



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:46 AM JST

PDB ID : 8Z1Z / pdb_00008z1z
EMDB ID : EMD-39741
Title : Cryo-EM structure of Escherichia coli DppAR383D+D436RBCDF in pre-catalytic state
Authors : Li, P.; Huang, Y.
Deposited on : 2024-04-12
Resolution : 3.26 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

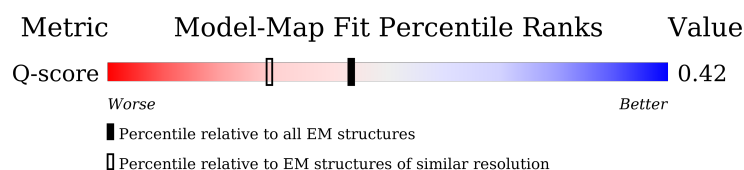
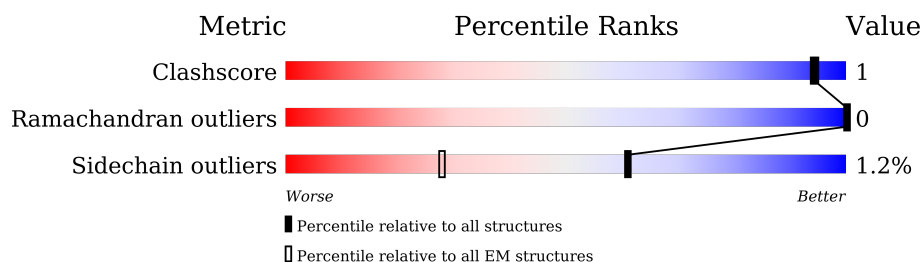
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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	14557 (2.76 - 3.76)

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	339	
2	B	300	
3	C	327	
4	D	334	

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Mol	Chain	Length	Quality of chain
5	F	535	87% 7% • 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13652 atoms, of which 0 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 Dipeptide transport system permease protein DppB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	298	Total	C	N	O	S	0	0
			2317	1526	390	384	17		

- Molecule 2 is a protein called Dipeptide transport system permease protein DppC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	289	Total	C	N	O	S	0	0
			2187	1445	359	369	14		

- Molecule 3 is a protein called Dipeptide transport ATP-binding protein DppD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2486	1559	447	463	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	179	GLN	GLU	conflict	UNP P0AAG0

- Molecule 4 is a protein called Dipeptide transport ATP-binding protein DppF.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	322	Total	C	N	O	S	0	0
			2537	1597	460	463	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	187	GLN	GLU	conflict	UNP P37313

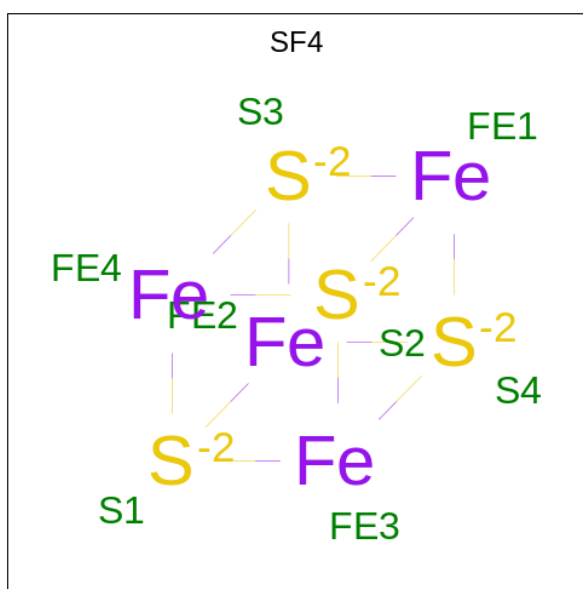
- Molecule 5 is a protein called Dipeptide-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	507	Total	C	N	O	S	0	0
			4047	2584	676	768	19		

There are 2 discrepancies between the modelled and reference sequences:

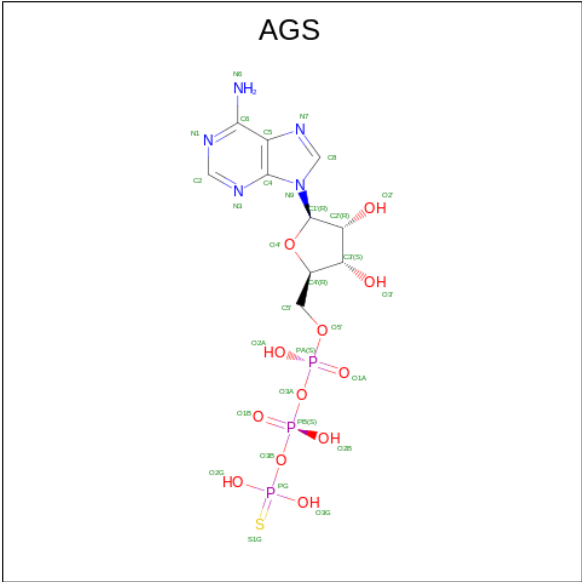
Chain	Residue	Modelled	Actual	Comment	Reference
F	383	ASP	ARG	engineered mutation	UNP P23847
F	436	ARG	ASP	engineered mutation	UNP P23847

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	Fe	S	0
			8	4	4	
6	D	1	Total	Fe	S	0
			8	4	4	

- Molecule 7 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).

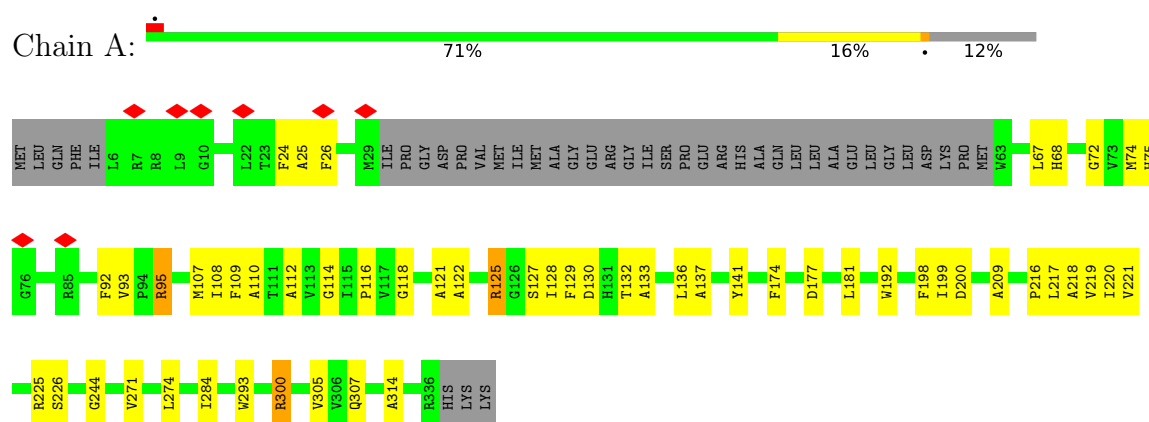


Mol	Chain	Residues	Atoms						AltConf
7	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

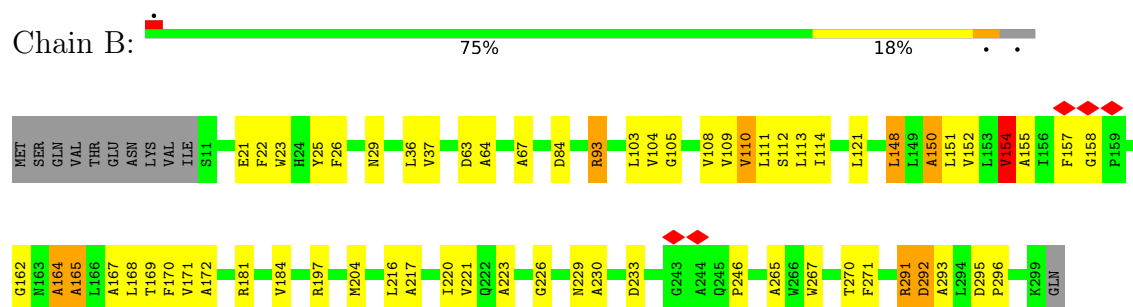
3 Residue-property plots [i](#)

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

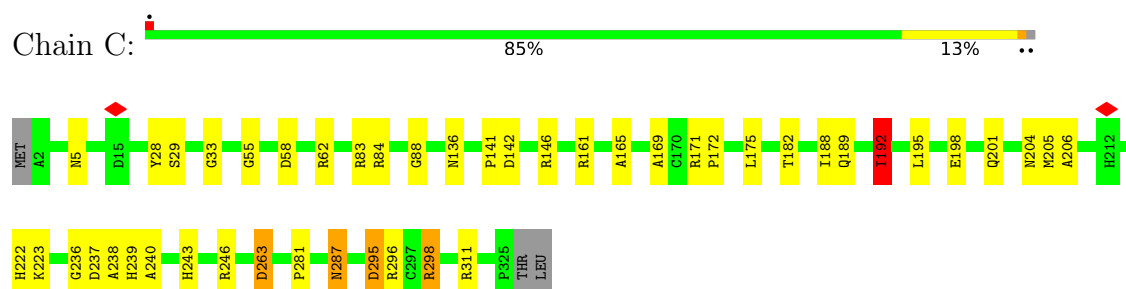
- Molecule 1: Dipeptide transport system permease protein DppB



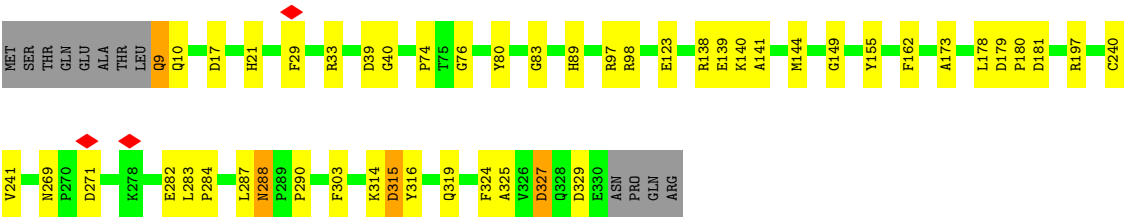
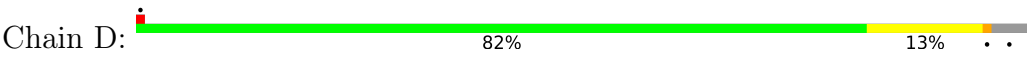
- Molecule 2: Dipeptide transport system permease protein DppC



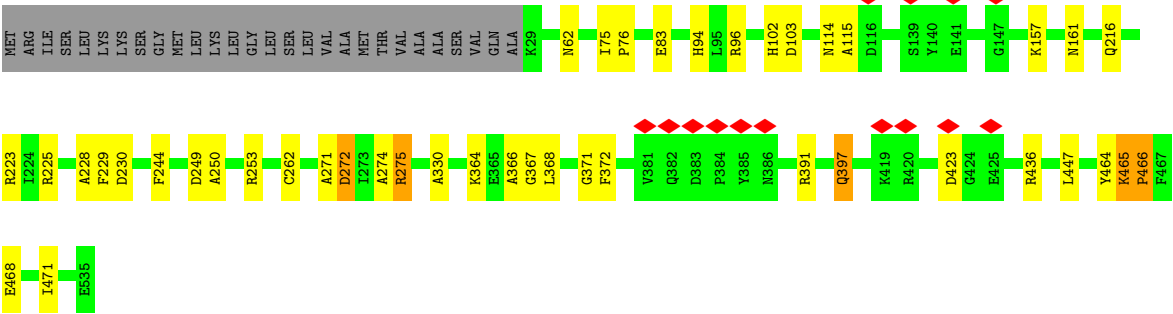
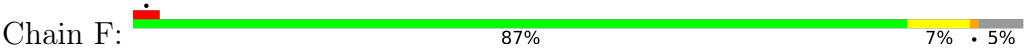
- Molecule 3: Dipeptide transport ATP-binding protein DppD



- Molecule 4: Dipeptide transport ATP-binding protein DppF



● Molecule 5: Dipeptide-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375658	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.387	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, AGS

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	1.47	20/2371 (0.8%)	1.74	58/3234 (1.8%)
2	B	1.68	23/2240 (1.0%)	1.79	67/3062 (2.2%)
3	C	1.46	20/2530 (0.8%)	1.66	47/3427 (1.4%)
4	D	1.54	21/2584 (0.8%)	1.74	49/3486 (1.4%)
5	F	1.23	25/4152 (0.6%)	1.53	35/5630 (0.6%)
All	All	1.45	109/13877 (0.8%)	1.68	256/18839 (1.4%)

