



wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 03:43 AM EDT

PDB ID : 7RKZ / pdb_00007rkz
EMDB ID : EMD-24511
Title : Structure of ACLY D1026A-substrates-asym-int
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2021-07-22
Resolution : 2.60 Å(reported)

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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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

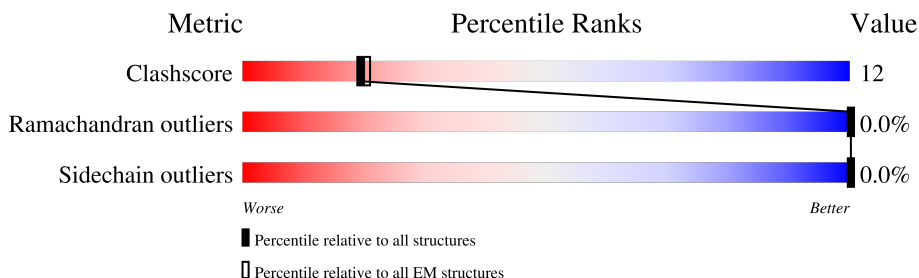
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 32610 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.

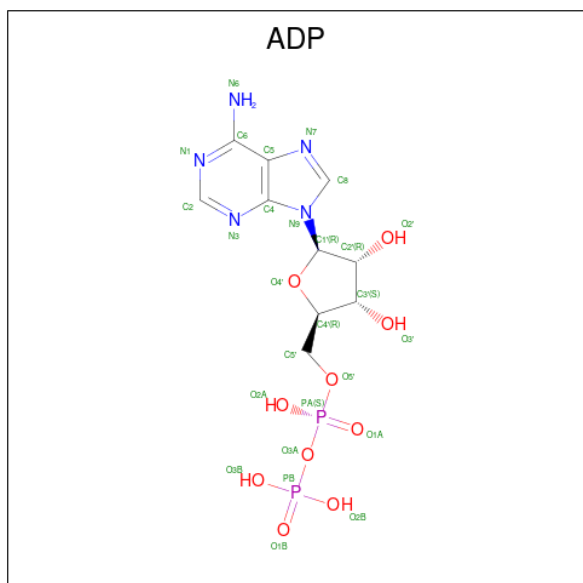
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1032	Total	C	N	O	S	2	0
			7989	5114	1354	1474	47		
1	B	1032	Total	C	N	O	S	2	0
			7989	5114	1354	1474	47		
1	C	1032	Total	C	N	O	S	2	0
			7989	5114	1354	1474	47		
1	D	1030	Total	C	N	O	S	2	0
			7974	5105	1350	1472	47		

There are 4 discrepancies between the modelled and reference sequences:

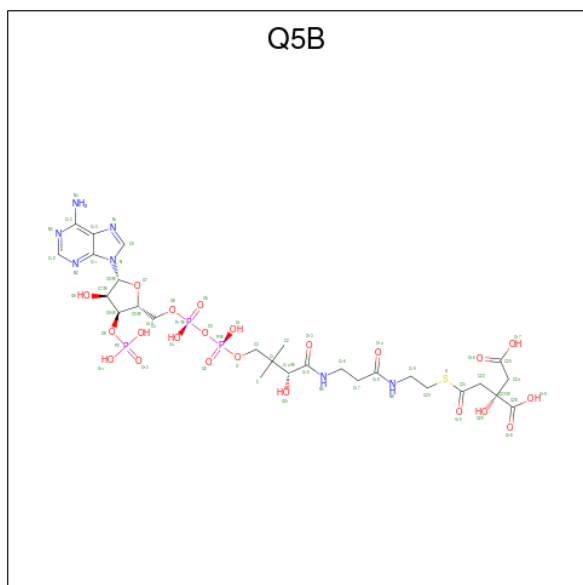
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	ASP	engineered mutation	UNP P53396
B	1026	ALA	ASP	engineered mutation	UNP P53396
C	1026	ALA	ASP	engineered mutation	UNP P53396
D	1026	ALA	ASP	engineered mutation	UNP P53396

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is (3S)-citryl-Coenzyme A (CCD ID: Q5B) (formula: $C_{27}H_{42}N_7O_{22}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).

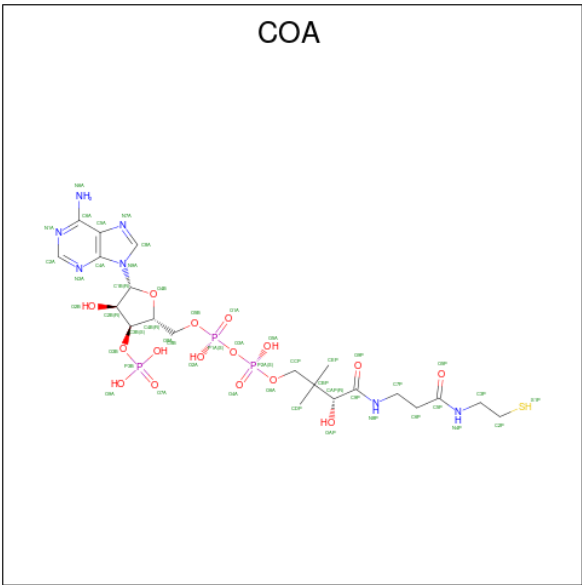


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			13	6	7	
4	B	1	Total	C	O	0
			13	6	7	
4	C	1	Total	C	O	0
			13	6	7	
4	D	1	Total	C	O	0
			13	6	7	

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			1	1	
5	C	1	Total	C	0
			1	1	

- Molecule 6 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
6	B	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
6	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
6	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

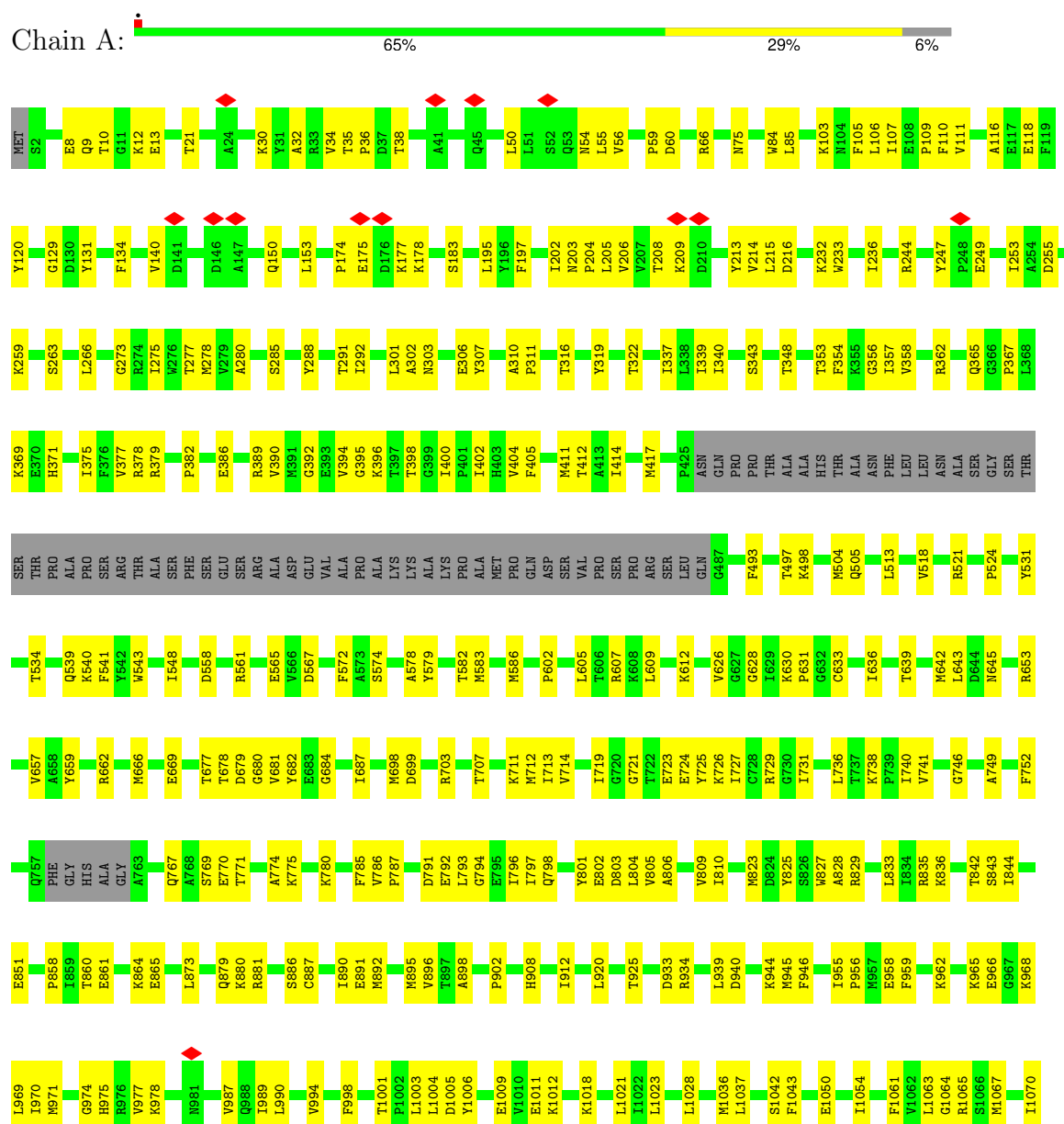
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	35	Total	O	0
			35	35	
7	B	47	Total	O	0
			47	47	
7	C	37	Total	O	0
			37	37	
7	D	43	Total	O	0
			43	43	

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.

