Full wwPDB EM Validation Report

Mar 25, 2026 – 10:05 PM UTC

PDB ID	:	7LIW / pdb_00007liw
EMDB ID	:	EMD-23387
Title	:	Local refinement of human ATP citrate lyase E599Q mutant ASH domain
Authors	:	Wei, X.; Marmorstein, R.
Deposited on	:	2021-01-28
Resolution	:	2.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

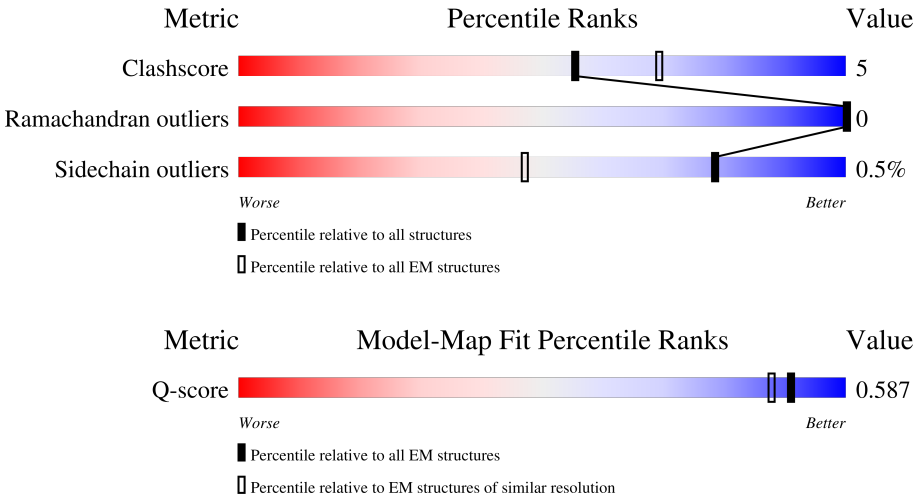
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.85 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	11965 (2.35 - 3.35)

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 <=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	22% · 75%
1	B	1101	· 80% 13% 6%
1	C	1101	23% · 75%
1	D	1101	21% · 75%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14598 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.

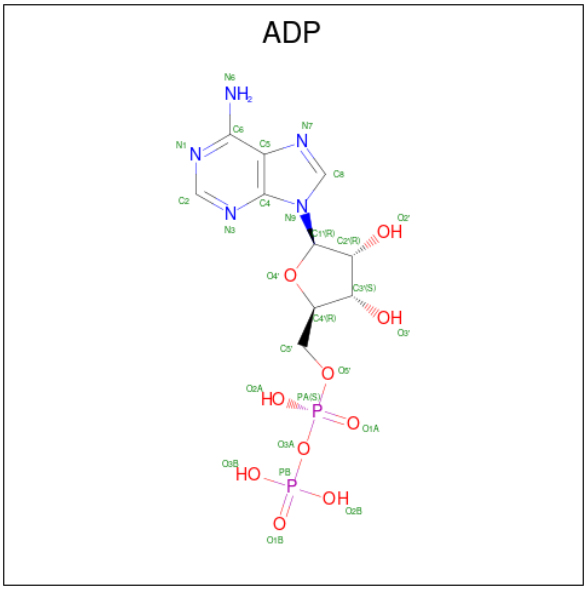
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	279	Total	C	N	O	S	0	0
			2163	1389	369	387	18		
1	B	1034	Total	C	N	O	S	8	0
			8011	5127	1360	1478	46		
1	C	279	Total	C	N	O	S	0	0
			2166	1390	370	388	18		
1	D	279	Total	C	N	O	S	0	0
			2166	1390	370	388	18		

There are 4 discrepancies between the modelled and reference sequences:

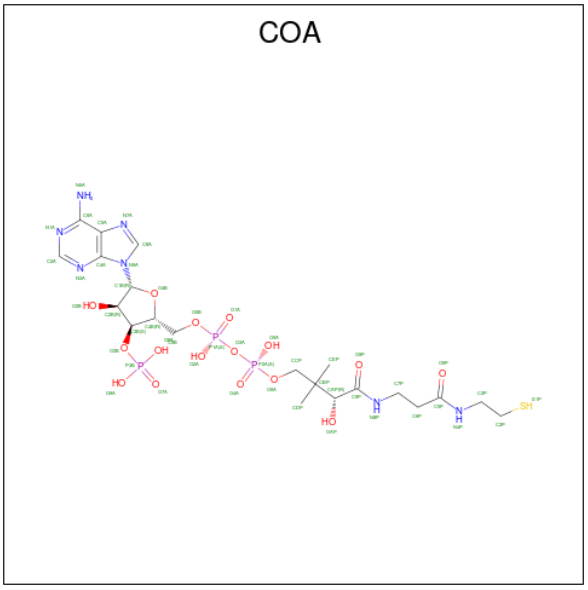
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	GLN	GLU	engineered mutation	UNP P53396
B	599	GLN	GLU	engineered mutation	UNP P53396
C	599	GLN	GLU	engineered mutation	UNP P53396
D	599	GLN	GLU	engineered mutation	UNP P53396