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
3	C	0	3
5	F	0	1
All	All	0	6

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	21	HIS	ND1-CE1	-9.60	1.23	1.32
5	F	94	HIS	CE1-NE2	-8.87	1.23	1.32
3	C	239	HIS	CE1-NE2	-8.86	1.23	1.32
1	A	75	HIS	ND1-CE1	-8.85	1.23	1.32
5	F	102	HIS	CE1-NE2	-8.78	1.23	1.32
1	A	68	HIS	CE1-NE2	-8.75	1.23	1.32
3	C	222	HIS	CE1-NE2	-8.71	1.23	1.32
3	C	243	HIS	CE1-NE2	-8.70	1.23	1.32
5	F	225	ARG	CZ-NH2	-8.31	1.22	1.33
5	F	96	ARG	CZ-NH2	-8.30	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	223	ARG	CZ-NH2	-8.25	1.22	1.33
5	F	275	ARG	CZ-NH2	-8.25	1.22	1.33
4	D	138	ARG	CZ-NH2	-8.21	1.22	1.33
3	C	298	ARG	CZ-NH2	-8.19	1.22	1.33
2	B	217	ALA	CA-CB	-8.17	1.42	1.53
2	B	291	ARG	CZ-NH2	-8.14	1.22	1.33
1	A	125	ARG	CZ-NH2	-8.10	1.23	1.33
5	F	94	HIS	CD2-NE2	-8.07	1.28	1.37
3	C	243	HIS	CD2-NE2	-8.06	1.28	1.37
1	A	68	HIS	CD2-NE2	-8.06	1.28	1.37
3	C	239	HIS	CD2-NE2	-8.05	1.28	1.37
3	C	222	HIS	CD2-NE2	-8.02	1.29	1.37
5	F	102	HIS	CD2-NE2	-7.97	1.29	1.37
3	C	236	GLY	N-CA	-7.79	1.38	1.45
2	B	64	ALA	CA-CB	-7.76	1.42	1.53
2	B	67	ALA	CA-CB	-7.45	1.41	1.53
4	D	173	ALA	CA-CB	-7.20	1.42	1.53
5	F	228	ALA	CA-CB	-7.16	1.42	1.53
1	A	25	ALA	CA-CB	-7.14	1.42	1.53
2	B	150	ALA	CA-CB	-7.14	1.42	1.53
5	F	330	ALA	CA-CB	-7.14	1.42	1.53
5	F	250	ALA	CA-CB	-7.13	1.42	1.53
4	D	141	ALA	CA-CB	-7.09	1.42	1.53
2	B	165	ALA	CA-CB	-7.09	1.42	1.53
1	A	137	ALA	CA-CB	-7.05	1.42	1.53
1	A	218	ALA	CA-CB	-7.05	1.42	1.53
1	A	314	ALA	CA-CB	-7.04	1.42	1.53
3	C	165	ALA	CA-CB	-7.04	1.42	1.53
3	C	240	ALA	CA-CB	-7.03	1.42	1.53
4	D	325	ALA	CA-CB	-7.03	1.42	1.53
3	C	238	ALA	CA-CB	-7.02	1.42	1.53
5	F	271	ALA	CA-CB	-7.01	1.42	1.53
1	A	133	ALA	CA-CB	-7.00	1.42	1.53
1	A	209	ALA	CA-CB	-7.00	1.42	1.53
4	D	290	PRO	CA-CB	-6.97	1.47	1.53
2	B	223	ALA	CA-CB	-6.95	1.42	1.53
2	B	167	ALA	CA-CB	-6.92	1.42	1.53
1	A	122	ALA	CA-CB	-6.83	1.42	1.53
5	F	225	ARG	CZ-NH1	-6.74	1.23	1.32
5	F	371	GLY	N-CA	-6.73	1.37	1.45
3	C	287	ASN	CA-CB	-6.72	1.48	1.54
5	F	223	ARG	CZ-NH1	-6.72	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	96	ARG	CZ-NH1	-6.71	1.23	1.32
2	B	265	ALA	CA-CB	-6.70	1.42	1.52
2	B	155	ALA	CA-CB	-6.70	1.42	1.53
3	C	206	ALA	CA-CB	-6.67	1.42	1.53
3	C	298	ARG	CZ-NH1	-6.67	1.23	1.32
1	A	110	ALA	CA-CB	-6.66	1.42	1.53
2	B	172	ALA	CA-CB	-6.64	1.42	1.53
4	D	138	ARG	CZ-NH1	-6.63	1.23	1.32
5	F	275	ARG	CZ-NH1	-6.62	1.23	1.32
5	F	115	ALA	CA-CB	-6.61	1.42	1.53
1	A	125	ARG	CZ-NH1	-6.59	1.23	1.32
2	B	291	ARG	CZ-NH1	-6.51	1.23	1.32
2	B	230	ALA	CA-CB	-6.46	1.42	1.53
4	D	89	HIS	CE1-NE2	-6.42	1.26	1.32
1	A	72	GLY	N-CA	-6.36	1.38	1.45
1	A	114	GLY	N-CA	-6.31	1.38	1.45
2	B	293	ALA	CA-CB	-6.31	1.42	1.53
2	B	105	GLY	N-CA	-6.30	1.38	1.45
2	B	158	GLY	N-CA	-6.27	1.36	1.43
3	C	88	GLY	N-CA	-6.22	1.37	1.45
5	F	366	ALA	CA-CB	-6.20	1.42	1.53
4	D	288	ASN	CA-CB	-6.20	1.46	1.53
1	A	121	ALA	CA-CB	-6.10	1.42	1.53
1	A	93	VAL	CA-CB	-6.10	1.51	1.54
2	B	226	GLY	N-CA	-6.06	1.38	1.45
4	D	89	HIS	CD2-NE2	-5.95	1.31	1.37
2	B	271	PHE	N-CA	-5.80	1.41	1.46
5	F	96	ARG	CD-NE	-5.71	1.38	1.46
4	D	241	VAL	N-CA	-5.67	1.41	1.46
1	A	118	GLY	N-CA	-5.63	1.38	1.45
3	C	281	PRO	CA-CB	-5.62	1.46	1.53
2	B	291	ARG	CD-NE	-5.62	1.38	1.46
5	F	225	ARG	CD-NE	-5.61	1.38	1.46
4	D	138	ARG	CD-NE	-5.58	1.38	1.46
4	D	288	ASN	CG-ND2	-5.52	1.21	1.33
2	B	162	GLY	N-CA	-5.46	1.38	1.45
3	C	298	ARG	CD-NE	-5.45	1.38	1.46
3	C	55	GLY	N-CA	-5.39	1.37	1.45
1	A	125	ARG	CD-NE	-5.37	1.38	1.46
5	F	275	ARG	CD-NE	-5.36	1.38	1.46
5	F	223	ARG	CD-NE	-5.34	1.38	1.46
3	C	142	ASP	N-CA	-5.27	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	217	ALA	N-CA	-5.26	1.41	1.46
4	D	76	GLY	N-CA	-5.23	1.40	1.45
4	D	180	PRO	CA-CB	-5.17	1.46	1.53
1	A	244	GLY	N-CA	-5.14	1.38	1.45
4	D	284	PRO	CA-CB	-5.14	1.46	1.53
4	D	97	ARG	CZ-NH2	-5.13	1.26	1.33
2	B	296	PRO	CA-CB	-5.12	1.46	1.53
5	F	367	GLY	N-CA	-5.12	1.38	1.45
4	D	33	ARG	CZ-NH2	-5.11	1.26	1.33
5	F	94	HIS	CA-CB	-5.09	1.46	1.52
3	C	33	GLY	N-CA	-5.07	1.37	1.45
4	D	40	GLY	N-CA	-5.07	1.38	1.45
2	B	197	ARG	CZ-NH2	-5.05	1.26	1.33
4	D	98	ARG	CZ-NH2	-5.05	1.26	1.33
4	D	74	PRO	CA-CB	-5.01	1.47	1.53

