



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:55 AM UTC

PDB ID : 7WTC / pdb_00007wtc
EMDB ID : EMD-32778
Title : Cryo-EM structure of human pyruvate carboxylase with acetyl-CoA in the ground state
Authors : Chai, P.; Lan, P.; Wu, J.; Lei, M.
Deposited on : 2022-02-04
Resolution : 4.00 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

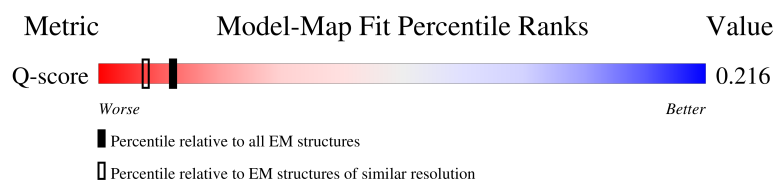
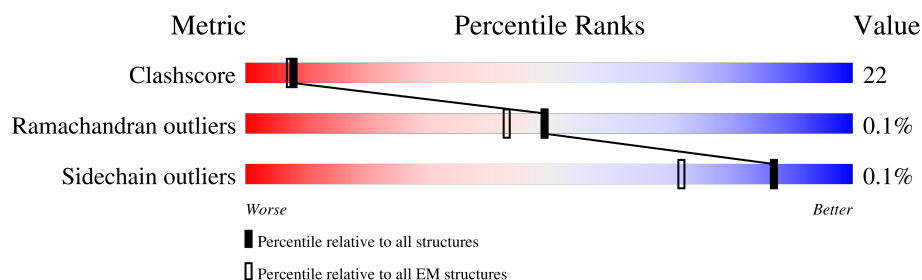
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	1178	
1	B	1178	
1	C	1178	
1	D	1178	

2 Entry composition [i](#)

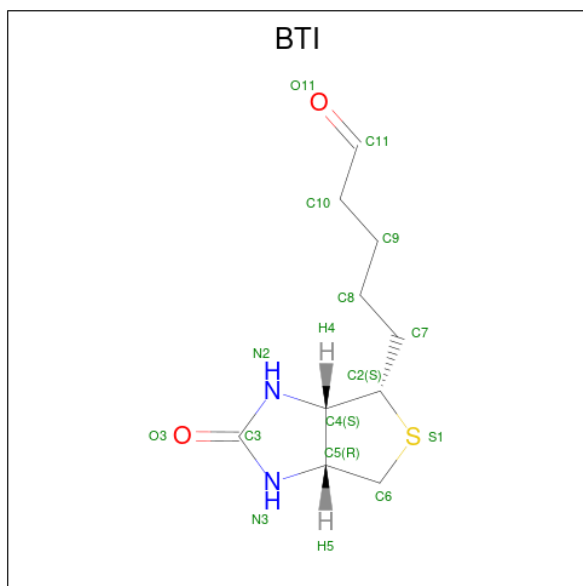
There are 3 unique types of molecules in this entry. The entry contains 28418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1146	Total	C	N	O	S	0	0
			8869	5612	1559	1651	47		
1	B	1147	Total	C	N	O	S	0	0
			8877	5618	1560	1652	47		
1	C	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		
1	D	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



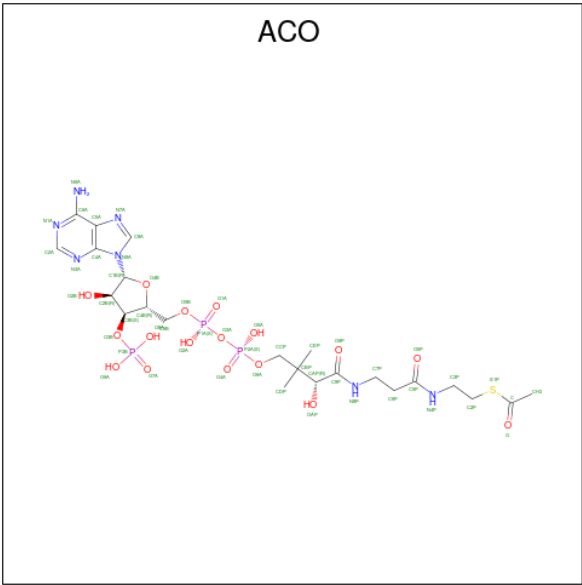
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	B	1	Total	C	N	O	S	0
			15	10	2	2	1	

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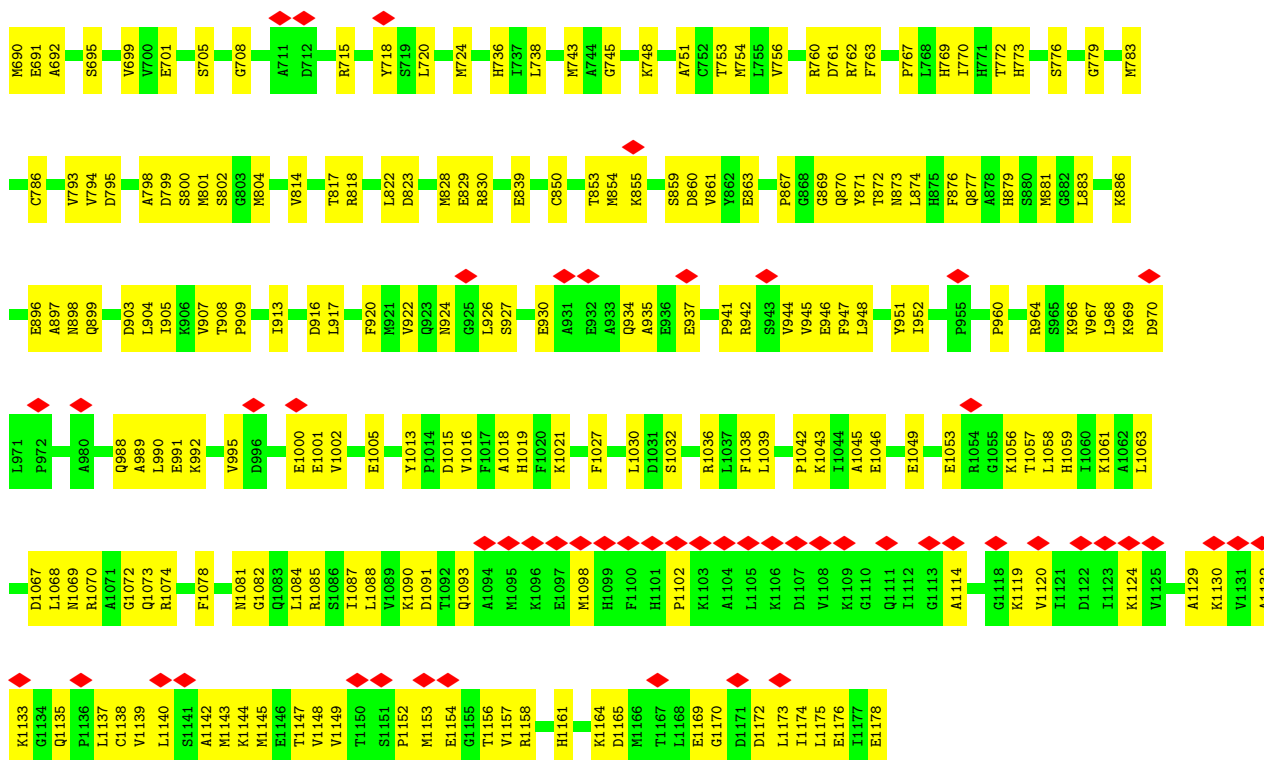
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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	D	1	Total	C	N	O	S	0
			15	10	2	2	1	