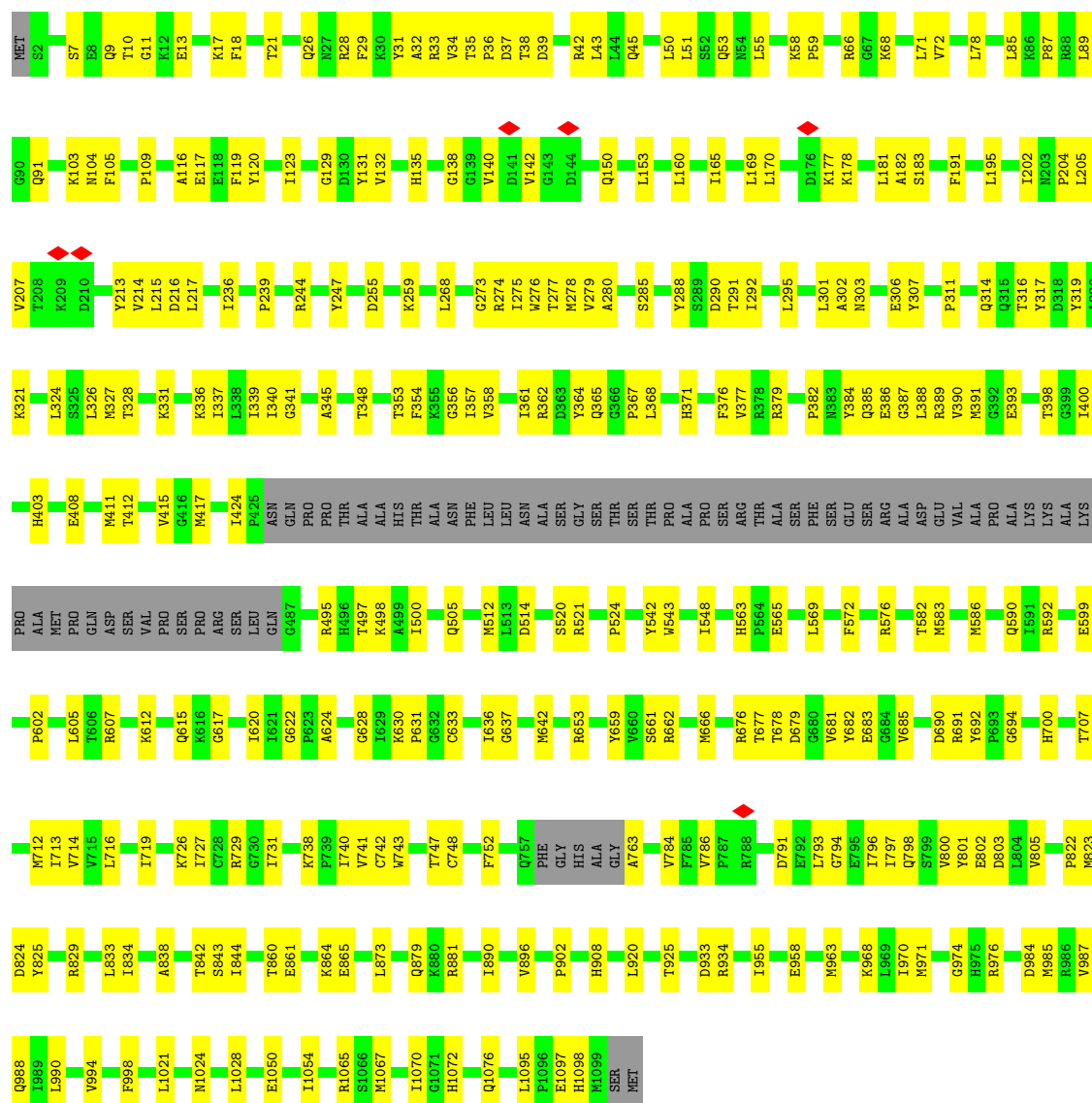
• Molecule 1: ATP-citrate synthase





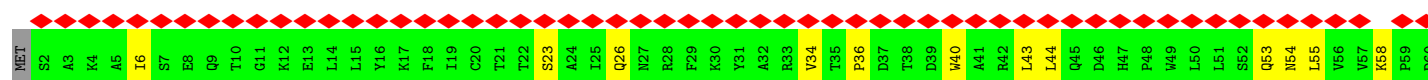
● Molecule 1: ATP-citrate synthase

Chain B: 67% 27% 6%



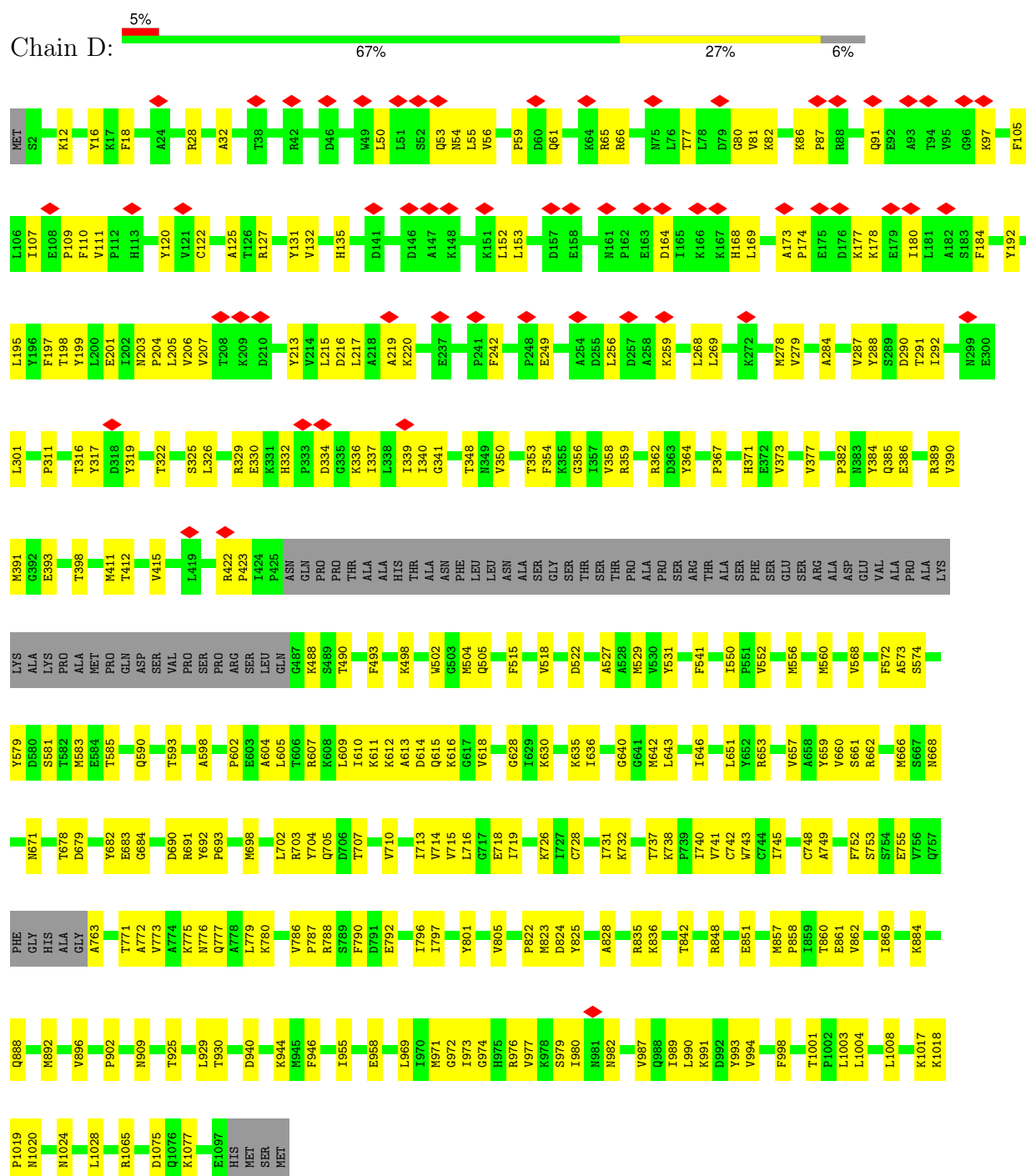
● Molecule 1: ATP-citrate synthase

Chain C: 46% 67% 27% 6%



L1008	E861	F785	V714	I629	H563	K488	PRO	G366	Y304	P241	L181	V121	Q61
I1013	V862	V786	V715	C633	P664	S489	PRO	P367	G305	F242	A182	C122	L62
S1016	F863	F787	L716	F634	E565	T490	THR	L368	E306	G243	S183	I123	I63
N1024	I869	R788	G717	K635	V566	T491	ALA	K369	S307	R244	F184	Y124	K64
L1028	L873	S789	E718	I636	D567	H496	HIS	E370	S308	E245	I185	A125	R65
F1043	F878	F790	I719	I637	V568	H499	THR	H371	G309	A246	S186	T126	R66
E1047	Q879	D791	G720	N638	L569	A499	ALA	A310	A310	Y247	G187	R127	G67
F1061	E792	E792	T722	L647	N571	V501	ASN	E372	F311	P248	L188	E128	K68
G1064	G794	G794	E723	A648	S574	V502	LEU	T374	S312	E249	F189	G129	L69
R1065	E795	S649	T725	A649	L575	G503	LEU	V503	E313	E250	N190	D130	G70
S1066	T796	K650	K726	K650	R576	M504	ASN	F376	Q314	A251	F191	Y131	L71
R1085	T797	L651	T727	L651	S577	L513	GLY	V377	Q315	Y252	Y192	V132	V72
V1094	Q798	Y652	C728	Y652	A578	V517	THR	R379	T316	I253	E193	L133	G73
SER	Y801	R653	R729	R654	V579	V518	THR	G380	Y317	A254	D194	F134	V74
MET	E802	P654	R730	P654	V580	R521	THR	G381	D318	D255	L195	H135	N75
	D803	V657	I731	V657	S581	D522	PRO	P382	Y319	L256	Y196	H136	L76
	L804	G664	K732	G664	T582	E523	ALA	N383	A320	D257	F197	E137	T77
	A806	G665	E733	G665	N583	P524	PRO	E386	K321	A258	T198	G138	L78
	M807	M666	G734	M666	E584	S525	SER	G387	T322	K259	Y199	G139	D79
	G808	S667	R735	S667	V526	V526	ARG	L388	I323	S260	L200	V140	G80
	Y809	H668	L736	H668	A527	A527	THR	L389	L324	G261	E201	D141	V81
	L810	E669	T737	E669	A528	A528	ALA	V390	S325	A262	I202	V142	K82
	V811	N671	R738	N671	V529	V529	SER	K391	L326	S263	N203	G143	S83
	P812	I674	I740	I674	Q590	Q590	GLU	G392	T328	L264	P204	D144	W84
	A813	T677	V741	T677	I591	I591	SER	E393	R329	L266	V206	V145	L85
	Q814	T678	I745	T678	R592	R592	ARG	V394	E330	L267	V207	D146	K86
	E815	T679		T679	T594	T594	ALA	G395	ASP	T267	T208	D147	P87
	V816	D679		D679	A595	A595	GLU	K396	H332	L268	R88	K148	R88
	P817	G680		G680	E599	E599	VAL	T397	P333	L269	K209	A149	L89
	L818	V681		V681	A598	A598	ALA	T398	G335	N270	D210	Q150	G90
	P819	E682		E682	E599	E599	PRO	G399	G336	P271	G211	K151	Q91
	T820	E683		E683	P602	P602	ALA	L400	I337	K272	V212	L152	E92
	V821	G684		G684	E603	E603	LYS	P401	L338	R274	Y213	L153	A93
	P822	V685		V685	F541	F541	LYS	I402	G341	I275	V214	V154	T94
	M823	G688		G688	Y542	Y542	PRO	H403	G342	W276	D216	G155	V95
	Y825	R691		R691	A604	A604	ALA	F405	G343	T277	L217	V156	G96
	S826	V692		V692	L605	L605	MET	E408	G344	M278	D157	D157	K97
	R827	G693		G693	T606	T606	GLN	T409	I344	V279	A218	E158	A98
	A828	F697		F697	R607	R607	ASP	H410	A345	G281	A219	K159	T99
	R829	M698		M698	L609	L609	SER	M411	N346	G282	K220	L160	G100
	L831	D699		D699	T610	T610	VAL	T412	F347	G283	V221	P161	F101
	G832	H700		H700	K611	K611	SER	A413	T348		D222	P162	L102
	T834	V701		V701	L549	L549	PRO	L414		V286	A223	E163	K103
	R835	L702		L702	V551	V551	ARG	V415	A352	V287	T224	D164	N104
	T842	R703		R703	V552	V552	SER	G416	T353	Y288	A225	I165	F105
	L844	Q705		Q705	F553	F553	GLN	M417	F354	S289	D226	K166	L106
	G856	K711		K711	K554	K554		A418	K355	I292	Y227	K167	I107
	M857	M712		M712	N555	N555		L419	I357		I228	H168	E108
	T860	I713		I713	N556	N556		G420	V358		K230	L170	P109
					A559	A559		H421	R359	G296	V171	H172	F110
					N560	N560		A422	A360	G297	K231	H173	V111
					R561	R561		P423	I361	V298	K232	A173	H113
					K562	K562		T424	R362	N299	W233	P174	S114
					G628	G628		P425	D363	E300	G234	E175	Q115
								ASN	Y364	L301	I236	D176	A116
								GLN	Q365	A302	E237	K177	E117
										N303	F238	E179	F119
											P239	K178	E118
													Y120