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



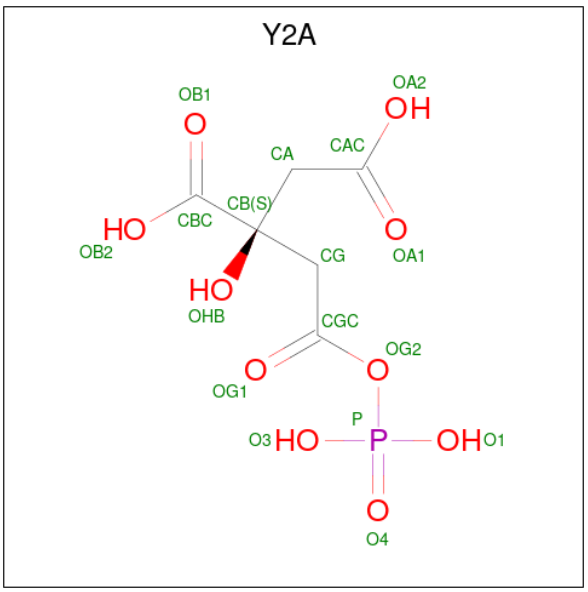
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 4 is (2S)-2-hydroxy-2-[2-oxo-2-(phosphonooxy)ethyl]butanedioic acid (CCD ID: Y2A) (formula: $C_6H_9O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	O	P	0
			17	6	10	1	

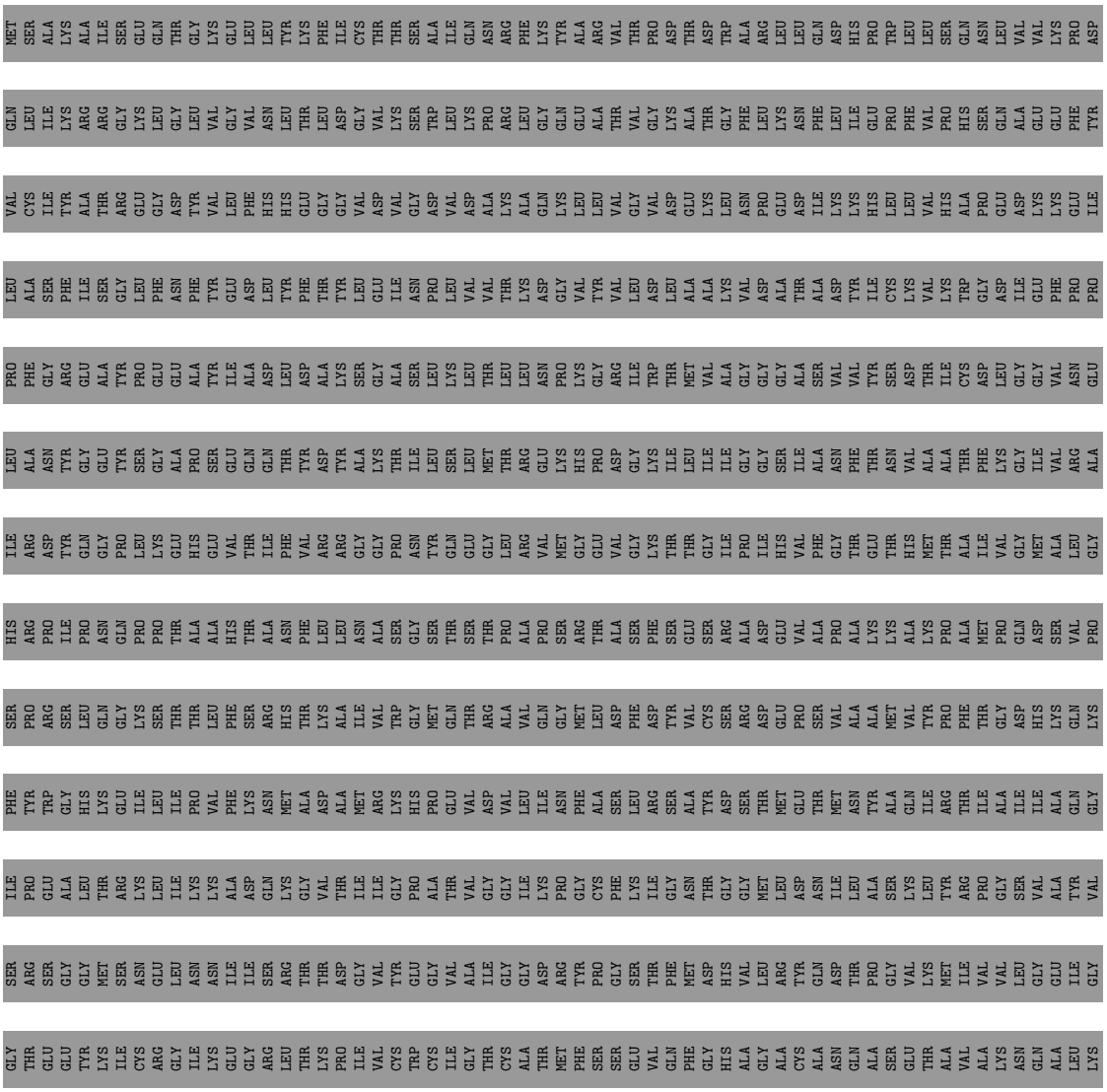
3 Residue-property plots (i)

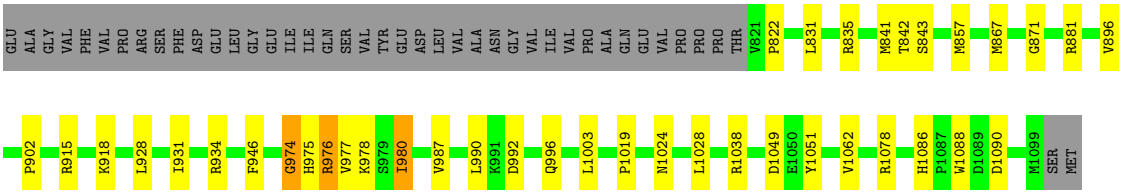
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: ATP-citrate synthase

Chain A:



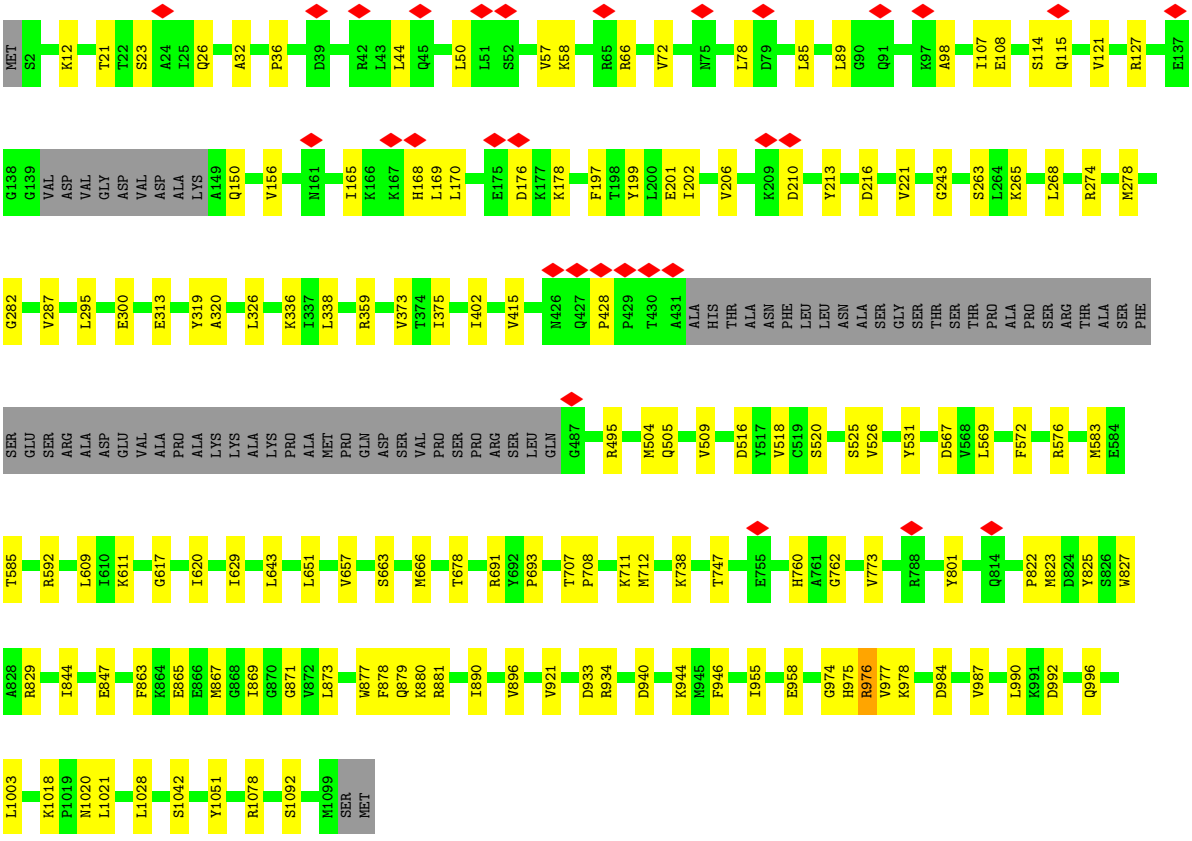




• Molecule 1: ATP-citrate synthase

Chain B:



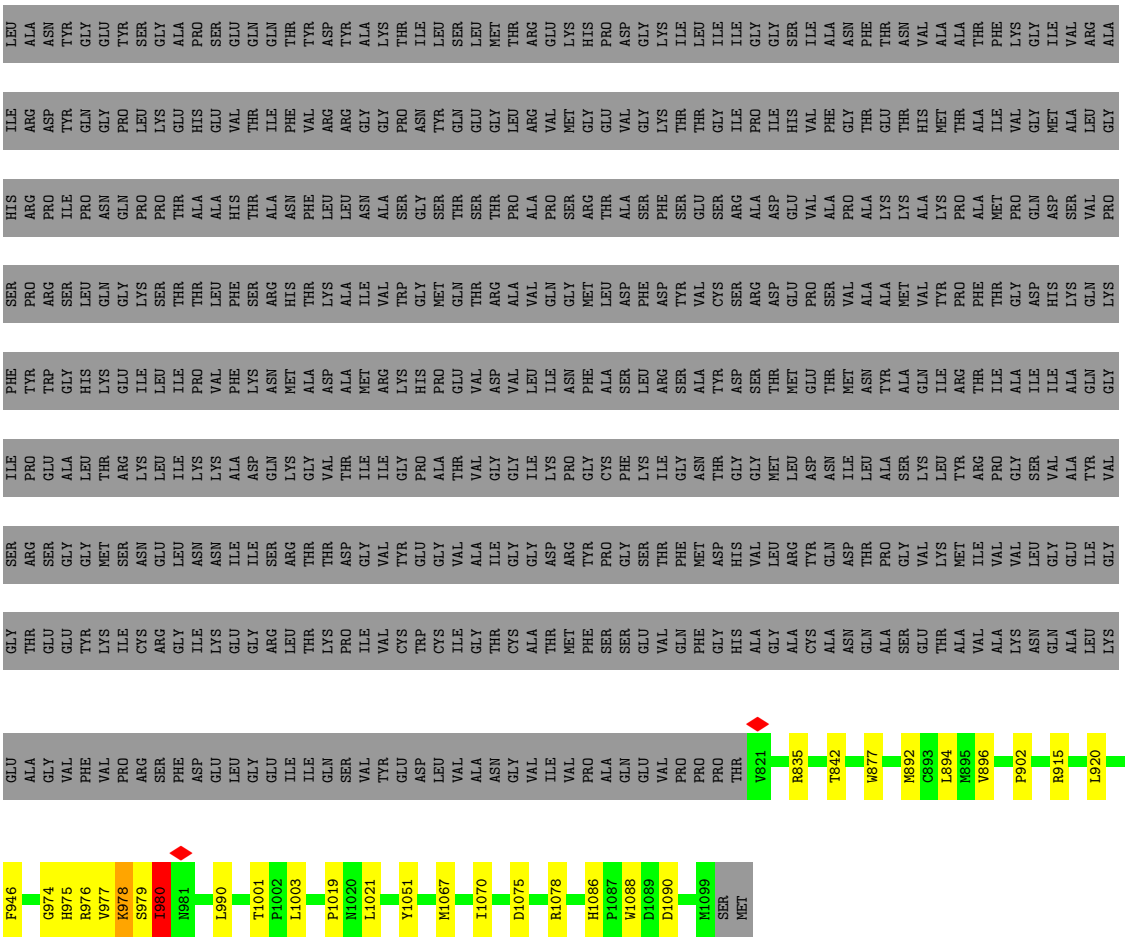


• Molecule 1: ATP-citrate synthase

Chain C:



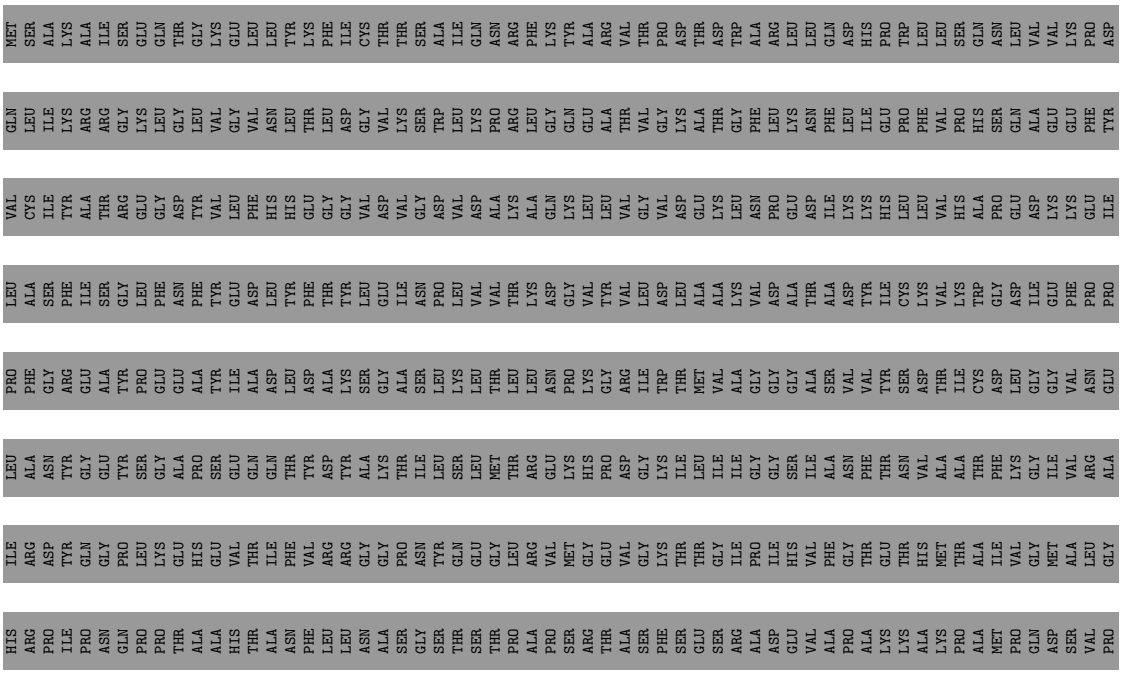


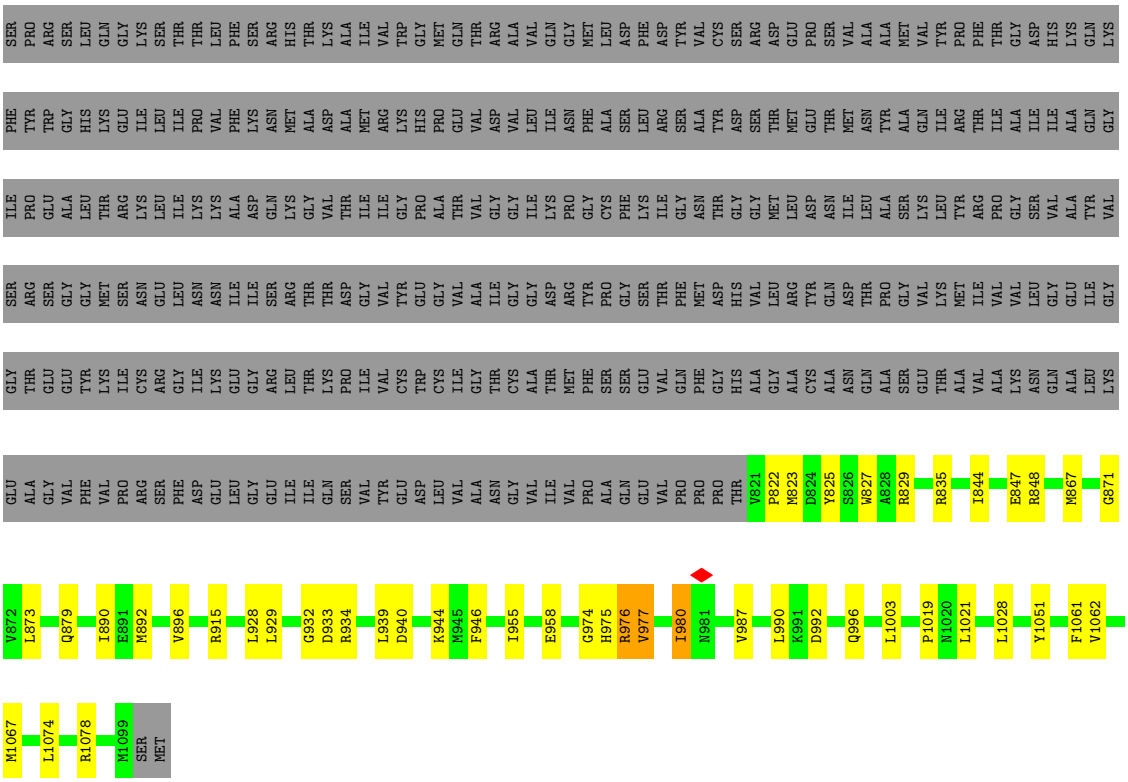


• Molecule 1: ATP-citrate synthase

Chain D:






SER PRO ARG SER LEU GLN GLY LYS SER THR THR LEU PHE SER ARG HIS THR LYS ALA ILE VAL TRP GLY MET GLN THR ARG ALA VAL GLN GLY MET LEU ASP PHE ASP TYR VAL CYS SER ARG ASP GLU PRO SER VAL ALA ALA MET VAL TYR PRO PHE THR GLY ASP LYS GLN GLY
PHE TYR TRP GLY HIS LYS GLU ILE LEU ILE PRO VAL PHE LYS ASN MET ALA ASP ALA MET ARG LYS HIS PRO GLU VAL ASP VAL LEU ILE ASN PHE ALA SER LEU ARG SER ALA TYR ASP SER THR MET GLU THR MET ASN TYR ALA GLN ILE ARG THR ILE ALA ILE ILE ALA GLN GLY
ILE PRO GLU ALA LEU THR ARG LYS LEU ILE LYS LYS ALA ASP GLN LYS GLY VAL THR ILE ILE GLY PRO ALA THR VAL GLY GLY ILE LYS PRO GLY CYS PHE LYS ILE GLY ASN THR GLY GLY MET LEU ASP ASN ILE LEU ALA SER LYS LEU TYR ARG PRO GLY SER VAL ALA ALA TYR
SER ARG SER GLY GLY MET SER ASN GLU LEU ASN ASN ILE ILE SER ARG THR THR ASP GLY VAL TYR GLU GLY VAL ALA ILE GLY GLY ASP ARG TYR PRO GLY SER THR PHE MET ASP HIS VAL LEU ARG TYR GLN ASP THR PRO GLY VAL LYS MET ILE VAL VAL LEU GLY GLU ILE GLY
GLY THR GLU GLU TYR LYS ILE CYS ARG GLY ILE LYS GLU GLY ARG LEU THR LYS PRO ILE VAL CYS TRP CYS ILE GLY THR CYS ALA THR MET PHE SER SER GLU VAL GLN PHE GLY HIS ALA GLY ALA CYS ALA ASN GLN ALA SER GLU THR ALA VAL ALA LYS ASN GLN ALA LEU LYS
GLU ALA GLY VAL PHE VAL PRO ARG SER PHE ASP GLU LEU GLY GLU ILE ILE GLN SER VAL TYR GLU ASP LEU VAL ALA ASN GLY VAL ILE VAL PRO ALA GLN GLU VAL PRO PRO PRO THR V821 P822 M823 D824 Y825 S826 W827 A828 R829 R835 I844 E847 R848 M867 G871
V872 L873 Q879 I890 E891 M892 V896 R915 L928 L929 G932 D933 R934 L939 D940 K944 N945 F946 I955 E958 G974 H975 R976 V977 I980 N981 V987 L990 K991 D992 Q996 L1003 P1019 N1020 L1021 L1028 Y1051 F1061 V1062
M1067 L1074 R1078 M1099 SER MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	800000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	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	4.587	Depositor
Minimum map value	-2.876	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.199	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	191.4, 191.4, 191.4	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86999995, 0.86999995, 0.86999995	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y2A, ADP, COA

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	0.46	1/2209 (0.0%)	0.61	0/2979
1	B	0.35	0/8231	0.56	1/11143 (0.0%)
1	C	0.48	2/2212 (0.1%)	0.69	7/2983 (0.2%)
1	D	0.44	1/2212 (0.0%)	0.64	3/2983 (0.1%)
All	All	0.40	4/14864 (0.0%)	0.60	11/20088 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	974	GLY	CA-C	-6.30	1.47	1.52
1	C	978	LYS	C-O	-5.66	1.16	1.23
1	C	979	SER	C-O	-5.37	1.19	1.24
1	D	975	HIS	C-O	-5.22	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	978	LYS	N-CA-C	8.16	121.45	110.35
1	B	976	ARG	N-CA-C	8.08	119.72	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	980	ILE	N-CA-CB	-6.81	98.69	110.13
1	C	979	SER	CB-CA-C	-6.20	99.38	112.82
1	C	980	ILE	N-CA-C	5.92	118.15	109.63
1	C	980	ILE	CB-CA-C	5.82	120.81	111.32
1	C	980	ILE	CA-C-N	5.59	131.83	123.05
1	C	980	ILE	C-N-CA	5.59	131.83	123.05
1	D	976	ARG	N-CA-C	5.55	117.33	111.28
1	D	848	ARG	CA-CB-CG	5.52	125.14	114.10
1	D	977	VAL	N-CA-C	5.39	116.65	112.12

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	831	LEU	Peptide
1	A	980	ILE	Peptide
1	B	428	PRO	Peptide
1	D	980	ILE	Peptide

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	2163	0	2180	28	0
1	B	8011	0	8044	84	0
1	C	2166	0	2184	24	0
1	D	2166	0	2184	30	0
2	B	27	0	12	1	0
3	B	48	0	32	2	0
4	B	17	0	0	3	0
All	All	14598	0	14636	145	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 5.