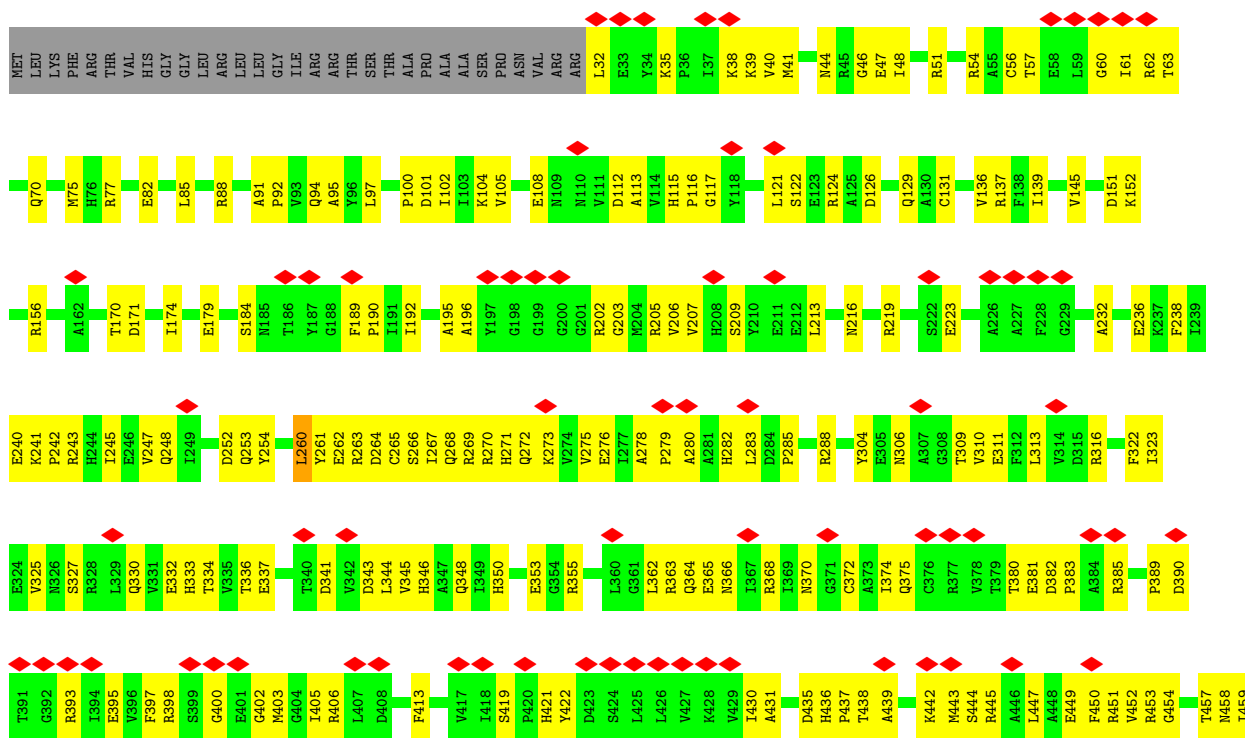
- Molecule 3 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).

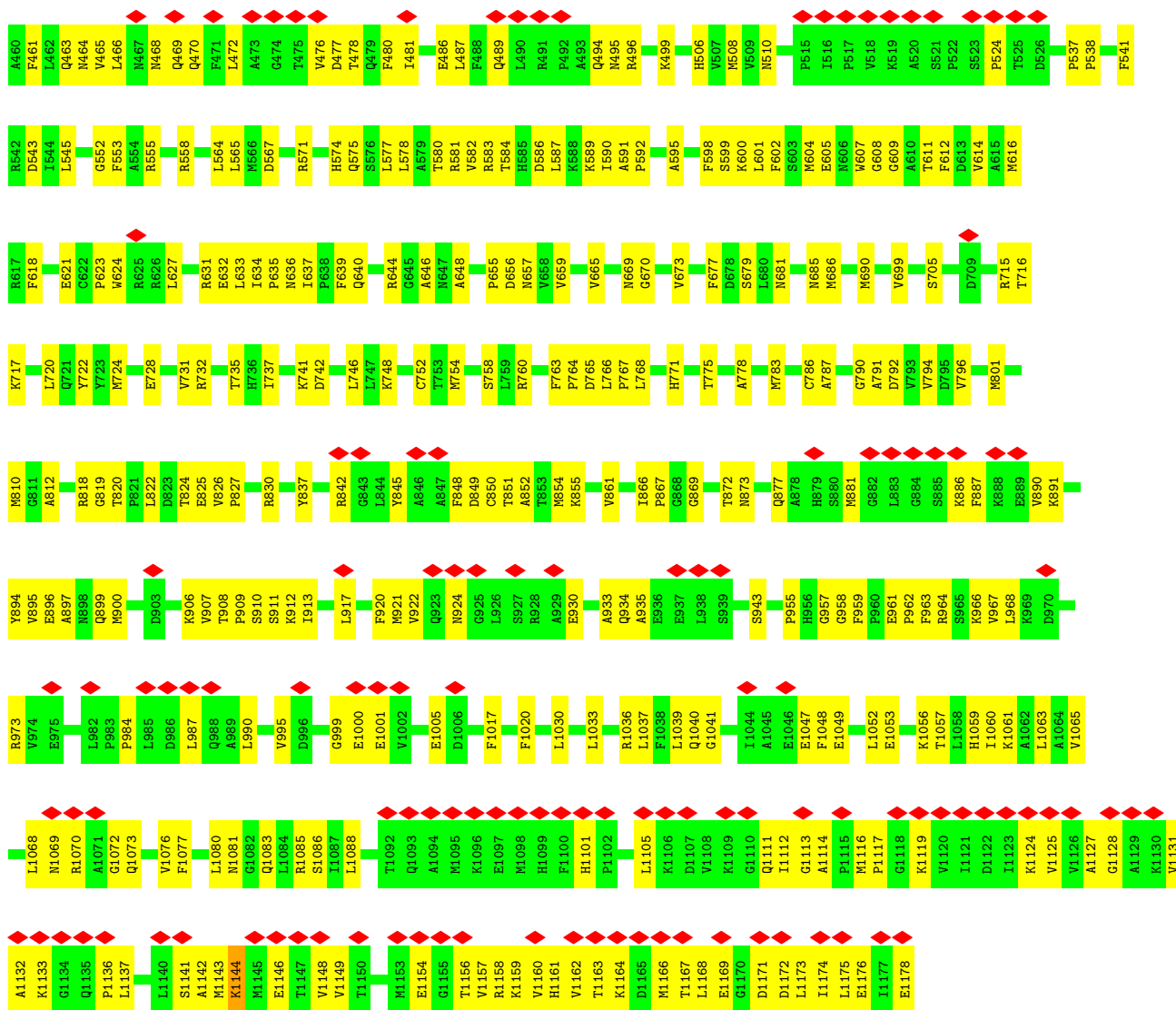


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
3	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

