.31	113.20
4	B	801	ATP	C6-C5-N7	2.15	136.24	132.09
4	B	801	ATP	C2-N1-C6	2.15	122.26	118.73
6	C	801	DEX	C22-C16-C17	2.11	119.23	114.96
6	C	801	DEX	O4-C20-C21	-2.10	115.83	119.73
6	C	801	DEX	C22-C16-C15	-2.08	109.92	113.39
6	C	801	DEX	C9-C10-C1	2.07	112.53	109.98
4	B	801	ATP	O2B-PB-O3A	-2.05	101.74	107.27

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	ATP	C5'-O5'-PA-O2A
4	A	801	ATP	C5'-O5'-PA-O3A
6	C	801	DEX	C13-C17-C20-C21
6	C	801	DEX	C13-C17-C20-O4
6	C	801	DEX	C17-C20-C21-O5
6	C	801	DEX	O4-C20-C21-O5
4	A	801	ATP	O4'-C4'-C5'-O5'
4	A	801	ATP	C3'-C4'-C5'-O5'
4	A	801	ATP	PG-O3B-PB-O1B
4	B	801	ATP	PB-O3B-PG-O1G
6	C	801	DEX	O3-C17-C20-O4
4	A	801	ATP	PG-O3B-PB-O2B
4	B	801	ATP	PB-O3B-PG-O2G
4	B	801	ATP	PB-O3B-PG-O3G
6	C	801	DEX	O3-C17-C20-C21

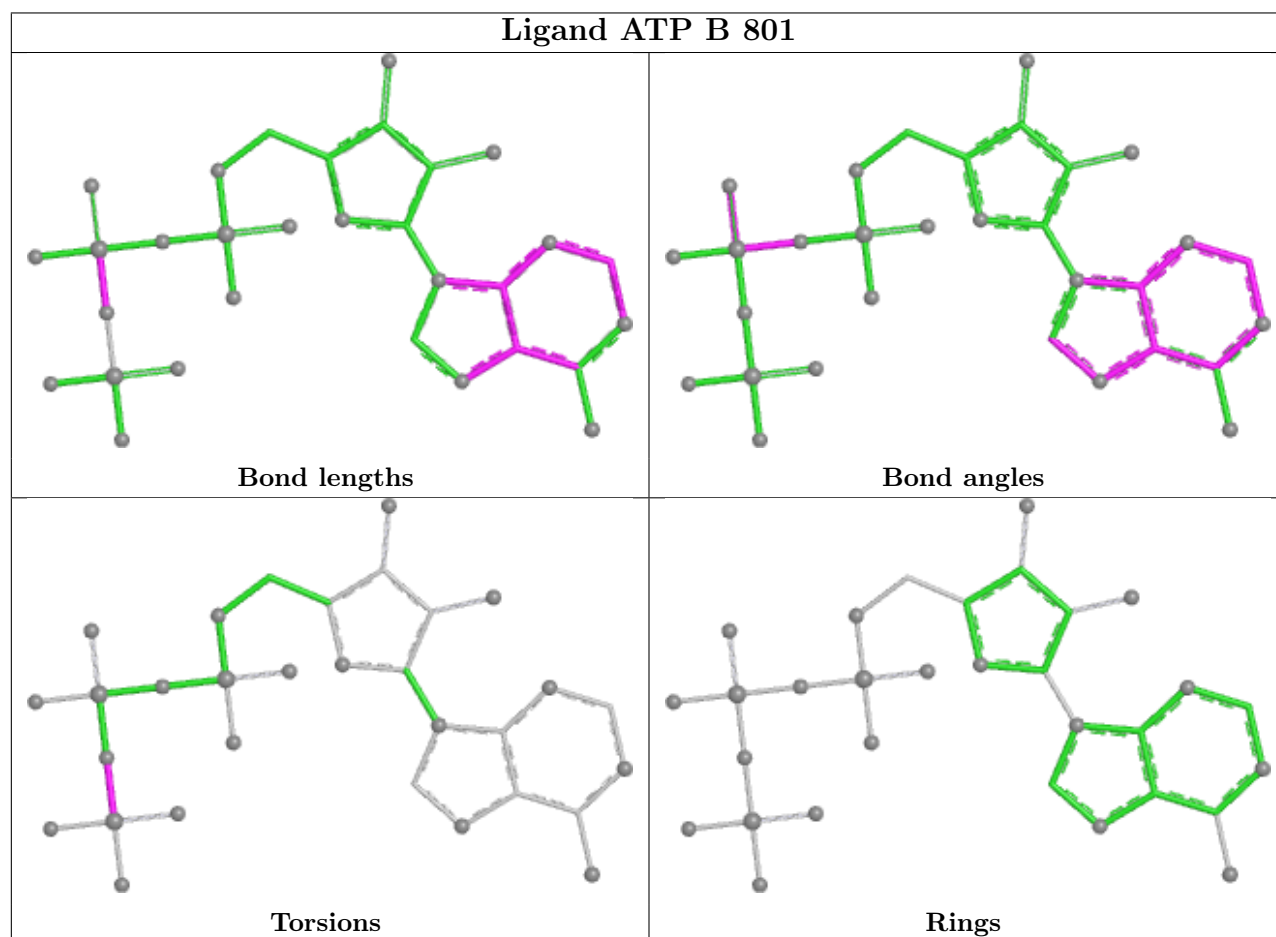
There are no ring outliers.