• Molecule 1: ATP-citrate synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	237362	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.024	Depositor
Minimum map value	-1.514	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.157	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: UNL, ADP, Q5B, COA, FLC

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	0.14	0/8167	0.34	0/11054
1	B	0.17	0/8167	0.35	0/11054
1	C	0.13	0/8167	0.31	0/11054
1	D	0.15	0/8151	0.33	0/11032
All	All	0.15	0/32652	0.33	0/44194

There are no bond length outliers.

There are no bond angle outliers.

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	7989	0	8040	222	0
1	B	7989	0	8040	208	0
1	C	7989	0	8040	201	0
1	D	7974	0	8031	210	0
2	A	27	0	12	6	0
2	B	27	0	12	2	0
2	D	27	0	12	2	0
3	A	60	0	0	1	0
3	B	60	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	60	0	0	1	0
4	A	13	0	5	1	0
4	B	13	0	5	1	0
4	C	13	0	5	1	0
4	D	13	0	5	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	48	0	32	4	0
6	B	48	0	32	3	0
6	C	96	0	64	11	0
7	A	35	0	0	0	0
7	B	47	0	0	0	0
7	C	37	0	0	1	0
7	D	43	0	0	0	0
All	All	32610	0	32335	804	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 12.

The worst 5 of 804 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:279:VAL:HG12	1:D:341:GLY:H	1.36	0.89
1:C:1085:ARG:HE	6:C:2102:COA:H62A	1.21	0.86
1:A:719:ILE:HD11	1:A:746:GLY:HA3	1.59	0.83
1:D:316:THR:HG21	1:D:353:THR:HA	1.60	0.82
1:C:835:ARG:HG3	1:D:822:PRO:HB2	1.62	0.81

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	1028/1101 (93%)	994 (97%)	34 (3%)	0	100	100
1	B	1028/1101 (93%)	997 (97%)	31 (3%)	0	100	100
1	C	1028/1101 (93%)	1002 (98%)	26 (2%)	0	100	100
1	D	1026/1101 (93%)	991 (97%)	34 (3%)	1 (0%)	48	71
All	All	4110/4404 (93%)	3984 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	690	ASP

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%)	852 (100%)	0	100	100
1	B	852/908 (94%)	852 (100%)	0	100	100
1	C	852/908 (94%)	852 (100%)	0	100	100
1	D	851/908 (94%)	850 (100%)	1 (0%)	92	98
All	All	3407/3632 (94%)	3406 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	691	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	115	GLN
1	C	668	ASN
1	D	988	GLN

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Mol	Chain	Res	Type
1	C	645	ASN
1	C	988	GLN

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 16 ligands modelled in this entry, 2 are unknown - leaving 14 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	FLC	B	1203	-	12,12,12	1.11	0	17,17,17	1.38	1 (5%)
3	Q5B	A	1202	-	56,62,62	3.05	18 (32%)	74,93,93	1.50	10 (13%)
6	COA	C	2101	-	43,50,50	0.84	1 (2%)	56,75,75	1.02	2 (3%)
2	ADP	B	1201	-	24,29,29	0.91	0	29,45,45	1.28	3 (10%)
2	ADP	D	1201	-	24,29,29	0.88	0	29,45,45	1.19	2 (6%)
4	FLC	C	2103	-	12,12,12	1.10	0	17,17,17	1.32	1 (5%)
6	COA	B	1204	-	43,50,50	0.81	0	56,75,75	1.08	2 (3%)
4	FLC	A	1203	-	12,12,12	1.10	0	17,17,17	1.37	1 (5%)
6	COA	C	2102	-	43,50,50	0.82	0	56,75,75	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Q5B	B	1202	-	56,62,62	2.93	19 (33%)	74,93,93	1.67	13 (17%)
4	FLC	D	1203	-	12,12,12	1.10	0	17,17,17	1.34	1 (5%)
6	COA	A	1205	-	43,50,50	0.82	0	56,75,75	1.03	3 (5%)
2	ADP	A	1201	-	24,29,29	0.92	1 (4%)	29,45,45	1.16	2 (6%)
3	Q5B	D	1202	-	56,62,62	3.05	18 (32%)	74,93,93	1.51	10 (13%)

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	FLC	B	1203	-	-	2/16/16/16	-
3	Q5B	A	1202	-	-	20/62/83/83	0/3/3/3
6	COA	C	2101	-	-	8/44/64/64	0/3/3/3
2	ADP	B	1201	-	-	6/12/32/32	0/3/3/3
2	ADP	D	1201	-	-	3/12/32/32	0/3/3/3
4	FLC	C	2103	-	-	12/16/16/16	-
6	COA	B	1204	-	-	15/44/64/64	0/3/3/3
4	FLC	A	1203	-	-	7/16/16/16	-
6	COA	C	2102	-	-	14/44/64/64	0/3/3/3
3	Q5B	B	1202	-	-	21/62/83/83	0/3/3/3
4	FLC	D	1203	-	-	7/16/16/16	-
6	COA	A	1205	-	-	19/44/64/64	0/3/3/3
2	ADP	A	1201	-	-	3/12/32/32	0/3/3/3
3	Q5B	D	1202	-	-	22/62/83/83	0/3/3/3

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	Q5B	P1-O3	9.46	1.69	1.59
3	A	1202	Q5B	P1-O3	9.38	1.69	1.59
3	B	1202	Q5B	P1-O3	8.40	1.68	1.59
3	A	1202	Q5B	P-O3	8.26	1.68	1.59
3	D	1202	Q5B	P-O3	8.20	1.68	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	Q5B	N2-C12-N3	-6.49	119.86	128.67
3	A	1202	Q5B	N2-C12-N3	-5.83	120.76	128.67
3	D	1202	Q5B	N2-C12-N3	-5.73	120.90	128.67
3	A	1202	Q5B	C22-C21-S	5.13	120.03	113.56
3	D	1202	Q5B	C22-C21-S	5.01	119.88	113.56

There are no chirality outliers.

5 of 159 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	O4'-C4'-C5'-O5'
2	B	1201	ADP	C5'-O5'-PA-O1A
2	B	1201	ADP	C5'-O5'-PA-O3A
2	B	1201	ADP	O4'-C4'-C5'-O5'
2	B	1201	ADP	C3'-C4'-C5'-O5'