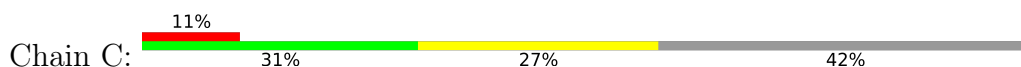


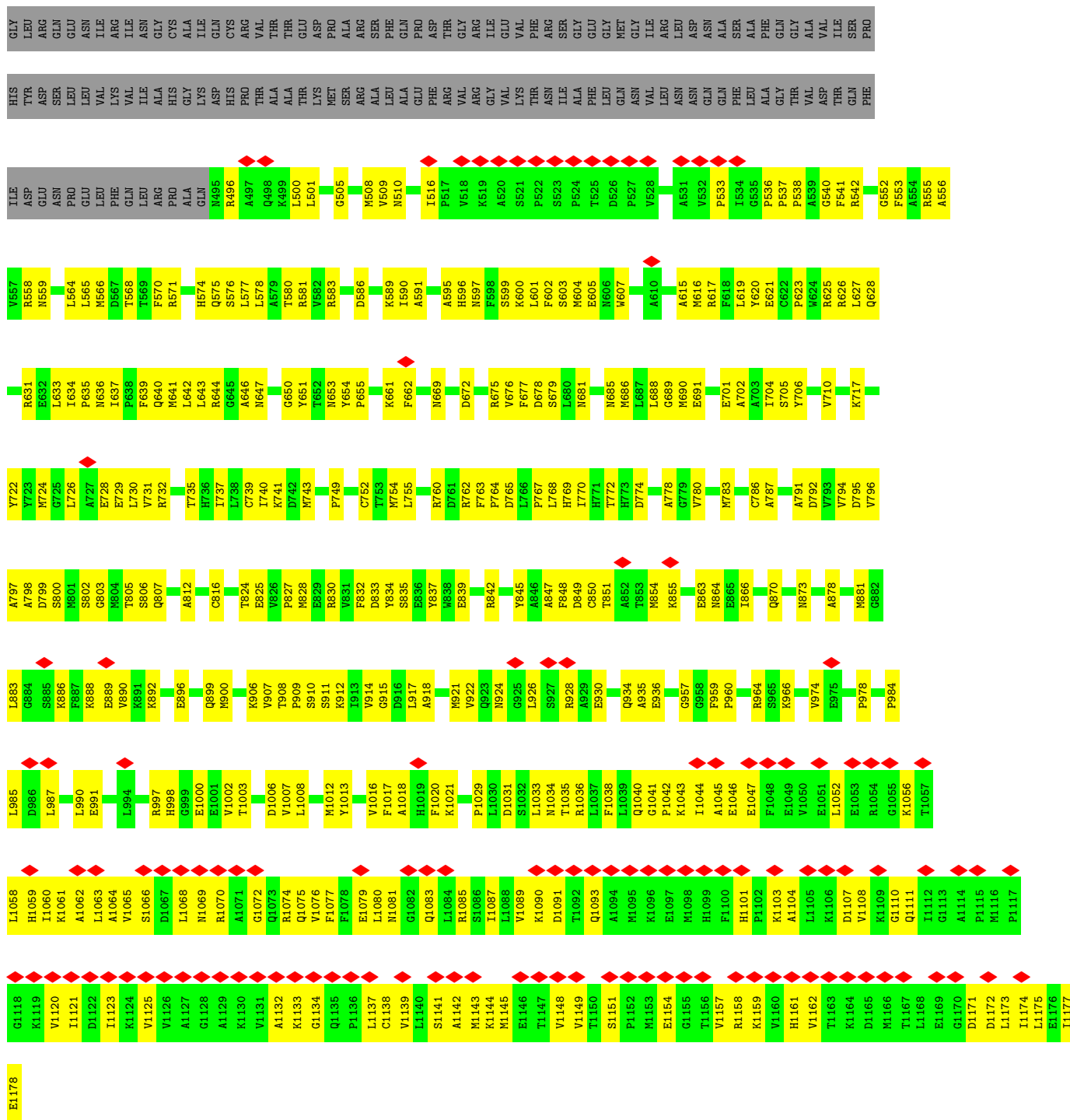
• Molecule 1: Pyruvate carboxylase, mitochondrial



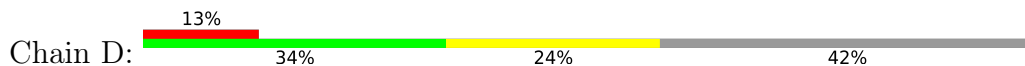


- Molecule 1: Pyruvate carboxylase, mitochondrial

[illegible]



- Molecule 1: Pyruvate carboxylase, mitochondrial

[illegible]

D1107	P1042	L971	V796	A702	B621	P550	ILE	HIS	GLY	GLN	LYS	HIS	GLY	LEU
V1108	K1043	P972	A797	A703	C622	F550	ASP	TYR	LEU	VAL	PRO	GLU	ARG	SER
K1109	K1043	P978	A798	I704	P623	F553	GLU	ASP	LEU	GLN	ARG	GLY	ARG	GLU
G1110	I1044	P978	D799	S705	W624	R558	ASN	SER	LEU	GLY	ILE	ASN	ARG	ALA
Q1111	A1045	S981	G882	Y706	R625	R558	PRO	LEU	VAL	ASN	GLY	ASN	ASP	ASP
I1112	E1046	L982	G884	L720	L627	G582	LEU	VAL	VAL	ALA	VAL	VAL	PHE	PHE
G1113	E1047	L985	S806	M724	Q628	L583	PHE	LYS	GLY	GLY	GLN	GLY	ALA	ALA
A1114	E1048	L986	Q807	G725	R631	L584	GLN	VAL	ILE	THR	ILE	THR	PHE	GLN
P1115	E1049	L987	P808	L726	R631	L585	ARG	VAL	ILE	VAL	GLY	VAL	PRO	ALA
M1116	V1050	Q988	S809	L736	L633	L586	LEU	ALA	GLY	VAL	GLY	GLY	CYS	CYS
P1117	E1051	A989	M810	A727	L633	L587	PRO	HIS	CYS	PHE	ASP	ILE	GLN	GLN
G1118	L1052	A989	V814	E728	L634	D587	ALA	GLY	CYS	VAL	GLN	PHE	ASP	ASP
K1119	E1053	L990	A815	E729	F635	R571	GLN	LYS	LYS	VAL	TYR	LYS	ALA	ALA
V1120	R1054	E991	C816	L730	M636	H574	N495	ASP	GLY	ASP	GLY	ALA	VAL	VAL
I1121	G1055	K992	T817	R732	F639	O575	R496	HIS	ILE	CYS	ILE	ALA	ARG	ARG
T1122	K1056	E993	R818	A733	Q640	O576	A497	PRO	GLY	ARG	GLY	TYR	ARG	GLY
D1123	K1057	Y995	L822	G734	M641	L577	Q498	ALA	THR	VAL	GLY	GLY	PHE	ILE
K1124	L1058	D996	D823	H735	L642	L578	L500	ALA	THR	HIS	LEU	GLY	GLY	GLY
V1125	H1059	G915	D823	H736	L643	L578	L501	THR	GLY	THR	LEU	GLY	PRO	PRO
V1126	I1060	D916	P827	L738	G645	R581	H503	LYS	ASP	GLY	GLY	GLY	ARG	GLY
A1127	K1061	Q919	M828	L738	A646	V582	F503	MET	ALA	VAL	ASP	GLY	GLY	GLY
G1128	L1063	M921	E829	T740	M647	R583	G505	ARG	ALA	VAL	CYS	VAL	VAL	VAL
A1129	A1064	V922	R330	K741	T652	H585	Y507	LEU	LEU	ARG	SER	VAL	ARG	ARG
V1065	V1065	V922	V831	M743	T652	H585	Y507	ALA	GLN	GLN	LYS	VAL	ARG	GLY
K1130	S1066	G925	Y834	K748	D656	H586	M508	PHE	GLY	GLY	ARG	GLY	GLY	GLY
D1067	D1067	L926	W838	T750	D657	K588	Y509	PHE	ASP	THR	GLY	GLY	GLY	GLY
R1070	R1070	L1006	Y834	K748	N657	K589	G511	ARG	ARG	THR	GLY	GLY	GLY	GLY
A1071	G1072	S927	W838	T750	N657	K589	P512	VAL	ARG	THR	GLY	GLY	GLY	GLY
Q1073	Q1073	A931	R842	C752	A591	L590	P517	GLY	GLY	THR	GLY	GLY	GLY	GLY
R1074	R1074	Y1013	G843	T753	A591	L590	P517	GLY	GLY	THR	GLY	GLY	GLY	GLY
F1077	F1077	D1015	A846	M754	L755	H596	V518	THR	THR	ASN	ILE	THR	THR	THR
G1078	G1078	V1016	A847	L759	L755	H596	K519	ASN	ASN	ASN	ALA	ALA	ALA	ALA
E1079	E1079	F1017	F848	D761	P522	S599	A520	ILE	ALA	ALA	ALA	ALA	ALA	ALA
L1084	L1084	F1019	D849	R762	F674	L601	S523	GLN	LEU	GLY	GLY	GLY	GLY	GLY
R1085	R1085	F1020	C850	R675	F602	F602	P524	ASN	ASN	GLY	GLY	GLY	GLY	GLY
S1086	S1086	K1021	T851	P676	S603	S603	T525	VAL	VAL	VAL	VAL	VAL	VAL	VAL
I1087	I1087	L948	A852	F677	M604	M604	T525	VAL	VAL	VAL	VAL	VAL	VAL	VAL
L1088	L1088	Q949	T853	D678	E605	E605	D526	LEU	LEU	LEU	LEU	LEU	LEU	LEU
V1089	V1089	G950	M854	D678	E605	E605	P527	ASN	ASN	ASN	ASN	ASN	ASN	ASN
K1144	K1144	T1024	M854	D678	E605	E605	V528	GLN	GLN	GLN	GLN	GLN	GLN	GLN
M1145	M1145	A1025	S859	T772	L680	V607	V528	GLN	GLN	GLN	GLN	GLN	GLN	GLN
E1146	E1146	T1025	S859	H773	M681	G608	T534	GLN	GLN	GLN	GLN	GLN	GLN	GLN
T1147	T1147	F1027	Y862	D774	Y682	G609	G535	PHE	PHE	VAL	VAL	VAL	VAL	VAL
V1148	M1095	G1028	E863	V780	L683	A610	G535	LEU	LEU	THR	THR	THR	THR	THR
V1149	K1096	P1029	N864	C766	M686	T611	P536	ALA	ALA	ALA	ALA	ALA	ALA	ALA
T1150	E1087	D1031	E865	A787	L687	D613	P537	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S1151	M1098	S1032	I866	A791	M690	V614	P538	THR	THR	VAL	VAL	VAL	VAL	VAL
P1152	H1099	L1033	G869	A791	M690	A615	F541	ASP	ASP	VAL	VAL	VAL	VAL	VAL
M1153	K1099	L1033	Q870	A791	M690	A615	R542	LYS	LYS	LYS	LYS	LYS	LYS	LYS
E1154	F1100	N1034	X871	A791	M690	A615	D543	LEU	LEU	LEU	LEU	LEU	LEU	LEU
G1155	H1101	R1036	T872	A791	M690	A615	L544	PRO	PRO	PRO	PRO	PRO	PRO	PRO
T1156	K1103	L1037	N873	A791	M690	A615	L544	ASP	ASP	ASP	ASP	ASP	ASP	ASP
V1157	V1157	F1038	N873	A791	M690	A615	L544	GLN	GLN	GLN	GLN	GLN	GLN	GLN
R1158	R1158	L1039	N873	A791	M690	A615	L544	THR	THR	THR	THR	THR	THR	THR
K1159	K1159	L1105	N873	A791	M690	A615	L544	VAL	VAL	VAL	VAL	VAL	VAL	VAL
V1160	V1160	L1105	N873	A791	M690	A615	L544	ASP	ASP	ASP	ASP	ASP	ASP	ASP
V1162	V1162	T1163	N873	A791	M690	A615	L544	GLN	GLN	GLN	GLN	GLN	GLN	GLN
T1163	T1163	T1163	N873	A791	M690	A615	L544	THR	THR	THR	THR	THR	THR	THR
K1164	K1164	K1164	N873	A791	M690	A615	L544	VAL	VAL	VAL	VAL	VAL	VAL	VAL
D1165	D1165	M1166	N873	A791	M690	A615	L544	ASP	ASP	ASP	ASP	ASP	ASP	ASP
M1166	M1166	M1166	N873	A791	M690	A615	L544	GLN	GLN	GLN	GLN	GLN	GLN	GLN