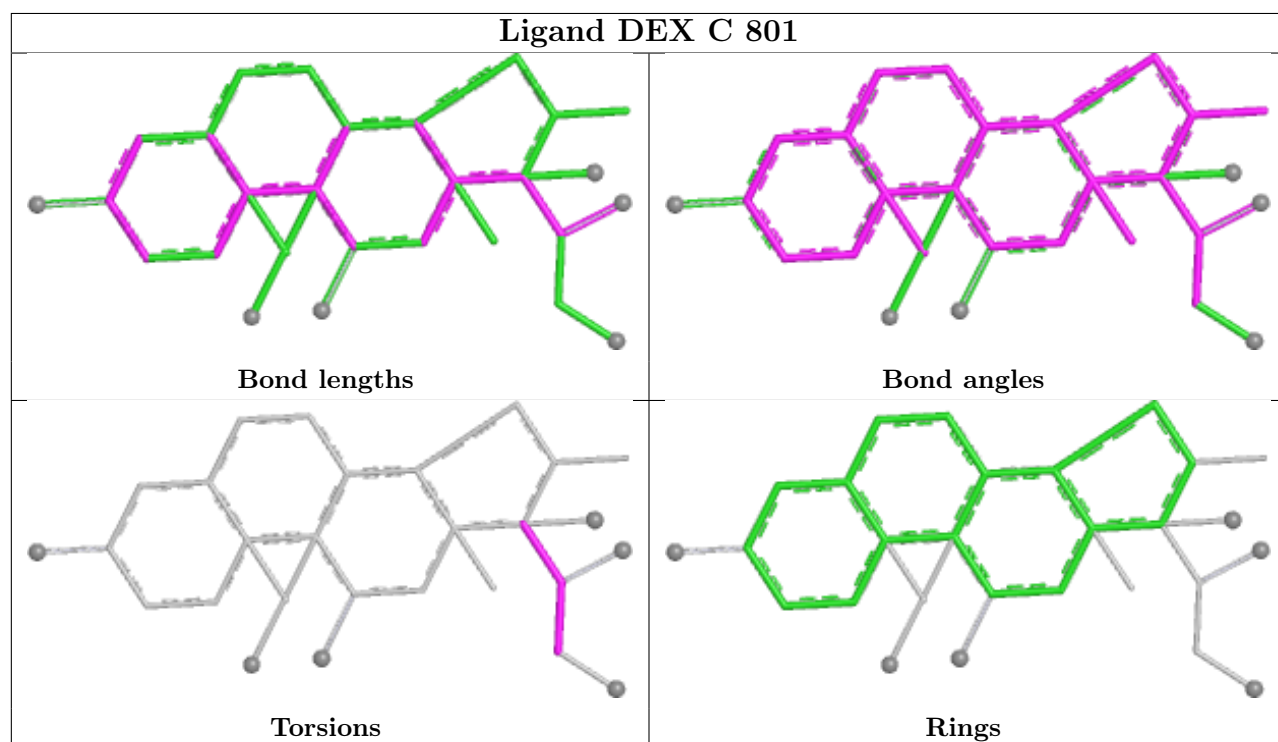
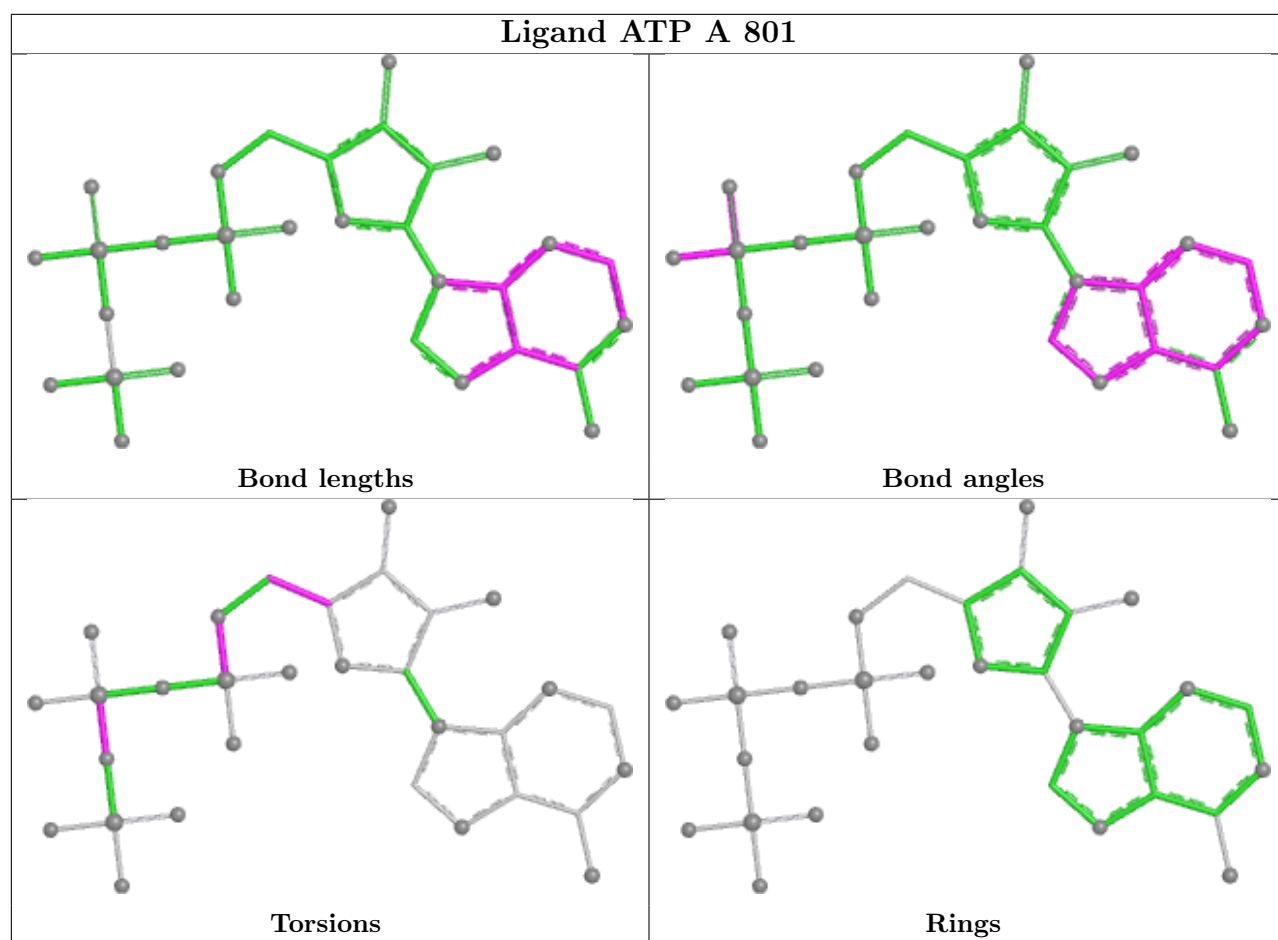
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	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.

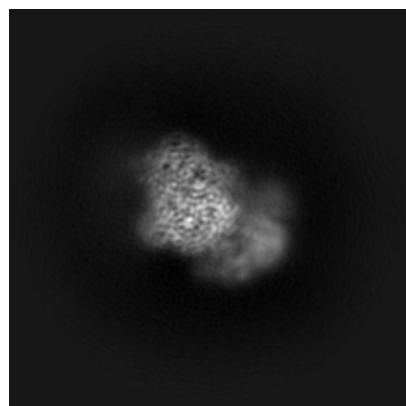
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29068. These allow visual inspection of the internal detail of the map and identification of artifacts.

