



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:40 AM UTC

PDB ID : 8G1E / pdb_00008g1e
EMDB ID : EMD-29668
Title : Structure of ACLY-D1026A-products-asm
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2023-02-02
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary 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

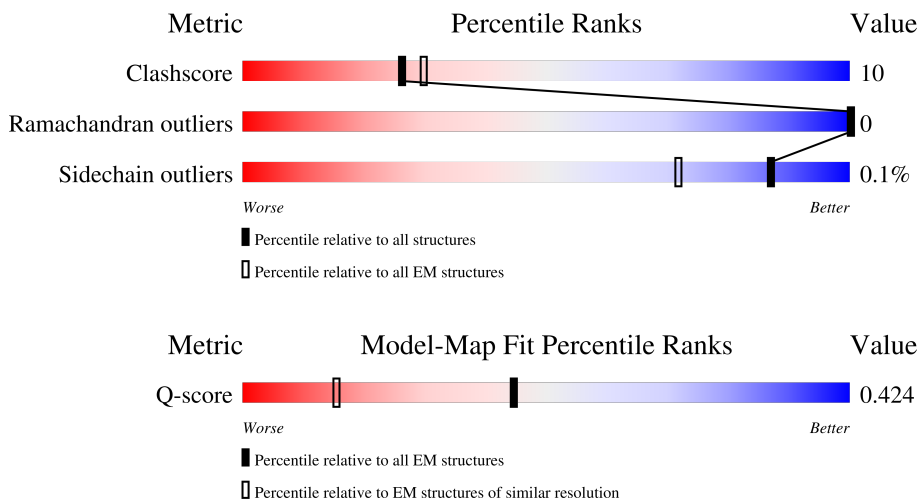
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	1101	
1	B	1101	
1	C	1101	
1	D	1101	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNL	B	2301	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 32649 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.

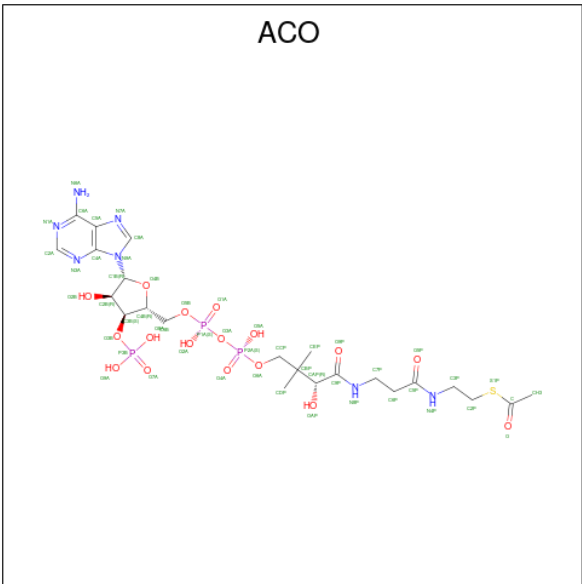
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	B	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	C	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	D	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		

There are 4 discrepancies between the modelled and reference sequences:

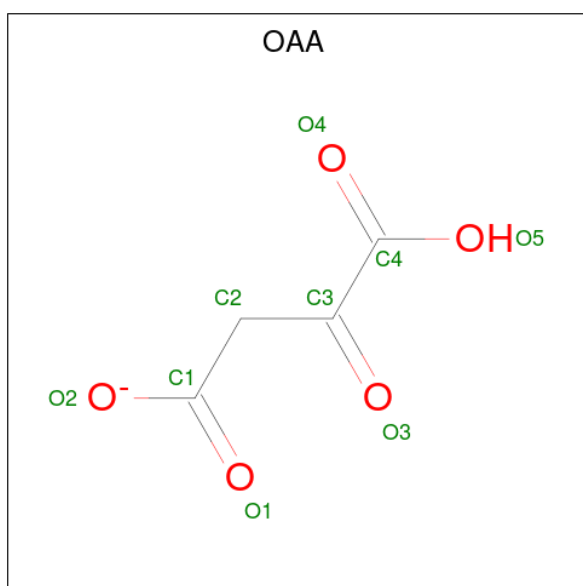
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	ASP	engineered mutation	UNP P53396
B	1026	ALA	ASP	engineered mutation	UNP P53396
C	1026	ALA	ASP	engineered mutation	UNP P53396
D	1026	ALA	ASP	engineered mutation	UNP P53396

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	C	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	D	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

- Molecule 3 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			9	4	5	
3	A	1	Total	C	O	0
			9	4	5	
3	C	1	Total	C	O	0
			9	4	5	
3	D	1	Total	C	O	0
			9	4	5	

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

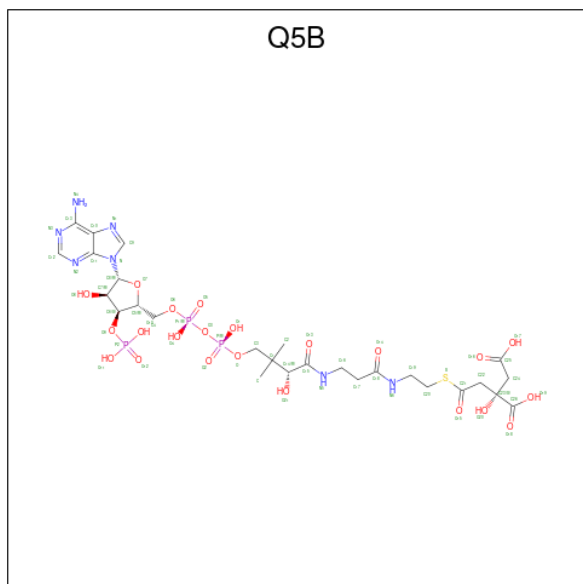
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	C	0
			1	1	

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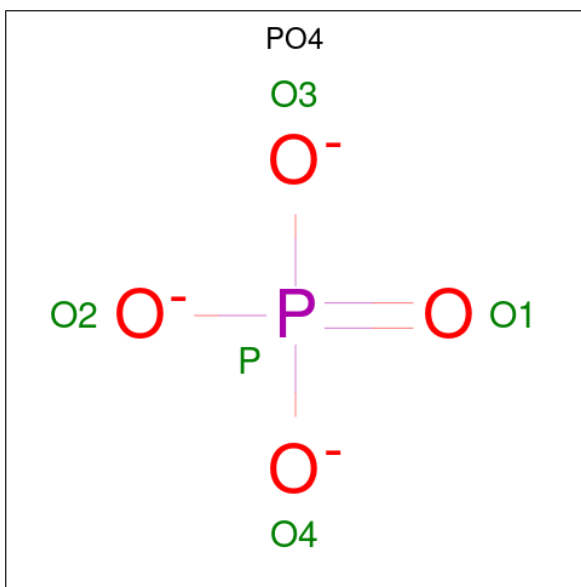
Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	C	0
			1	1	

- Molecule 5 is (3S)-citryl-Coenzyme A (CCD ID: Q5B) (formula: $C_{27}H_{42}N_7O_{22}P_3S$).



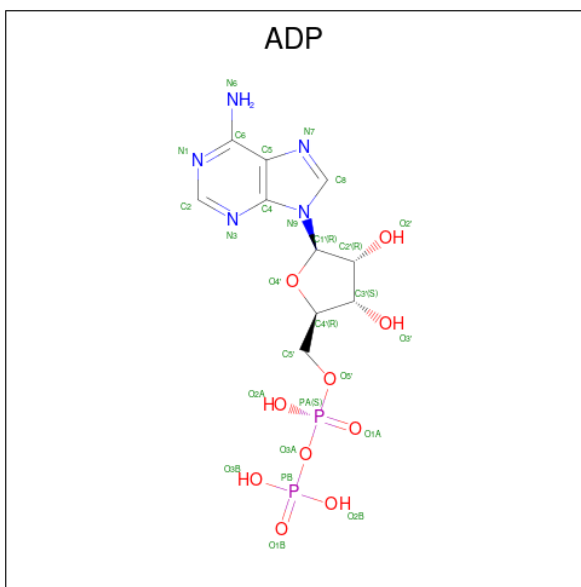
Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
5	C	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
5	D	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	O	P	0
			5	4	1	
6	C	1	Total	O	P	0
			5	4	1	
6	D	1	Total	O	P	0
			5	4	1	

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

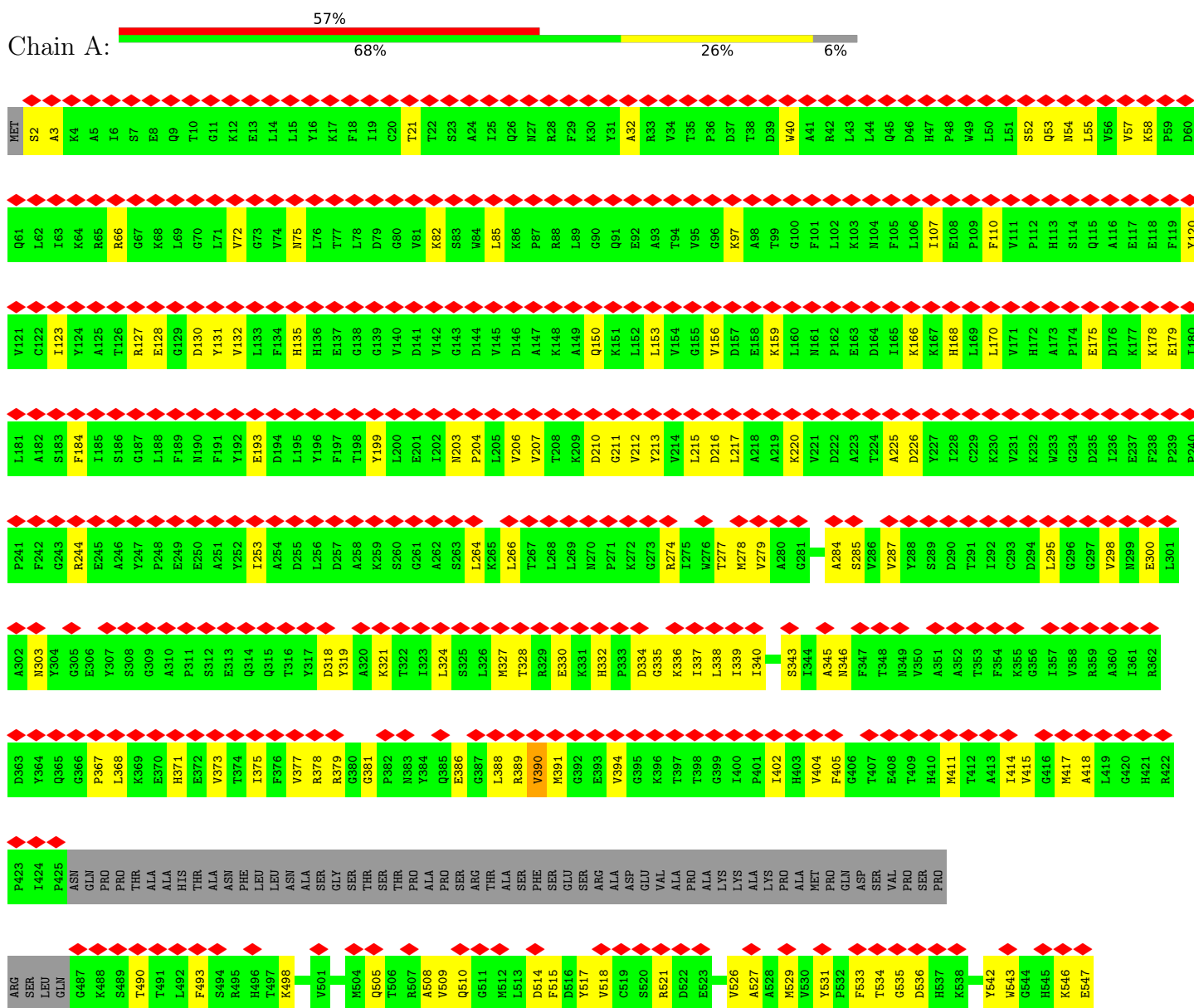
- Molecule 8 is water.