T1167	L1168	E1169	G1170	D1171	D1172	L1173	I1174	L1175	E1176	I1177	E1178
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143019	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size ($\text{\AA}$)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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: BTI, ACO

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	0.19	0/9060	0.43	0/12277
1	B	0.21	0/9068	0.46	4/12288 (0.0%)
1	C	0.23	1/5373 (0.0%)	0.49	3/7284 (0.0%)
1	D	0.18	0/5373	0.45	1/7284 (0.0%)
All	All	0.20	1/28874 (0.0%)	0.45	8/39133 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	536	PRO	CG-CD	-7.58	1.25	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	536	PRO	N-CD-CG	-11.05	86.62	103.20
1	C	536	PRO	CA-N-CD	-6.92	102.32	112.00
1	C	536	PRO	CA-CB-CG	-6.38	92.39	104.50
1	B	260	LEU	CA-C-N	5.85	132.72	121.54
1	B	260	LEU	C-N-CA	5.85	132.72	121.54

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	8869	0	8829	409	0
1	B	8877	0	8840	391	0
1	C	5255	0	5248	273	0
1	D	5255	0	5248	230	0
2	A	15	0	15	1	0
2	B	15	0	15	2	0
2	C	15	0	15	4	0
2	D	15	0	15	5	0
3	A	51	0	34	7	0
3	B	51	0	34	10	0
All	All	28418	0	28293	1271	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 22.

The worst 5 of 1271 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:C:574:HIS:HB3	1:C:580:THR:HA	1.47	0.95
1:D:586:ASP:HA	1:D:589:LYS:HD3	1.49	0.93
1:A:542:ARG:NH1	1:A:634:ILE:O	2.06	0.89
1:A:381:GLU:HA	1:A:389:PRO:HA	1.56	0.87
1:A:465:VAL:HG22	1:A:487:LEU:HD23	1.55	0.87

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	1144/1178 (97%)	1041 (91%)	102 (9%)	1 (0%)	48 81
1	B	1145/1178 (97%)	1050 (92%)	95 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	682/1178 (58%)	626 (92%)	56 (8%)	0	100	100
1	D	682/1178 (58%)	642 (94%)	38 (6%)	2 (0%)	36	70
All	All	3653/4712 (78%)	3359 (92%)	291 (8%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1095	MET
1	A	495	ASN
1	D	1099	HIS

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	942/968 (97%)	942 (100%)	0	100	100
1	B	943/968 (97%)	940 (100%)	3 (0%)	86	85
1	C	564/968 (58%)	564 (100%)	0	100	100
1	D	564/968 (58%)	564 (100%)	0	100	100
All	All	3013/3872 (78%)	3010 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1143	MET
1	B	1144	LYS
1	B	1146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	898	ASN

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Mol	Chain	Res	Type
1	D	1093	GLN
1	C	949	GLN
1	D	498	GLN
1	B	364	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](#)

6 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	$\# Z > 2$
3	ACO	B	2001	-	51,53,53	0.38	0	73,79,79	0.49	1 (1%)
2	BTI	B	2002	1	15,16,16	6.45	11 (73%)	20,21,21	2.83	9 (45%)
3	ACO	A	1202	-	51,53,53	0.47	0	73,79,79	0.52	1 (1%)
2	BTI	D	1900	1	15,16,16	6.44	11 (73%)	20,21,21	2.80	9 (45%)
2	BTI	C	1900	1	15,16,16	6.45	11 (73%)	20,21,21	2.78	8 (40%)
2	BTI	A	1201	1	15,16,16	6.43	11 (73%)	20,21,21	2.83	9 (45%)

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
3	ACO	B	2001	-	-	11/51/67/67	0/3/3/3
2	BTI	B	2002	1	-	2/6/27/27	0/2/2/2
3	ACO	A	1202	-	-	23/51/67/67	0/3/3/3
2	BTI	D	1900	1	-	4/6/27/27	0/2/2/2
2	BTI	C	1900	1	-	5/6/27/27	0/2/2/2
2	BTI	A	1201	1	-	3/6/27/27	0/2/2/2

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1900	BTI	C6-S1	-13.25	1.44	1.81
2	B	2002	BTI	C6-S1	-13.17	1.44	1.81
2	A	1201	BTI	C6-S1	-13.14	1.44	1.81
2	D	1900	BTI	C6-S1	-13.13	1.44	1.81
2	A	1201	BTI	C3-N3	12.46	1.58	1.35