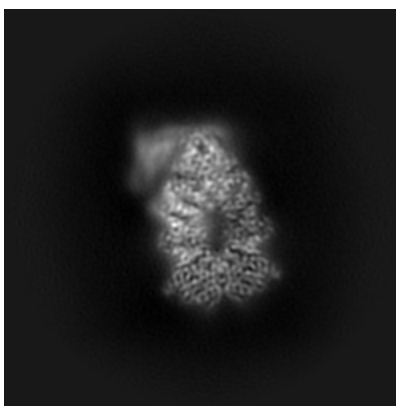
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

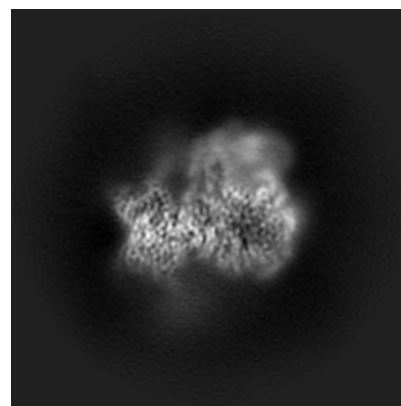
6.1.1 Primary map



X

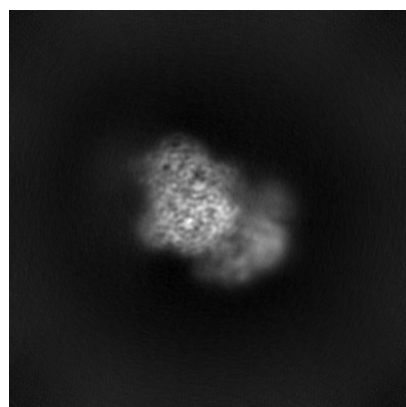


Y

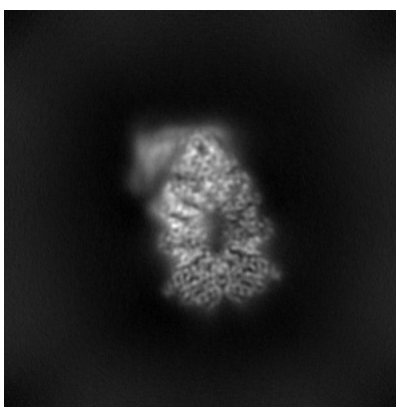


Z

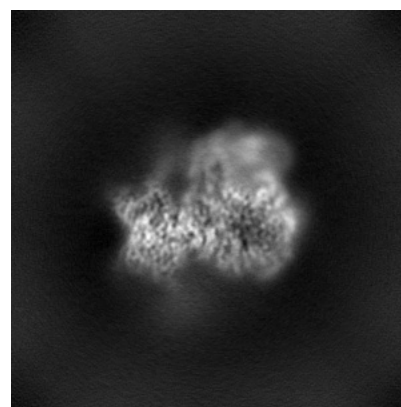
6.1.2 Raw map



X



Y

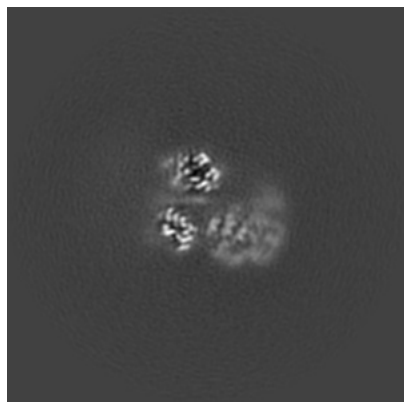


Z

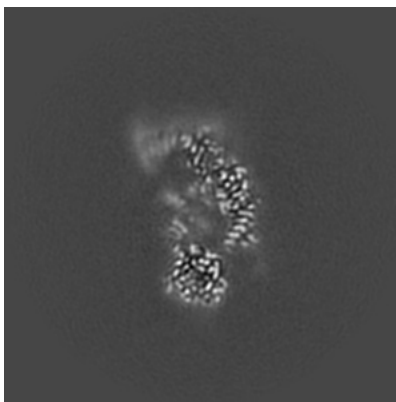
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

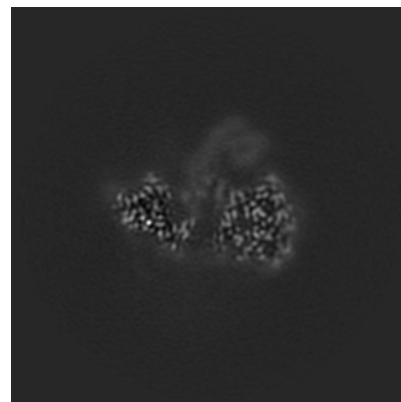
6.2.1 Primary map



X Index: 160

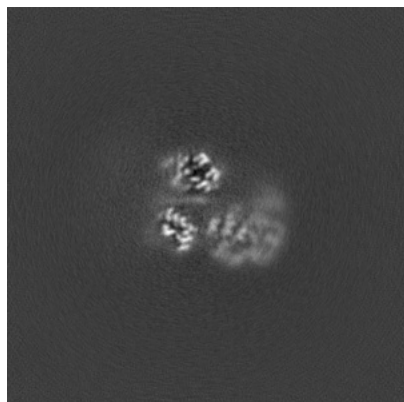


Y Index: 160

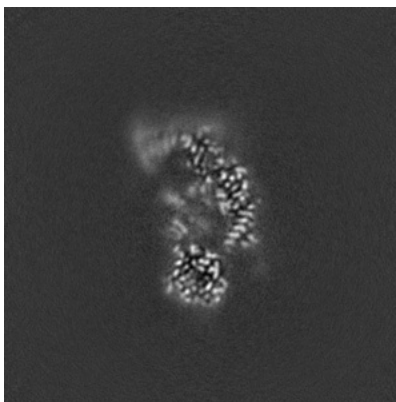


Z Index: 160

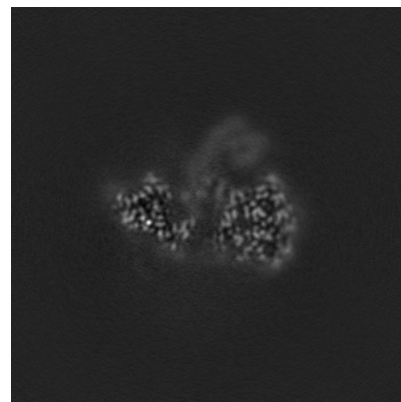
6.2.2 Raw map



X Index: 160



Y Index: 160

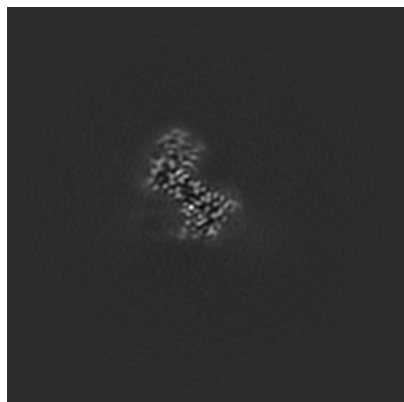


Z Index: 160

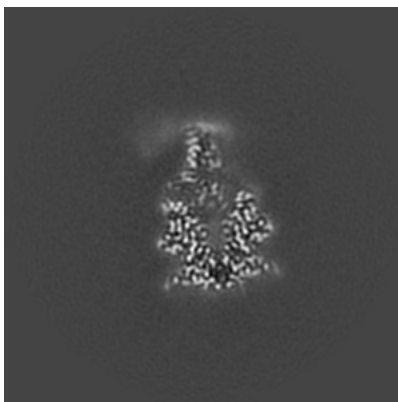
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