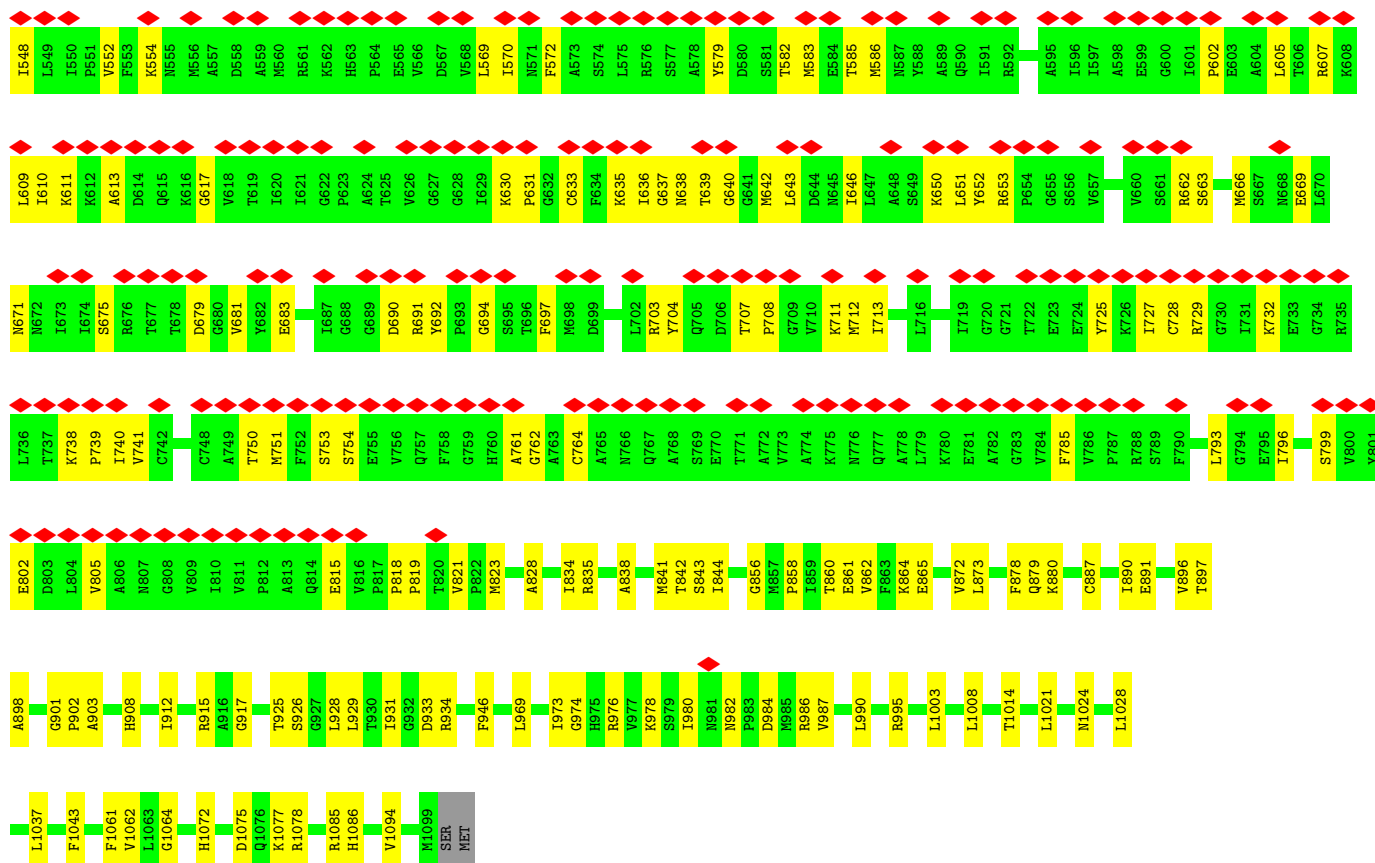
Mol	Chain	Residues	Atoms		AltConf
8	A	23	Total	O	0
			23	23	
8	B	18	Total	O	0
			18	18	
8	C	29	Total	O	0
			29	29	
8	D	20	Total	O	0
			20	20	

3 Residue-property plots

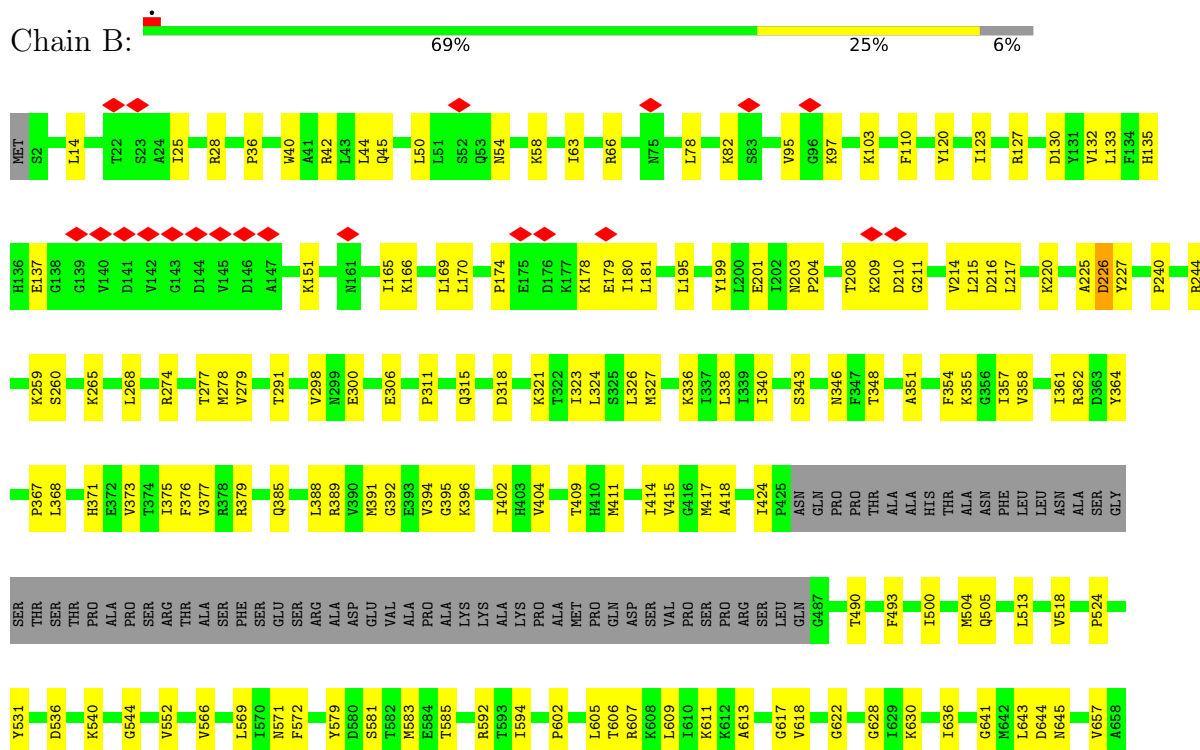
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP-citrate synthase