All (145) 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:B:975:HIS:O	1:B:1020:ASN:OD1	1.69	1.10
1:C:975:HIS:ND1	1:C:978:LYS:HB2	1.97	0.79
3:B:2002:COA:S1P	4:B:2003:Y2A:OG1	2.48	0.70
1:A:976:ARG:HG3	1:A:977:VAL:HG23	1.74	0.68
1:A:975:HIS:HE1	1:A:978:LYS:HE2	1.58	0.67
1:B:992:ASP:O	1:B:996:GLN:NE2	2.29	0.65
1:B:880:LYS:HD3	1:B:1042:SER:HB3	1.80	0.63
1:B:32:ALA:HB3	1:B:107:ILE:HB	1.80	0.63
1:B:583:MET:HE2	1:B:609:LEU:HD23	1.80	0.63
1:A:992:ASP:O	1:A:996:GLN:NE2	2.31	0.62
1:B:278:MET:HE3	1:B:319:TYR:HD2	1.63	0.62
1:C:975:HIS:CE1	1:C:978:LYS:HG2	2.36	0.60
1:B:877:TRP:O	1:D:1078:ARG:NH2	2.35	0.59
1:B:156:VAL:HB	1:B:611:LYS:HD2	1.85	0.59
1:B:57:VAL:HG21	1:B:85:LEU:HD11	1.85	0.59
1:D:823:MET:HE2	1:D:827:TRP:HD1	1.68	0.59
1:B:170:LEU:O	1:B:178:LYS:NZ	2.36	0.58
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.84	0.58
1:B:12:LYS:NZ	1:B:108:GLU:OE1	2.36	0.58
1:B:707:THR:O	1:B:738:LYS:NZ	2.37	0.58
1:B:921:VAL:HG12	1:D:929:LEU:HD23	1.86	0.57
1:A:934:ARG:NH1	1:D:915:ARG:O	2.37	0.56
1:A:835:ARG:HD3	1:D:822:PRO:HG2	1.86	0.56
1:D:987:VAL:HG13	1:D:1028:LEU:HD22	1.88	0.56
1:A:1088:TRP:NE1	1:B:847:GLU:OE1	2.37	0.56
1:B:869:ILE:HG23	1:D:1067:MET:HE1	1.88	0.56
1:B:865:GLU:OE1	1:B:881:ARG:NH1	2.39	0.56
1:B:263:SER:OG	1:B:265:LYS:NZ	2.40	0.55
1:A:1078:ARG:NH2	1:C:877:TRP:O	2.40	0.54
1:B:375:ILE:HB	1:B:402:ILE:HG12	1.89	0.54
1:A:915:ARG:O	1:D:934:ARG:NH1	2.41	0.54
1:B:974:GLY:HA2	1:B:1021:LEU:HA	1.88	0.54
1:B:978:LYS:HD2	1:B:984:ASP:HA	1.89	0.53
1:C:975:HIS:ND1	1:C:978:LYS:CB	2.71	0.53
1:A:974:GLY:O	1:A:1024:ASN:OD1	2.27	0.53
1:B:58:LYS:HG2	1:B:72:VAL:HG22	1.91	0.53
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.91	0.52
1:A:946:PHE:HB3	1:A:1003:LEU:HD11	1.92	0.52
1:A:841:MET:HG2	1:B:1092:SER:HB3	1.91	0.52
1:C:974:GLY:HA2	1:C:1021:LEU:HA	1.91	0.52
1:B:822:PRO:HG2	1:C:835:ARG:HD3	1.91	0.52
1:C:896:VAL:HG21	1:C:990:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:946:PHE:HB3	1:C:1003:LEU:HD11	1.91	0.52
1:D:825:TYR:OH	1:D:829:ARG:NH1	2.43	0.51
1:B:509:VAL:HG13	1:B:526:VAL:HG21	1.93	0.51
1:D:974:GLY:HA2	1:D:1021:LEU:HA	1.92	0.51
1:B:121[B]:VAL:HG23	1:B:202:ILE:HB	1.93	0.51
1:A:928:LEU:HD11	1:A:1062:VAL:HG13	1.91	0.50
1:B:940:ASP:OD2	1:B:944:LYS:NZ	2.39	0.50
1:B:282:GLY:N	4:B:2003:Y2A:O3	2.43	0.50
1:B:313:GLU:OE1	1:B:359:ARG:NH2	2.45	0.50
1:B:825:TYR:OH	1:B:829:ARG:NH1	2.43	0.50
1:B:287:VAL:HG21	1:B:666:MET:HE2	1.94	0.50
1:B:934:ARG:NH1	1:C:915:ARG:O	2.45	0.50
1:A:1078:ARG:HH21	1:C:1051:TYR:HE1	1.60	0.50
1:D:928:LEU:HD11	1:D:1062:VAL:HG13	1.93	0.50
1:A:1051:TYR:OH	1:C:1078:ARG:NH1	2.45	0.50
1:B:114:SER:OG	1:B:115:GLN:N	2.44	0.50
1:B:127:ARG:NH2	1:B:693:PRO:O	2.42	0.50
1:B:976:ARG:HG2	1:B:976:ARG:HH11	1.77	0.50
1:B:58:LYS:NZ	1:B:216:ASP:OD1	2.40	0.49
1:B:576:ARG:NH2	3:B:2002:COA:O7A	2.41	0.49
1:B:26:GLN:NE2	1:B:210:ASP:O	2.44	0.49
1:B:21:THR:HG22	1:B:23:SER:H	1.76	0.49
1:B:567:ASP:OD1	1:B:567:ASP:N	2.44	0.49
1:C:1001:THR:O	1:C:1001:THR:OG1	2.31	0.49
1:B:1078:ARG:NH1	1:D:1051:TYR:OH	2.45	0.48
1:A:857:MET:HE1	1:A:881:ARG:HD2	1.96	0.48
1:B:657:VAL:HG22	1:B:712:MET:HG3	1.96	0.48
1:B:1051:TYR:OH	1:D:1078:ARG:NH1	2.41	0.48
1:B:50:LEU:HB3	1:B:78:LEU:HD12	1.96	0.48
1:B:518:VAL:HG21	1:B:643:LEU:HD21	1.95	0.48
1:B:150:GLN:NE2	1:B:168:HIS:O	2.41	0.48
1:B:987:VAL:HG13	1:B:1028:LEU:HD22	1.96	0.48
1:B:933:ASP:OD1	1:B:933:ASP:N	2.43	0.48
1:C:975:HIS:CE1	1:C:978:LYS:CG	2.96	0.48
1:B:199:TYR:OH	1:B:201:GLU:OE1	2.27	0.47
1:B:878:PHE:HA	1:D:1078:ARG:HH22	1.80	0.47
1:C:975:HIS:ND1	1:C:978:LYS:CG	2.78	0.47
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.96	0.47
1:B:844:ILE:HG22	1:B:879:GLN:NE2	2.30	0.47