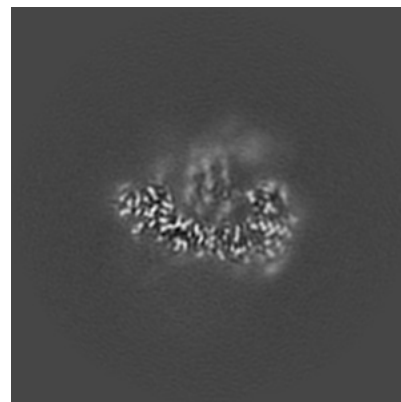
6.3.1 Primary map



X Index: 109

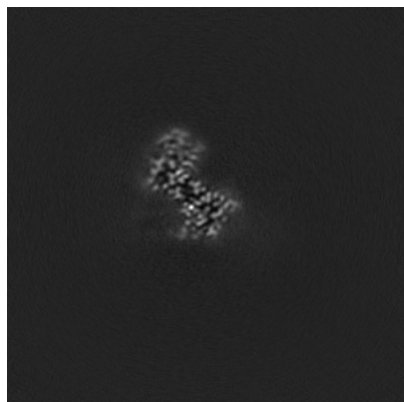


Y Index: 144

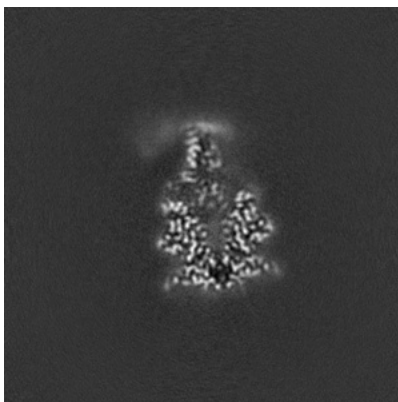


Z Index: 151

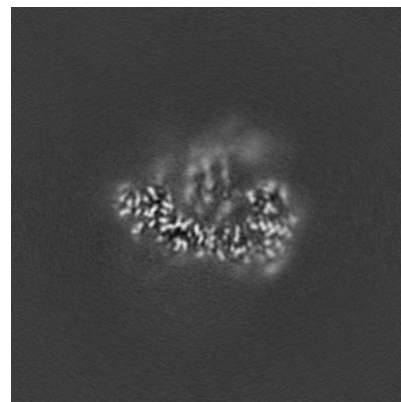
6.3.2 Raw map



X Index: 109



Y Index: 144

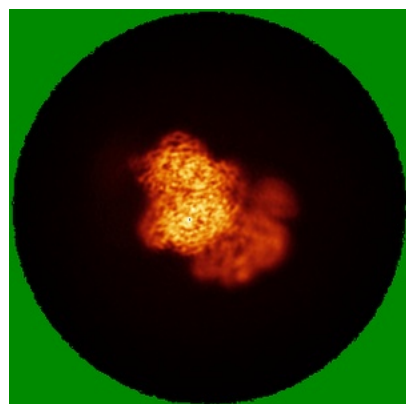


Z Index: 151

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

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

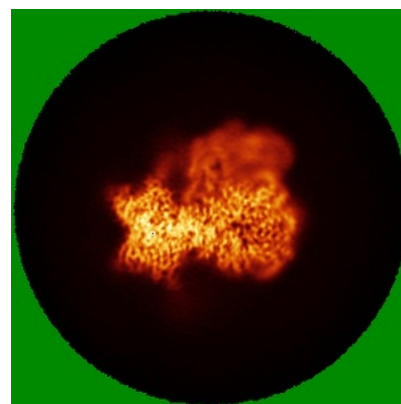
6.4.1 Primary map



X

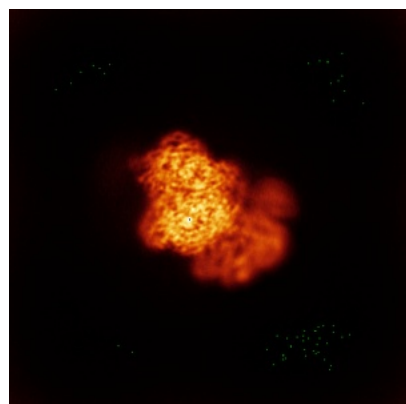


Y



Z

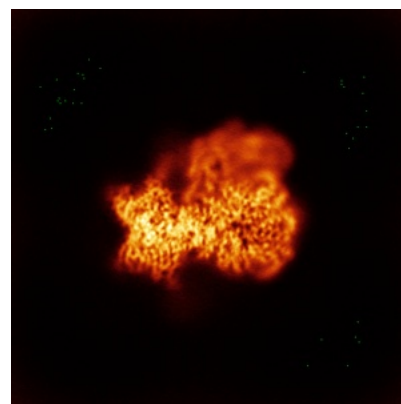
6.4.2 Raw map



X



Y

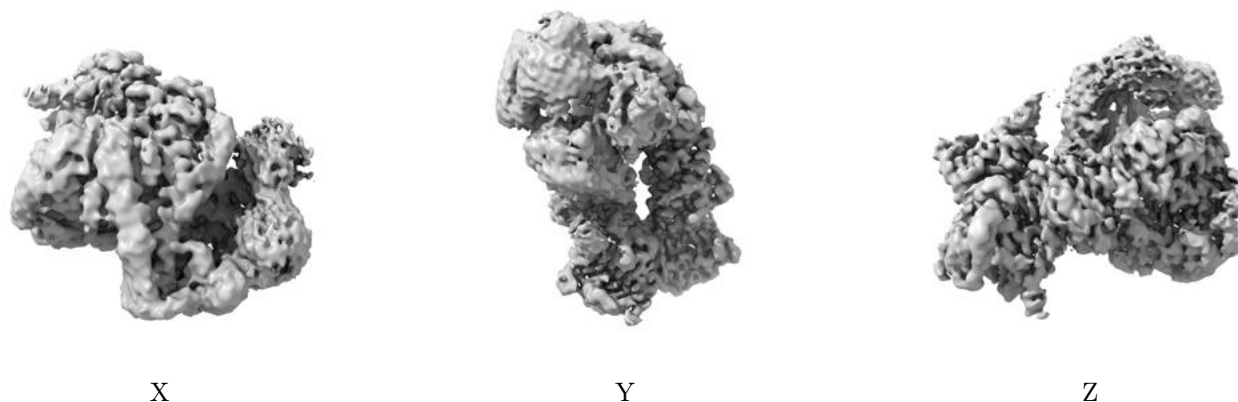


Z

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 0.2. 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.