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	BTI	C6-S1-C2	7.08	104.70	89.98
2	C	1900	BTI	C6-S1-C2	6.94	104.42	89.98
2	D	1900	BTI	C6-S1-C2	6.39	103.27	89.98
2	B	2002	BTI	C6-S1-C2	6.19	102.85	89.98
2	D	1900	BTI	C4-C5-N3	5.52	108.56	102.43

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

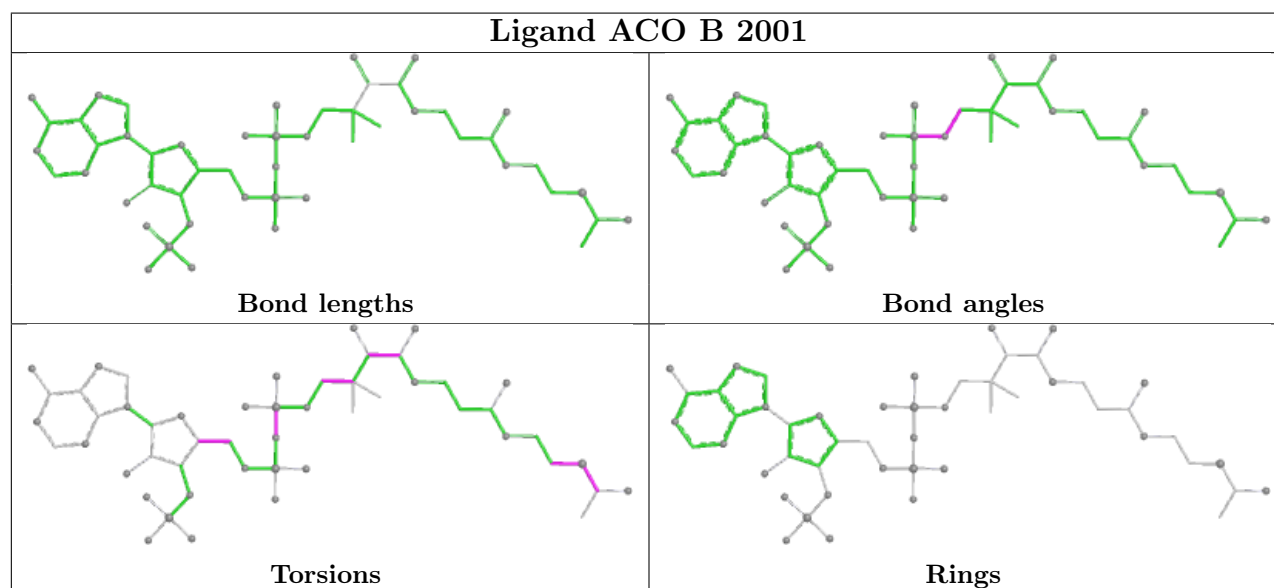
Mol	Chain	Res	Type	Atoms
2	A	1201	BTI	C9-C10-C11-O11
2	A	1201	BTI	S1-C2-C7-C8
2	A	1201	BTI	C4-C2-C7-C8
2	B	2002	BTI	S1-C2-C7-C8
2	B	2002	BTI	C4-C2-C7-C8

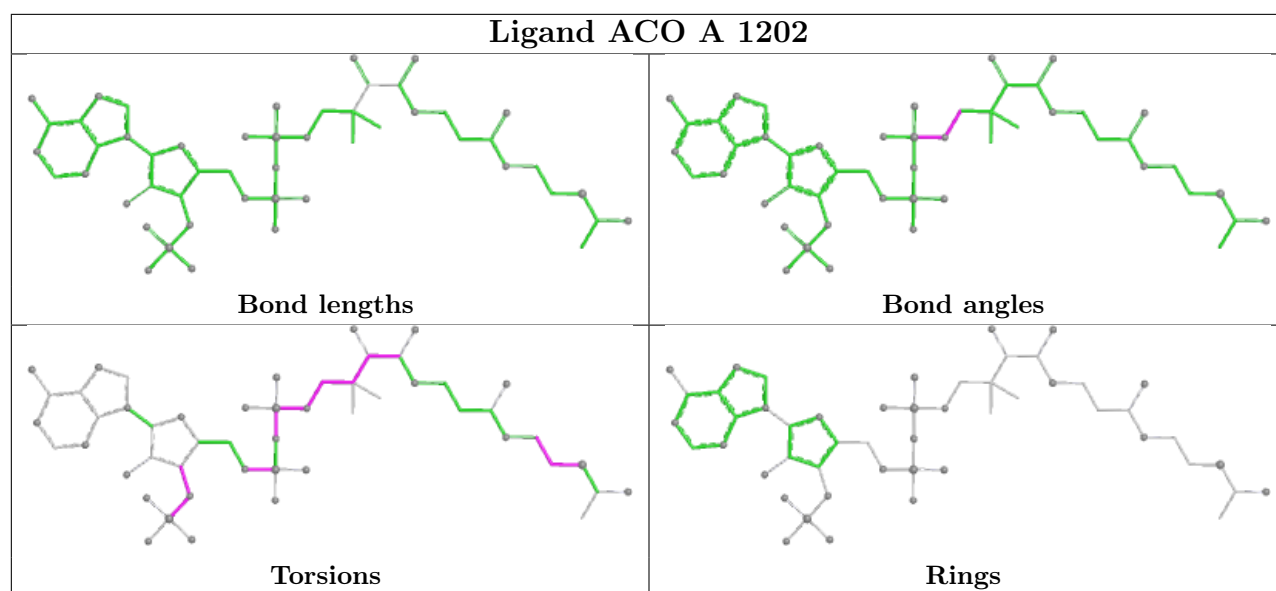
There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	ACO	10	0
2	B	2002	BTI	2	0
3	A	1202	ACO	7	0
2	D	1900	BTI	5	0
2	C	1900	BTI	4	0
2	A	1201	BTI	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.

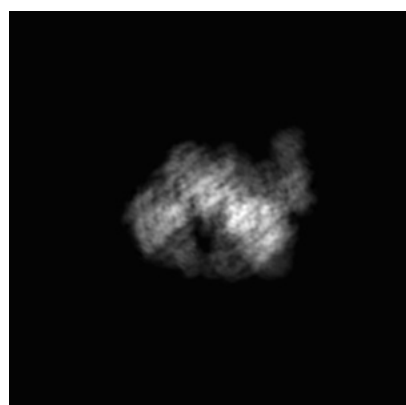
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32778. These allow visual inspection of the internal detail of the map and identification of artifacts.

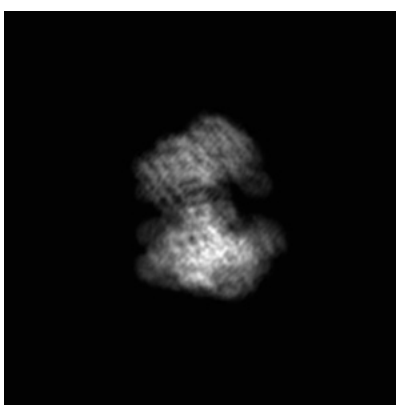
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

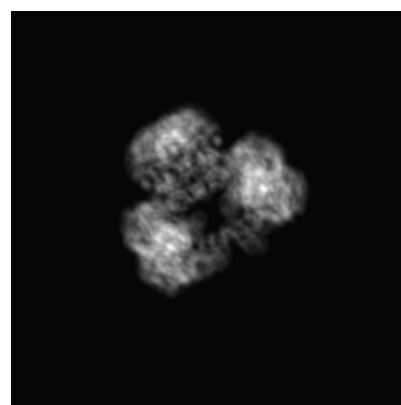
6.1.1 Primary map



X



Y



Z

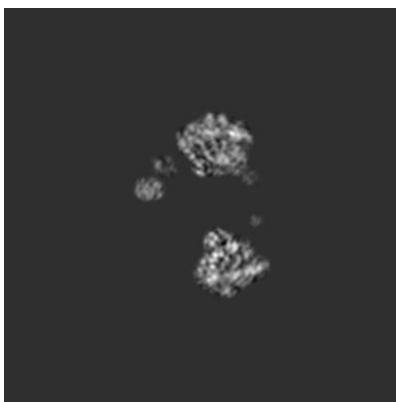
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