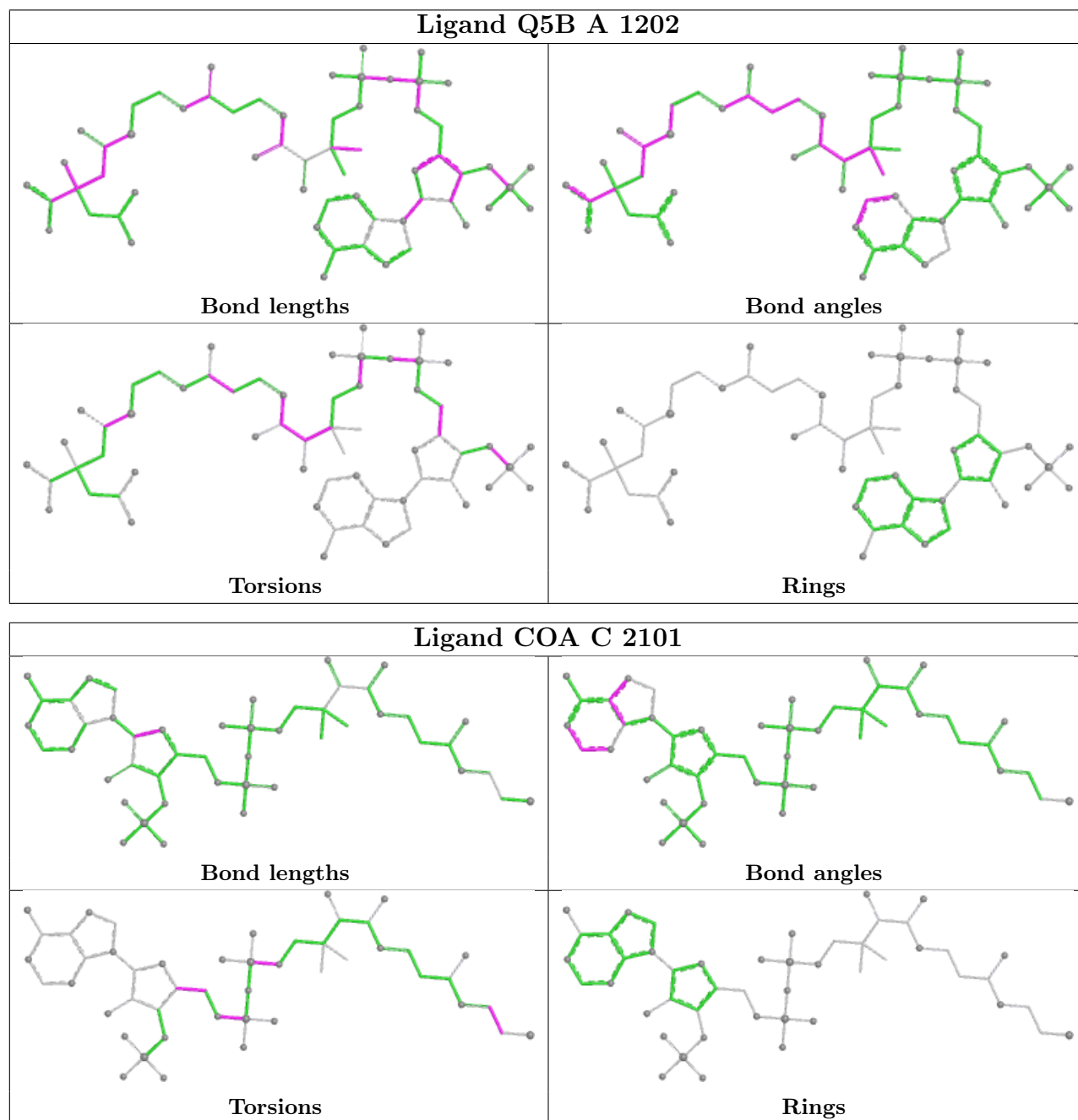
There are no ring outliers.

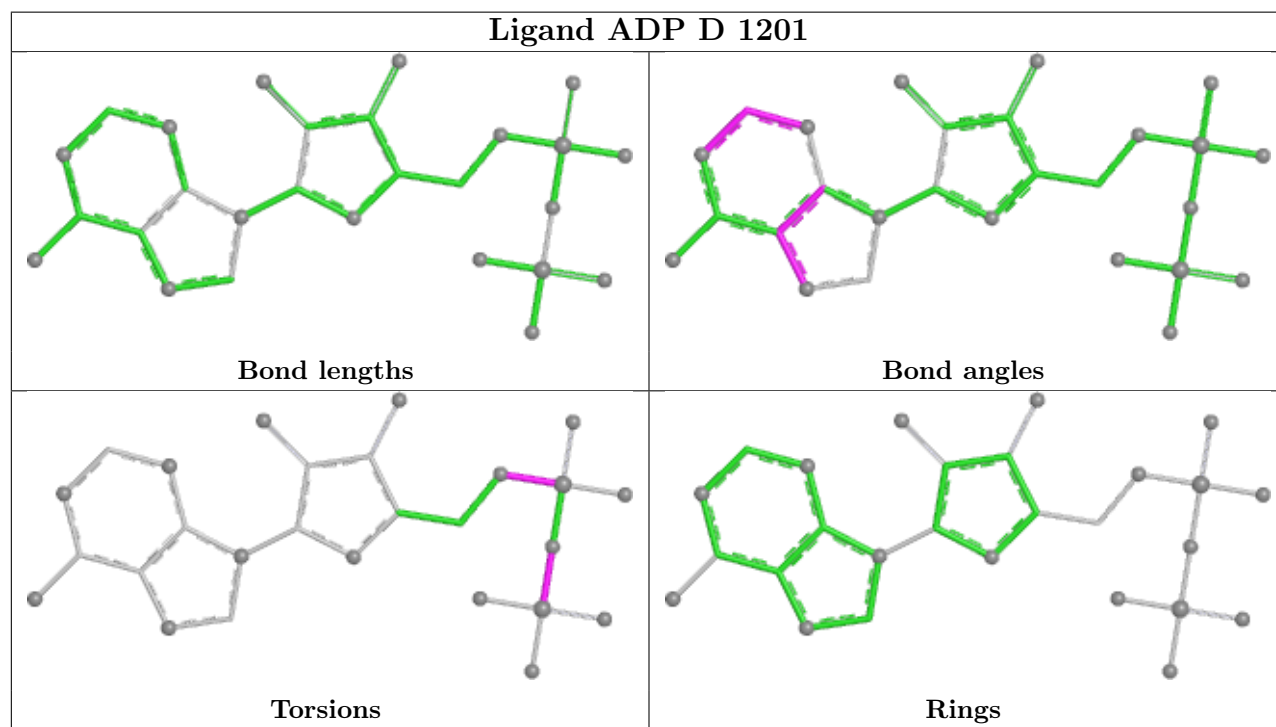
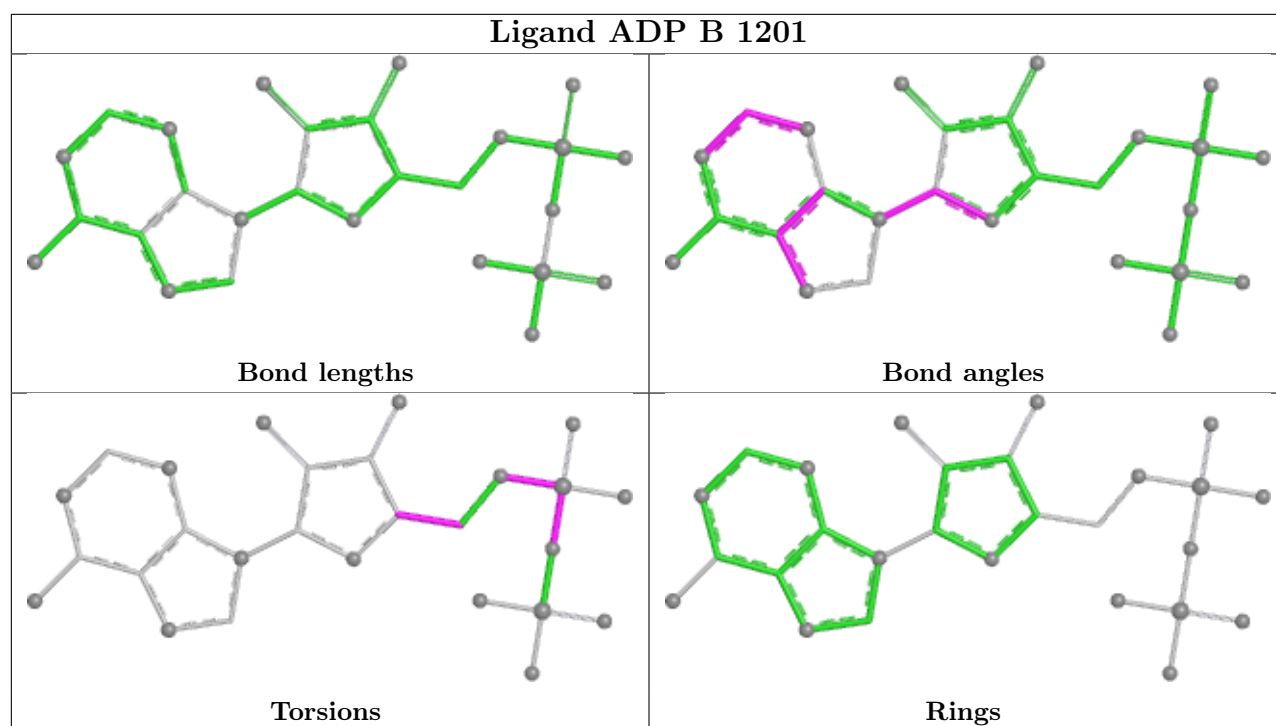
14 monomers are involved in 37 short contacts:

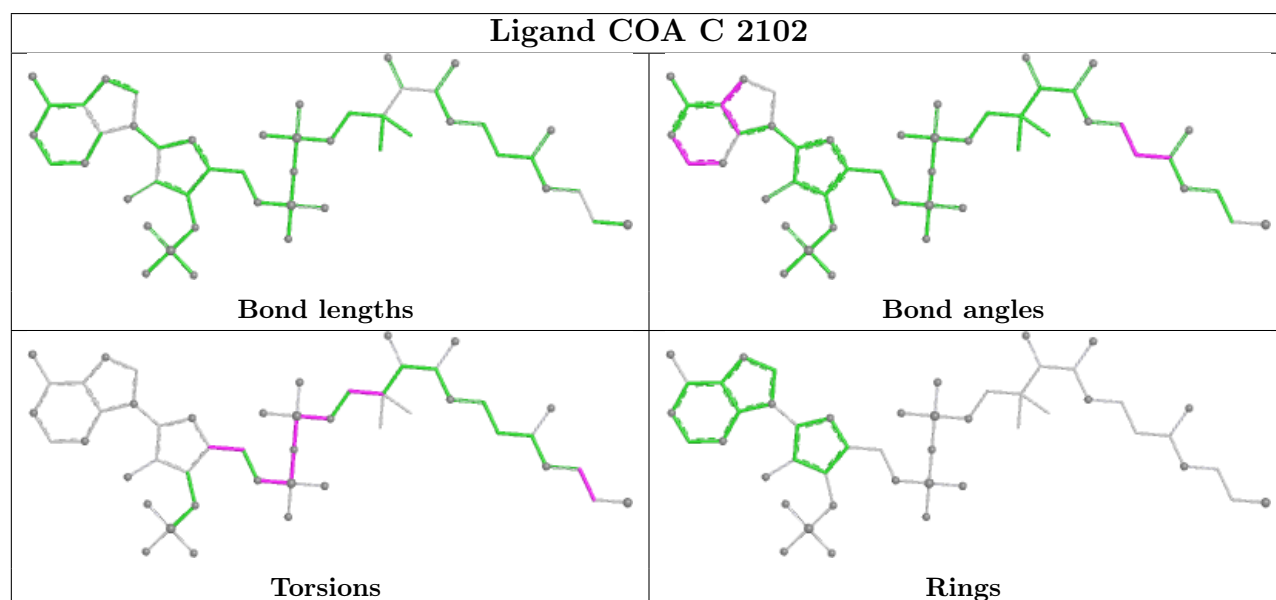
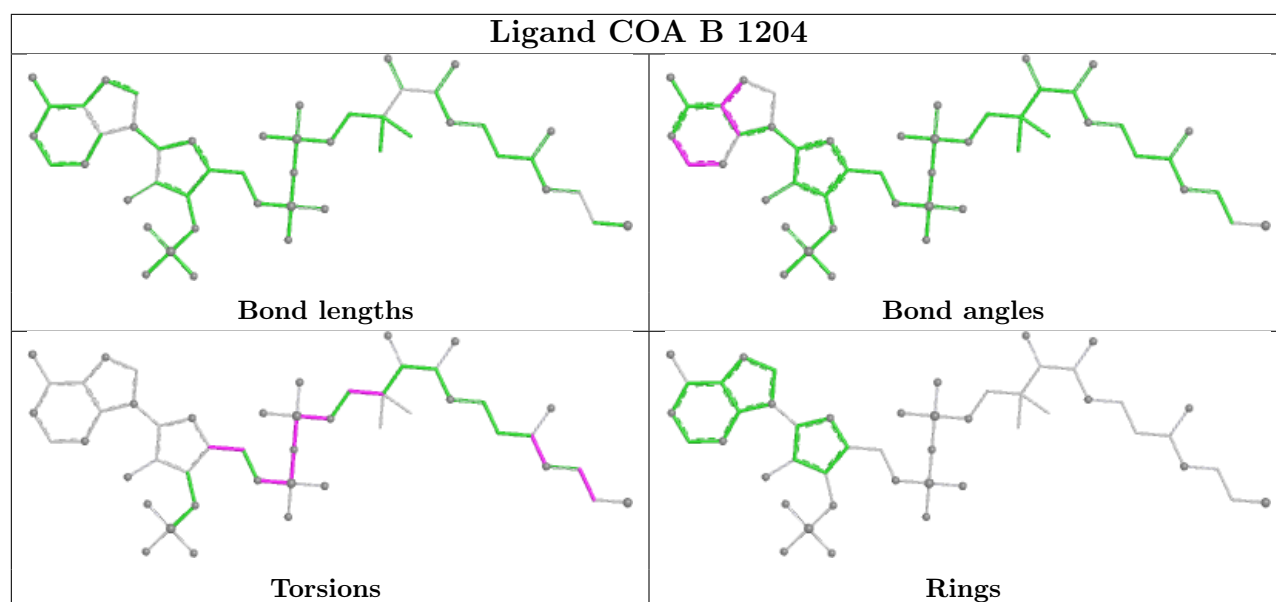
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1203	FLC	1	0
3	A	1202	Q5B	1	0
6	C	2101	COA	4	0
2	B	1201	ADP	2	0
2	D	1201	ADP	2	0
4	C	2103	FLC	1	0
6	B	1204	COA	3	0
4	A	1203	FLC	1	0
6	C	2102	COA	7	0
3	B	1202	Q5B	3	0
4	D	1203	FLC	1	0
6	A	1205	COA	4	0
2	A	1201	ADP	6	0
3	D	1202	Q5B	1	0

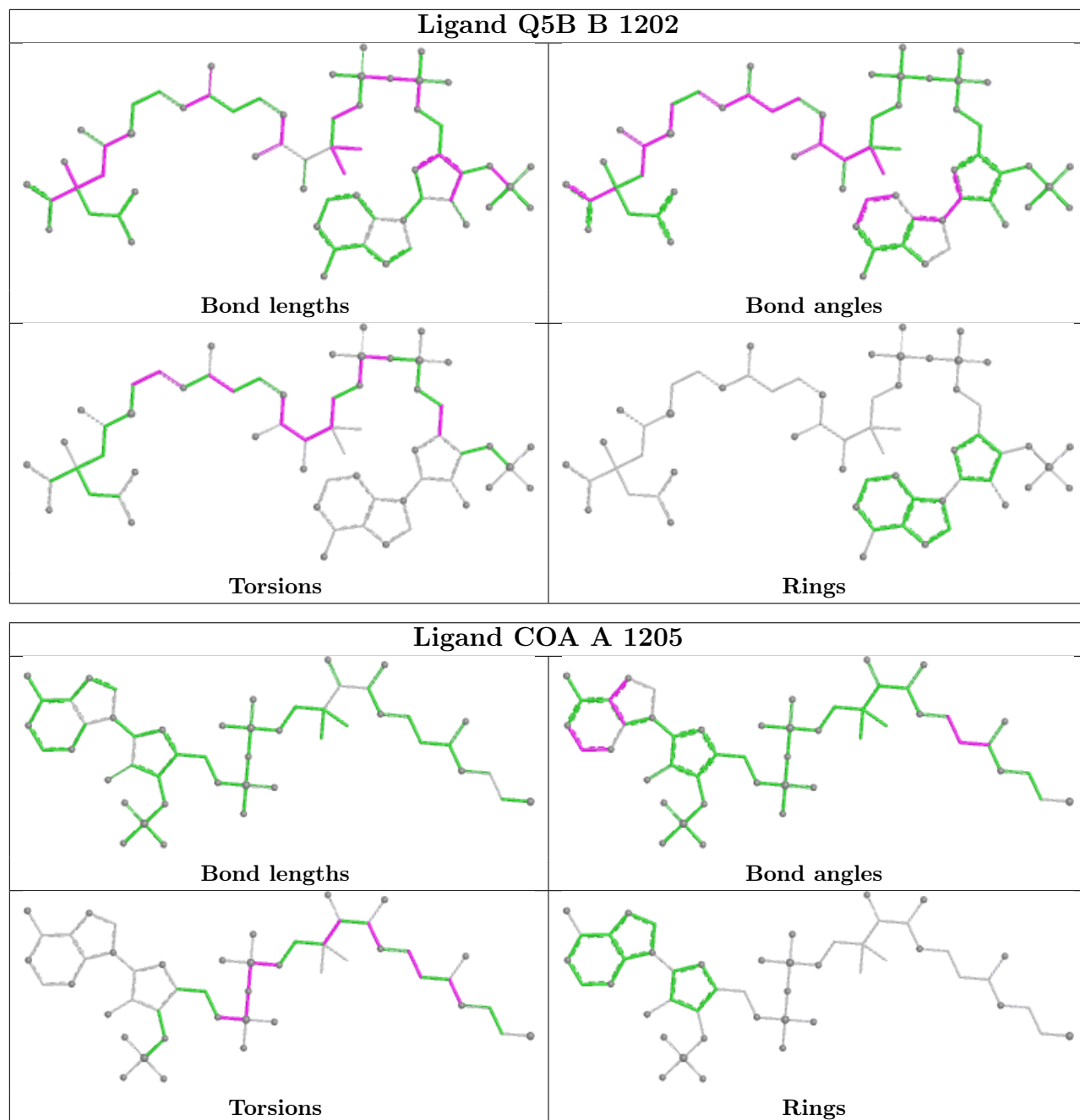
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

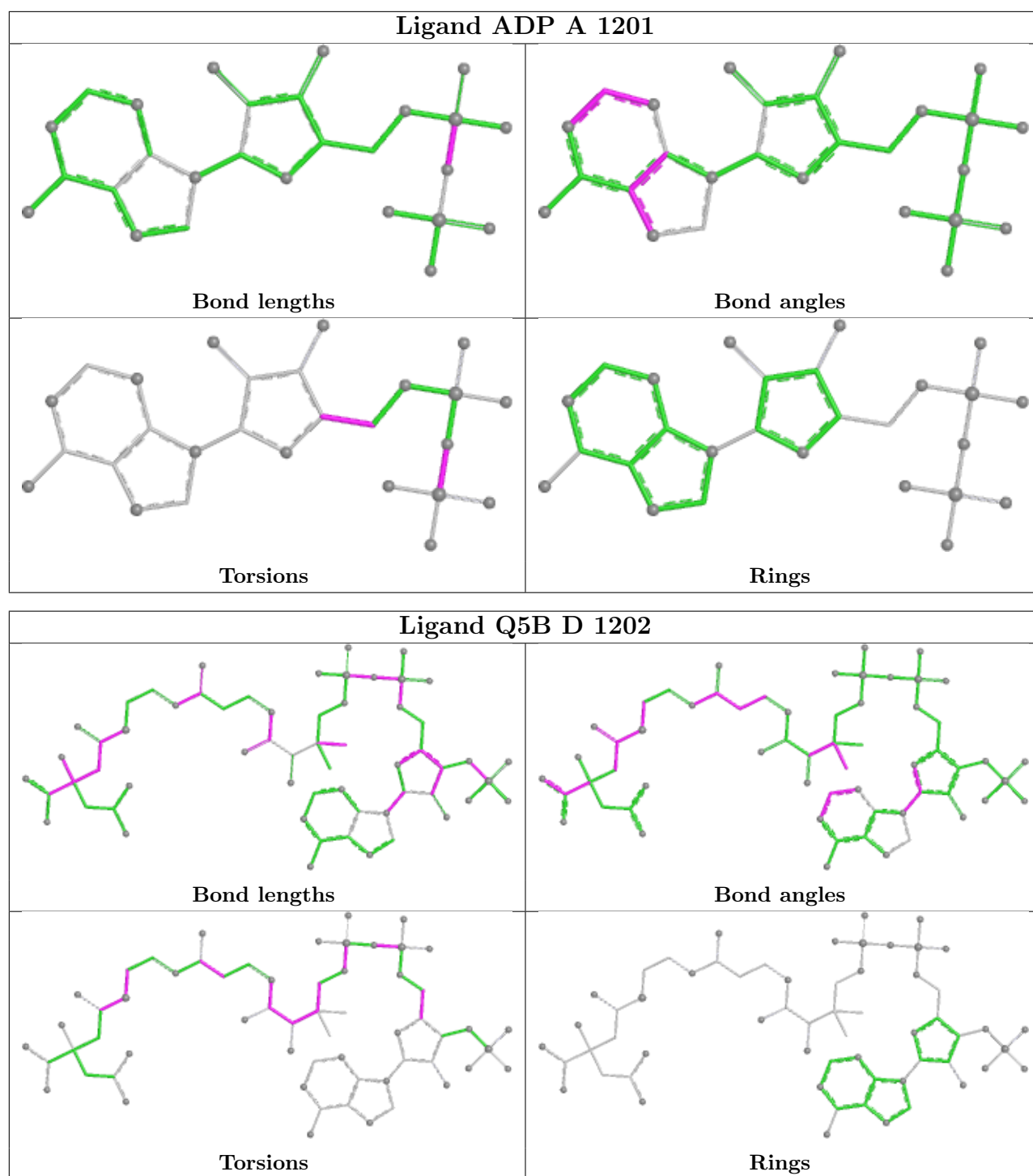
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents 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 ⓘ

There are no chain breaks in this entry.