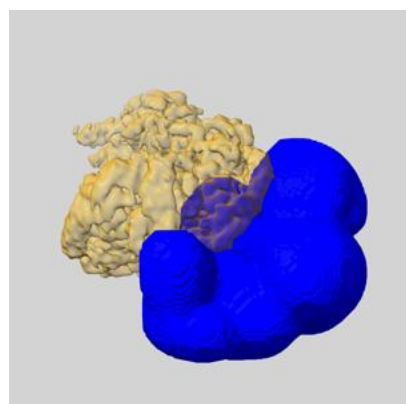
6.6 Mask visualisation [i](#)

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

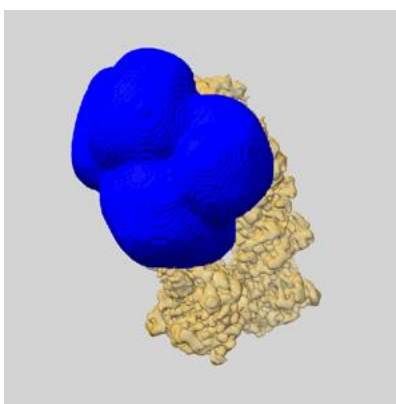
A mask typically either:

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

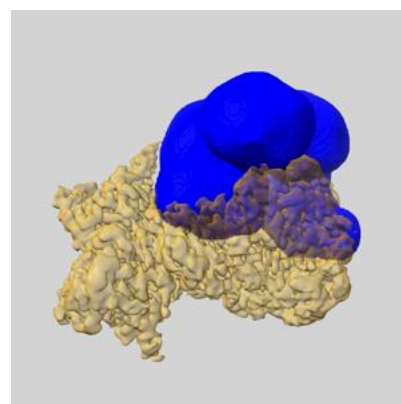
6.6.1 emd_29068_msk_3.map [i](#)



X

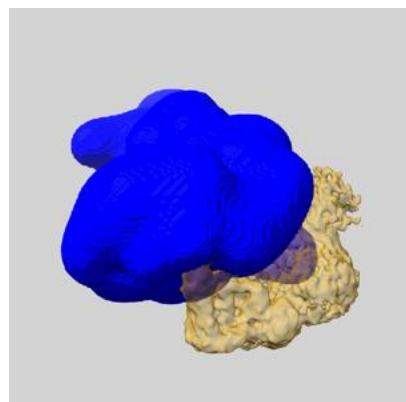


Y

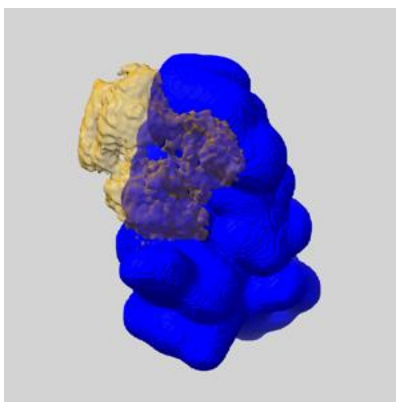


Z

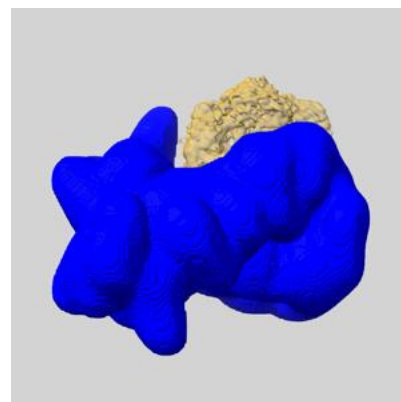
6.6.2 emd_29068_msk_2.map [i](#)



X

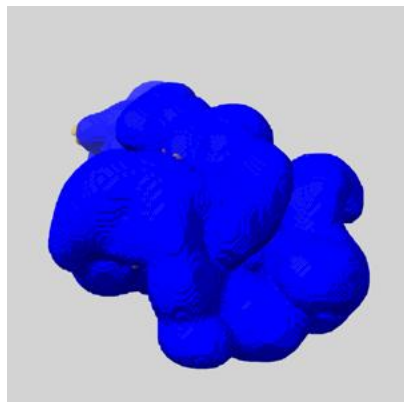


Y

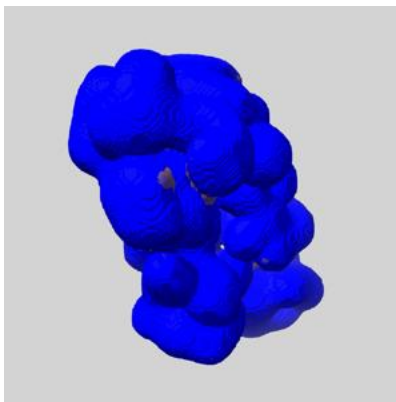


Z

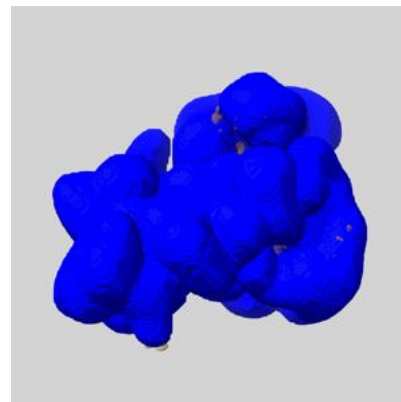
6.6.3 emd_29068_msk_1.map [i](#)