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	ASN	CA-C-N	8.10	130.66	122.96
3	C	5	ASN	C-N-CA	8.10	130.66	122.96
5	F	102	HIS	CA-CB-CG	7.65	121.45	113.80
4	D	21	HIS	CA-CB-CG	7.65	121.45	113.80
5	F	103	ASP	CA-CB-CG	7.54	120.14	112.60
3	C	237	ASP	CA-CB-CG	7.45	120.05	112.60
3	C	204	ASN	CA-CB-CG	7.39	119.99	112.60
2	B	246	PRO	N-CA-C	7.36	119.68	110.70
1	A	26	PHE	CA-CB-CG	7.31	121.11	113.80
2	B	292	ASP	CA-CB-CG	7.27	119.87	112.60
5	F	161	ASN	CA-CB-CG	7.27	119.87	112.60
4	D	162	PHE	CA-CB-CG	7.26	121.06	113.80
1	A	177	ASP	CA-CB-CG	7.25	119.86	112.60
4	D	288	ASN	CA-CB-CG	7.22	119.82	112.60
1	A	129	PHE	CA-CB-CG	7.18	120.98	113.80
4	D	327	ASP	CA-CB-CG	7.15	119.75	112.60
3	C	58	ASP	CA-CB-CG	7.08	119.68	112.60
3	C	222	HIS	CA-CB-CG	7.06	120.86	113.80
1	A	92	PHE	CA-C-N	7.06	125.97	120.33
1	A	92	PHE	C-N-CA	7.06	125.97	120.33
1	A	93	VAL	N-CA-CB	6.98	115.90	110.45
5	F	229	PHE	CA-CB-CG	6.97	120.77	113.80
2	B	26	PHE	CA-CB-CG	6.95	120.75	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	272	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	112	ALA	CA-C-N	6.87	130.46	122.35
1	A	112	ALA	C-N-CA	6.87	130.46	122.35
2	B	233	ASP	CA-CB-CG	6.84	119.44	112.60
2	B	170	PHE	CA-CB-CG	6.83	120.63	113.80
2	B	29	ASN	CA-CB-CG	6.81	119.41	112.60
5	F	423	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	68	HIS	CA-CB-CG	6.79	120.59	113.80
3	C	142	ASP	CA-CB-CG	6.78	119.38	112.60
5	F	114	ASN	CA-CB-CG	6.76	119.36	112.60
3	C	295	ASP	CA-CB-CG	6.76	119.36	112.60
2	B	271	PHE	CA-CB-CG	6.75	120.55	113.80
2	B	295	ASP	CA-CB-CG	6.74	119.34	112.60
5	F	230	ASP	CA-CB-CG	6.73	119.33	112.60
4	D	39	ASP	CA-CB-CG	6.71	119.31	112.60
4	D	269	ASN	CA-CB-CG	6.64	119.24	112.60
4	D	240	CYS	CA-C-N	6.62	129.48	122.14
4	D	240	CYS	C-N-CA	6.62	129.48	122.14
4	D	303	PHE	CA-CB-CG	6.59	120.39	113.80
4	D	287	LEU	CA-C-N	6.55	131.78	123.34
4	D	287	LEU	C-N-CA	6.55	131.78	123.34
2	B	157	PHE	CA-CB-CG	6.51	120.31	113.80
2	B	229	ASN	CA-CB-CG	6.50	119.10	112.60
3	C	287	ASN	CA-CB-CG	6.50	119.10	112.60
4	D	315	ASP	CA-CB-CG	6.46	119.06	112.60
4	D	329	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	200	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	24	PHE	CA-CB-CG	6.42	120.22	113.80
4	D	17	ASP	CA-CB-CG	6.39	118.99	112.60
3	C	161	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	A	130	ASP	CA-CB-CG	6.37	118.97	112.60
4	D	179	ASP	CA-CB-CG	6.33	118.93	112.60
4	D	181	ASP	CA-CB-CG	6.30	118.90	112.60
5	F	157	LYS	CA-C-N	6.29	129.74	120.74
5	F	157	LYS	C-N-CA	6.29	129.74	120.74
1	A	75	HIS	CA-CB-CG	6.27	120.07	113.80
2	B	22	PHE	CA-CB-CG	6.26	120.06	113.80
3	C	243	HIS	CA-CB-CG	6.19	119.99	113.80
5	F	223	ARG	CD-NE-CZ	6.17	133.04	124.40
3	C	136	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	125	ARG	CD-NE-CZ	6.09	132.93	124.40
5	F	466	PRO	O-C-N	-6.00	114.55	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	222	HIS	CA-C-N	5.99	131.92	122.94
3	C	222	HIS	C-N-CA	5.99	131.92	122.94
3	C	141	PRO	CA-C-N	5.97	127.53	122.28
3	C	141	PRO	C-N-CA	5.97	127.53	122.28
5	F	94	HIS	CA-CB-CG	5.97	119.77	113.80
1	A	225	ARG	NE-CZ-NH2	5.96	124.56	119.20
4	D	21	HIS	CE1-NE2-CD2	-5.92	103.08	109.00
1	A	109	PHE	CA-CB-CG	5.92	119.72	113.80
3	C	236	GLY	N-CA-C	5.90	119.07	110.63
5	F	372	PHE	CA-C-N	5.89	130.85	122.72
5	F	372	PHE	C-N-CA	5.89	130.85	122.72
4	D	149	GLY	CA-C-N	5.86	130.46	122.19
4	D	149	GLY	C-N-CA	5.86	130.46	122.19
2	B	36	LEU	CA-C-N	5.80	128.09	120.60
2	B	36	LEU	C-N-CA	5.80	128.09	120.60
3	C	204	ASN	CA-C-N	5.79	128.98	120.82
3	C	204	ASN	C-N-CA	5.79	128.98	120.82
4	D	21	HIS	ND1-CG-CD2	-5.79	100.31	106.10
4	D	21	HIS	CG-CD2-NE2	5.74	112.94	107.20
3	C	298	ARG	CD-NE-CZ	5.72	132.40	124.40
5	F	249	ASP	CA-C-N	5.68	128.21	120.54
5	F	249	ASP	C-N-CA	5.68	128.21	120.54
2	B	21	GLU	CA-C-N	5.64	127.77	120.44
2	B	21	GLU	C-N-CA	5.64	127.77	120.44
4	D	181	ASP	CA-C-N	5.64	130.53	123.14
4	D	181	ASP	C-N-CA	5.64	130.53	123.14
2	B	154	VAL	N-CA-CB	5.64	117.52	110.47
2	B	154	VAL	CA-C-N	5.63	128.28	120.29
2	B	154	VAL	C-N-CA	5.63	128.28	120.29
5	F	83	GLU	CA-C-N	5.63	130.81	122.99
5	F	83	GLU	C-N-CA	5.63	130.81	122.99
2	B	114	ILE	N-CA-CB	5.62	116.75	110.62
4	D	240	CYS	N-CA-CB	5.62	118.32	109.83
2	B	23	TRP	N-CA-CB	5.60	118.14	110.01
2	B	84	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	95	ARG	NE-CZ-NH2	5.58	124.22	119.20
2	B	181	ARG	NE-CZ-NH2	5.53	124.18	119.20
3	C	189	GLN	CA-CB-CG	5.53	125.16	114.10
4	D	314	LYS	CA-C-N	5.53	130.89	122.65
4	D	314	LYS	C-N-CA	5.53	130.89	122.65
3	C	33	GLY	CA-C-N	5.52	130.34	122.72
3	C	33	GLY	C-N-CA	5.52	130.34	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	29	SER	CA-C-N	5.51	130.80	122.98
3	C	29	SER	C-N-CA	5.51	130.80	122.98
2	B	216	LEU	CA-C-N	5.49	127.62	120.26
2	B	216	LEU	C-N-CA	5.49	127.62	120.26
2	B	108	VAL	N-CA-CB	5.49	116.39	110.62
2	B	26	PHE	CA-C-N	5.49	127.64	120.28
2	B	26	PHE	C-N-CA	5.49	127.64	120.28
3	C	201	GLN	CA-C-N	5.49	127.91	120.44
3	C	201	GLN	C-N-CA	5.49	127.91	120.44
4	D	197	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	B	155	ALA	CA-C-N	5.48	127.47	120.56
2	B	155	ALA	C-N-CA	5.48	127.47	120.56
1	A	127	SER	N-CA-CB	5.47	117.69	110.25
4	D	284	PRO	CA-C-N	5.47	129.22	121.61
4	D	284	PRO	C-N-CA	5.47	129.22	121.61
2	B	164	ALA	CA-C-N	5.45	127.89	120.54
2	B	164	ALA	C-N-CA	5.45	127.89	120.54
2	B	25	TYR	CA-C-N	5.44	128.01	120.29
2	B	25	TYR	C-N-CA	5.44	128.01	120.29
1	A	198	PHE	CA-C-N	5.42	127.60	120.60
1	A	198	PHE	C-N-CA	5.42	127.60	120.60
4	D	140	LYS	CA-C-N	5.41	127.48	120.44
4	D	140	LYS	C-N-CA	5.41	127.48	120.44
1	A	75	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
2	B	291	ARG	N-CA-CB	5.40	117.79	109.91
3	C	263	ASP	CA-CB-CG	5.39	117.99	112.60
5	F	229	PHE	CA-C-N	5.39	127.44	120.44
5	F	229	PHE	C-N-CA	5.39	127.44	120.44
3	C	223	LYS	CA-CB-CG	5.38	124.87	114.10
4	D	138	ARG	N-CA-CB	5.38	117.81	110.01
3	C	192	ILE	N-CA-CB	5.37	116.84	110.55
4	D	80	TYR	CA-C-N	5.36	130.89	123.07
4	D	80	TYR	C-N-CA	5.36	130.89	123.07
1	A	108	ILE	CA-C-N	5.36	127.72	120.44
1	A	108	ILE	C-N-CA	5.36	127.72	120.44
2	B	37	VAL	N-CA-CB	5.36	116.45	110.51
4	D	319	GLN	OE1-CD-NE2	-5.35	117.25	122.60
2	B	110	VAL	N-CA-CB	5.35	116.81	110.55
2	B	171	VAL	N-CA-CB	5.35	117.82	110.54
2	B	230	ALA	CA-C-N	5.34	129.55	121.65
2	B	230	ALA	C-N-CA	5.34	129.55	121.65
5	F	364	LYS	CA-CB-CG	5.33	124.75	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ALA	CA-C-N	5.31	127.25	120.56
1	A	218	ALA	C-N-CA	5.31	127.25	120.56
4	D	139	GLU	CA-C-N	5.31	127.34	120.44
4	D	139	GLU	C-N-CA	5.31	127.34	120.44
1	A	216	PRO	CA-C-N	5.31	127.65	120.38
1	A	216	PRO	C-N-CA	5.31	127.65	120.38
2	B	151	LEU	CA-C-N	5.30	127.24	120.56
2	B	151	LEU	C-N-CA	5.30	127.24	120.56
3	C	62	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	B	104	VAL	N-CA-CB	5.30	116.75	110.55
1	A	75	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	A	116	PRO	CA-C-N	5.29	127.33	120.56
1	A	116	PRO	C-N-CA	5.29	127.33	120.56
3	C	239	HIS	CA-C-N	5.29	127.31	120.44
3	C	239	HIS	C-N-CA	5.29	127.31	120.44
2	B	93	ARG	NE-CZ-NH2	5.26	123.94	119.20
4	D	282	GLU	CA-C-N	5.26	127.81	120.65
4	D	282	GLU	C-N-CA	5.26	127.81	120.65
3	C	296	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	219	VAL	CA-C-N	5.25	127.18	120.56
1	A	219	VAL	C-N-CA	5.25	127.18	120.56
3	C	240	ALA	CA-C-N	5.25	127.17	120.56
3	C	240	ALA	C-N-CA	5.25	127.17	120.56
2	B	112	SER	CA-C-N	5.24	127.26	120.44
2	B	112	SER	C-N-CA	5.24	127.26	120.44
1	A	75	HIS	CG-CD2-NE2	5.24	112.44	107.20
3	C	246	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	B	221	VAL	N-CA-CB	5.22	116.31	110.51
1	A	226	SER	N-CA-CB	5.22	117.53	109.91
5	F	275	ARG	N-CA-CB	5.21	117.57	110.01
2	B	265	ALA	CA-C-N	5.21	127.69	120.29
2	B	265	ALA	C-N-CA	5.21	127.69	120.29
5	F	102	HIS	CA-C-N	5.21	130.59	122.26
5	F	102	HIS	C-N-CA	5.21	130.59	122.26
1	A	125	ARG	N-CA-CB	5.21	117.55	109.48
2	B	103	LEU	N-CA-CB	5.21	117.56	110.01
1	A	300	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	B	93	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	125	ARG	CB-CG-CD	5.19	123.24	111.30
2	B	148	LEU	CA-C-N	5.19	127.18	120.44
2	B	148	LEU	C-N-CA	5.19	127.18	120.44
1	A	127	SER	CA-C-N	5.19	127.09	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	SER	C-N-CA	5.19	127.09	120.56
1	A	220	ILE	N-CA-CB	5.18	116.61	110.55
2	B	109	VAL	N-CA-CB	5.18	116.61	110.55
2	B	267	TRP	CA-C-N	5.18	127.56	120.46
2	B	267	TRP	C-N-CA	5.18	127.56	120.46
5	F	223	ARG	CA-CB-CG	5.17	124.44	114.10
3	C	223	LYS	CG-CD-CE	5.17	123.18	111.30
4	D	138	ARG	CA-C-N	5.17	127.16	120.44
4	D	138	ARG	C-N-CA	5.17	127.16	120.44
4	D	271	ASP	CA-CB-CG	5.16	117.76	112.60
3	C	169	ALA	CA-C-N	5.15	127.70	120.28
3	C	169	ALA	C-N-CA	5.15	127.70	120.28
1	A	199	ILE	N-CA-CB	5.15	116.22	110.51
2	B	220	ILE	N-CA-CB	5.15	116.57	110.55
1	A	220	ILE	CA-C-N	5.15	127.04	120.56
1	A	220	ILE	C-N-CA	5.15	127.04	120.56
2	B	22	PHE	N-CA-CB	5.14	117.47	110.01
5	F	244	PHE	CA-CB-CG	5.14	118.94	113.80
3	C	198	GLU	N-CA-CB	5.13	117.52	110.07
1	A	130	ASP	N-CA-CB	5.13	117.45	110.01
4	D	138	ARG	CB-CG-CD	5.13	123.09	111.30
4	D	139	GLU	N-CA-CB	5.13	117.44	110.01
2	B	220	ILE	CA-C-N	5.12	127.21	120.60
2	B	220	ILE	C-N-CA	5.12	127.21	120.60
5	F	397	GLN	OE1-CD-NE2	-5.11	117.49	122.60
4	D	83	GLY	CA-C-N	5.11	130.20	123.05
4	D	83	GLY	C-N-CA	5.11	130.20	123.05
1	A	136	LEU	CA-C-N	5.09	127.06	120.44
1	A	136	LEU	C-N-CA	5.09	127.06	120.44
2	B	29	ASN	CA-C-N	5.09	127.36	120.44
2	B	29	ASN	C-N-CA	5.09	127.36	120.44
4	D	324	PHE	CA-C-N	5.08	127.09	120.28
4	D	324	PHE	C-N-CA	5.08	127.09	120.28
2	B	113	LEU	N-CA-CB	5.08	117.38	110.01
2	B	293	ALA	CA-C-N	5.08	130.44	122.11
2	B	293	ALA	C-N-CA	5.08	130.44	122.11
5	F	96	ARG	CA-CB-CG	5.08	124.26	114.10
5	F	62	ASN	CA-CB-CG	5.08	117.68	112.60
2	B	103	LEU	CA-C-N	5.07	126.95	120.56
2	B	103	LEU	C-N-CA	5.07	126.95	120.56
3	C	237	ASP	CA-C-N	5.06	127.33	120.65
3	C	237	ASP	C-N-CA	5.06	127.33	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	195	LEU	N-CA-CB	5.06	117.35	110.01
5	F	391	ARG	NE-CZ-NH2	5.06	123.75	119.20
4	D	144	MET	N-CA-CB	5.06	117.34	110.01
1	A	307	GLN	OE1-CD-NE2	-5.05	117.55	122.60
3	C	236	GLY	CA-C-N	5.04	127.87	120.71
3	C	236	GLY	C-N-CA	5.04	127.87	120.71
2	B	148	LEU	N-CA-CB	5.04	117.32	110.01
1	A	217	LEU	N-CA-CB	5.03	117.61	110.06
3	C	182	THR	N-CA-C	5.03	116.45	111.07
5	F	274	ALA	CA-C-N	5.03	126.98	120.44
5	F	274	ALA	C-N-CA	5.03	126.98	120.44
1	A	128	ILE	CA-C-N	5.03	127.33	120.54
1	A	128	ILE	C-N-CA	5.03	127.33	120.54
5	F	216	GLN	CA-CB-CG	5.03	124.16	114.10
1	A	67	LEU	CA-C-N	5.02	126.97	120.44
1	A	67	LEU	C-N-CA	5.02	126.97	120.44
1	A	129	PHE	CA-C-N	5.02	126.97	120.44
1	A	129	PHE	C-N-CA	5.02	126.97	120.44
5	F	436	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	68	HIS	N-CA-CB	5.00	117.27	110.01
1	A	221	VAL	N-CA-CB	5.00	116.40	110.55
1	A	132	THR	CA-C-N	5.00	127.25	120.65
1	A	132	THR	C-N-CA	5.00	127.25	120.65