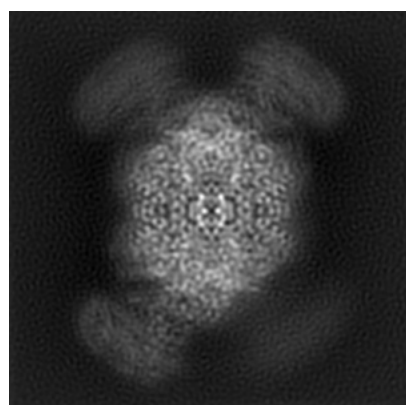
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24511. These allow visual inspection of the internal detail of the map and identification of artifacts.

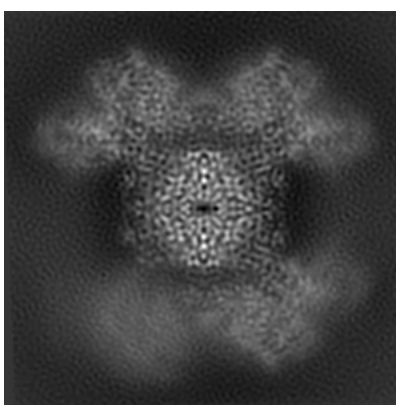
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

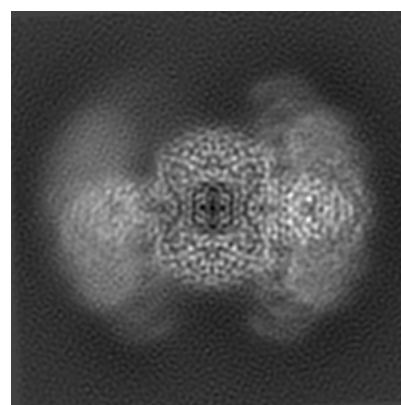
6.1.1 Primary map



X



Y

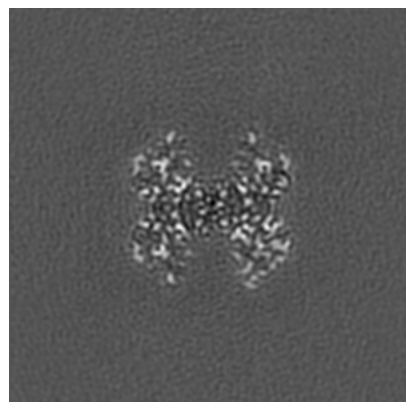


Z

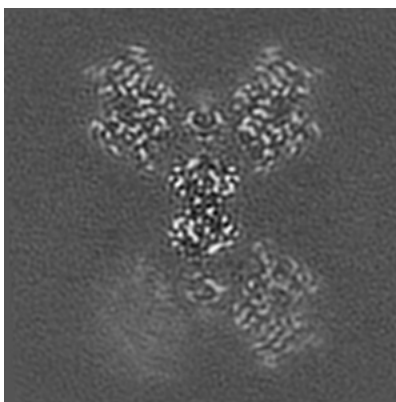
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

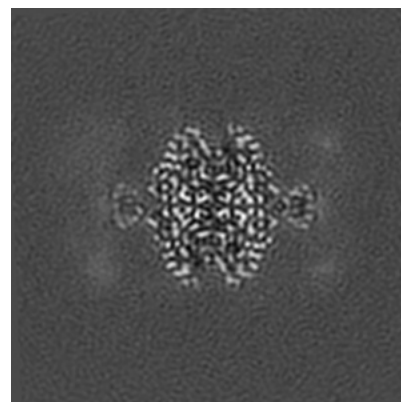
6.2.1 Primary map



X Index: 110



Y Index: 110

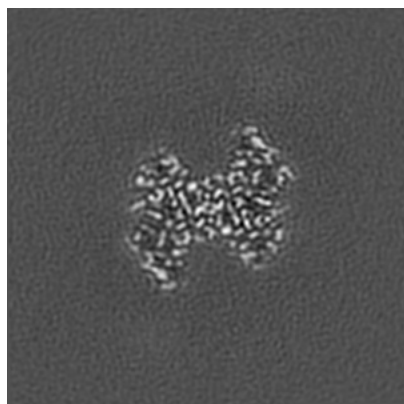


Z Index: 110

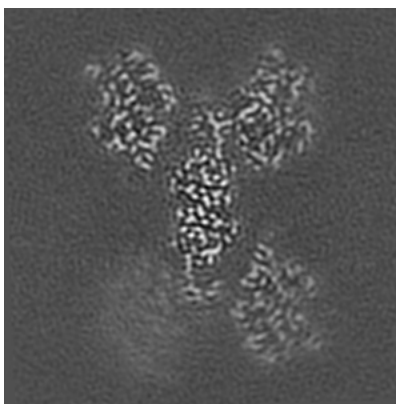
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

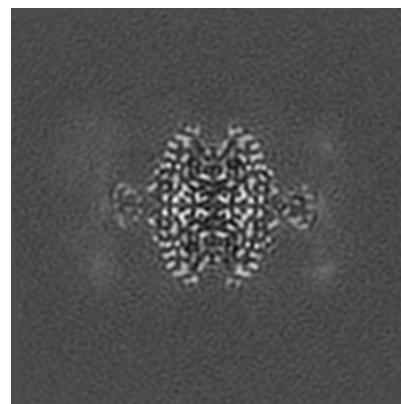
6.3.1 Primary map



X Index: 119



Y Index: 106

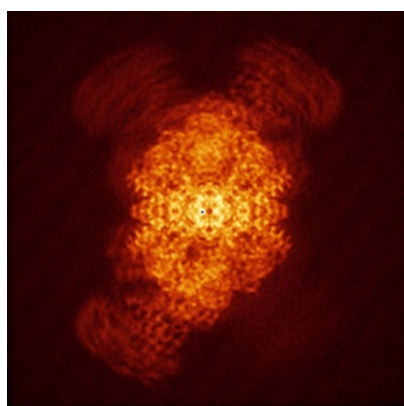


Z Index: 109

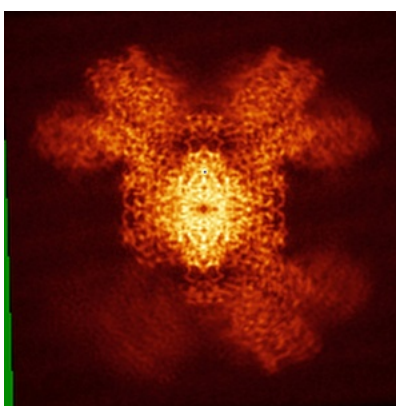
The images above show the largest variance slices of the map in three orthogonal directions.

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

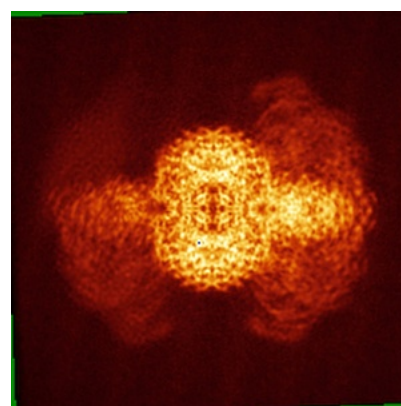
6.4.1 Primary map



X



Y

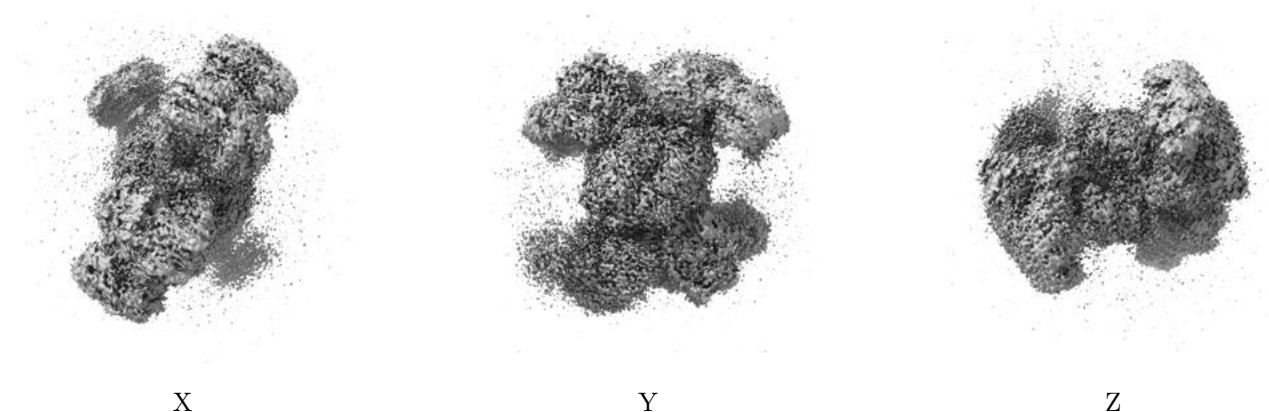


Z

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.