X



Y

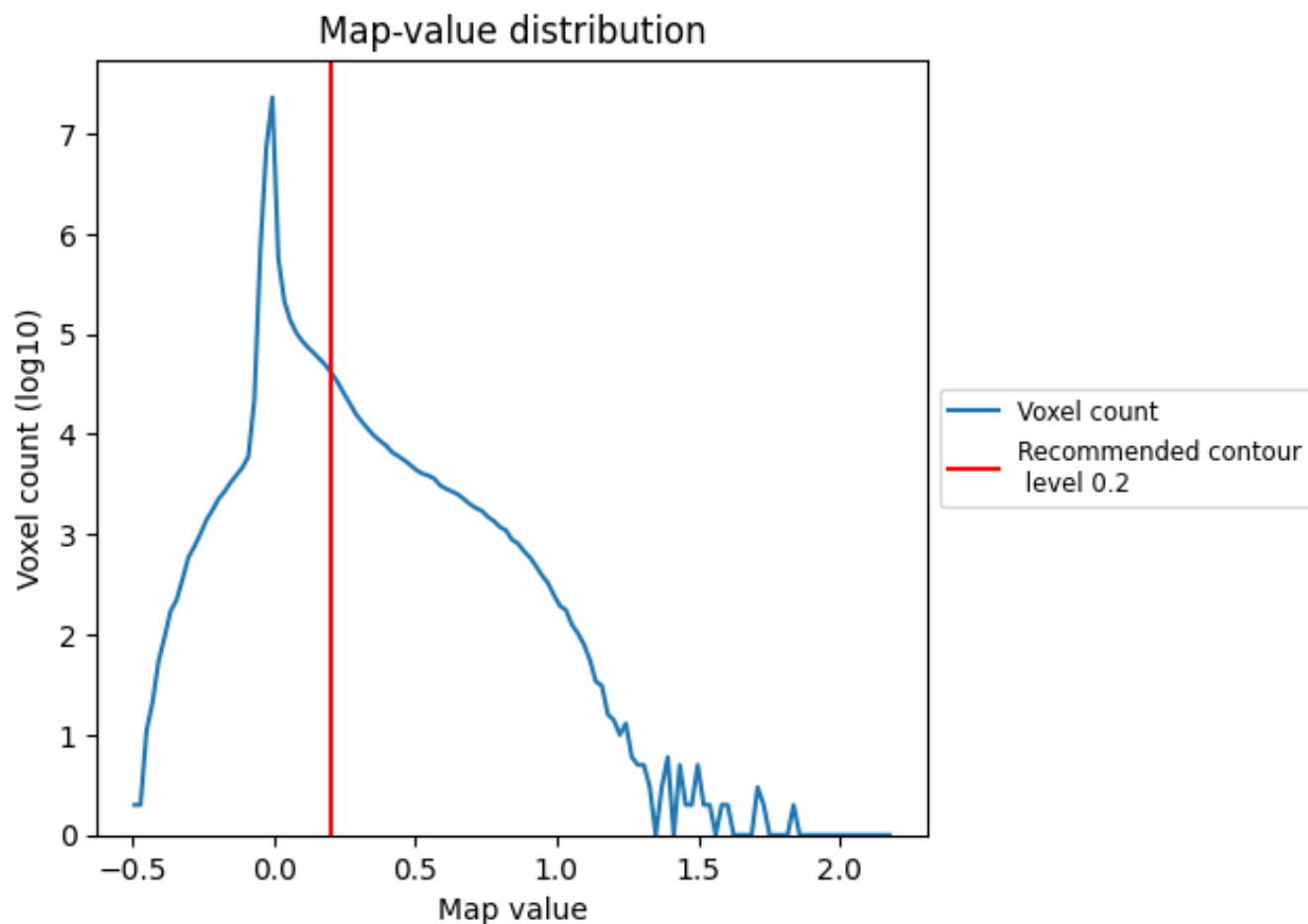


Z

7 Map analysis [i](#)

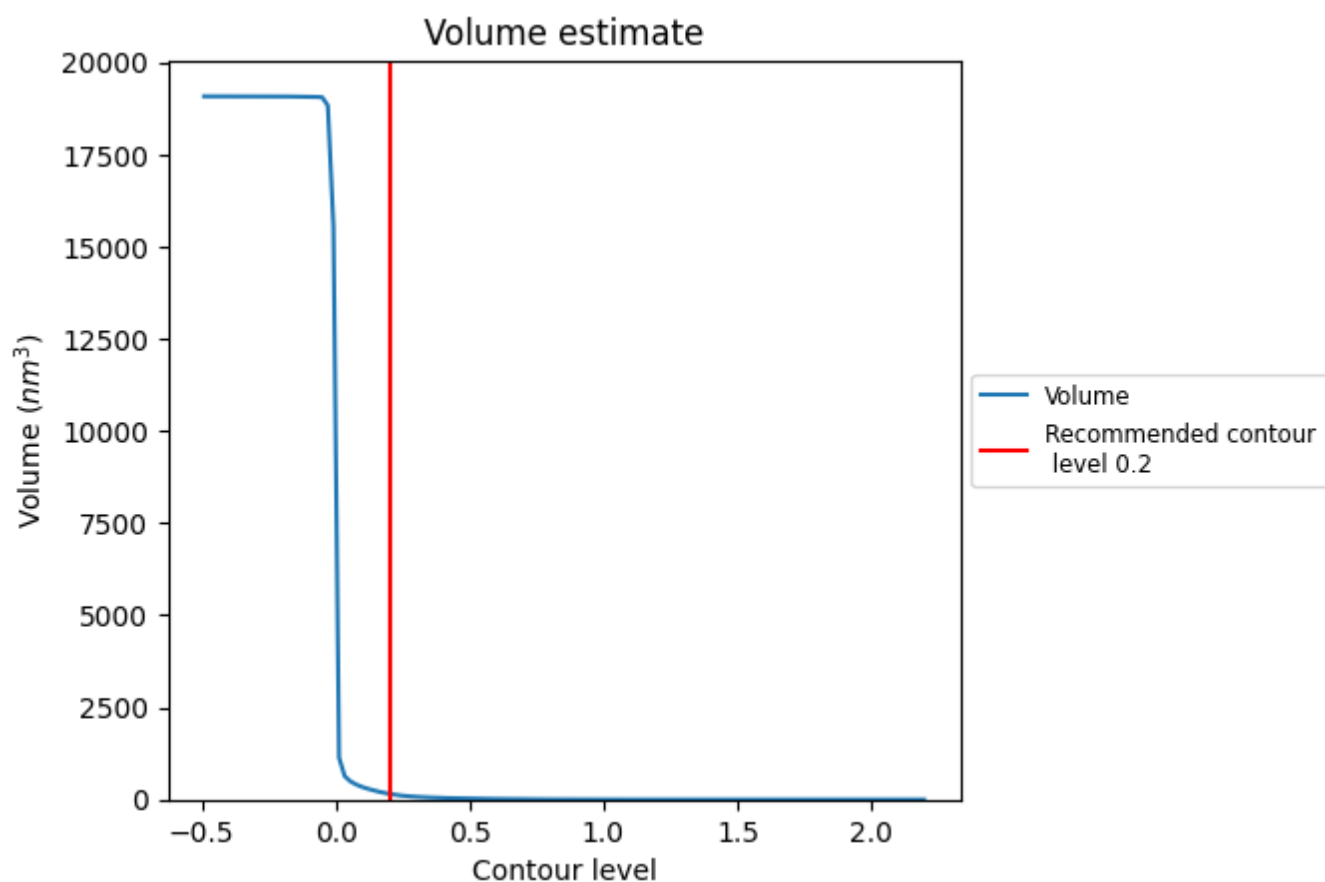
This section contains the results of statistical analysis of the map.

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.