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	300	ARG	Sidechain
3	C	146	ARG	Sidechain
3	C	28	TYR	Sidechain
3	C	311	ARG	Sidechain
5	F	253	ARG	Sidechain

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	2317	0	2428	6	0
2	B	2187	0	2275	12	0
3	C	2486	0	2513	6	0
4	D	2537	0	2589	6	0
5	F	4047	0	3945	5	0
6	C	8	0	0	0	0
6	D	8	0	0	0	0
7	C	31	0	12	0	0
7	D	31	0	12	0	0
All	All	13652	0	13774	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:B:204:MET:HE3	2:B:204:MET:H	1.35	0.90
2:B:165:ALA:O	2:B:169:THR:HG23	1.86	0.74
5:F:272:ASP:OD1	5:F:275:ARG:NH1	2.24	0.71
2:B:148:LEU:O	2:B:152:VAL:HG23	1.94	0.68
3:C:295:ASP:OD1	3:C:298:ARG:NH2	2.36	0.59
2:B:291:ARG:NH1	2:B:292:ASP:OD1	2.38	0.56
2:B:204:MET:H	2:B:204:MET:CE	2.15	0.55
5:F:464:TYR:O	5:F:465:LYS:C	2.52	0.53
2:B:150:ALA:O	2:B:154:VAL:HG23	2.08	0.53
5:F:465:LYS:HB3	5:F:466:PRO:HD3	1.91	0.52
4:D:315:ASP:OD1	4:D:316:TYR:N	2.43	0.52
3:C:287:ASN:C	3:C:287:ASN:OD1	2.55	0.50
3:C:188:ILE:O	3:C:192:ILE:HG12	2.12	0.49
2:B:93:ARG:HH21	2:B:93:ARG:HG3	1.78	0.48
3:C:175:LEU:HB3	3:C:205:MET:HE3	1.96	0.48
2:B:121:LEU:HD23	2:B:184:VAL:HG21	1.95	0.48
4:D:9:GLN:OE1	4:D:10:GLN:O	2.32	0.47
4:D:9:GLN:OE1	4:D:9:GLN:C	2.58	0.47
4:D:123:GLU:OE2	4:D:155:TYR:OH	2.33	0.47
1:A:293:TRP:CZ2	1:A:305:VAL:HG13	2.50	0.46
1:A:107:MET:HE2	1:A:274:LEU:HD22	1.98	0.46
1:A:125:ARG:NH2	2:B:292:ASP:OD2	2.46	0.46
2:B:110:VAL:HG13	2:B:111:LEU:N	2.32	0.44
4:D:316:TYR:OH	4:D:327:ASP:OD1	2.32	0.43
3:C:84:ARG:NE	3:C:84:ARG:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HD2	1:A:293:TRP:CD2	2.55	0.42
3:C:171:ARG:N	3:C:172:PRO:HD3	2.34	0.42
1:A:181:LEU:HA	1:A:192:TRP:CZ3	2.55	0.41
5:F:75:ILE:HB	5:F:76:PRO:HD2	2.02	0.41
4:D:29:PHE:O	4:D:29:PHE:CG	2.74	0.41
1:A:107:MET:HE3	1:A:271:VAL:HG23	2.02	0.41
2:B:63:ASP:C	2:B:63:ASP:OD1	2.63	0.41
2:B:164:ALA:O	2:B:168:LEU:HD22	2.21	0.40
5:F:468:GLU:HA	5:F:471:ILE:HG22	2.04	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	294/339 (87%)	287 (98%)	7 (2%)	0	100	100
2	B	287/300 (96%)	282 (98%)	5 (2%)	0	100	100
3	C	322/327 (98%)	314 (98%)	8 (2%)	0	100	100
4	D	320/334 (96%)	313 (98%)	7 (2%)	0	100	100
5	F	505/535 (94%)	482 (95%)	23 (5%)	0	100	100
All	All	1728/1835 (94%)	1678 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	249/283 (88%)	246 (99%)	3 (1%)	63	74
2	B	228/239 (95%)	226 (99%)	2 (1%)	70	76
3	C	267/270 (99%)	264 (99%)	3 (1%)	65	75
4	D	279/290 (96%)	275 (99%)	4 (1%)	59	72
5	F	434/456 (95%)	429 (99%)	5 (1%)	63	74
All	All	1457/1538 (95%)	1440 (99%)	17 (1%)	61	74

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	174	PHE
1	A	284	ILE
2	B	154	VAL
2	B	270	THR
3	C	83	ARG
3	C	192	ILE
3	C	263	ASP
4	D	9	GLN
4	D	178	LEU
4	D	283	LEU
4	D	288	ASN
5	F	262	CYS
5	F	368	LEU
5	F	397	GLN
5	F	447	LEU
5	F	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	258	ASN
2	B	20	GLN
2	B	72	GLN
2	B	210	ASN
2	B	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	263	GLN
2	B	284	ASN
3	C	103	ASN
3	C	152	HIS
3	C	312	GLN
4	D	44	ASN
4	D	136	GLN
4	D	160	HIS
5	F	114	ASN
5	F	258	GLN
5	F	298	ASN
5	F	311	GLN
5	F	495	HIS
5	F	505	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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
7	AGS	D	402	-	29,33,33	0.94	1 (3%)	39,52,52	1.33	7 (17%)
6	SF4	C	401	3	0,12,12	-	-	-	-	-
7	AGS	C	402	-	29,33,33	0.94	1 (3%)	39,52,52	1.42	8 (20%)
6	SF4	D	401	4	0,12,12	-	-	-	-	-

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
7	AGS	D	402	-	-	1/21/38/38	0/3/3/3
6	SF4	C	401	3	-	-	0/6/5/5
7	AGS	C	402	-	-	0/21/38/38	0/3/3/3
6	SF4	D	401	4	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	402	AGS	C5-C4	-2.16	1.35	1.39
7	C	402	AGS	C5-C4	-2.04	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	402	AGS	PA-O3A-PB	-3.64	120.32	132.83
7	C	402	AGS	PA-O3A-PB	-3.44	121.01	132.83
7	C	402	AGS	C5-C4-N3	-3.09	122.72	126.75
7	D	402	AGS	C5-C4-N3	-2.84	123.04	126.75
7	C	402	AGS	O2G-PG-O3B	-2.76	95.43	104.64
7	D	402	AGS	C4-C5-N7	2.72	113.93	110.62
7	C	402	AGS	C4-C5-N7	2.70	113.91	110.62
7	D	402	AGS	C5-C6-N1	2.62	123.02	117.39
7	C	402	AGS	C5-C6-N1	2.61	123.00	117.39
7	D	402	AGS	N6-C6-N1	-2.20	113.53	118.35
7	C	402	AGS	C2-N1-C6	-2.17	115.05	118.77
7	D	402	AGS	C2-N1-C6	-2.16	115.05	118.77
7	C	402	AGS	N3-C4-N9	2.09	130.53	127.08
7	D	402	AGS	N3-C4-N9	2.06	130.48	127.08
7	C	402	AGS	N6-C6-N1	-2.02	113.93	118.35

There are no chirality outliers.

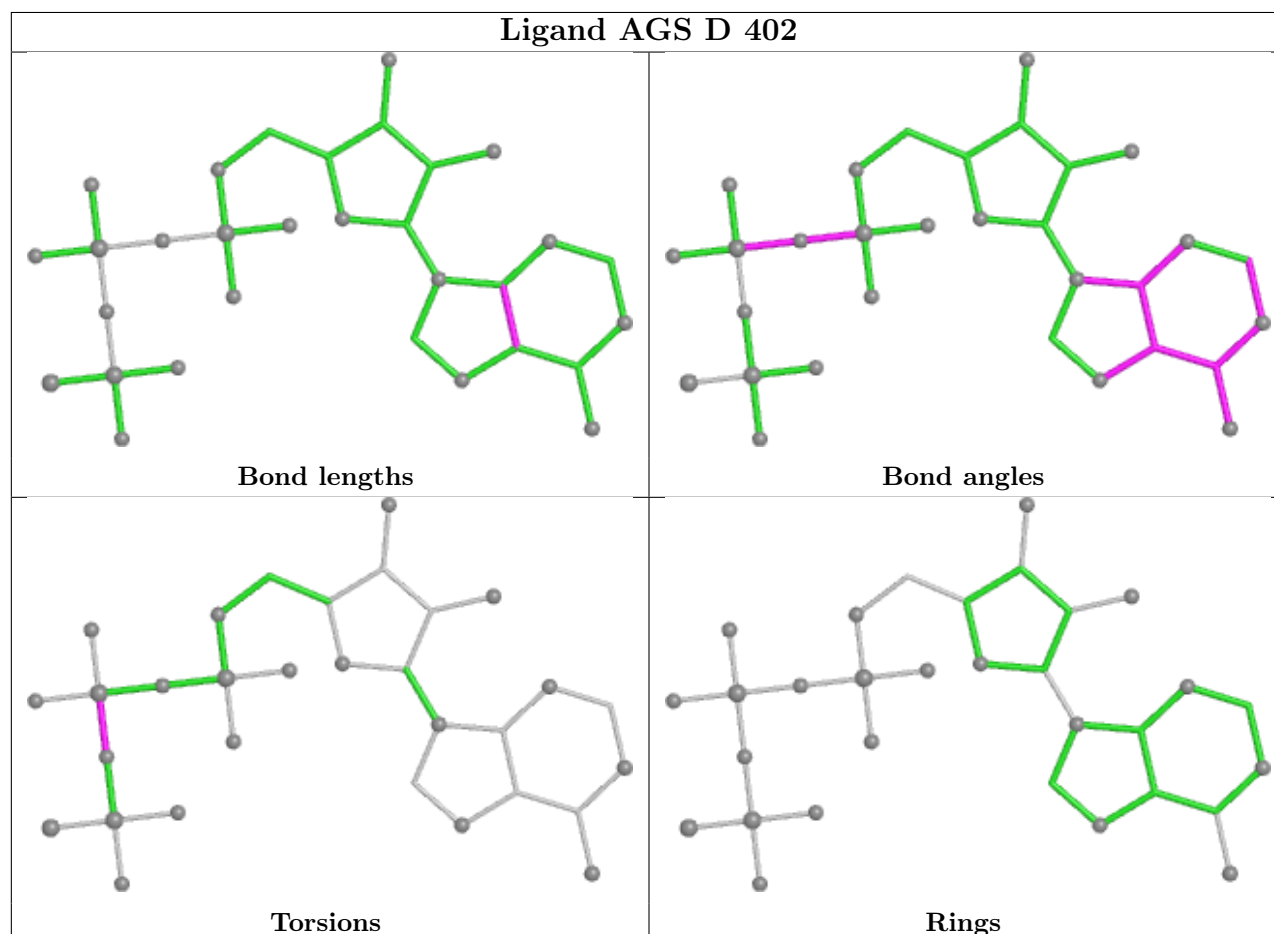
All (1) torsion outliers are listed below:

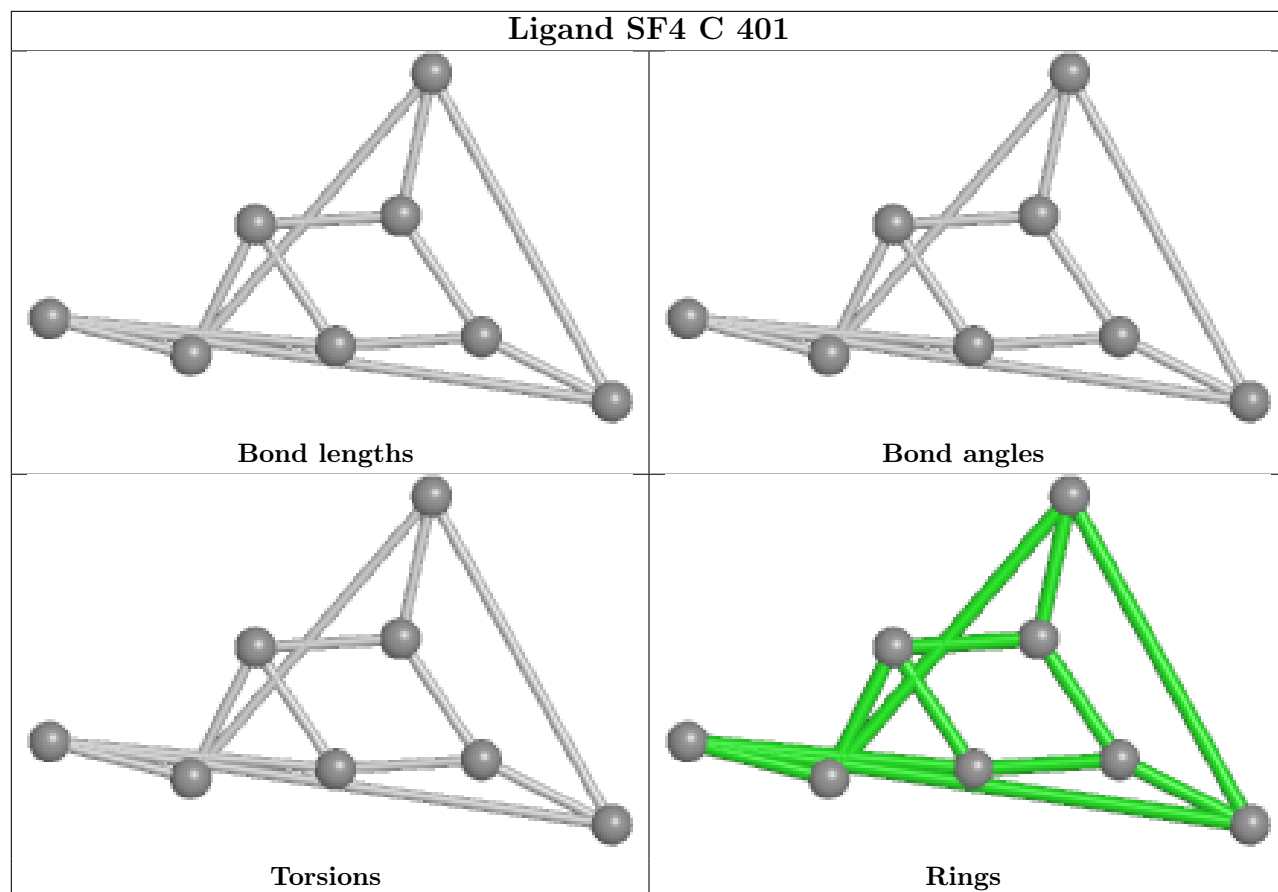
Mol	Chain	Res	Type	Atoms
7	D	402	AGS	PG-O3B-PB-O2B

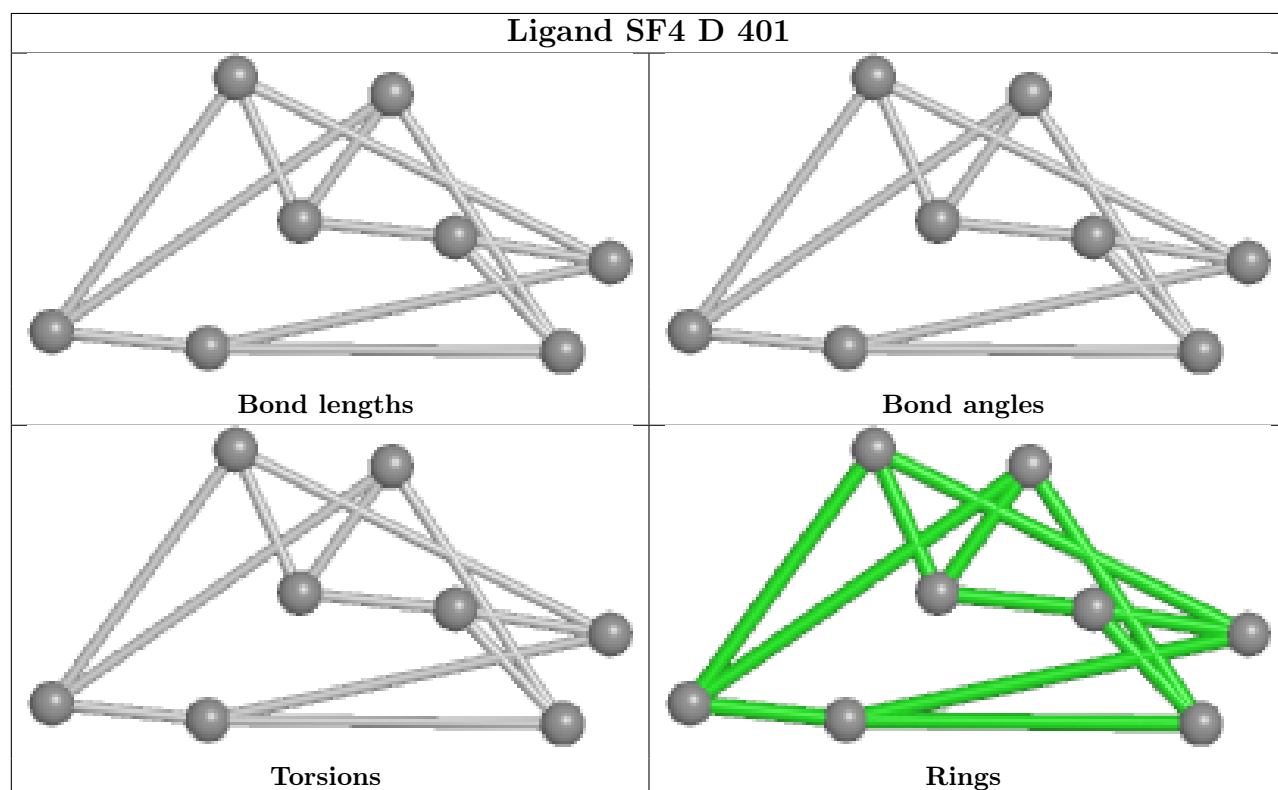
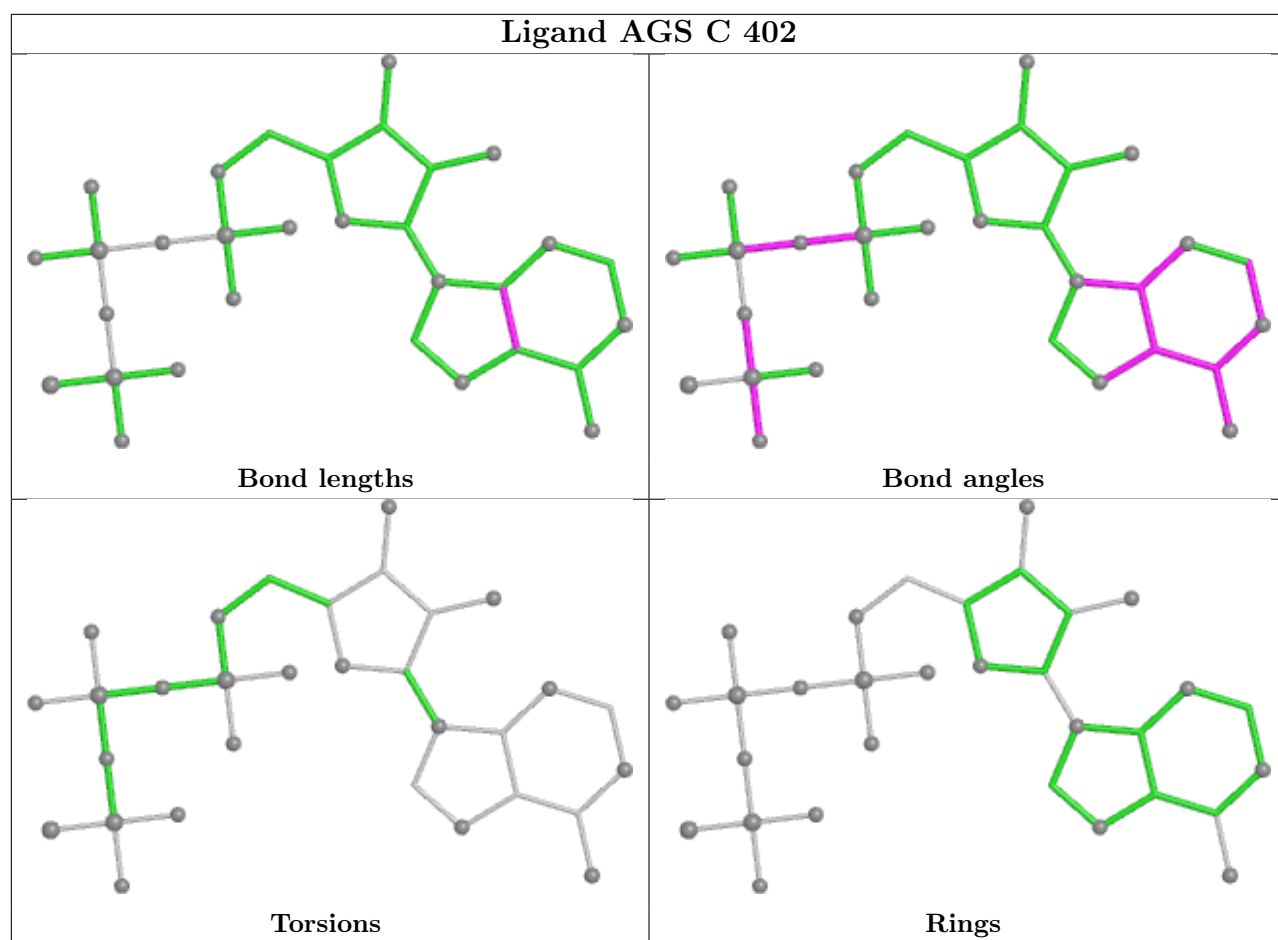
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

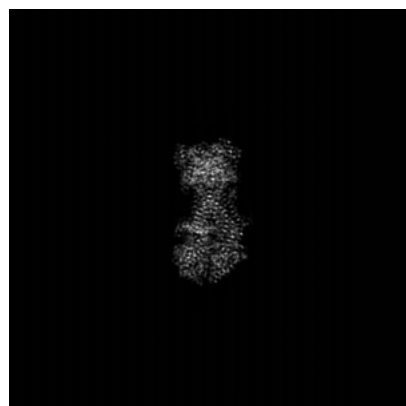
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39741. These allow visual inspection of the internal detail of the map and identification of artifacts.

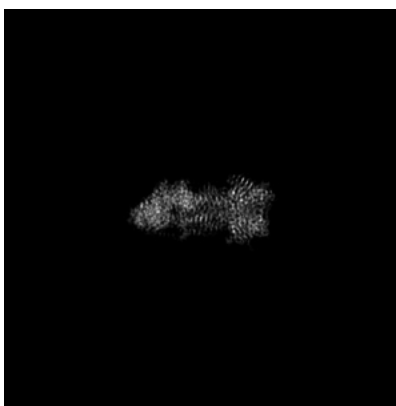
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