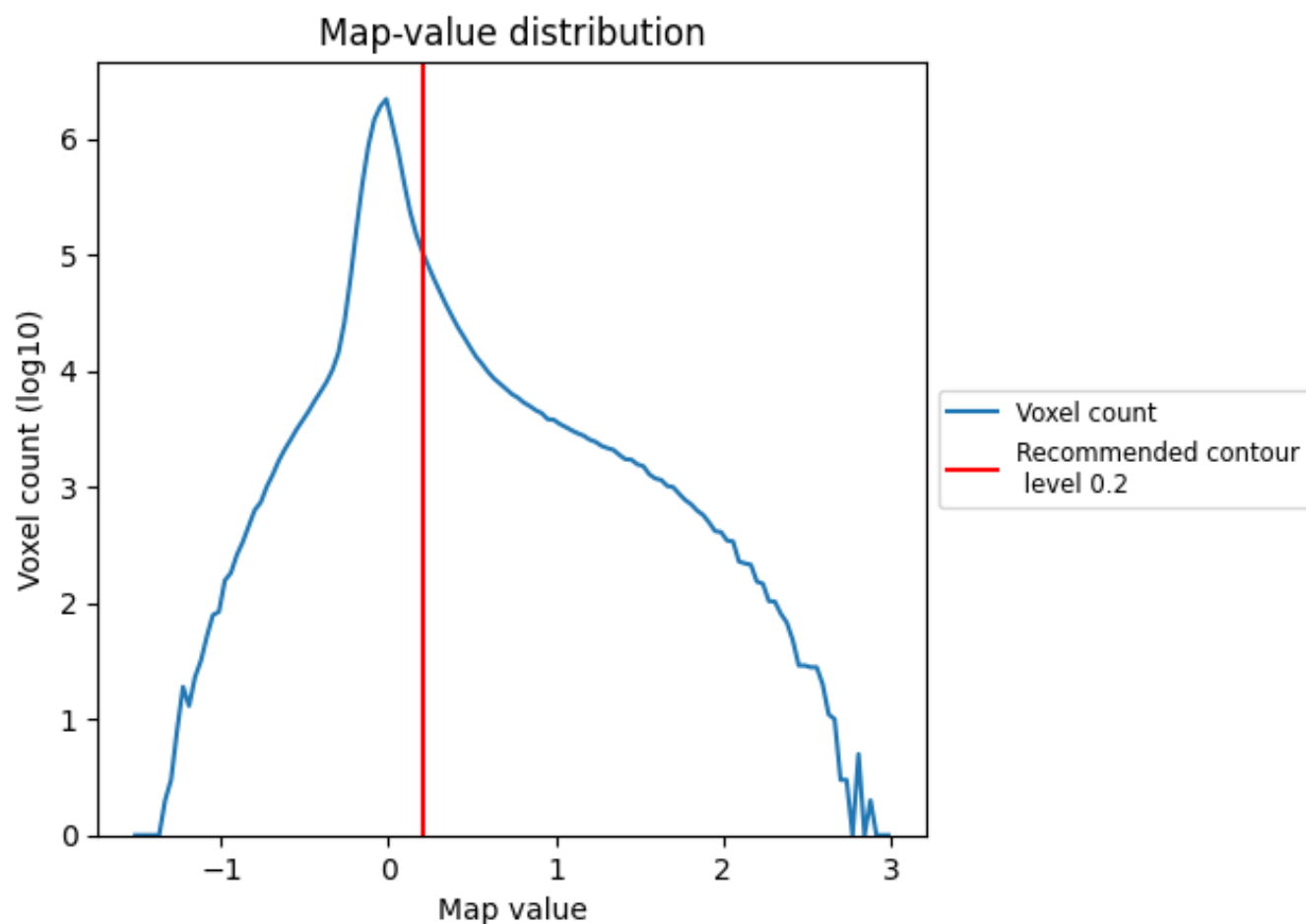
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

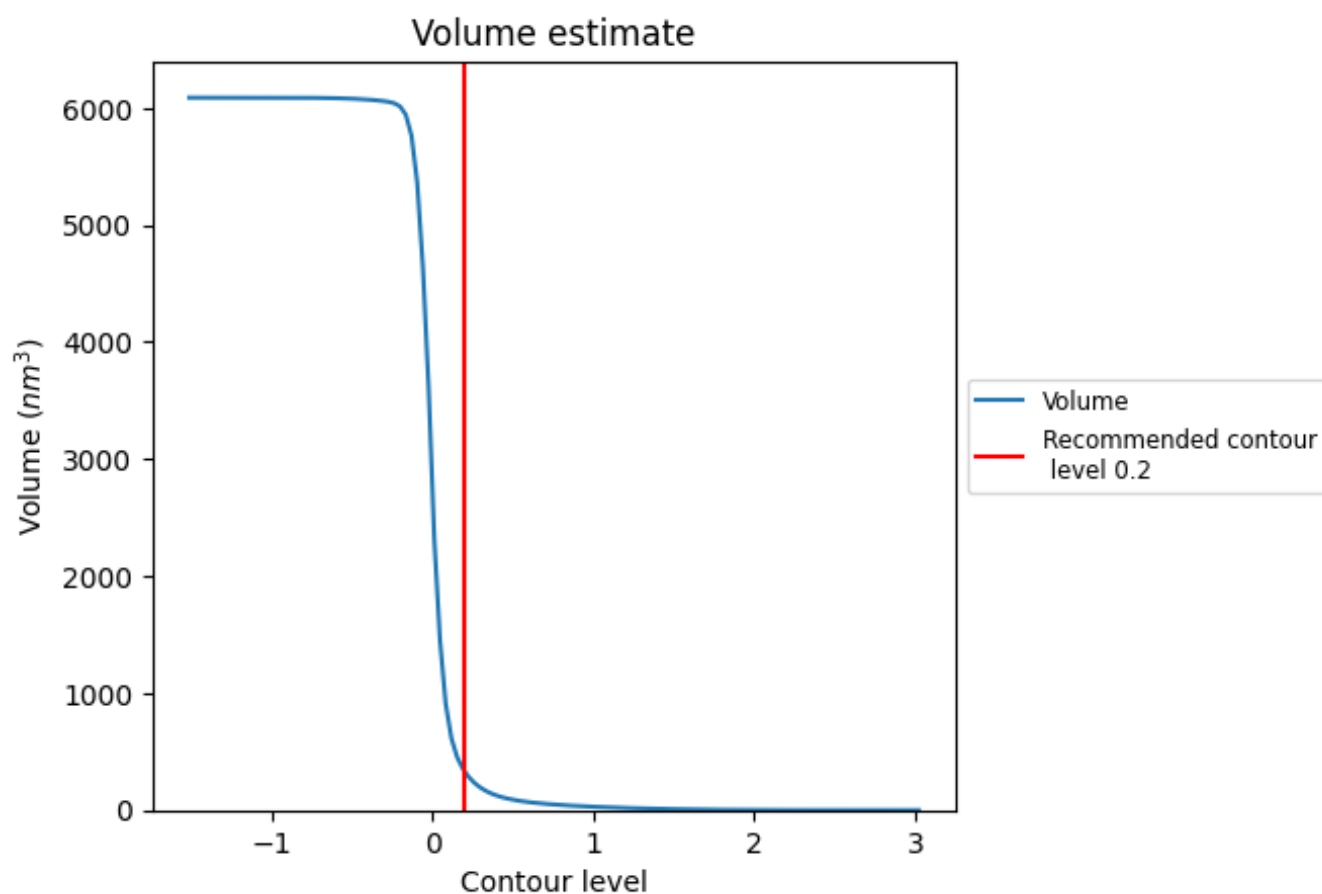
This section contains the results of statistical analysis of the map.

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.

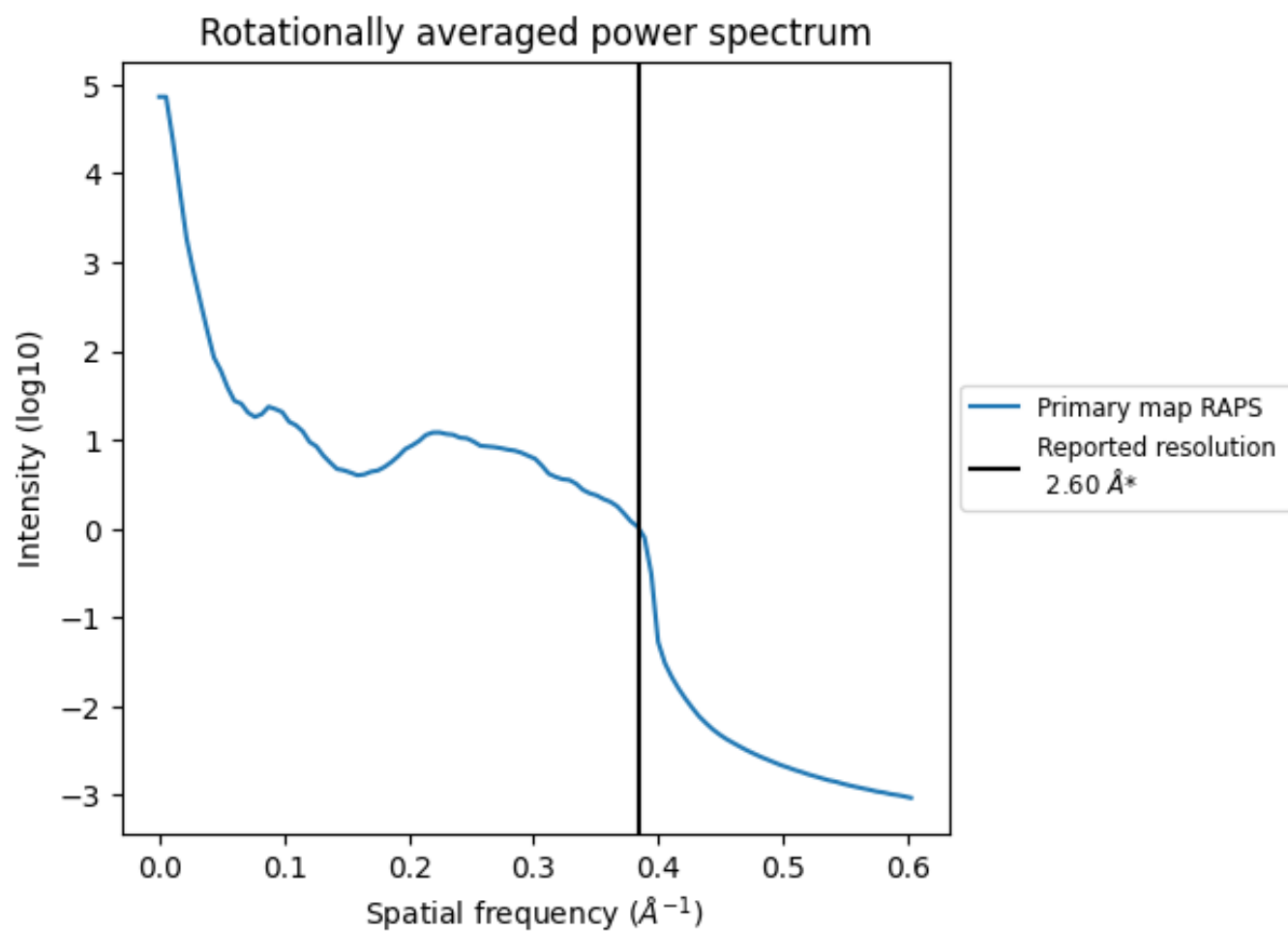
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm^3 ; this corresponds to an approximate mass of 299 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 0.385 Å⁻¹