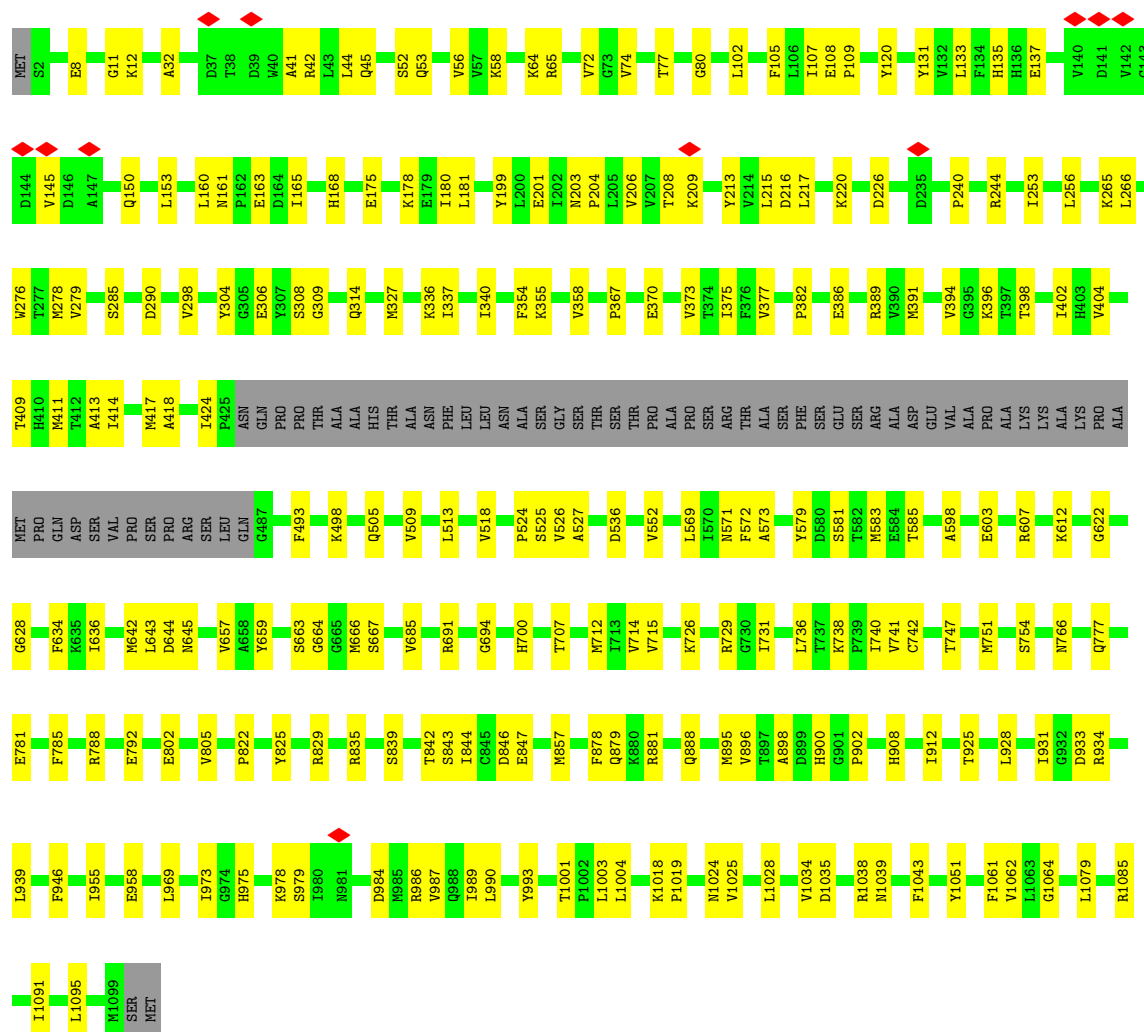


• Molecule 1: ATP-citrate synthase

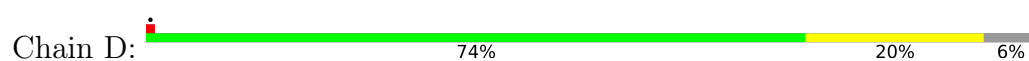




• Molecule 1: ATP-citrate synthase



• Molecule 1: ATP-citrate synthase



L1003	K864	R691	F493	PRO	L264	H135	MET
S1016	V872	Y692	Q505	PRO	K265	G139	S2
P1019	F878	S695	V509	ALA	L268	V140	Q9
N1020	Q879	H700	M512	HIS	T277	D141	E13
L1021	K880	P708	L513	THR	M278	V142	L14
N1024	R881	T707	D516	ALA	V279	D143	I25
V1025	Q888	P708	Y517	ASN	PHE	G144	Q26
A1026	Q888	K711	V518	THR	LEU	V145	N27
G1027	E891	M712	V518	ALA	LEU	D146	R28
L1028	M895	I713	P524	ASN	ALA	A147	F29
V1034	V896	V714	S525	ALA	N303	L153	K30
D1035	T897	E718	M529	SER	GLY	V156	Y31
R1038	A898	C728	F553	THR	E306	I165	A32
N1039	P902	I731	K562	SER	THR	K166	R33
F1043	H908	K732	D567	THR	S325	K167	V34
V1062	I912	R735	V568	ALA	L324	H168	L44
L1063	R915	L736	L569	ALA	S325	M327	Q53
G1064	A916	K738	F572	PRO	L338	L170	N54
H1072	G917	V741	T585	ARG	I339	P174	L55
D1075	T925	M751	M586	THR	I340	K178	K58
Q1076	L928	F752	E599	ALA	S343	E179	P59
K1077	F946	S754	K611	PHE	F354	D194	R66
I1091	M953	H760	K612	GLU	V358	Y199	V72
V1094	I970	F785	G628	SER	P367	N203	N75
H1098	M971	R788	F634	ARG	L368	L205	L78
N1099	G974	E792	K635	ASP	V206	V207	D79
SER	R975	L793	I636	GLU	T208	K209	L89
MET	V977	L793	G637	VAL	R377	Y213	Q91
	K978	I797	L643	ALA	R378	V214	K97
	S979	P822	D644	PRO	R379	L215	F101
	N981	R835	N645	ALA	R389	K220	L102
	N982	T842	V657	LYS	V390	N104	K103
	P983	S843	A658	LYS	M391	F105	N104
	D984	I844	Y659	ALA	G392	L106	F105
	M985	E851	R662	LYS	F393	Y227	L107
	R986	M857	S663	PRO	V394	K232	E108
	V987	P858	G664	VAL	G416	P240	P109
	Q988	I859	G665	SER	R422	R244	F110
	I989	T860	M666	ARG	P425	D255	Y120
	L990		S667	SER	ASN	L256	Y131
	Y993		V685	LEU	GLN	D257	L133
				GLN		A258	F134
				G487		K259	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183036	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 ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.003	Depositor
Minimum map value	-1.655	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	182.59999, 182.59999, 182.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: Q5B, UNL, OAA, ACO, PO4, ADP

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	0.11	0/8198	0.30	2/11098 (0.0%)
1	B	0.14	0/8198	0.31	0/11098
1	C	0.12	0/8198	0.30	0/11098
1	D	0.10	0/8198	0.29	0/11098
All	All	0.12	0/32792	0.30	2/44392 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	VAL	CA-C-N	-5.30	111.86	120.72
1	A	390	VAL	C-N-CA	-5.30	111.86	120.72

There are no chirality outliers.

There are no planarity outliers.

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	8017	0	8057	202	0
1	B	8017	0	8057	188	0
1	C	8017	0	8057	150	0
1	D	8017	0	8057	153	0
2	A	51	0	34	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	51	0	34	8	0
2	C	51	0	34	5	0
2	D	51	0	34	17	0
3	A	18	0	4	2	0
3	C	9	0	2	0	0
3	D	9	0	2	1	0
4	B	1	0	0	2	0
4	C	1	0	0	0	0
5	B	60	0	0	0	0
5	C	60	0	0	1	0
5	D	60	0	0	3	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
7	C	27	0	12	0	0
7	D	27	0	12	0	0
8	A	23	0	0	2	0
8	B	18	0	0	0	0
8	C	29	0	0	0	0
8	D	20	0	0	0	0
All	All	32649	0	32396	656	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 10.

The worst 5 of 656 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:D:976:ARG:HD2	2:D:3301:ACO:H2B	1.37	1.06
1:A:1085:ARG:HH11	2:B:2303:ACO:H62A	1.10	0.96
1:C:382:PRO:HA	1:C:642:MET:HE2	1.56	0.86
1:B:925:THR:HG23	1:D:925:THR:HG23	1.60	0.83
1:A:1085:ARG:NH1	2:B:2303:ACO:H62A	1.81	0.78

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1035/1101 (94%)	992 (96%)	43 (4%)	0	100	100
1	B	1035/1101 (94%)	999 (96%)	36 (4%)	0	100	100
1	C	1035/1101 (94%)	1003 (97%)	32 (3%)	0	100	100
1	D	1035/1101 (94%)	1007 (97%)	28 (3%)	0	100	100
All	All	4140/4404 (94%)	4001 (97%)	139 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	852/908 (94%)	850 (100%)	2 (0%)	87	96
1	B	852/908 (94%)	850 (100%)	2 (0%)	87	96
1	C	852/908 (94%)	850 (100%)	2 (0%)	87	96
1	D	852/908 (94%)	850 (100%)	2 (0%)	87	96
All	All	3408/3632 (94%)	3400 (100%)	8 (0%)	87	96

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	226[B]	ASP
1	D	226[A]	ASP
1	C	226[A]	ASP

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Mol	Chain	Res	Type
1	B	226[B]	ASP
1	C	226[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	383	ASN
1	D	777	GLN
1	C	638	ASN
1	D	1024	ASN
1	D	421	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are unknown - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	Q5B	B	2302	-	60,62,62	2.87	20 (33%)	87,93,93	1.85	19 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OAA	A	1203	-	8,8,8	1.36	1 (12%)	8,10,10	1.40	1 (12%)
2	ACO	D	3301	-	51,53,53	1.12	4 (7%)	73,79,79	1.50	8 (10%)
2	ACO	C	3301	-	51,53,53	1.11	5 (9%)	73,79,79	1.51	12 (16%)
3	OAA	A	1202	-	8,8,8	1.34	1 (12%)	8,10,10	1.42	1 (12%)
2	ACO	B	2303	-	51,53,53	1.13	5 (9%)	73,79,79	1.51	11 (15%)
5	Q5B	D	3303	-	60,62,62	2.91	21 (35%)	87,93,93	1.79	19 (21%)
6	PO4	C	3306	-	4,4,4	0.97	0	6,6,6	0.35	0
3	OAA	D	3302	-	8,8,8	1.37	1 (12%)	8,10,10	1.43	1 (12%)
2	ACO	A	1201	-	51,53,53	1.16	5 (9%)	73,79,79	1.47	11 (15%)
7	ADP	C	3303	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
6	PO4	D	3305	-	4,4,4	0.96	0	6,6,6	0.45	0
7	ADP	D	3304	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
5	Q5B	C	3305	-	60,62,62	2.87	21 (35%)	87,93,93	1.76	20 (22%)
6	PO4	B	2304	-	4,4,4	0.97	0	6,6,6	0.46	0
3	OAA	C	3302	-	8,8,8	1.35	1 (12%)	8,10,10	1.41	1 (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
5	Q5B	B	2302	-	-	10/66/83/83	0/3/3/3
3	OAA	A	1203	-	-	4/8/8/8	-
2	ACO	D	3301	-	-	15/51/67/67	0/3/3/3
2	ACO	C	3301	-	-	20/51/67/67	0/3/3/3
3	OAA	A	1202	-	-	5/8/8/8	-
2	ACO	B	2303	-	-	13/51/67/67	0/3/3/3
5	Q5B	D	3303	-	-	21/66/83/83	0/3/3/3
7	ADP	C	3303	-	-	4/16/32/32	0/3/3/3
3	OAA	D	3302	-	-	6/8/8/8	-
2	ACO	A	1201	-	-	12/51/67/67	0/3/3/3
7	ADP	D	3304	-	-	5/16/32/32	0/3/3/3
5	Q5B	C	3305	-	-	15/66/83/83	0/3/3/3
3	OAA	C	3302	-	-	6/8/8/8	-

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3303	Q5B	P1-O3	8.54	1.68	1.59
5	C	3305	Q5B	P1-O3	8.26	1.68	1.59
5	D	3303	Q5B	C6-C5	-8.20	1.31	1.52
5	B	2302	Q5B	C6-C5	-8.17	1.31	1.52
5	B	2302	Q5B	P1-O3	8.12	1.68	1.59

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	3303	ADP	C5-C4-N3	-5.98	118.48	126.72
7	D	3304	ADP	C5-C4-N3	-5.87	118.64	126.72
2	D	3301	ACO	C5A-C4A-N3A	-5.84	118.68	126.72
2	A	1201	ACO	C5A-C4A-N3A	-5.68	118.89	126.72
2	B	2303	ACO	C5A-C4A-N3A	-5.56	119.06	126.72

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ACO	CCP-O6A-P2A-O3A
2	A	1201	ACO	CCP-O6A-P2A-O4A
2	A	1201	ACO	CCP-O6A-P2A-O5A
2	A	1201	ACO	C6P-C5P-N4P-C3P
2	A	1201	ACO	O-C-S1P-C2P

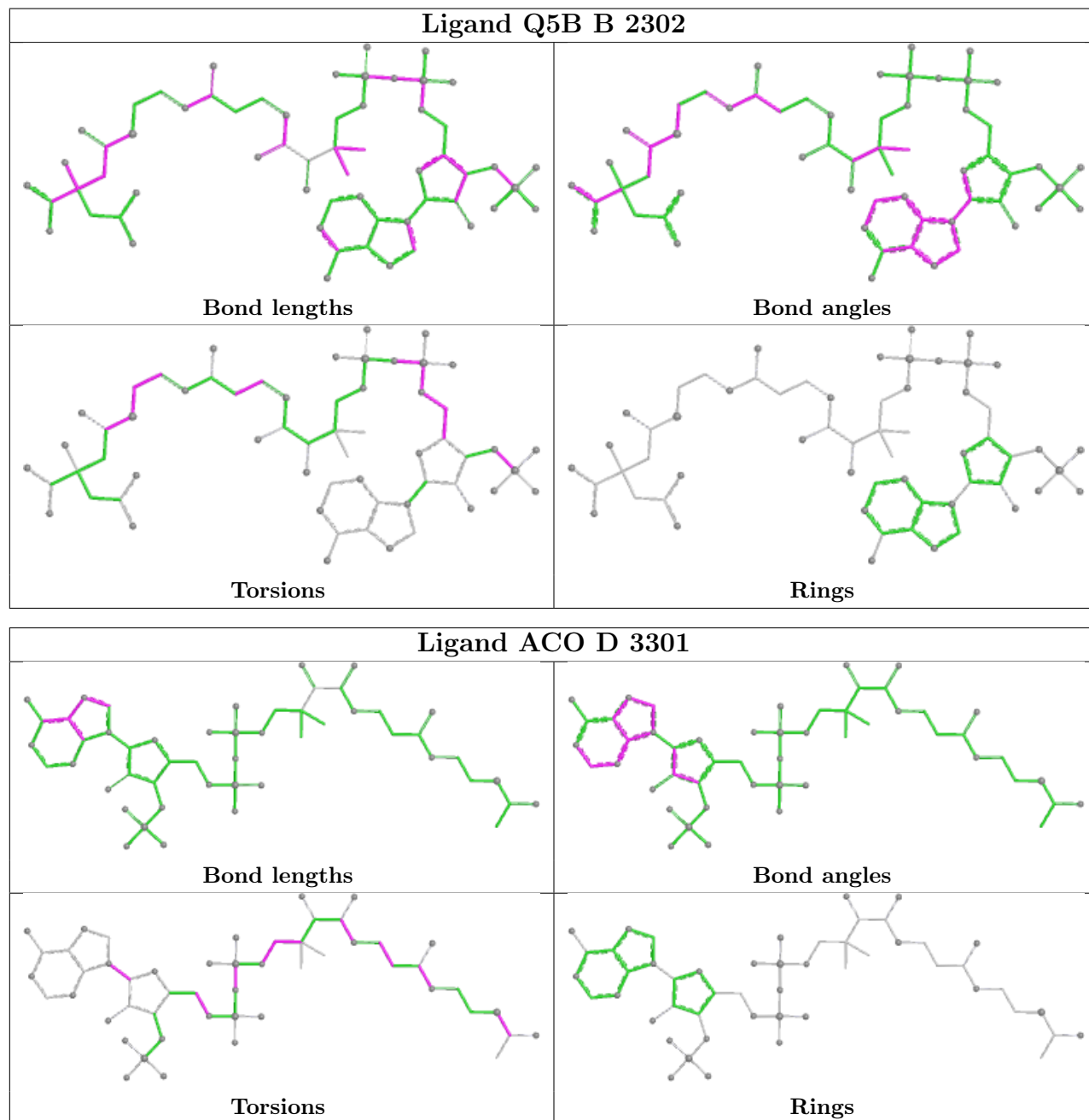
There are no ring outliers.