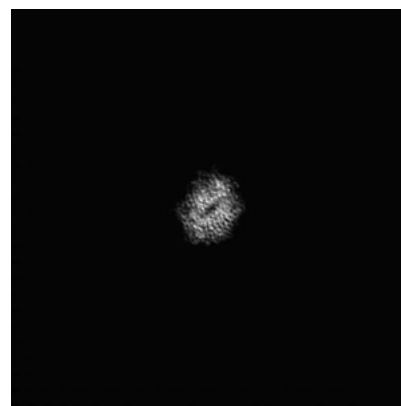
6.1.1 Primary map



X

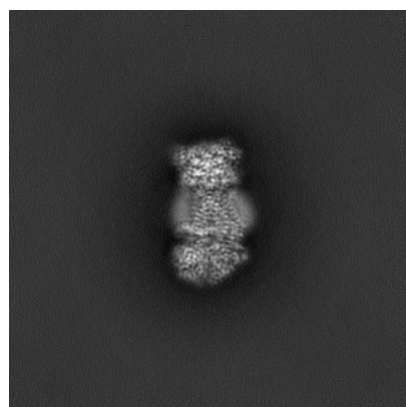


Y

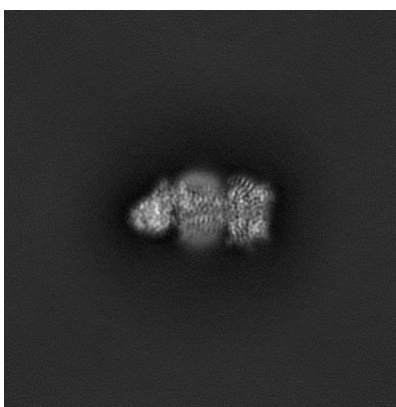


Z

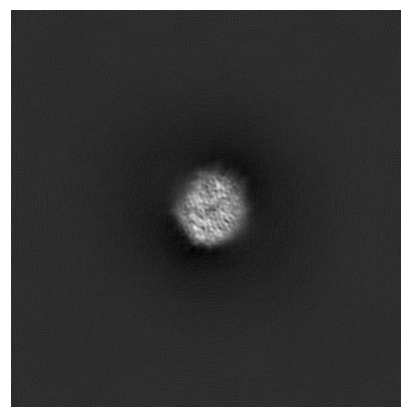
6.1.2 Raw map



X



Y

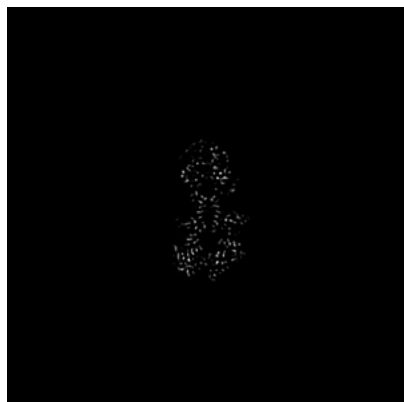


Z

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

6.2 Central slices [i](#)

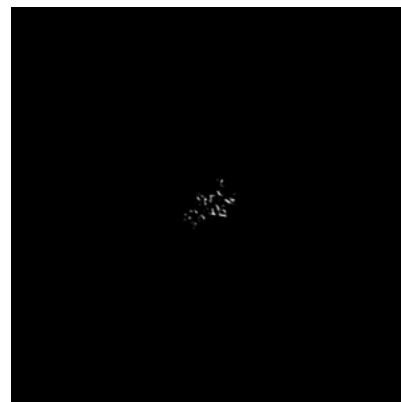
6.2.1 Primary map



X Index: 192

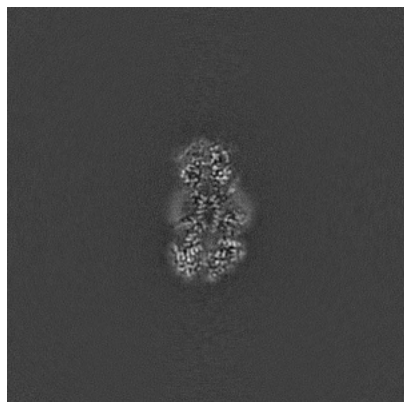


Y Index: 192

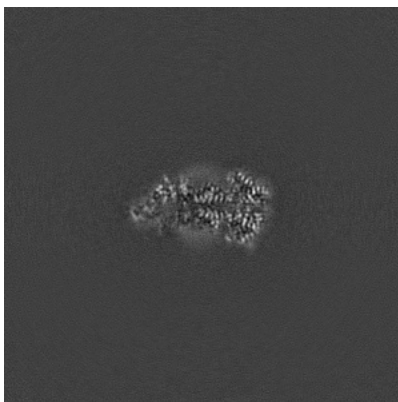


Z Index: 192

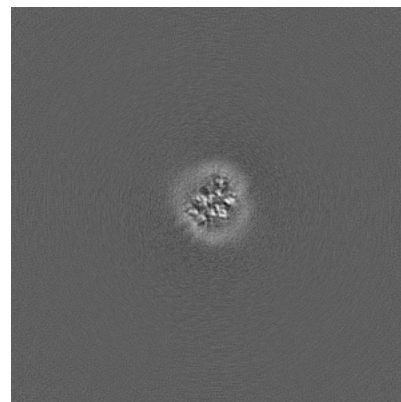
6.2.2 Raw map



X Index: 192



Y Index: 192

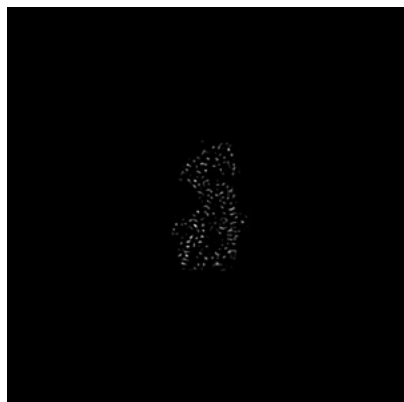


Z Index: 192

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

6.3 Largest variance slices [i](#)

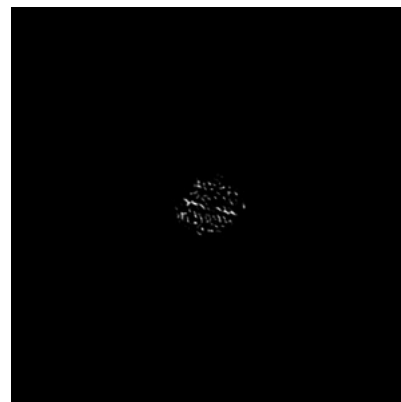
6.3.1 Primary map



X Index: 198

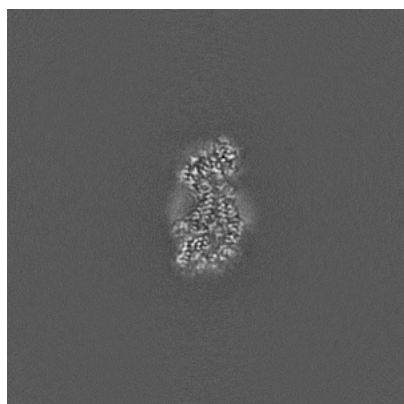


Y Index: 181

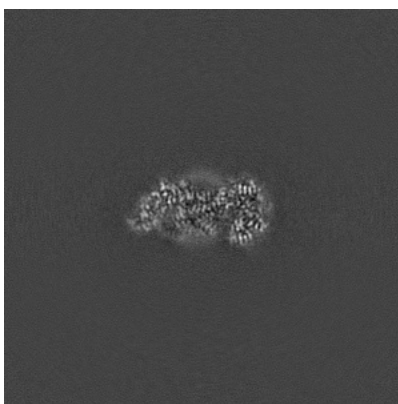


Z Index: 226

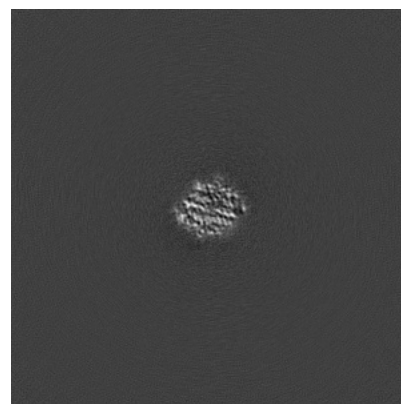
6.3.2 Raw map



X Index: 200



Y Index: 185

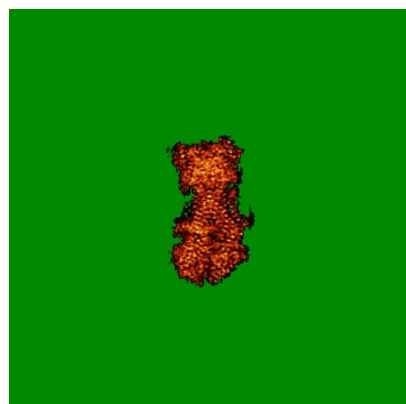


Z Index: 226

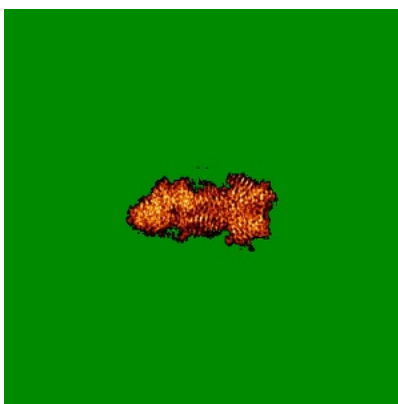
The images above show the largest variance slices of the map in three orthogonal directions.

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

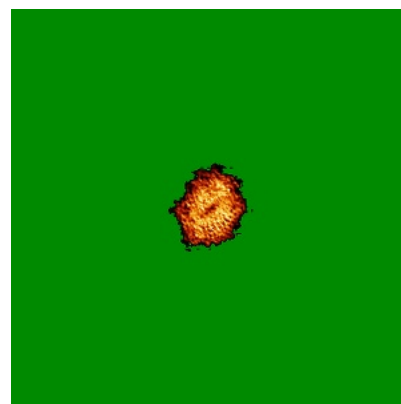
6.4.1 Primary map



X

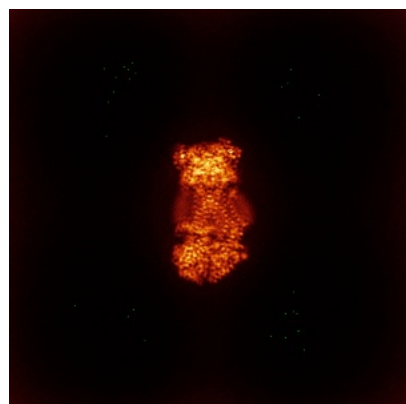


Y

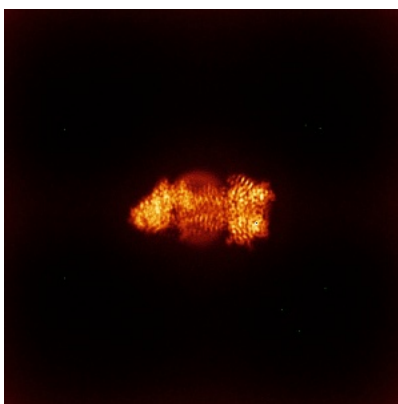


Z

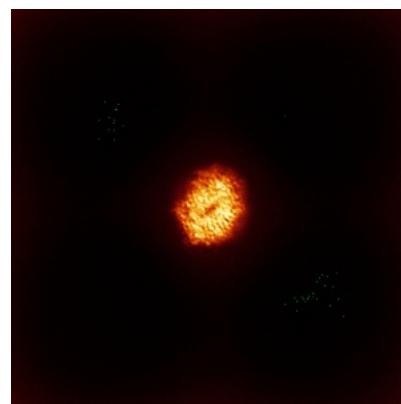
6.4.2 Raw map



X



Y

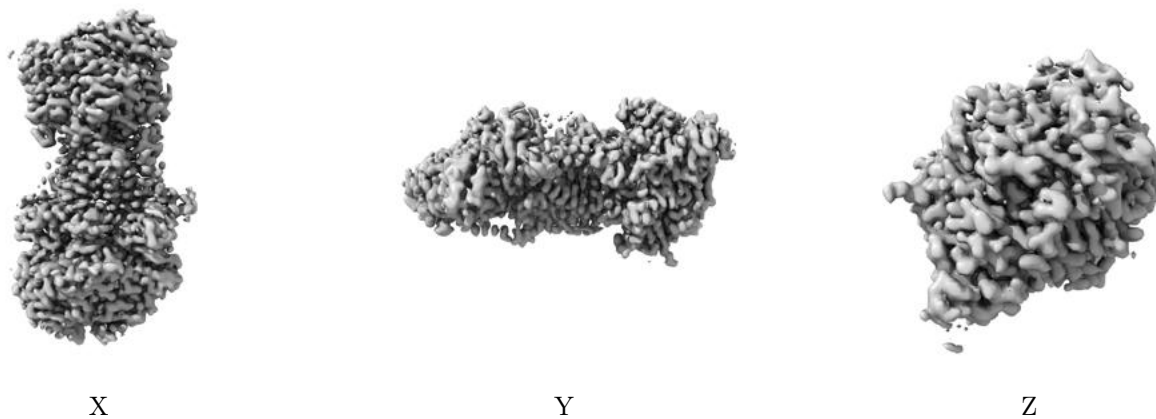


Z

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.