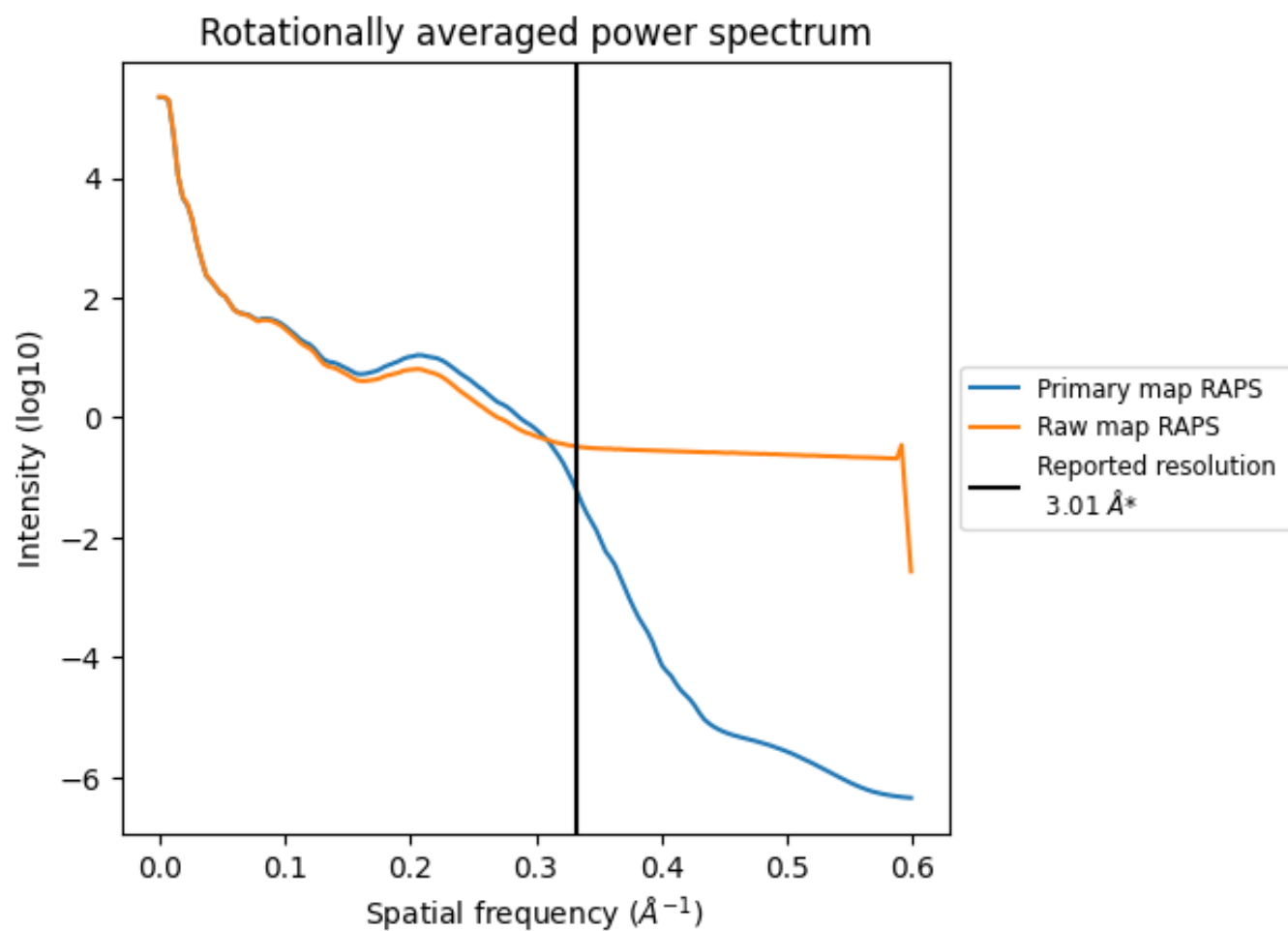
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 ⓘ

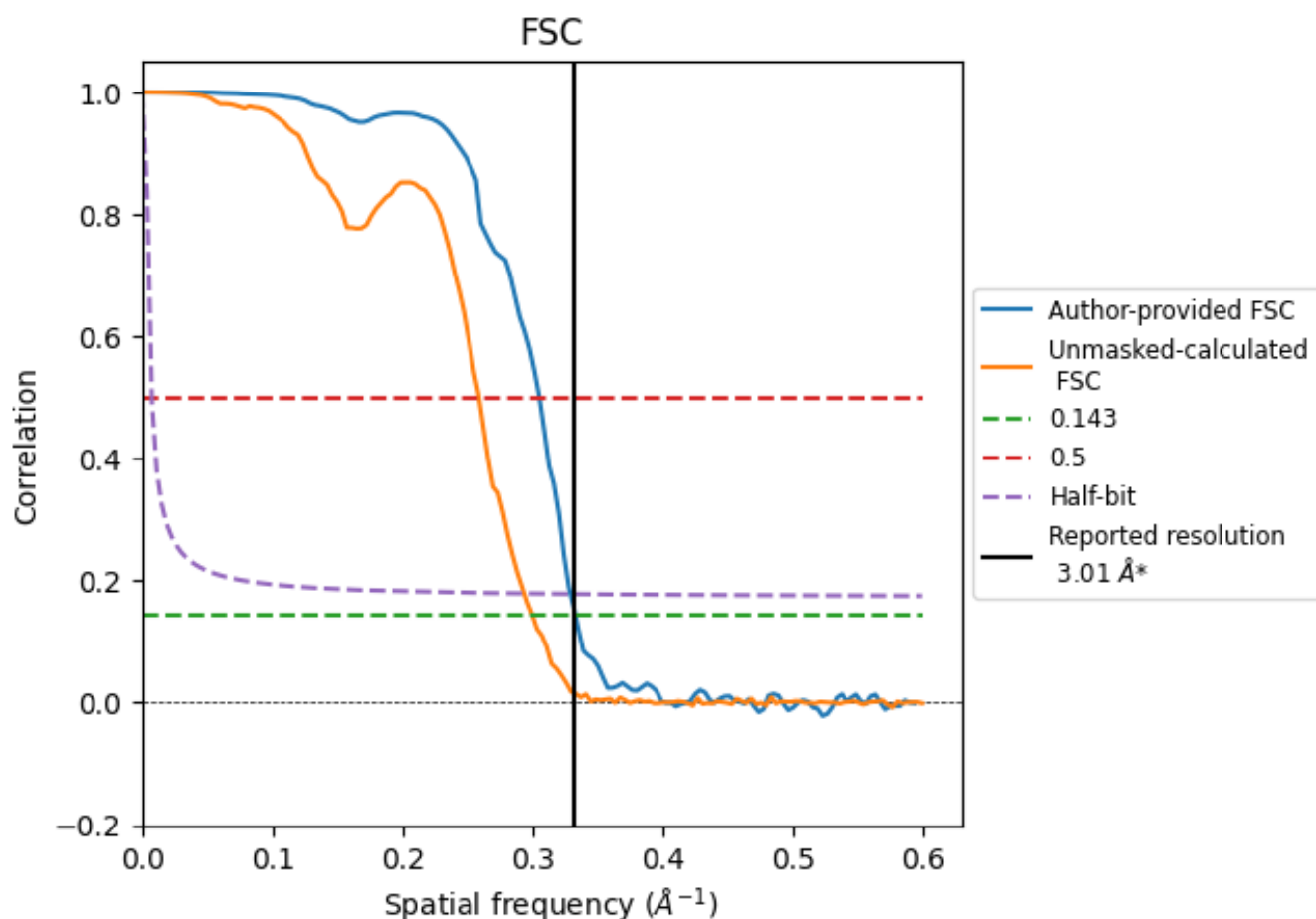


*Reported resolution corresponds to spatial frequency of $0.332 \text{ \AA}^{-1}$

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 $0.332 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

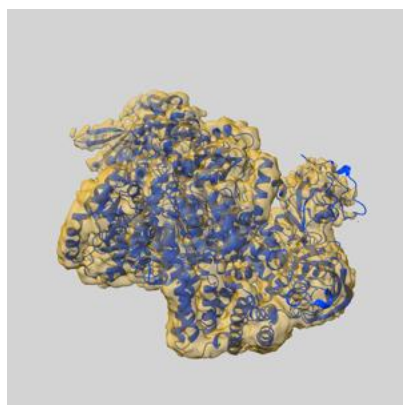
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.28	3.04
Unmasked-calculated*	3.34	3.87	3.41

*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 3.34 differs from the reported value 3.01 by more than 10 %

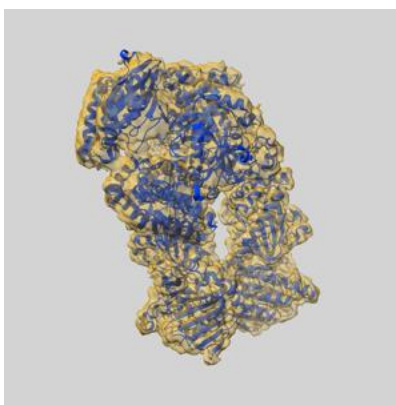
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29068 and PDB model 8FFV. Per-residue inclusion information can be found in section 3 on page 6.