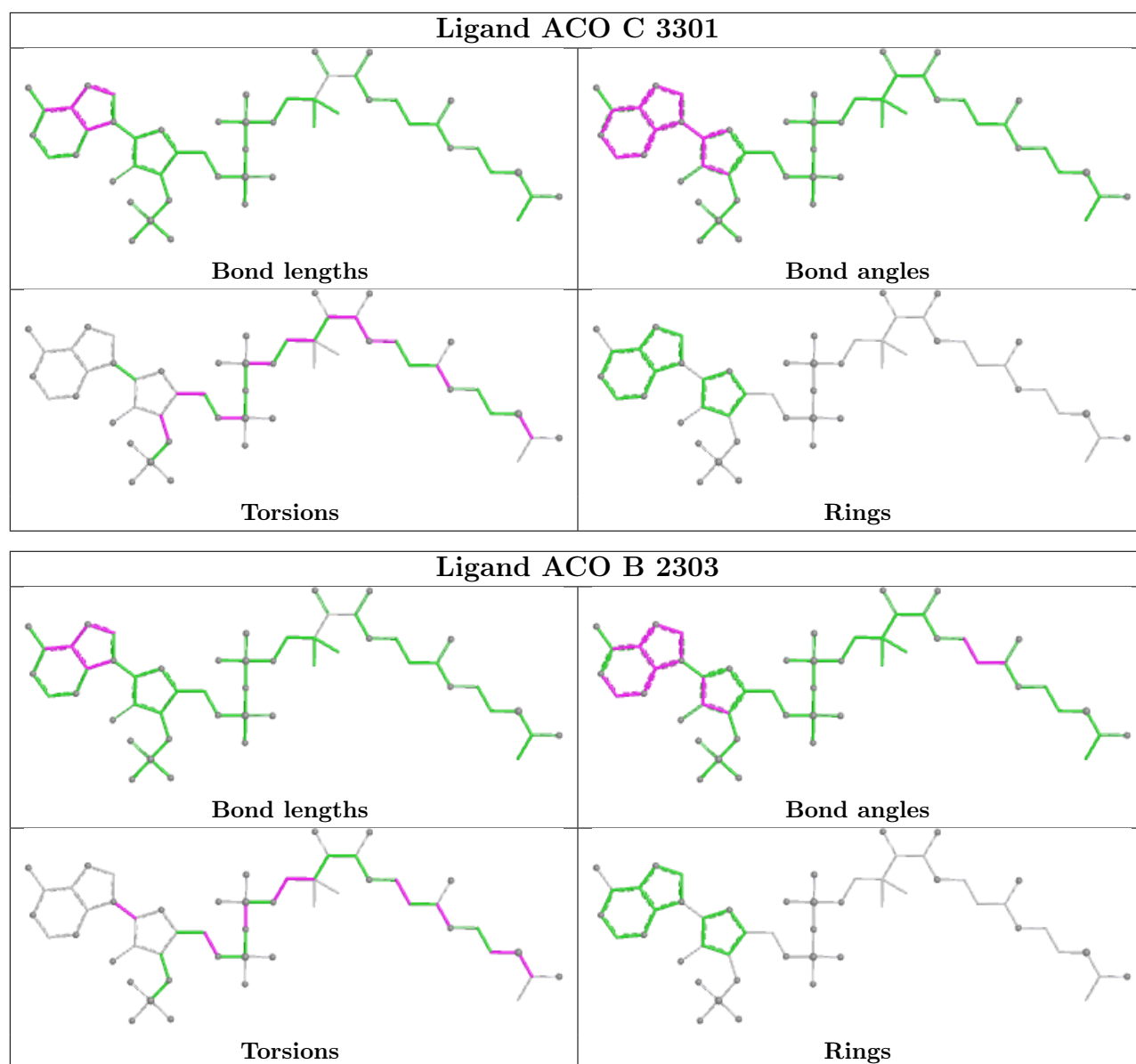
10 monomers are involved in 45 short contacts:

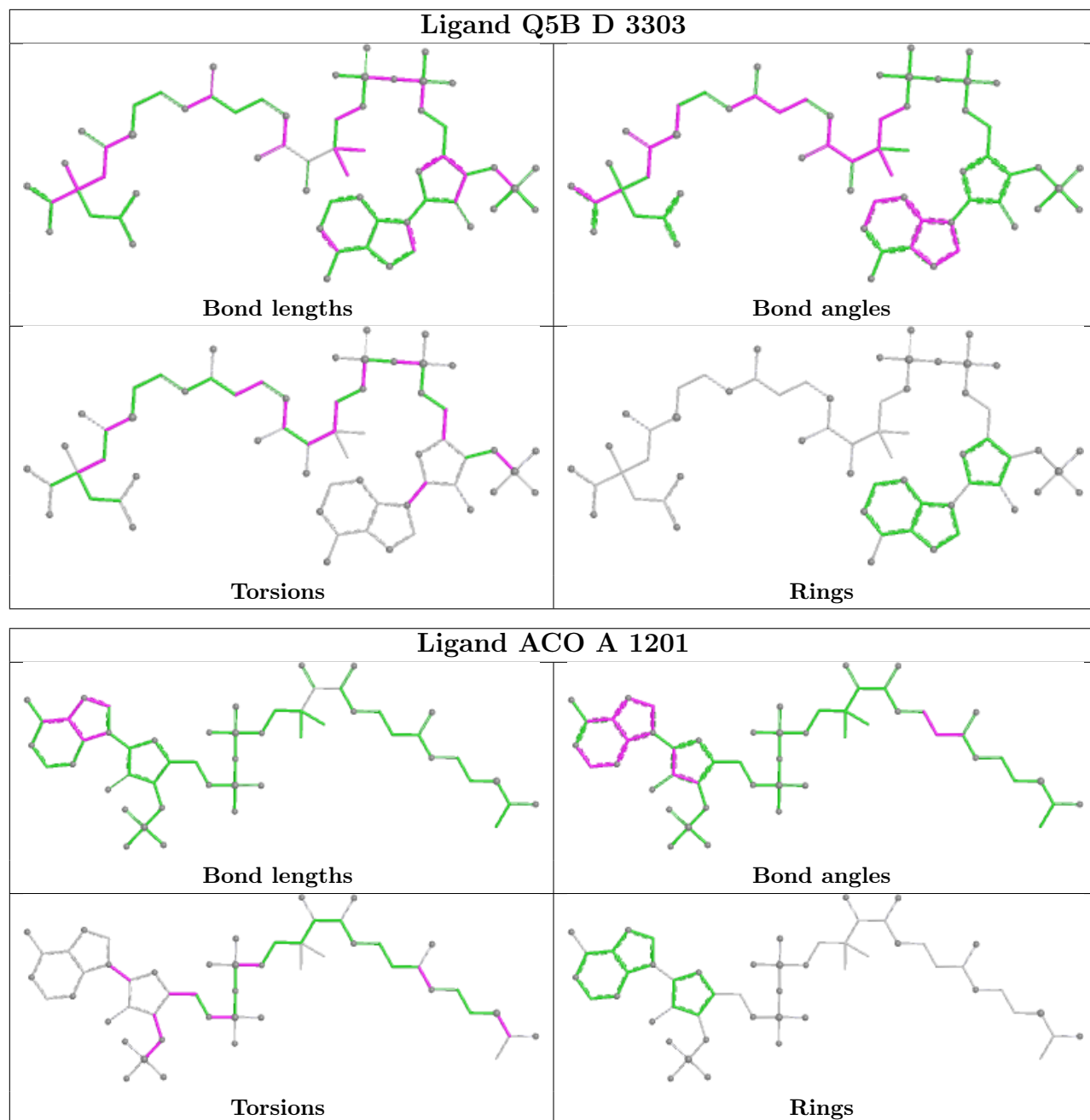
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1203	OAA	1	0
2	D	3301	ACO	17	0
2	C	3301	ACO	5	0
3	A	1202	OAA	1	0
2	B	2303	ACO	8	0
5	D	3303	Q5B	3	0
3	D	3302	OAA	1	0
2	A	1201	ACO	9	0
6	D	3305	PO4	1	0
5	C	3305	Q5B	1	0

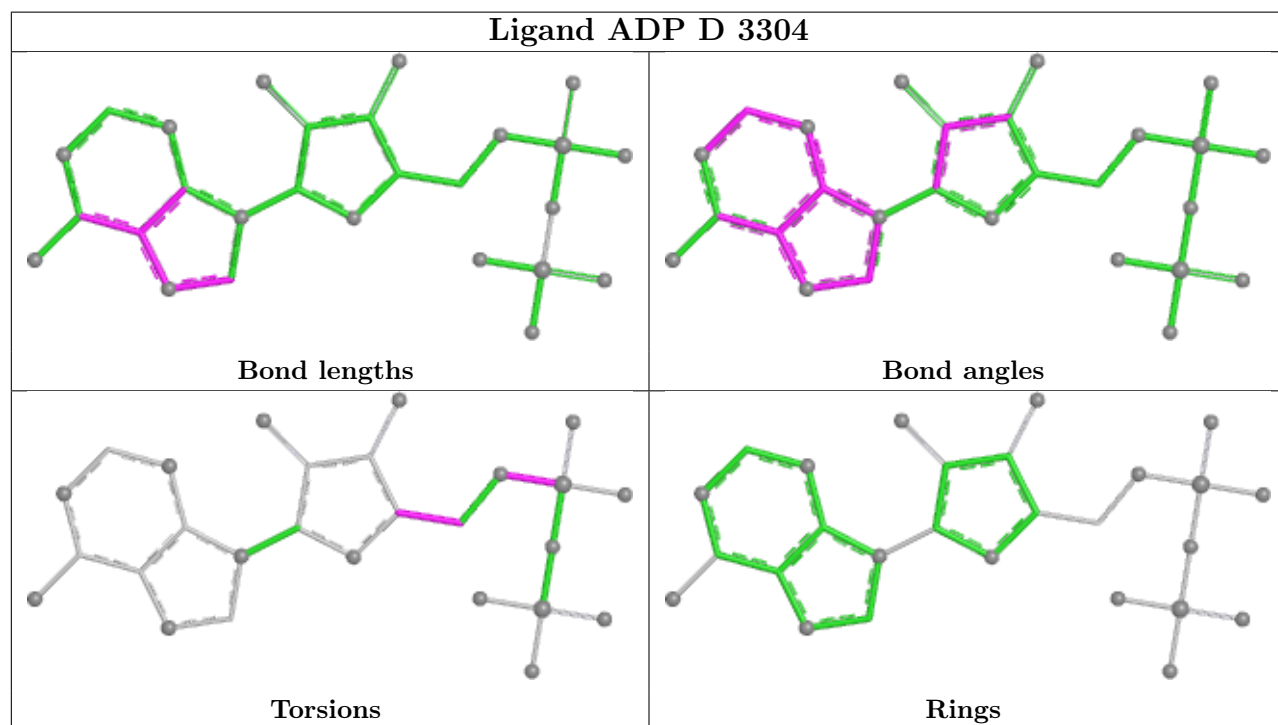
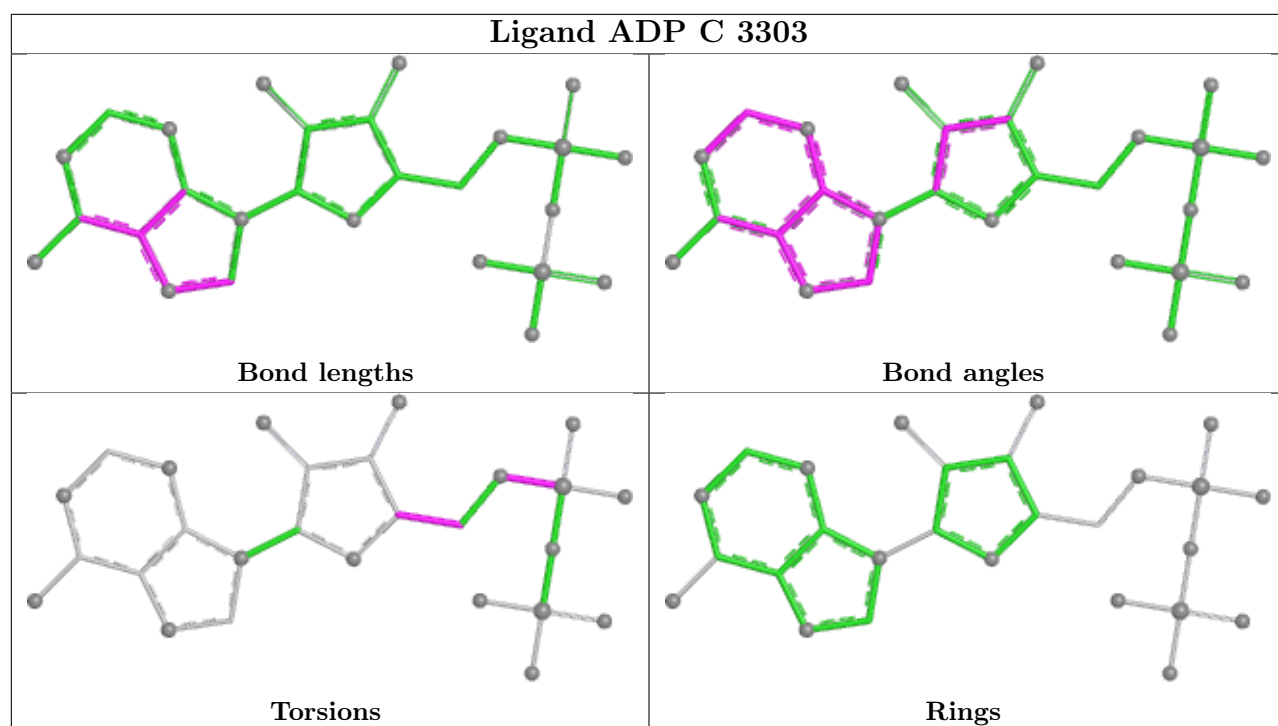
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