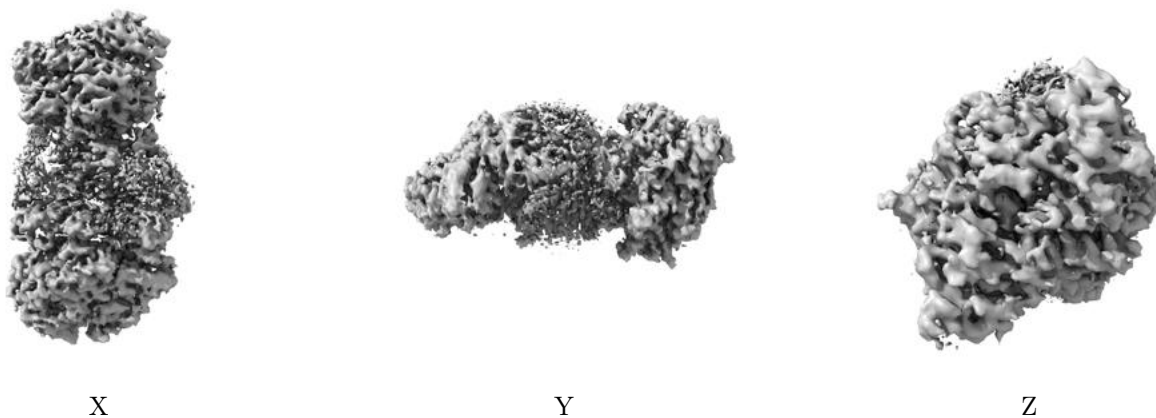
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

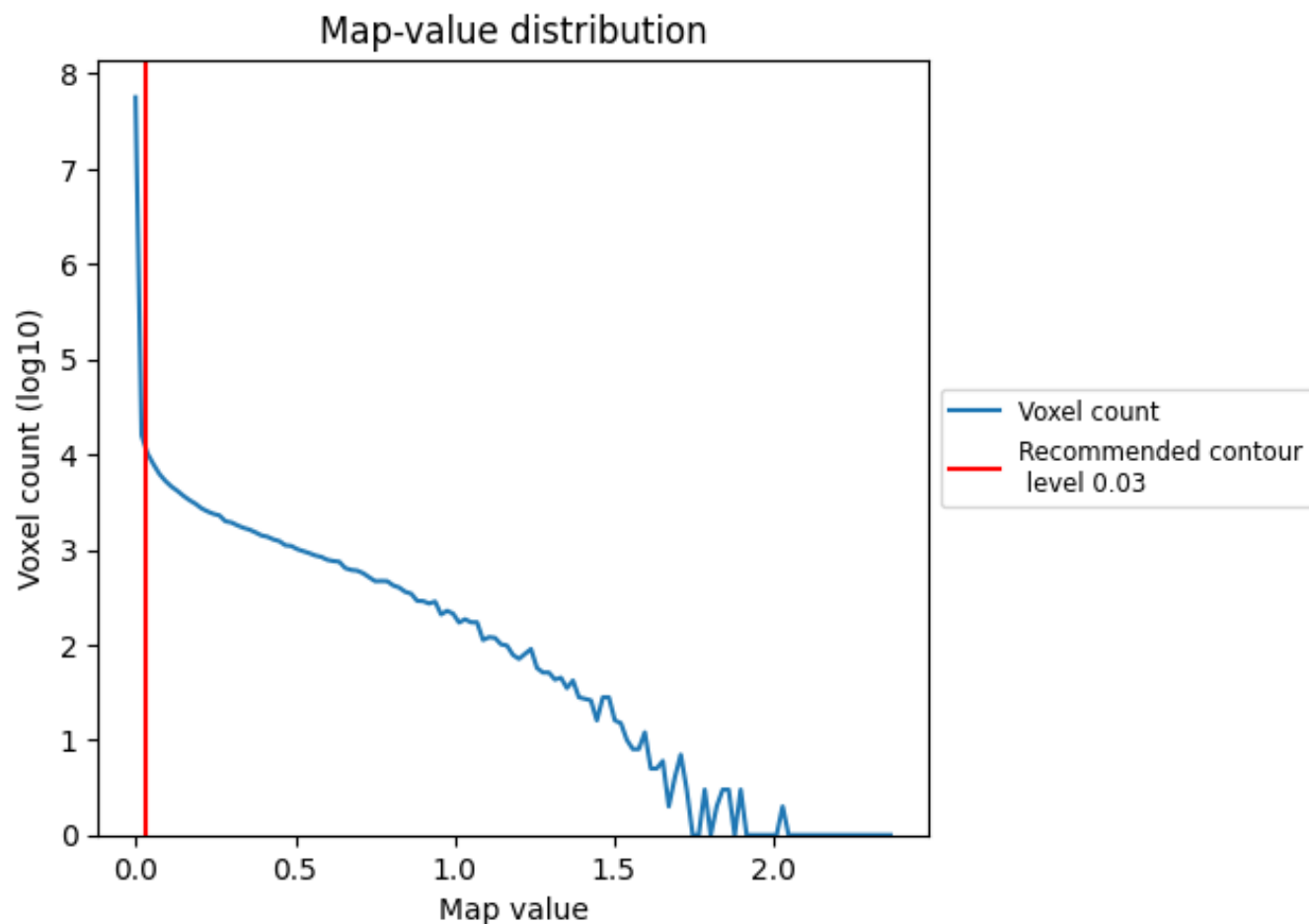
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

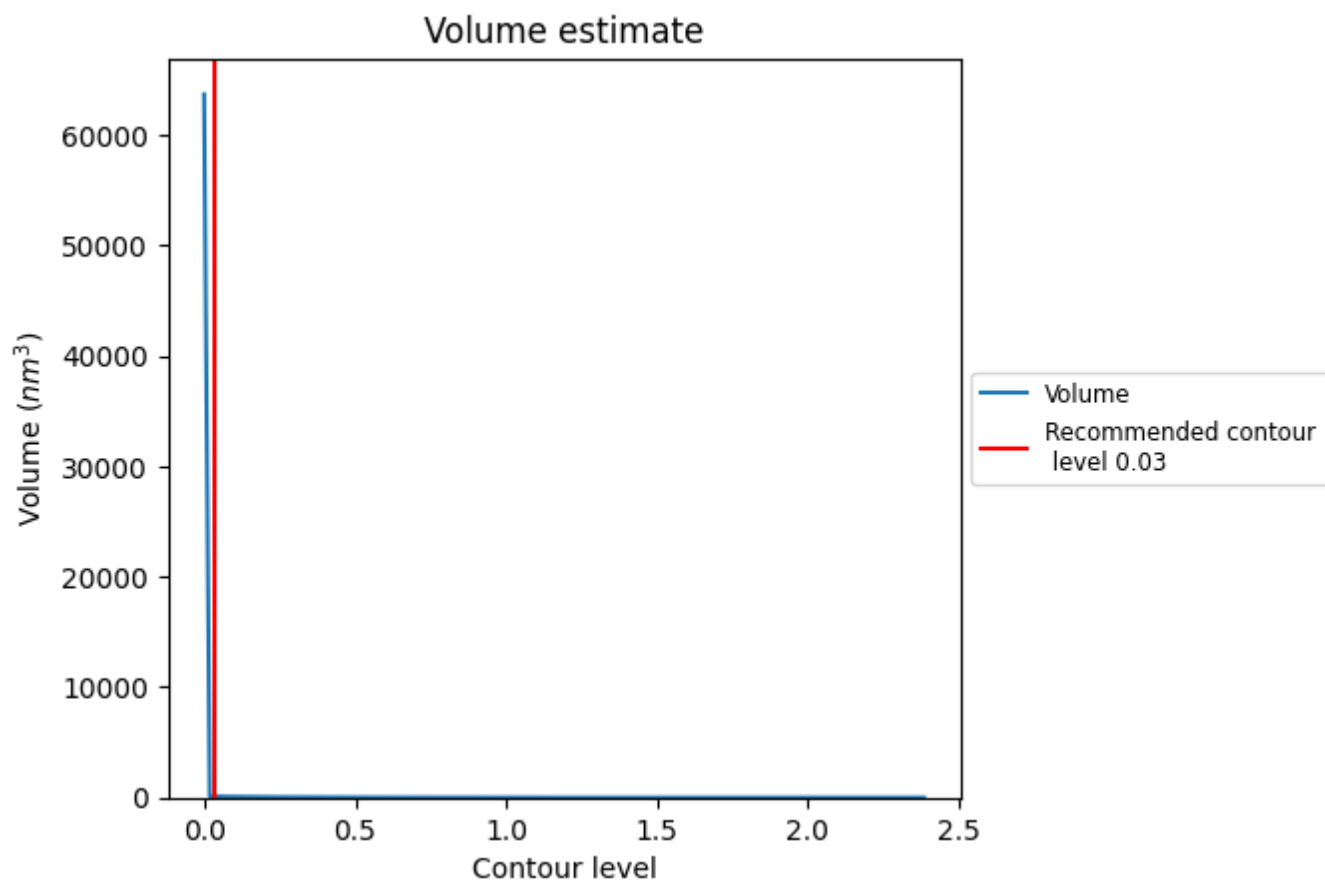
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

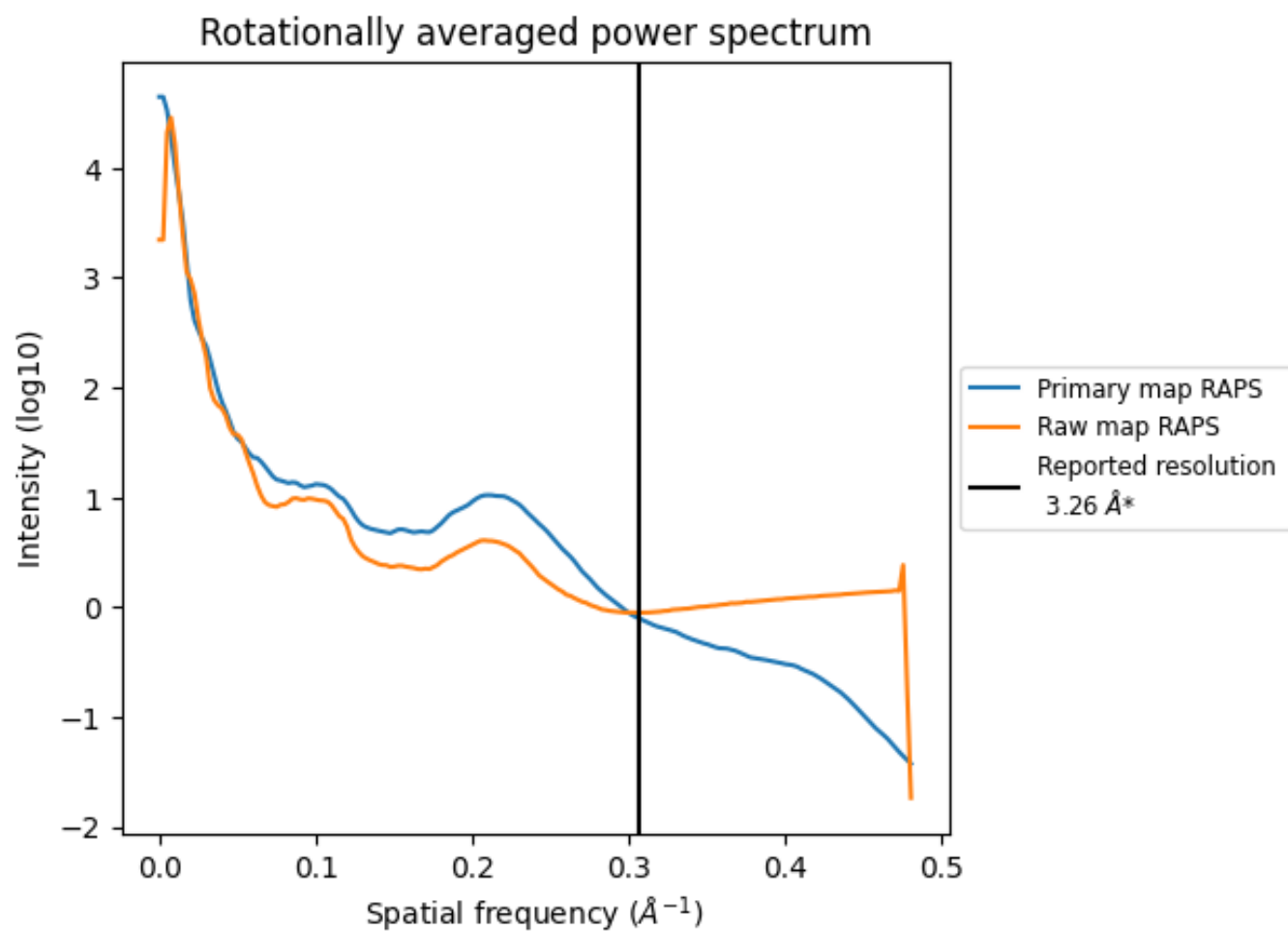
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm³; this corresponds to an approximate mass of 99 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 ⓘ