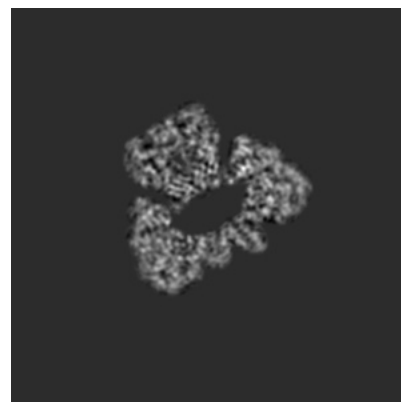
6.2.1 Primary map



X Index: 144



Y Index: 144

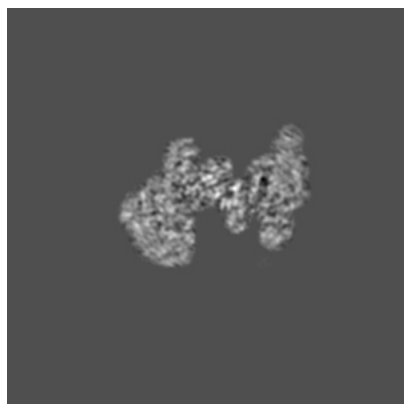


Z Index: 144

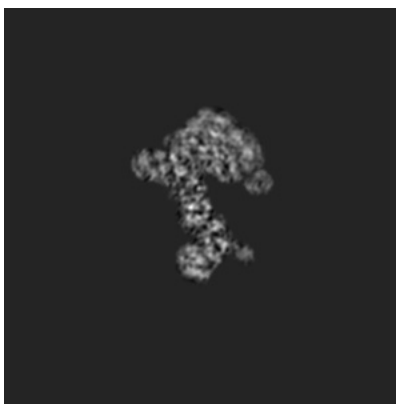
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

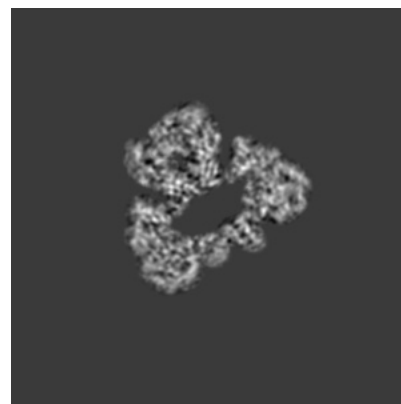
6.3.1 Primary map



X Index: 114



Y Index: 161

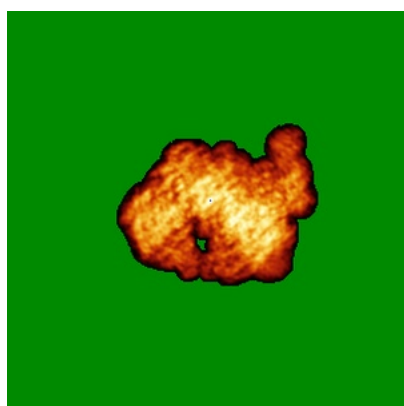


Z Index: 146

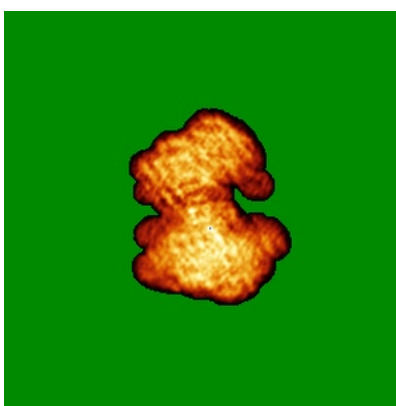
The images above show the largest variance slices of the map in three orthogonal directions.

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

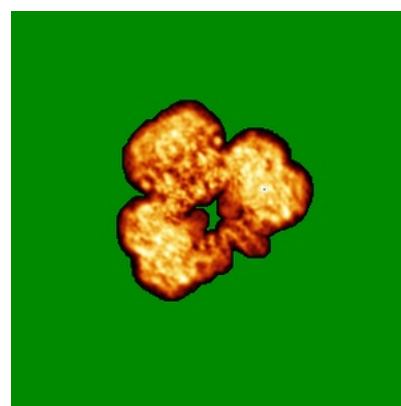
6.4.1 Primary map



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

This section was not generated.