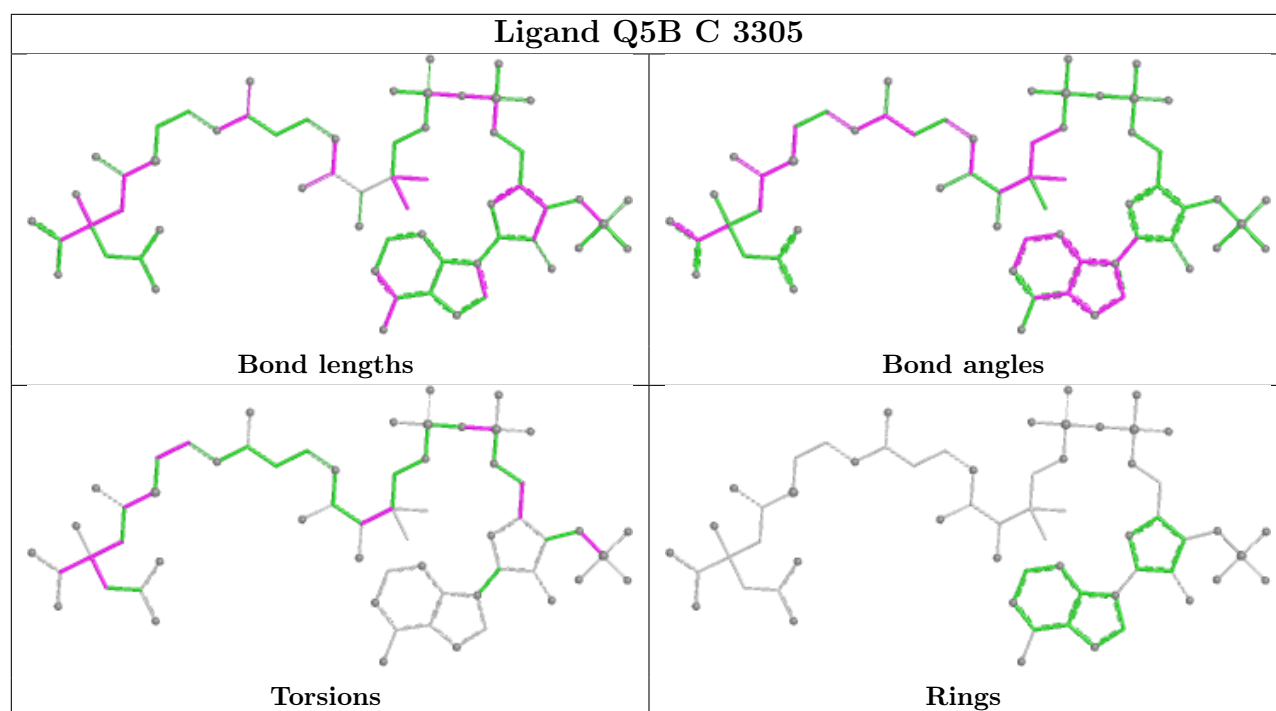
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

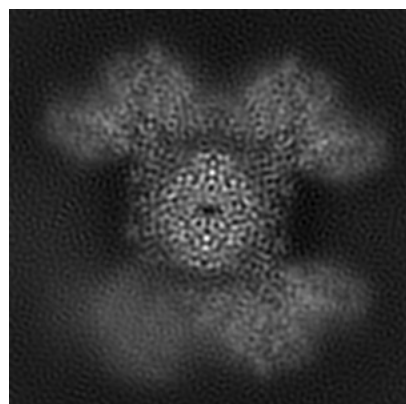
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29668. These allow visual inspection of the internal detail of the map and identification of artifacts.

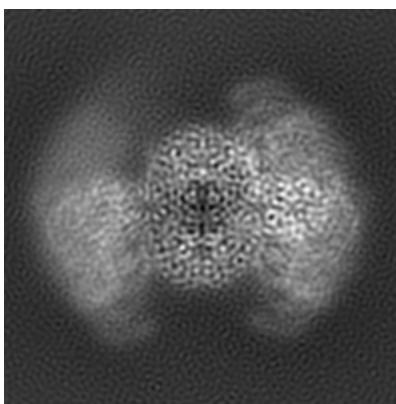
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

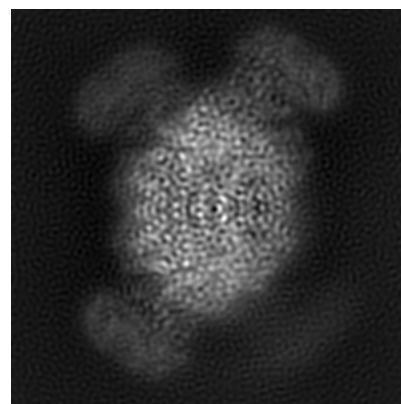
6.1.1 Primary map



X

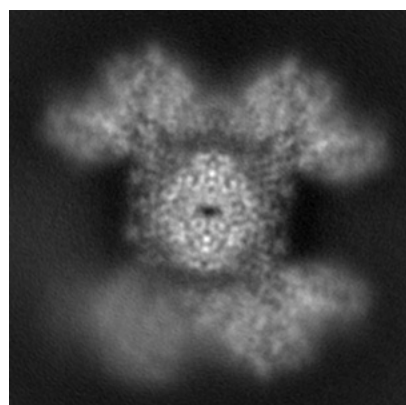


Y

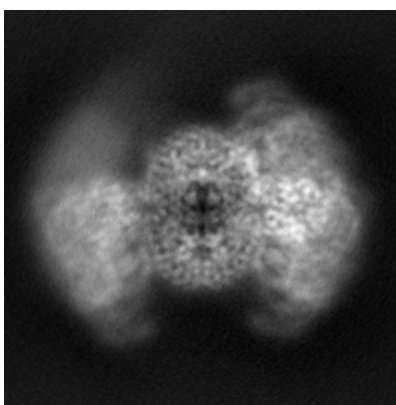


Z

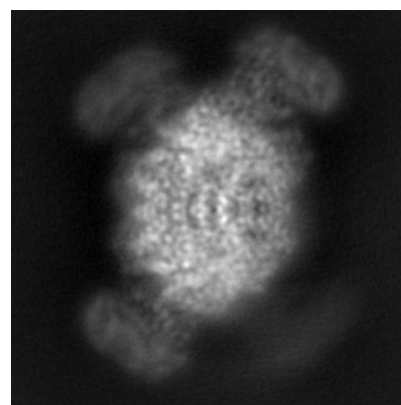
6.1.2 Raw map



X



Y

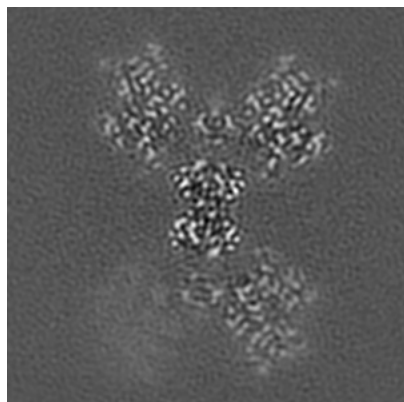


Z

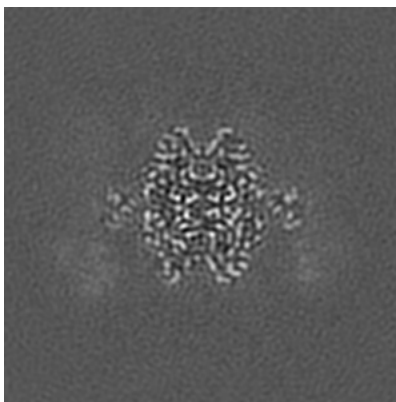
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

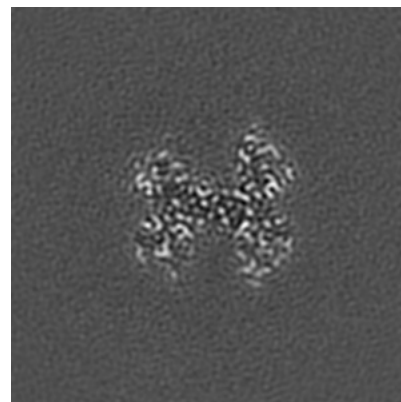
6.2.1 Primary map



X Index: 110

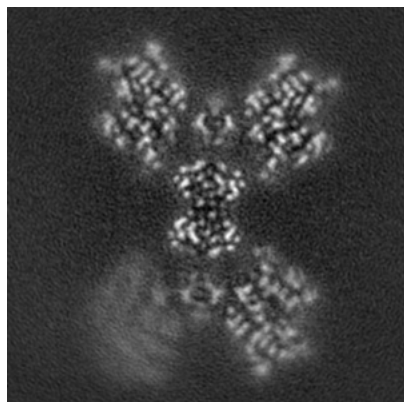


Y Index: 110

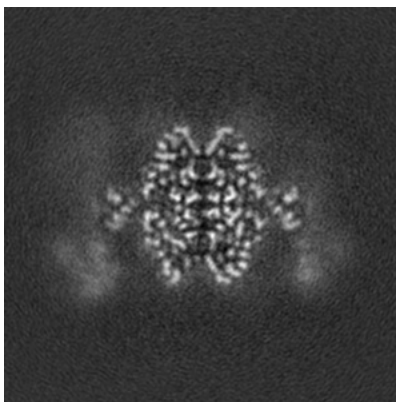


Z Index: 110

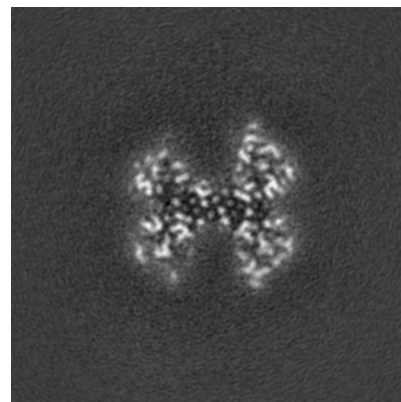
6.2.2 Raw map



X Index: 110



Y Index: 110

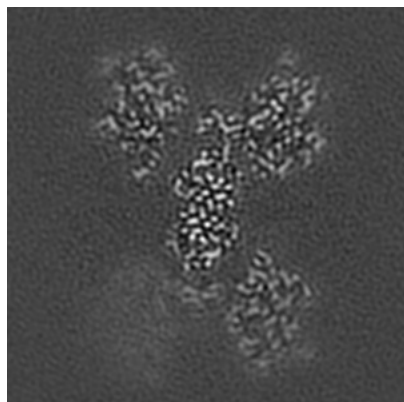


Z Index: 110

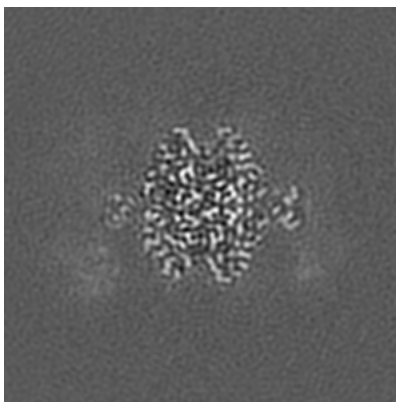
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