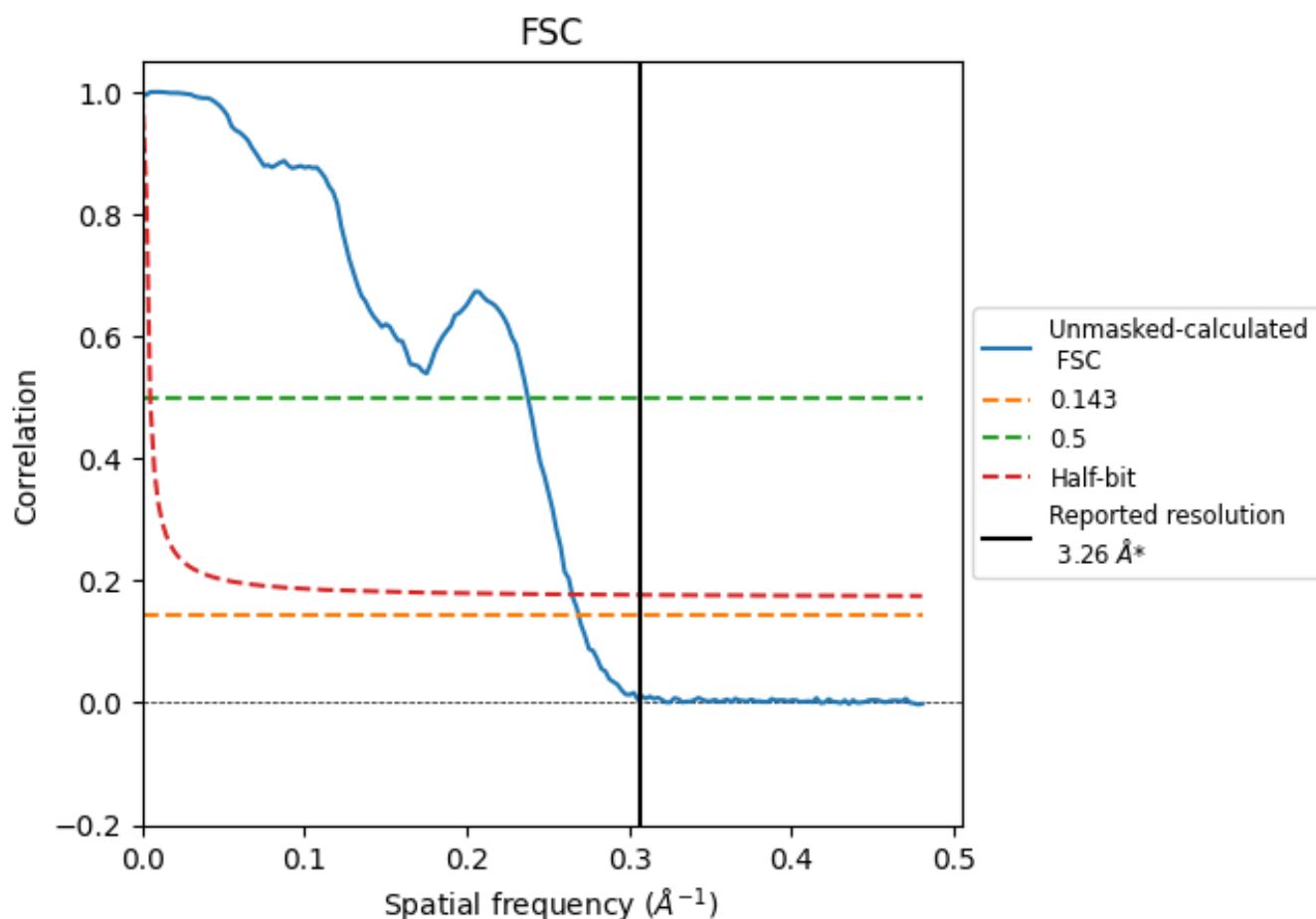


*Reported resolution corresponds to spatial frequency of 0.307 $\text{\AA}^{-1}$

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 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

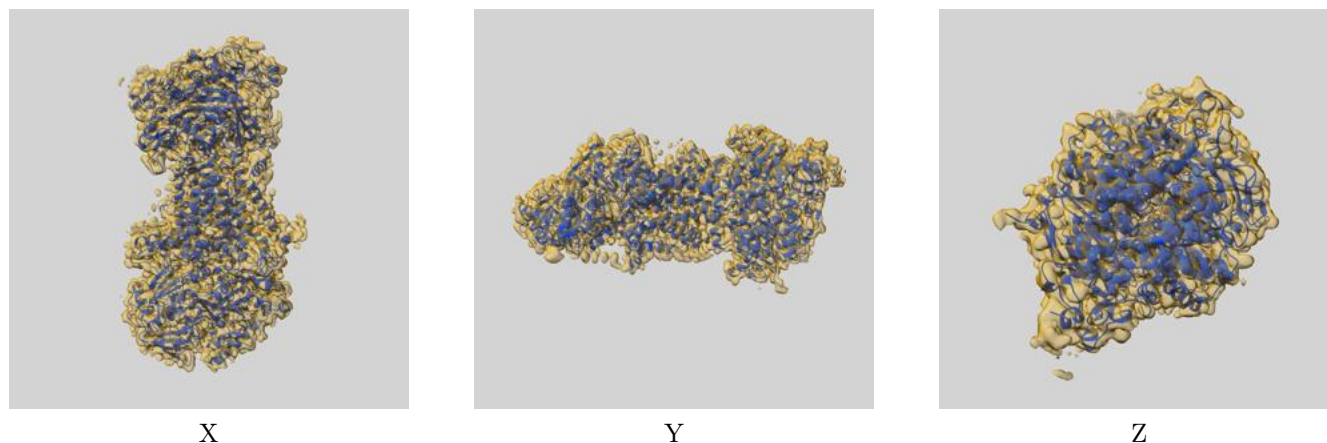
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.21	3.77

*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 3.72 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

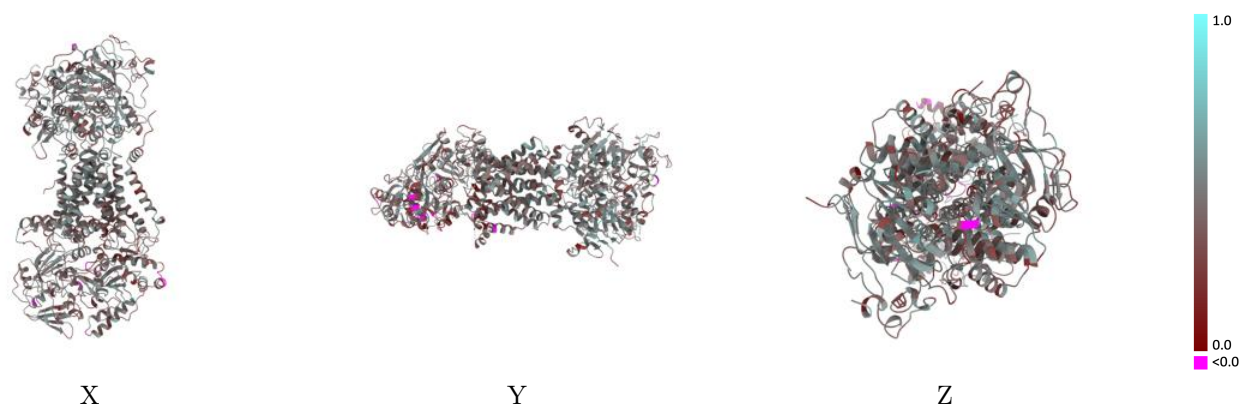
This section contains information regarding the fit between EMDB map EMD-39741 and PDB model 8Z1Z. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



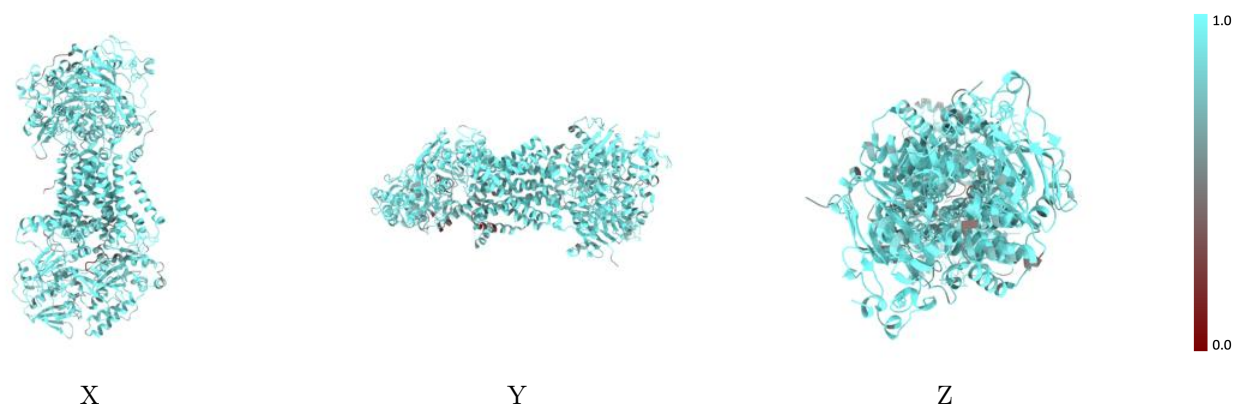
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



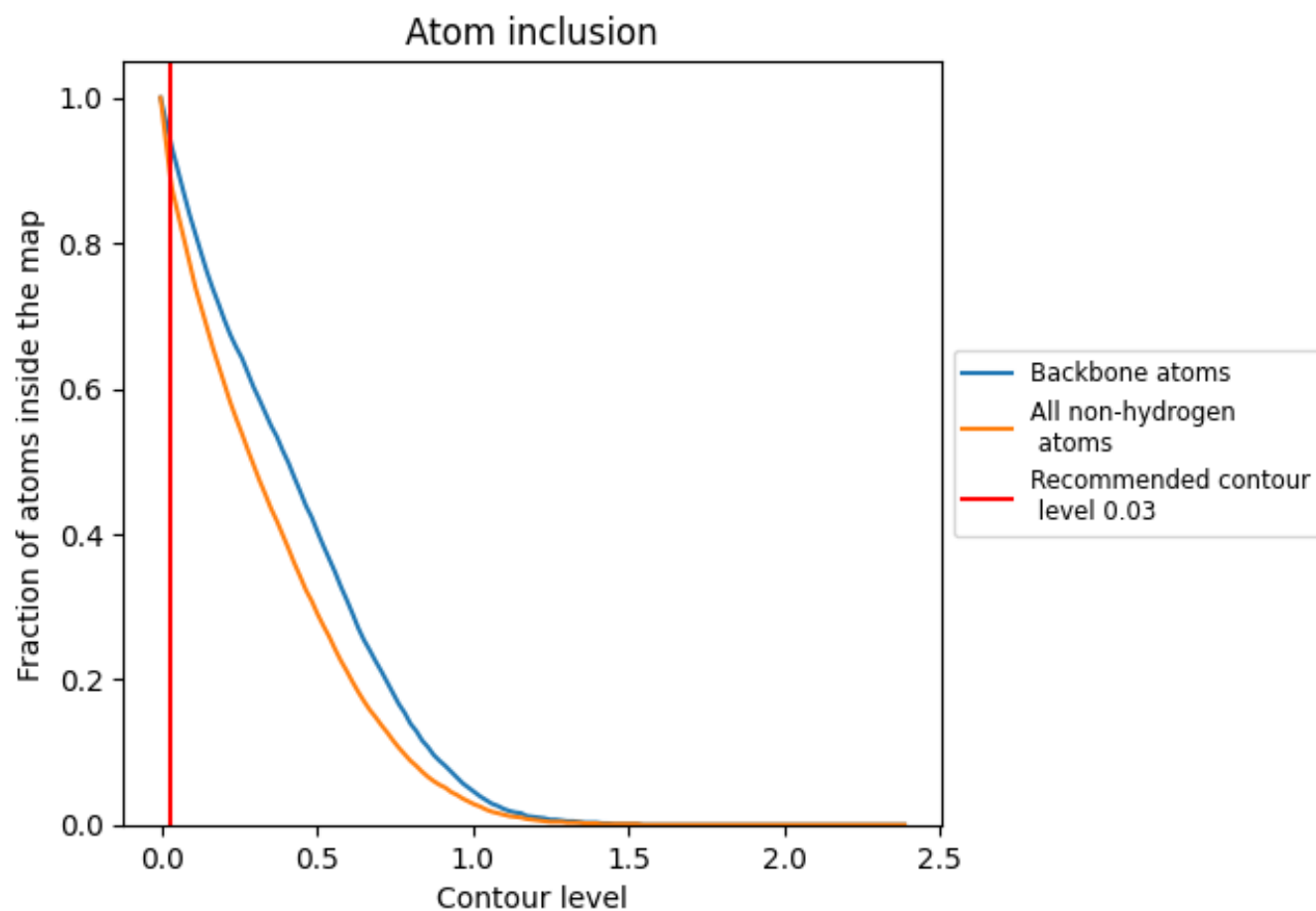
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.4200
A	0.8920	0.4240
B	0.9060	0.4190
C	0.9060	0.4340
D	0.9070	0.4540
F	0.8560	0.3870