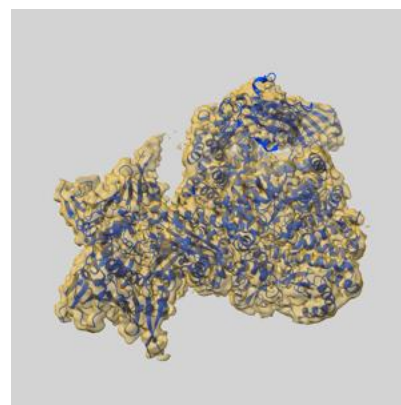
9.1 Map-model overlay [i](#)



X



Y



Z

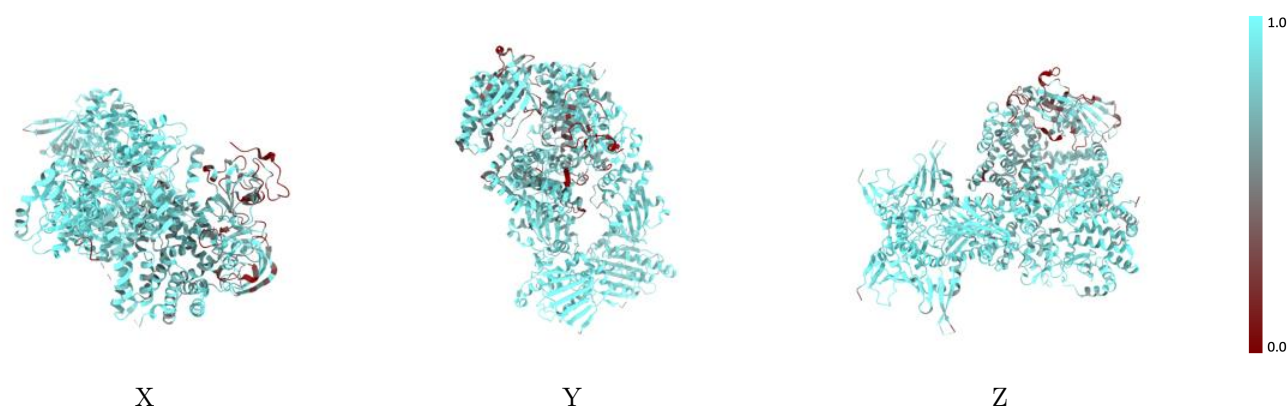
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



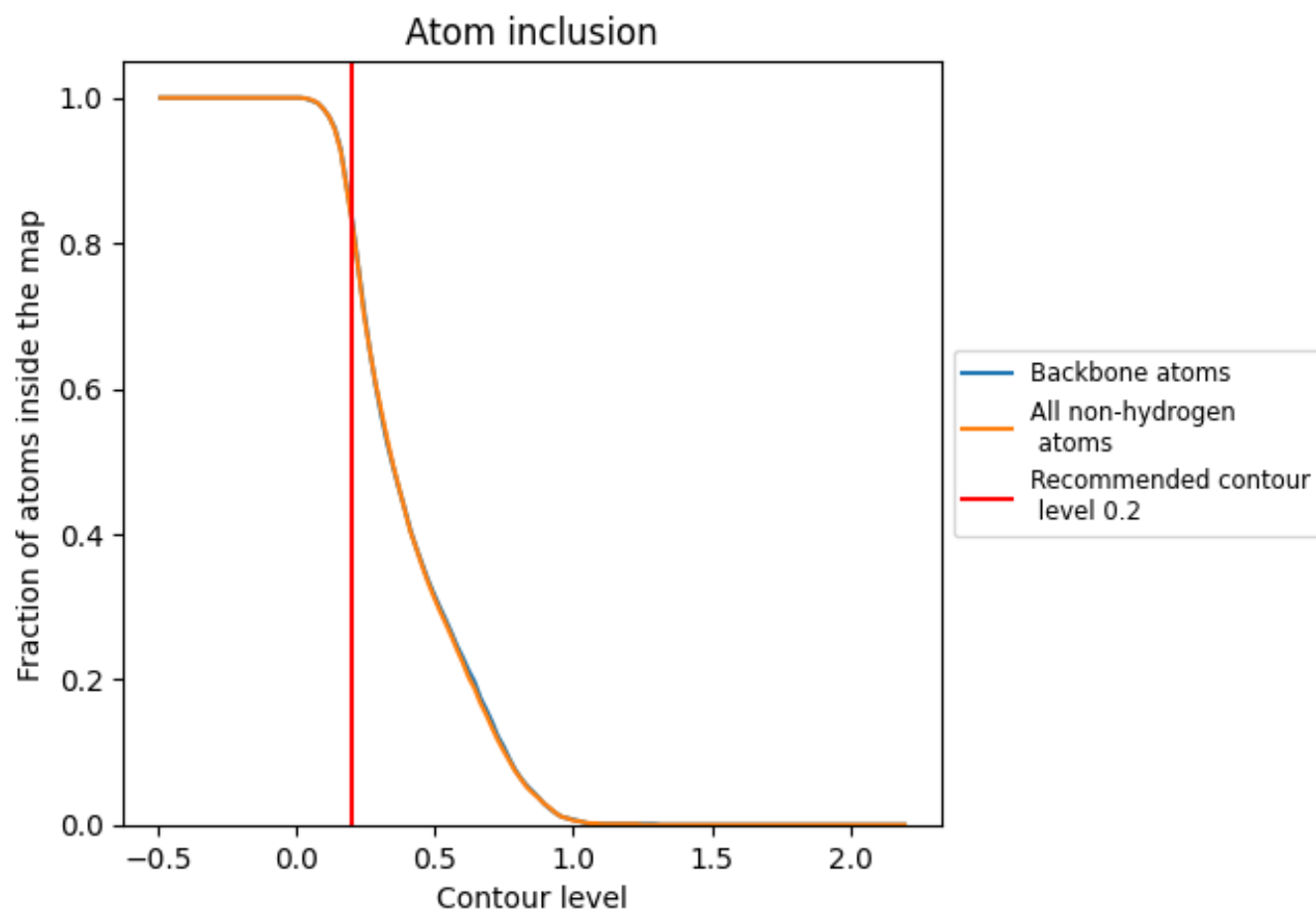
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.4000
A	0.9150	0.4950
B	0.9030	0.4950
C	0.7600	0.2820
D	0.6630	0.1760