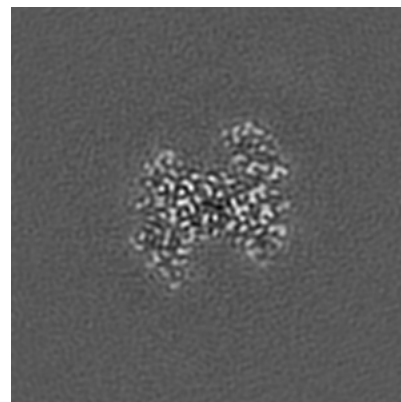
6.3.1 Primary map



X Index: 105

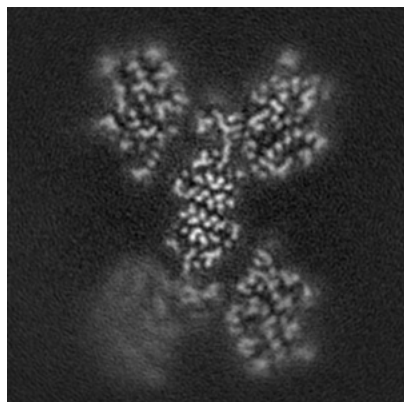


Y Index: 111

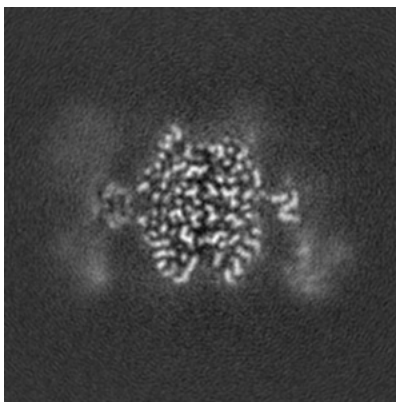


Z Index: 119

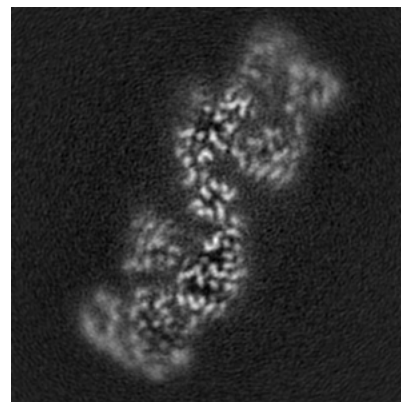
6.3.2 Raw map



X Index: 105



Y Index: 106

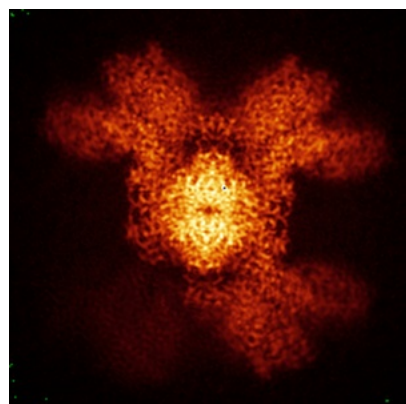


Z Index: 154

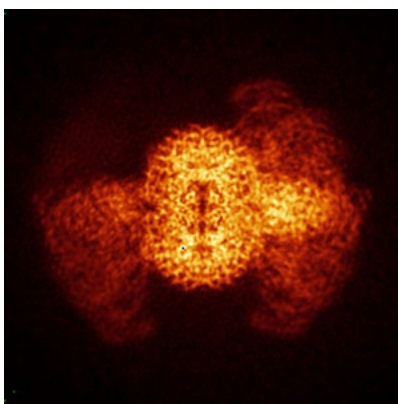
The images above show the largest variance slices of the map in three orthogonal directions.

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

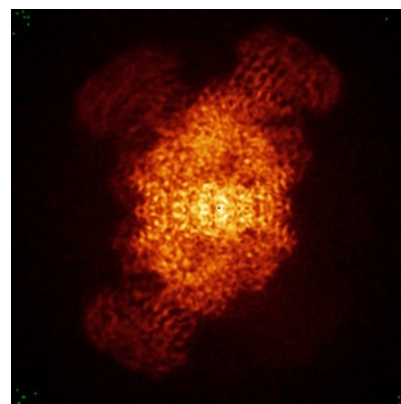
6.4.1 Primary map



X

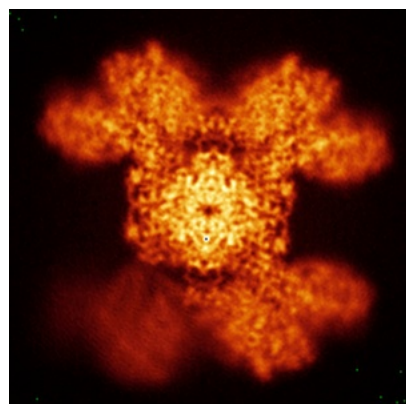


Y

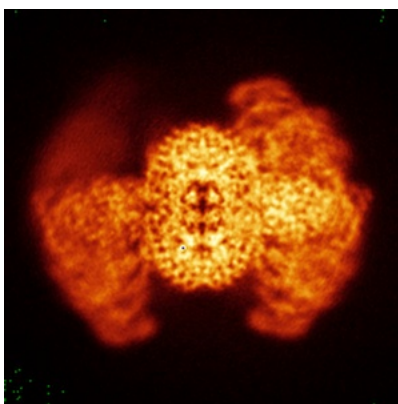


Z

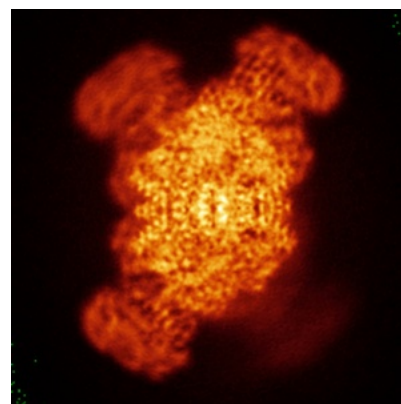
6.4.2 Raw map



X



Y

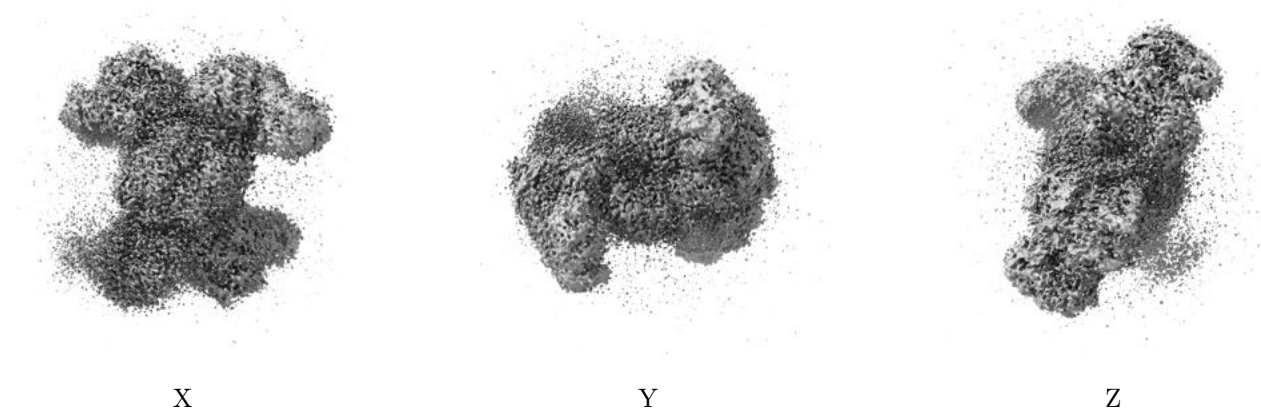


Z

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.

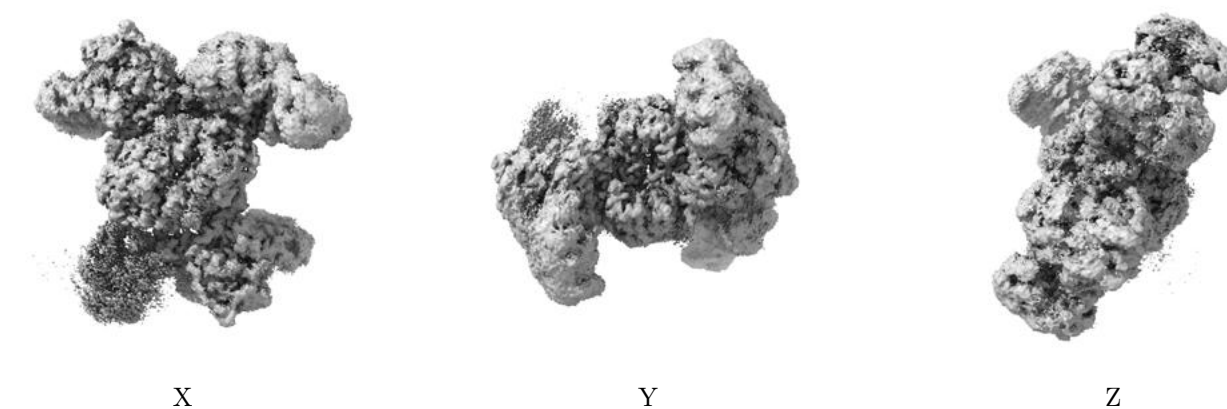
6.5 Orthogonal surface views [i](#)

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.