1:B:823:MET:HE2	1:B:827:TRP:CD1	2.50	0.46
1:C:1086:HIS:NE2	1:C:1090:ASP:OD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:OD1	1:B:176:ASP:N	2.46	0.46
1:D:955:ILE:HG13	1:D:958:GLU:H	1.81	0.46
1:B:747:THR:HG23	1:B:773:VAL:HG22	1.98	0.45
1:D:980:ILE:HG22	1:D:1019:PRO:HB3	1.97	0.45
1:B:268:LEU:HD21	1:B:326:LEU:HD13	1.98	0.45
1:A:1086:HIS:NE2	1:A:1090:ASP:OD2	2.39	0.45
1:B:691:ARG:HD2	1:B:762:GLY:HA2	1.98	0.45
1:B:44:LEU:HD11	1:B:78:LEU:HD11	1.98	0.45
1:D:940:ASP:OD2	1:D:944:LYS:NZ	2.49	0.45
1:C:980:ILE:HD11	1:C:1019:PRO:HB3	1.99	0.44
1:B:516:ASP:OD2	1:B:525:SER:N	2.51	0.44
1:B:867:MET:HB2	1:B:871:GLY:HA3	1.99	0.44
1:C:892:MET:HE2	1:C:990:LEU:HD23	1.99	0.44
1:D:933:ASP:OD1	1:D:933:ASP:N	2.40	0.44
1:D:867:MET:HB2	1:D:871:GLY:HA3	2.00	0.44
1:A:918:LYS:HD3	1:D:932:GLY:HA3	2.00	0.44
1:C:1088:TRP:NE1	1:D:847:GLU:OE2	2.50	0.43
1:A:902:PRO:HG3	1:C:842:THR:HG21	2.01	0.43
1:D:844:ILE:HG22	1:D:879:GLN:NE2	2.33	0.43
1:B:66:ARG:N	2:B:2001:ADP:O2B	2.44	0.43
1:B:278:MET:HE1	1:B:320:ALA:HB2	2.01	0.43
1:A:867:MET:HE2	1:A:867:MET:HB3	1.72	0.43
1:D:1074:LEU:O	1:D:1078:ARG:HG3	2.19	0.43
1:B:336:LYS:HB2	1:B:373:VAL:HG22	2.01	0.43
1:B:708:PRO:O	1:B:711:LYS:NZ	2.41	0.43
1:B:165:ILE:HG23	1:B:169:LEU:HD12	2.01	0.43
4:B:2003:Y2A:OA1	4:B:2003:Y2A:OHB	2.35	0.42
1:D:946:PHE:HB3	1:D:1003:LEU:HD11	2.01	0.42
1:A:928:LEU:HD12	1:A:931:ILE:HD12	2.02	0.42
1:B:197:PHE:HA	1:B:221:VAL:HA	2.02	0.42
1:A:1038:ARG:NH2	1:A:1049:ASP:OD1	2.53	0.42
1:B:36:PRO:HD3	1:B:89:LEU:HD11	2.01	0.42
1:B:505:GLN:HG3	1:B:572:PHE:CG	2.54	0.42
1:C:980:ILE:H	1:C:980:ILE:HG13	1.29	0.42
1:B:946:PHE:HB3	1:B:1003:LEU:HD11	2.02	0.42
1:B:495:ARG:NH2	1:B:520:SER:O	2.53	0.42
1:B:504:MET:HE3	1:B:531:TYR:HB2	2.02	0.42
1:B:678:THR:HG23	1:B:801:TYR:CD1	2.55	0.41
1:D:873:LEU:HD22	1:D:890:ILE:HG21	2.02	0.41
1:B:98:ALA:HB1	1:B:243:GLY:HA3	2.02	0.41
1:B:295:LEU:HD12	1:B:415:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:HB	1:B:213:TYR:HB2	2.02	0.41
1:B:592:ARG:NH2	1:B:617:GLY:O	2.53	0.41
1:A:822:PRO:HG2	1:D:835:ARG:HD2	2.03	0.41
1:A:980:ILE:HG22	1:A:1019:PRO:HB3	2.03	0.41
1:A:867:MET:HB2	1:A:871:GLY:HA3	2.03	0.41
1:B:663:SER:HB3	1:B:760:HIS:HE1	1.85	0.41
1:B:338:LEU:HD23	1:B:375:ILE:HG12	2.01	0.41
1:B:629:ILE:HD13	1:B:651:LEU:HD13	2.03	0.41
1:B:873:LEU:HD22	1:B:890:ILE:HG21	2.03	0.41
1:A:987:VAL:HG13	1:A:1028:LEU:HD13	2.03	0.41
1:B:863:PHE:CE1	1:D:892:MET:HG3	2.55	0.41
1:B:955:ILE:HG13	1:B:958:GLU:H	1.85	0.41
1:D:939:LEU:HD23	1:D:1061:PHE:HB2	2.01	0.41
1:B:1018:LYS:HB2	1:B:1021:LEU:HG	2.03	0.40
1:C:894:LEU:HB3	1:C:1067:MET:HE1	2.03	0.40
1:B:569:LEU:HD22	1:B:585:THR:HG21	2.03	0.40
1:A:843:SER:OG	1:C:1075:ASP:OD1	2.39	0.40
1:B:274:ARG:HG2	1:B:300:GLU:HB3	2.02	0.40
1:C:920:LEU:HD11	1:C:1070:ILE:HG23	2.02	0.40
1:D:992:ASP:O	1:D:996:GLN:HG3	2.21	0.40
1:A:896:VAL:HG21	1:A:990:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/1101 (25%)	268 (97%)	9 (3%)	0	100	100
1	B	1036/1101 (94%)	1006 (97%)	30 (3%)	0	100	100
1	C	277/1101 (25%)	266 (96%)	11 (4%)	0	100	100
1	D	277/1101 (25%)	265 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1867/4404 (42%)	1805 (97%)	62 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	229/909 (25%)	228 (100%)	1 (0%)	84 92
1	B	858/909 (94%)	855 (100%)	3 (0%)	86 93
1	C	230/909 (25%)	227 (99%)	3 (1%)	61 79
1	D	230/909 (25%)	228 (99%)	2 (1%)	70 84
All	All	1547/3636 (42%)	1538 (99%)	9 (1%)	78 89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	976	ARG
1	B	620[A]	ILE
1	B	620[B]	ILE
1	B	977	VAL
1	C	976	ARG
1	C	977	VAL
1	C	980	ILE
1	D	976	ARG
1	D	977	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	900	HIS
1	A	975	HIS
1	A	996	GLN