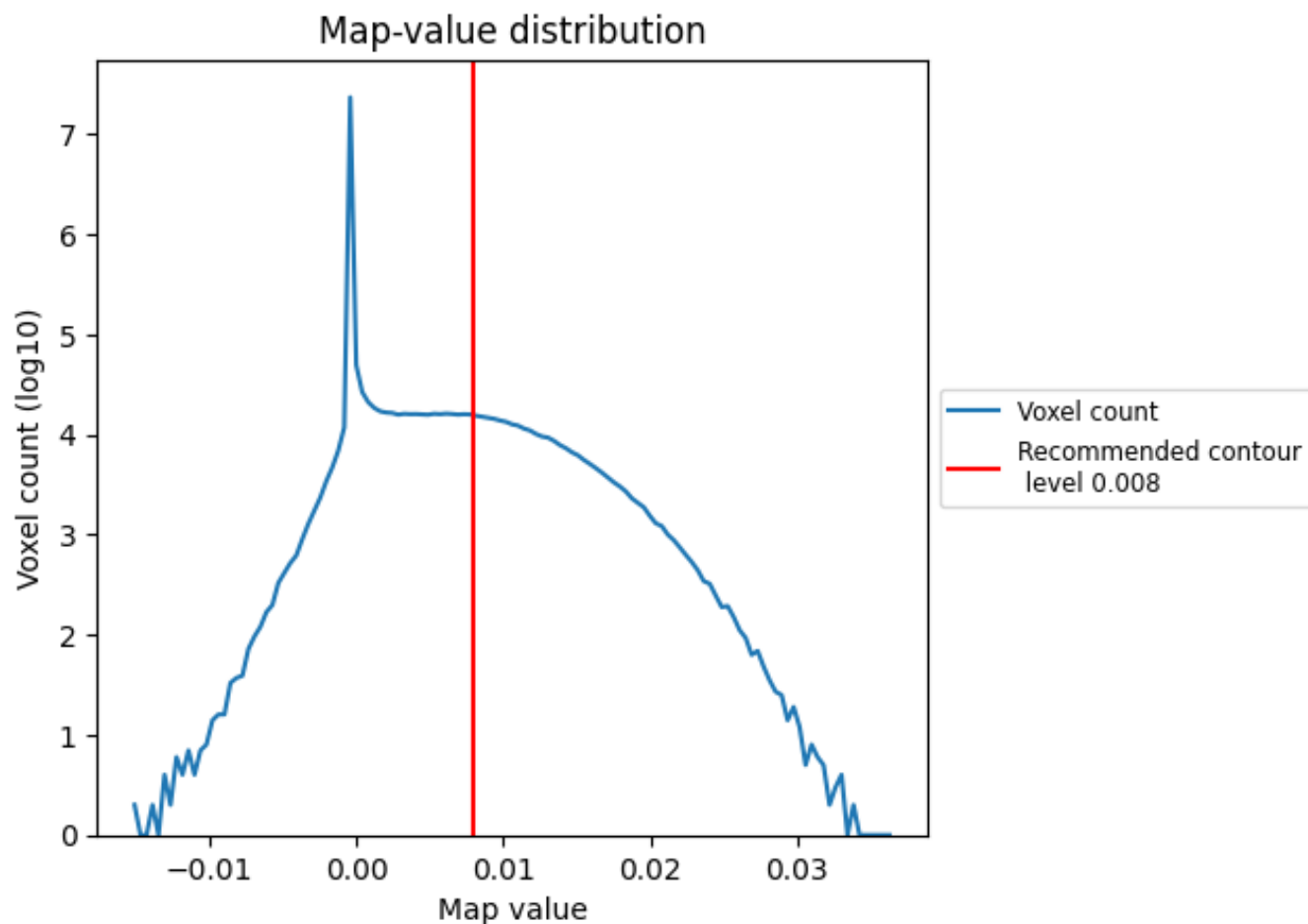
6.6 Mask visualisation

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

7 Map analysis [i](#)

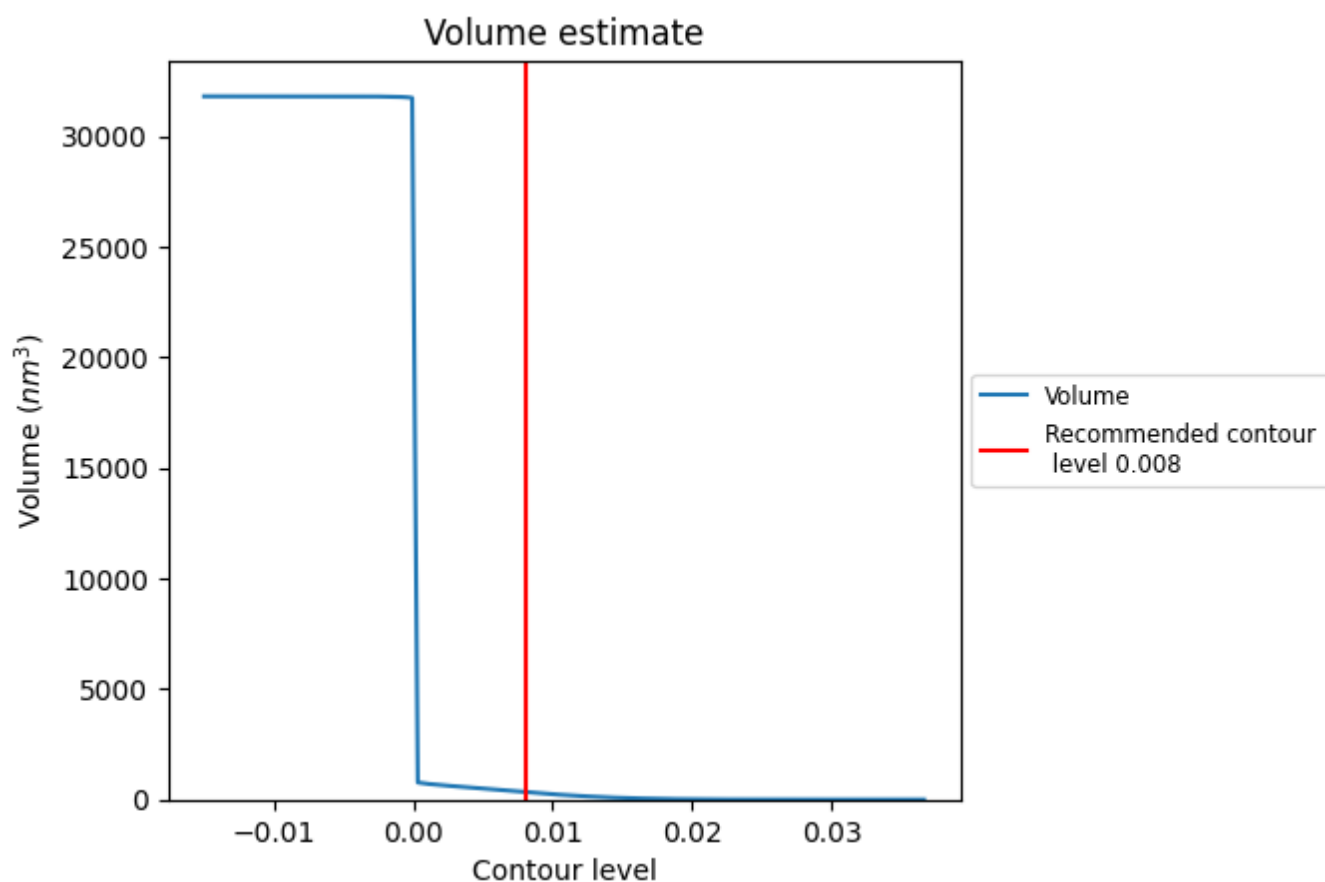
This section contains the results of statistical analysis of the map.

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.

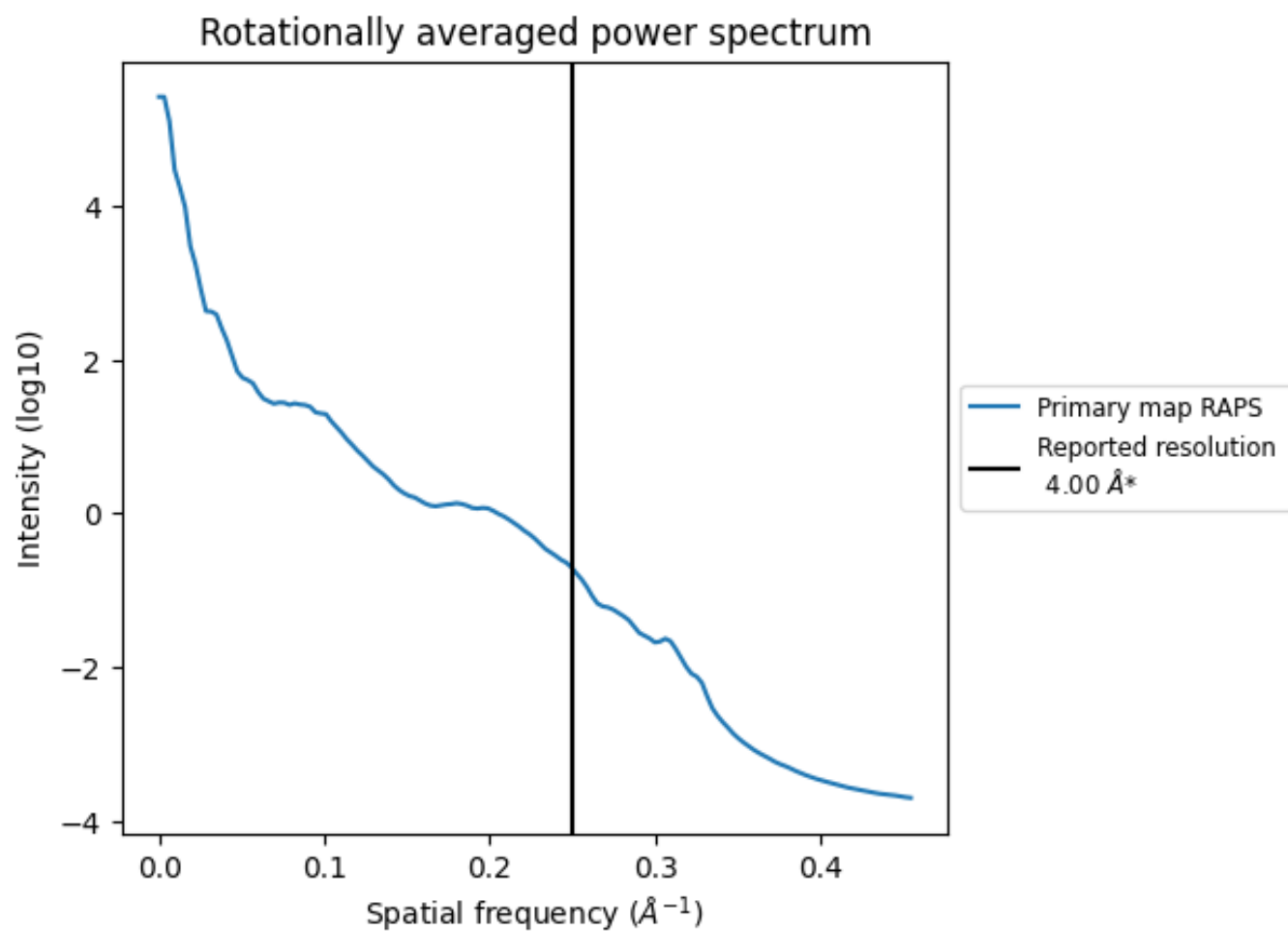
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 306 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 0.250 Å⁻¹