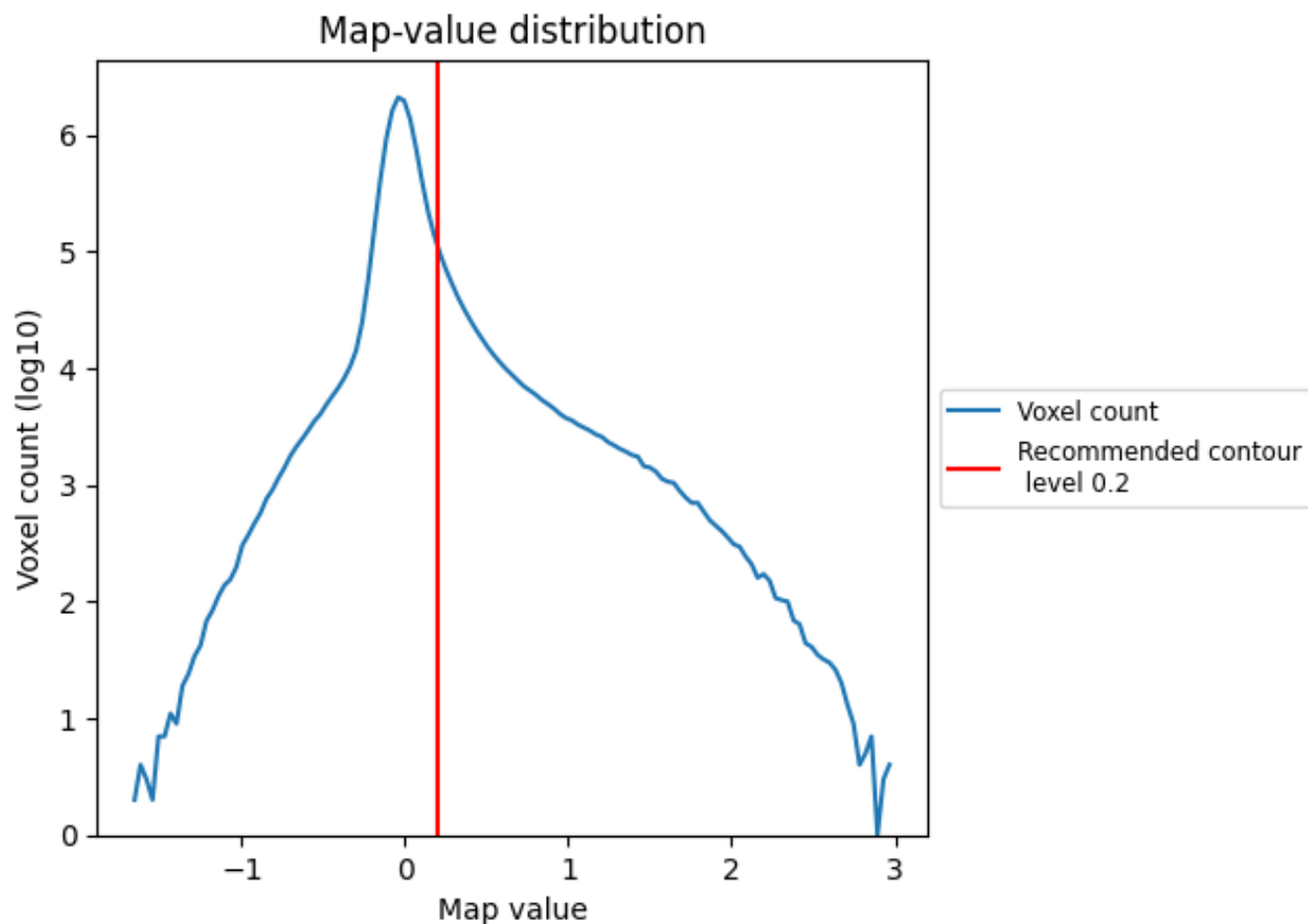
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

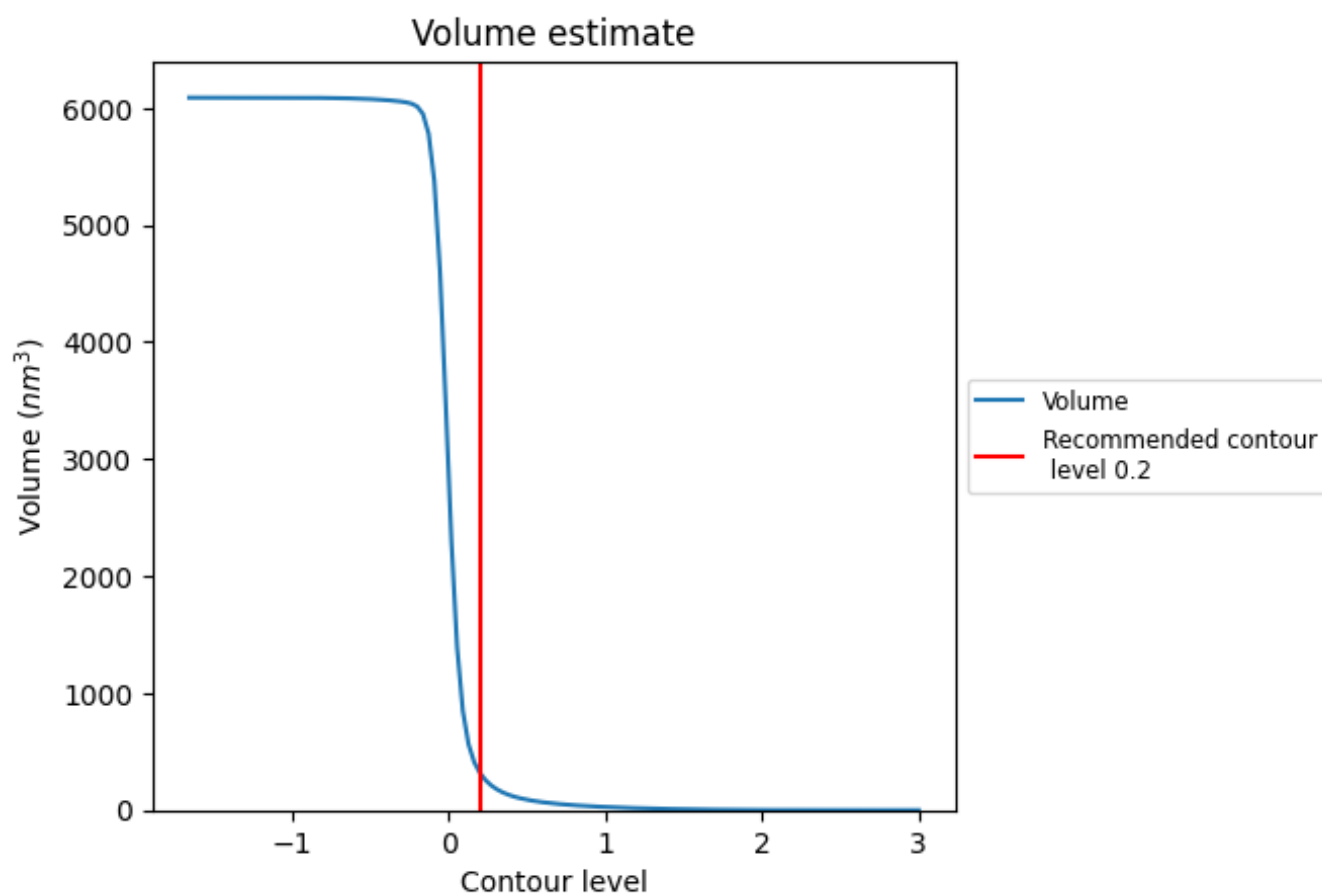
This section contains the results of statistical analysis of the map.

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.

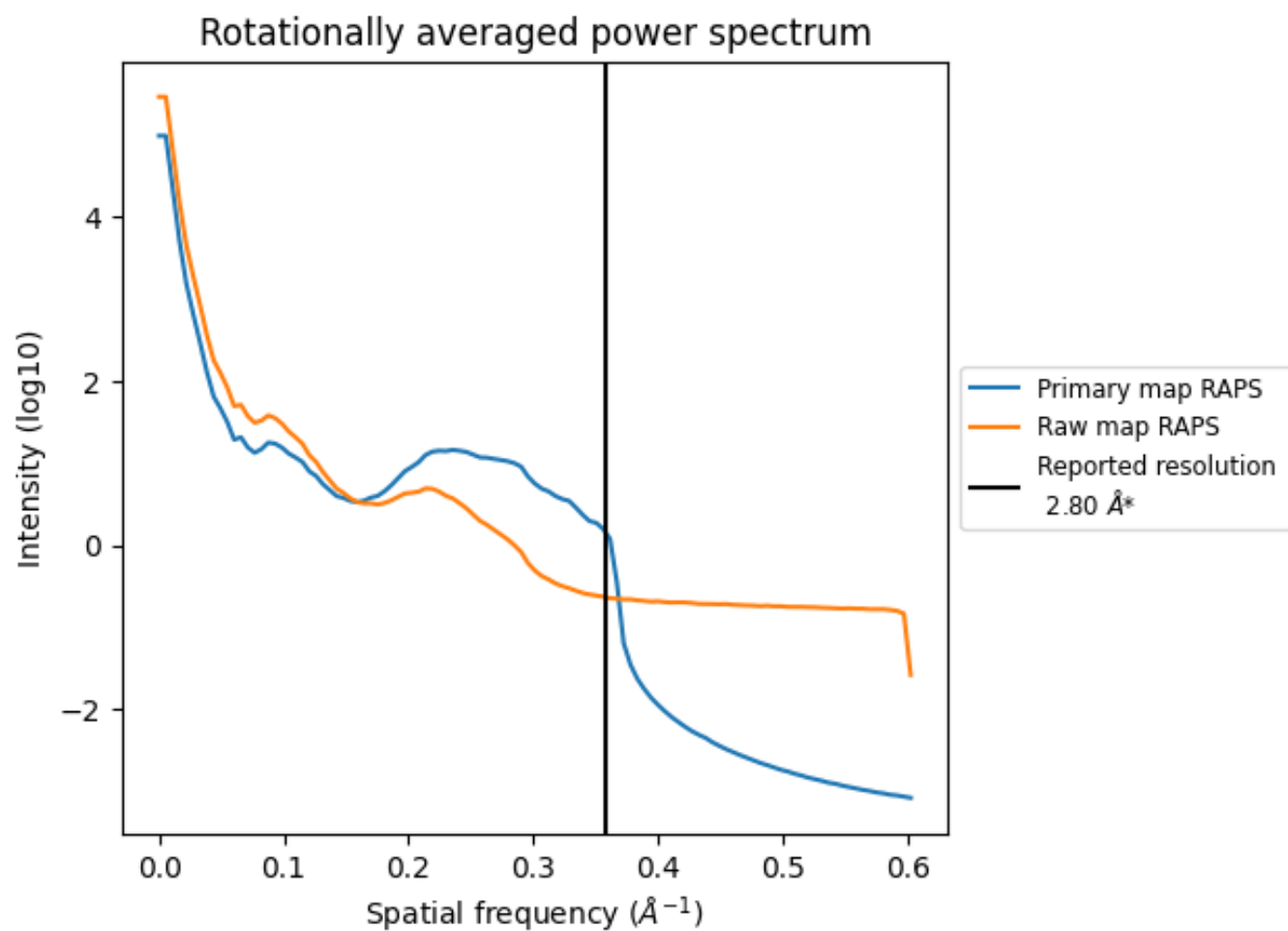
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm³; this corresponds to an approximate mass of 289 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 ⓘ