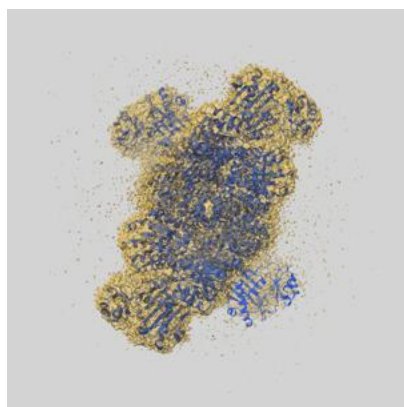
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

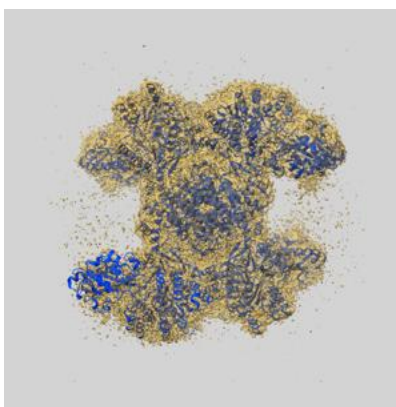
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24511 and PDB model 7RKZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

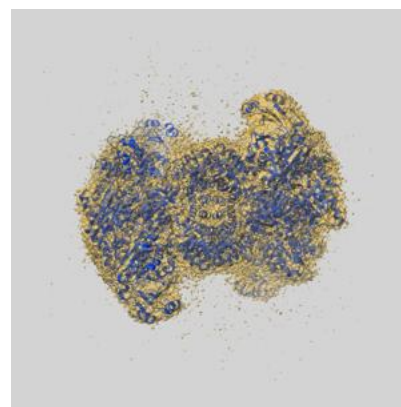
9.1 Map-model overlay [i](#)



X



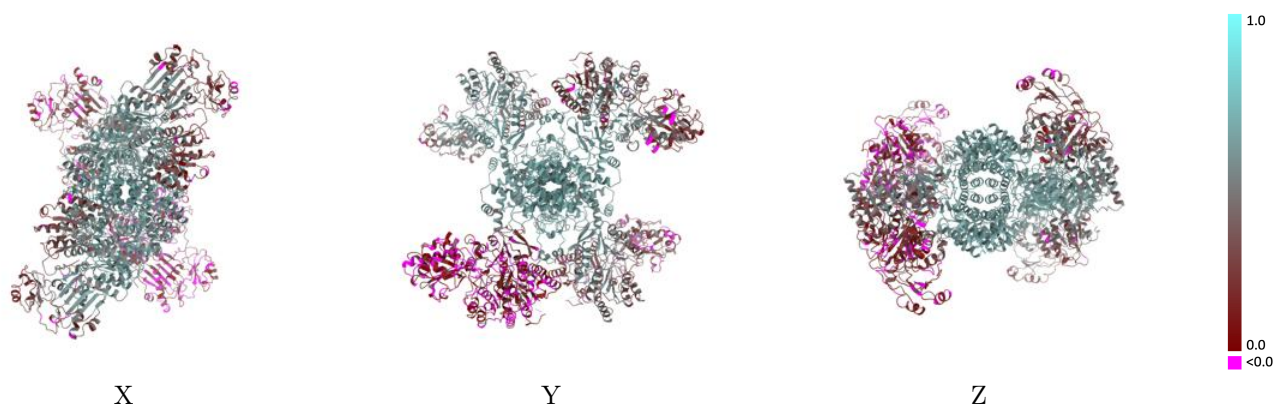
Y



Z

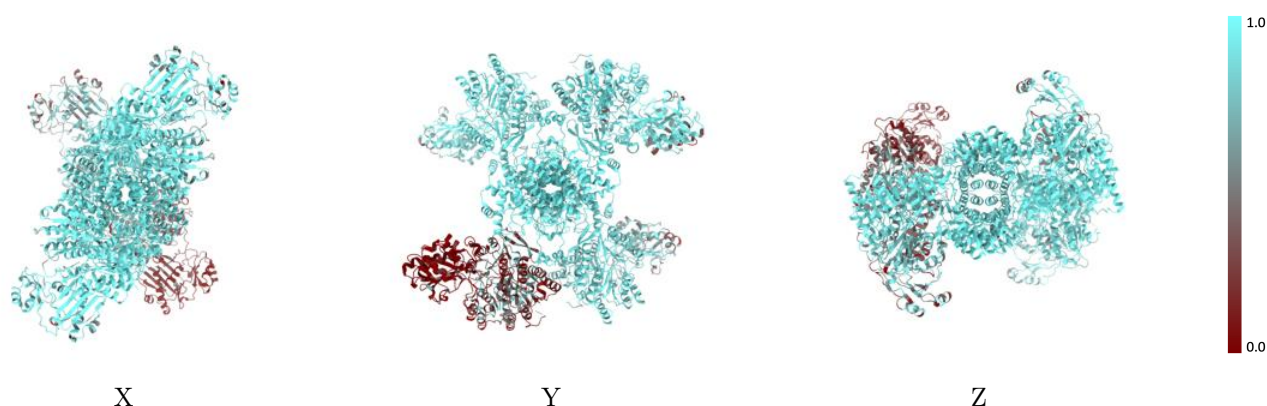
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



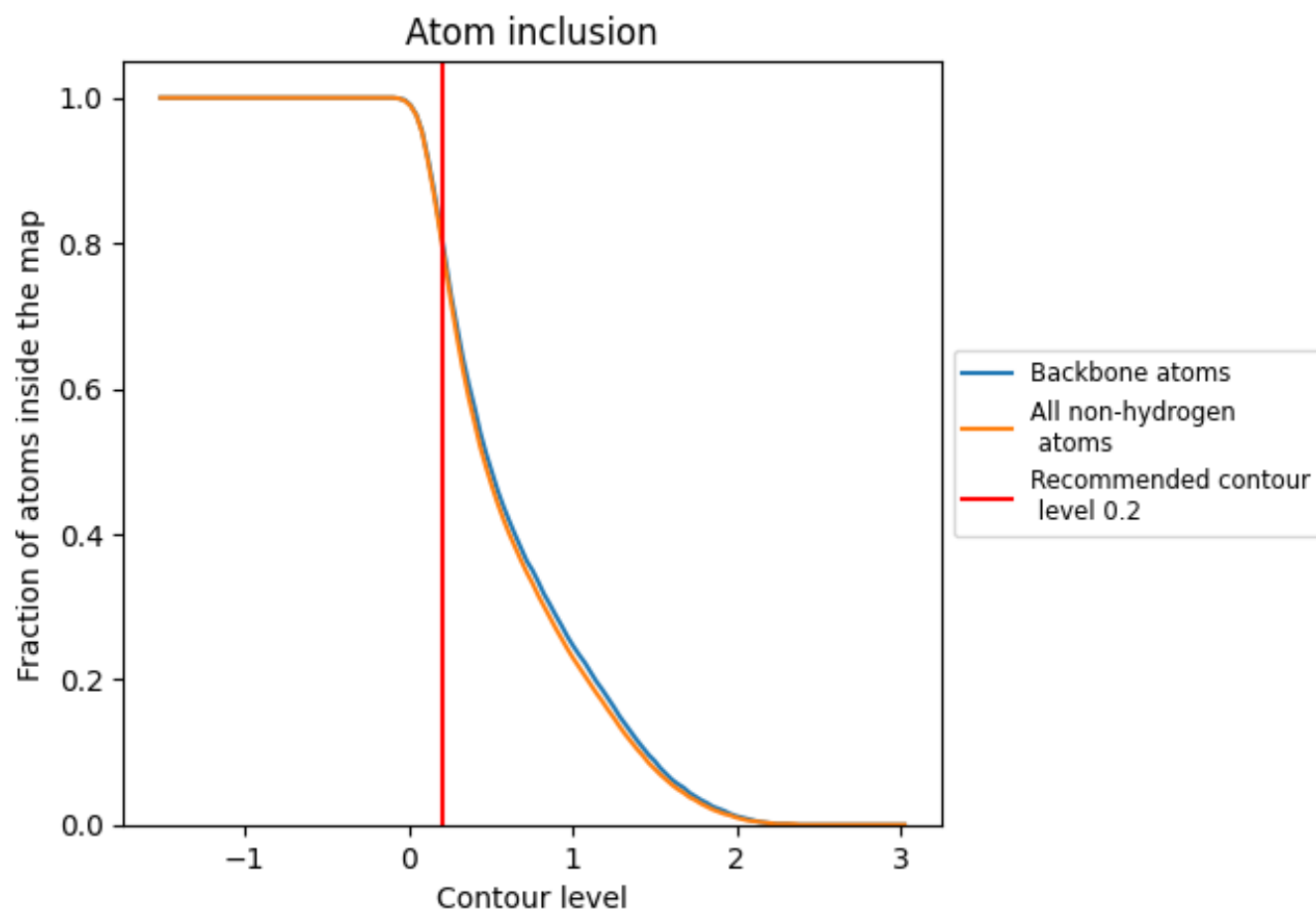
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% 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	<div></div> 0.8030	<div></div> 0.4120
A	<div></div> 0.9280	<div></div> 0.4910
B	<div></div> 0.9450	<div></div> 0.5230
C	<div></div> 0.4900	<div></div> 0.2380
D	<div></div> 0.8530	<div></div> 0.3970