8 Fourier-Shell correlation

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

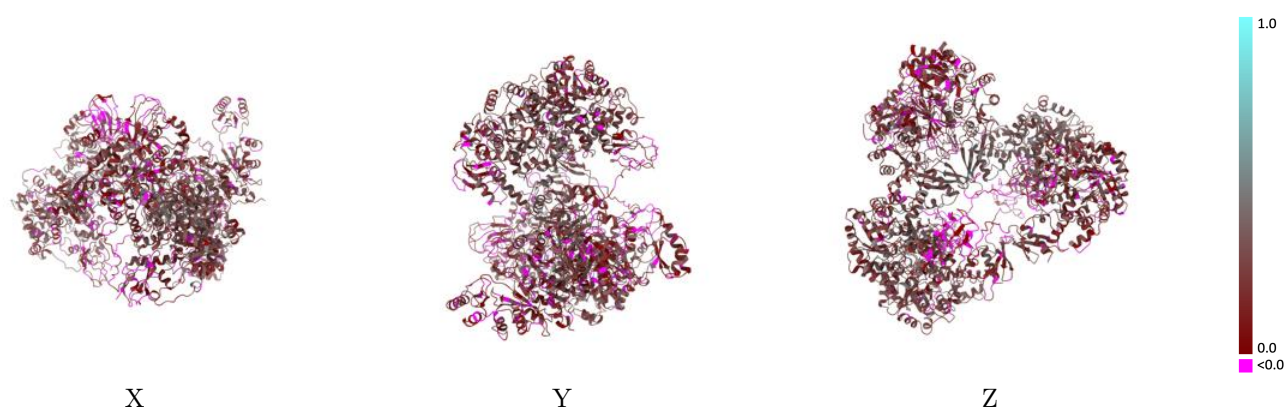
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32778 and PDB model 7WTC. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

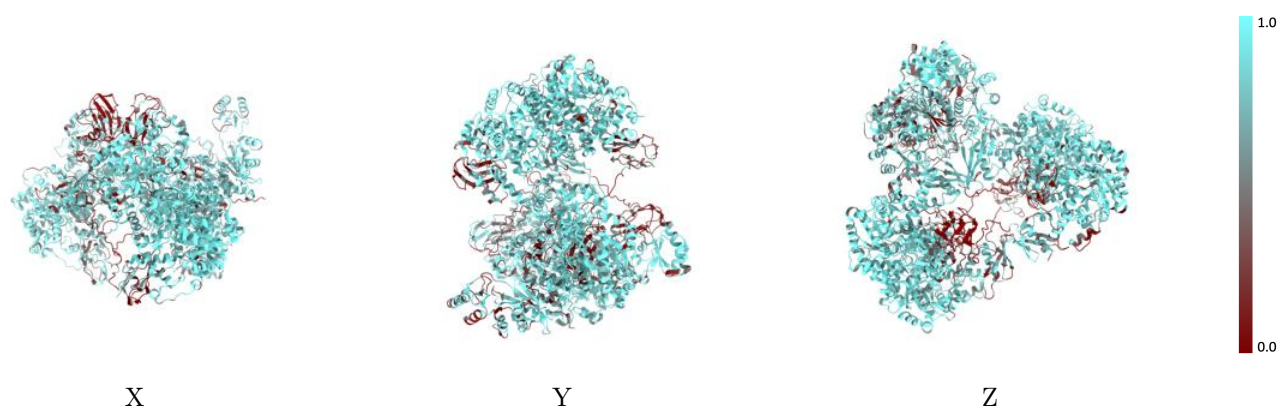
This section was not generated.

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



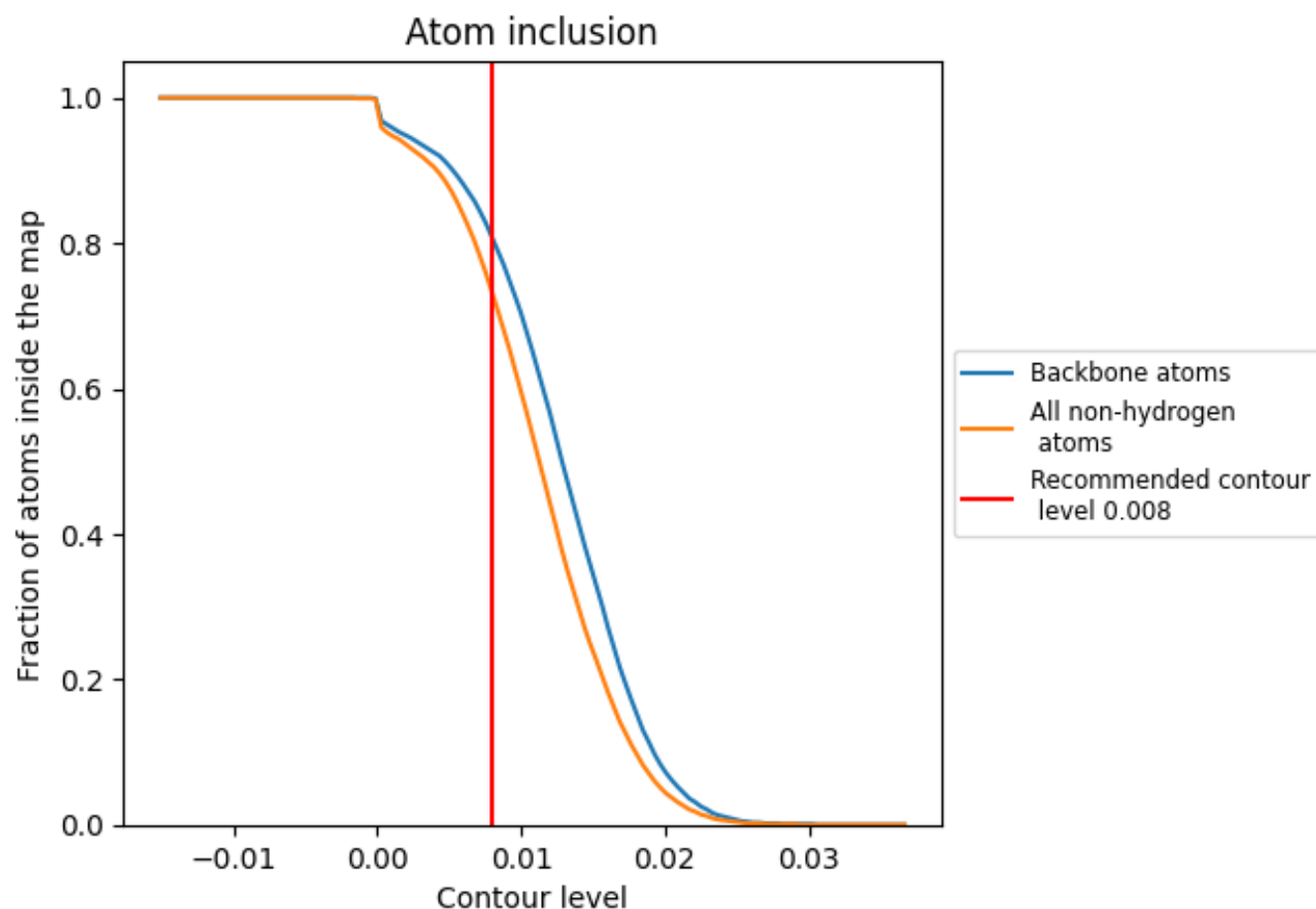
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7320	0.2160
A	0.7570	0.2280
B	0.7290	0.2240
C	0.7310	0.2070
D	0.6970	0.1920