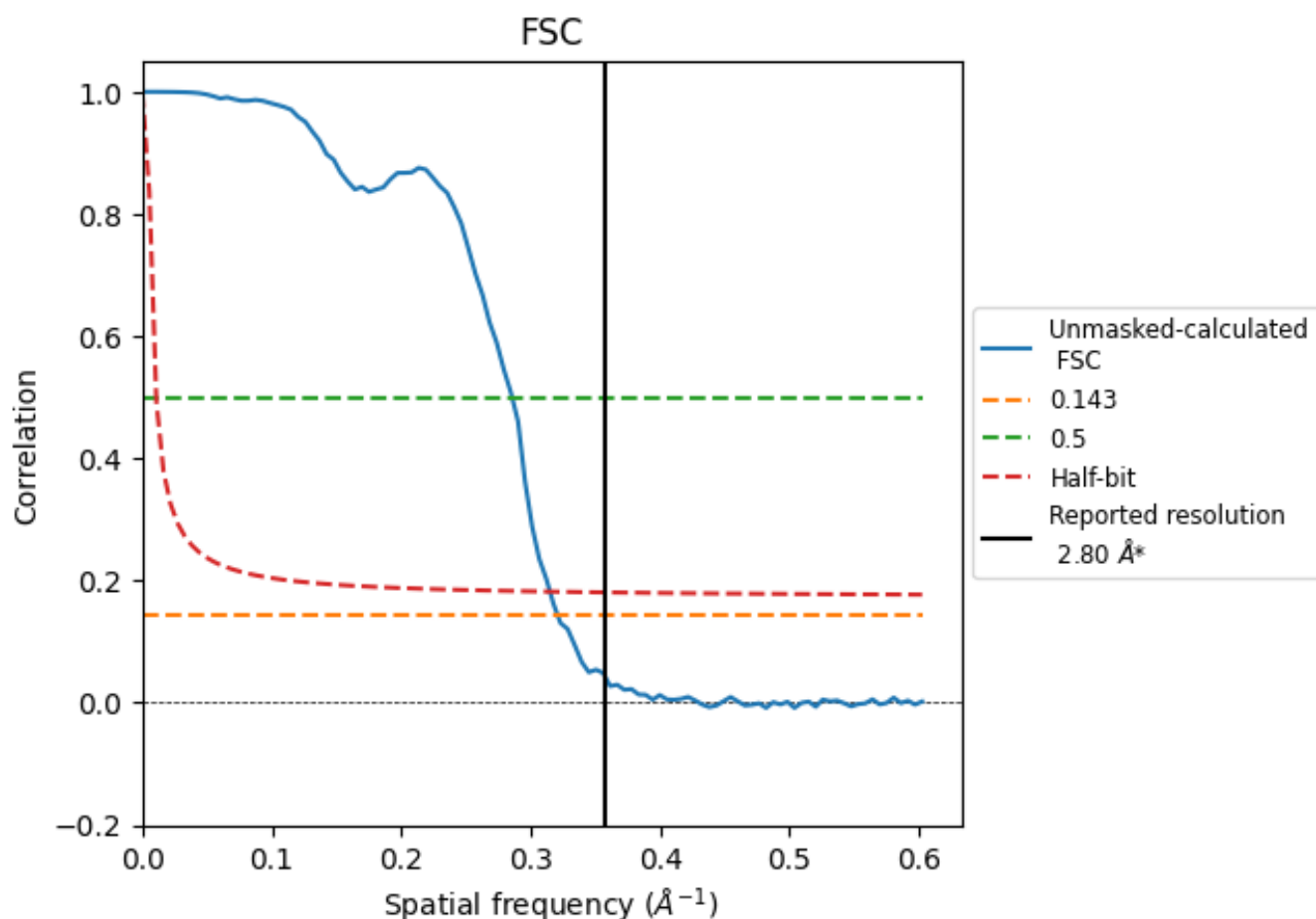


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

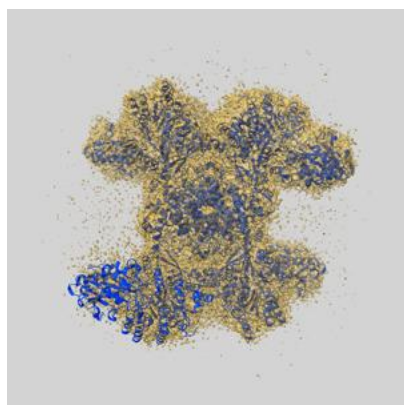
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.50	3.18

*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 3.12 differs from the reported value 2.8 by more than 10 %

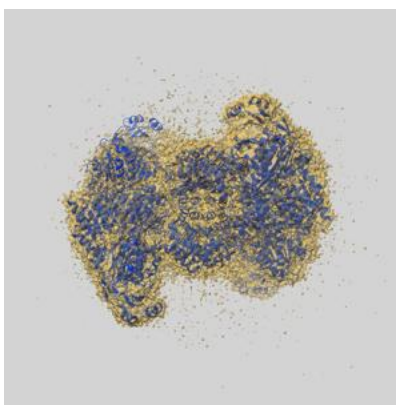
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29668 and PDB model 8G1E. Per-residue inclusion information can be found in section [3](#) on page [9](#).

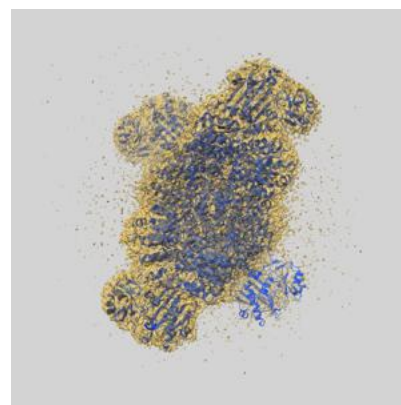
9.1 Map-model overlay [i](#)



X



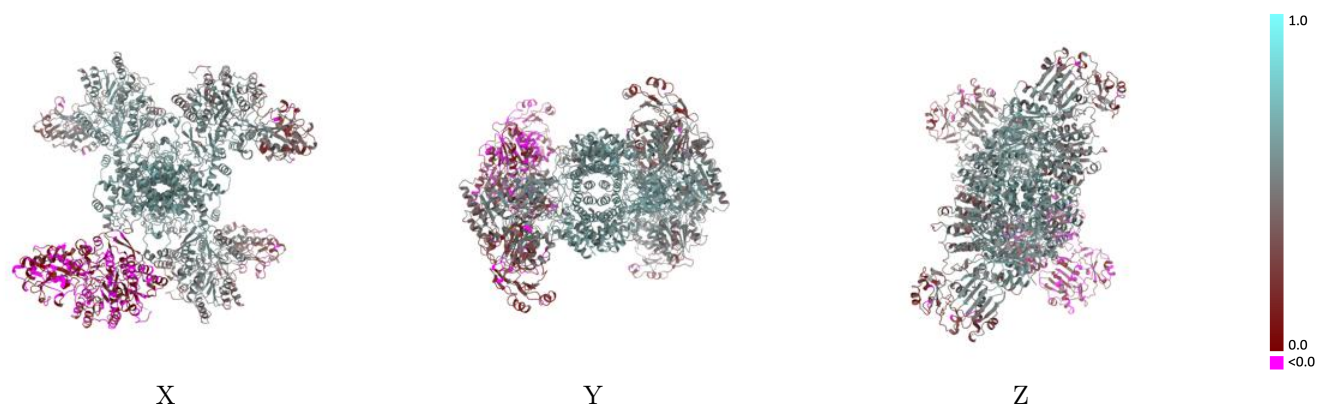
Y



Z

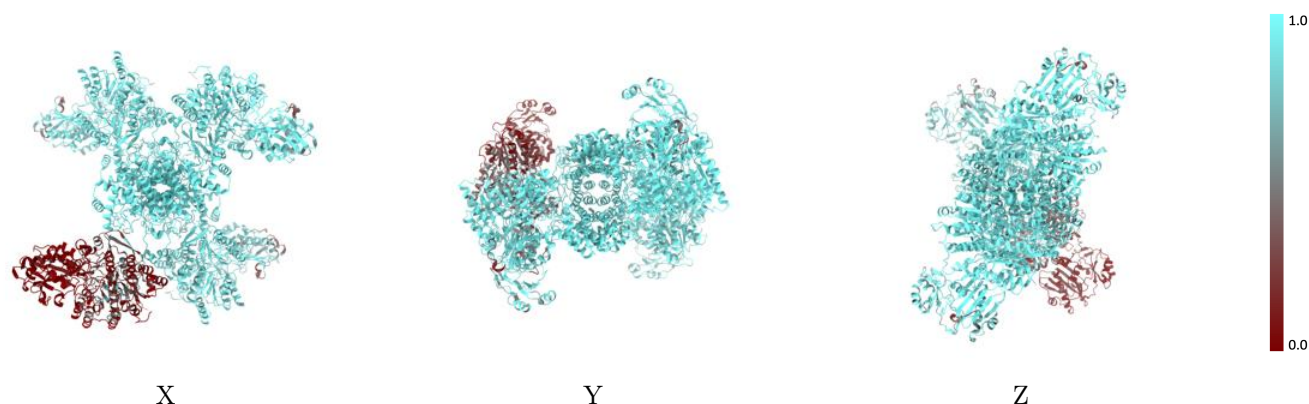
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



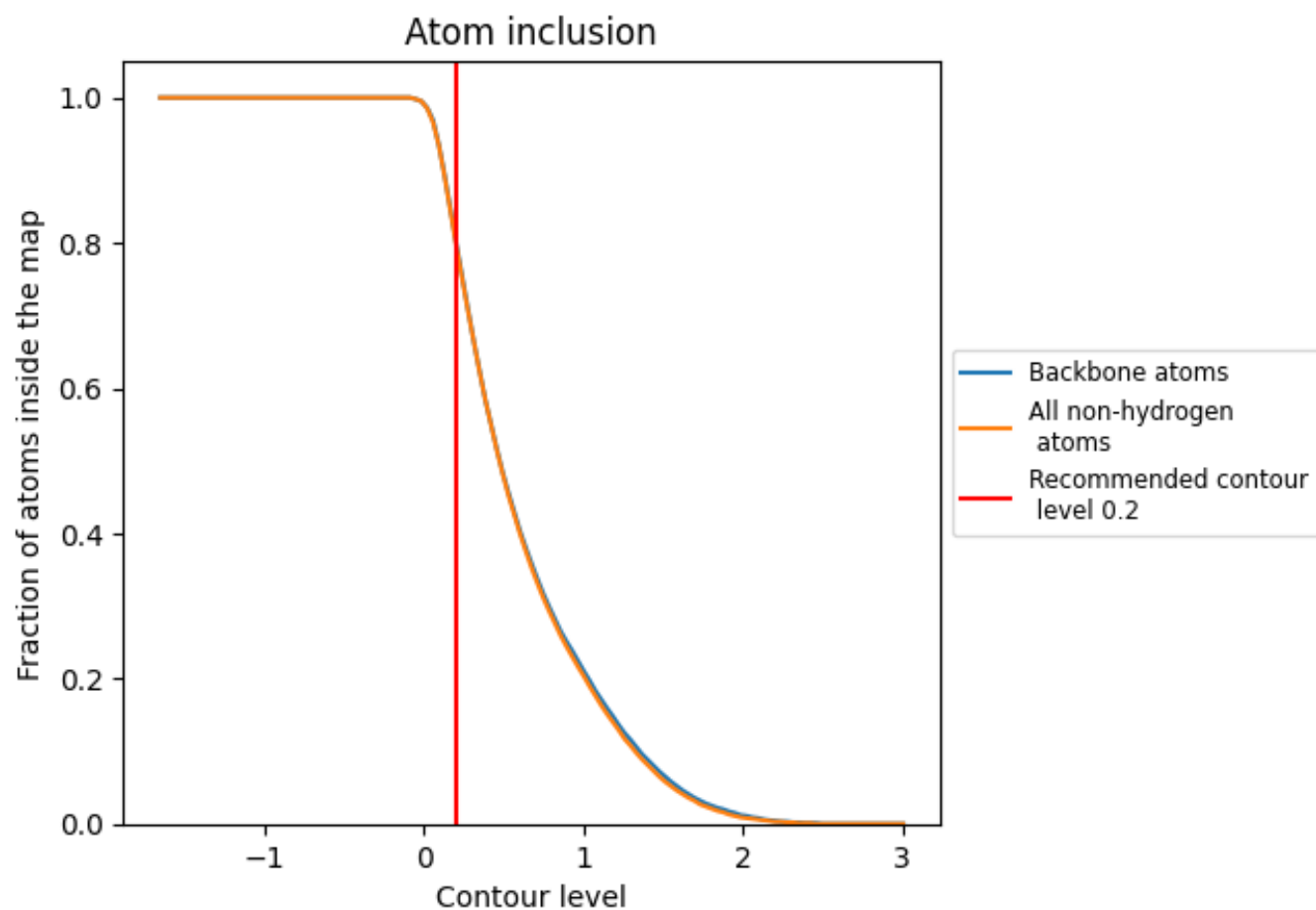
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

Chain	Atom inclusion	Q-score
All	0.7970	0.4240
A	0.4030	0.2090
B	0.9010	0.4570
C	0.9450	0.5150
D	0.9420	0.5120