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Mol	Chain	Res	Type
1	A	1024	ASN
1	A	1058	ASN
1	B	161	ASN
1	B	332	HIS
1	B	365	GLN
1	B	563	HIS
1	B	638	ASN
1	B	645	ASN
1	B	814	GLN
1	B	900	HIS
1	B	1020	ASN
1	B	1058	ASN
1	C	888	GLN
1	C	1058	ASN
1	C	1081	GLN
1	D	900	HIS
1	D	988	GLN
1	D	1039	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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	$\#\|Z\| > 2$
4	Y2A	B	2003	-	15,16,16	1.33	1 (6%)	21,24,24	1.32	1 (4%)
2	ADP	B	2001	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	11 (25%)
3	COA	B	2002	-	47,50,50	2.02	19 (40%)	69,75,75	1.95	17 (24%)

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	Y2A	B	2003	-	-	10/19/21/21	-
2	ADP	B	2001	-	-	5/16/32/32	0/3/3/3
3	COA	B	2002	-	-	16/48/64/64	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ADP	C5-C4	4.46	1.47	1.39
3	B	2002	COA	C5A-N7A	-3.90	1.32	1.39
3	B	2002	COA	P3B-O8A	-3.72	1.41	1.54
3	B	2002	COA	C8A-N9A	-3.54	1.31	1.37
3	B	2002	COA	P3B-O9A	-3.51	1.41	1.54
3	B	2002	COA	C4A-N9A	-3.43	1.30	1.37
3	B	2002	COA	P3B-O3B	-3.39	1.53	1.59
4	B	2003	Y2A	P-OG2	3.03	1.65	1.59
3	B	2002	COA	C2A-N1A	-2.85	1.28	1.33
3	B	2002	COA	O4B-C4B	-2.71	1.39	1.45
3	B	2002	COA	C2A-N3A	-2.60	1.29	1.33
2	B	2001	ADP	C5-C6	2.57	1.48	1.41
3	B	2002	COA	C6A-N1A	-2.55	1.28	1.35
3	B	2002	COA	C5P-N4P	-2.47	1.27	1.33
3	B	2002	COA	CDP-CBP	-2.45	1.48	1.53
2	B	2001	ADP	C5-N7	-2.38	1.34	1.39
3	B	2002	COA	C2B-C1B	-2.36	1.46	1.53
2	B	2001	ADP	C8-N7	2.26	1.36	1.31
3	B	2002	COA	OAP-CAP	-2.24	1.38	1.42
3	B	2002	COA	CEP-CBP	-2.23	1.49	1.53
3	B	2002	COA	O5P-C5P	-2.21	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	COA	P1A-O2A	-2.18	1.45	1.55
2	B	2001	ADP	C4-N9	-2.08	1.33	1.37
3	B	2002	COA	P2A-O3A	-2.03	1.57	1.59
3	B	2002	COA	O9P-C9P	-2.01	1.19	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2002	COA	C5A-C4A-N3A	-5.80	118.73	126.72
2	B	2001	ADP	C5-C4-N3	-5.62	118.98	126.72
3	B	2002	COA	N3A-C4A-N9A	4.76	135.27	127.17
3	B	2002	COA	N3A-C2A-N1A	-4.76	121.38	128.58
2	B	2001	ADP	N3-C4-N9	4.44	134.71	127.17
3	B	2002	COA	OAP-CAP-CBP	-4.38	100.04	110.18
3	B	2002	COA	C7P-C6P-C5P	-4.24	105.33	112.39
3	B	2002	COA	C2A-N3A-C4A	4.20	122.10	111.83
4	B	2003	Y2A	OB2-CBC-CB	3.84	120.51	113.14
2	B	2001	ADP	C2-N3-C4	3.60	120.62	111.83
2	B	2001	ADP	C4-C5-N7	-3.42	106.68	110.58
2	B	2001	ADP	N3-C2-N1	-3.19	123.75	128.58
3	B	2002	COA	C4A-N9A-C8A	3.06	108.95	105.74
3	B	2002	COA	C2P-C3P-N4P	-2.89	105.74	112.31
2	B	2001	ADP	C4-N9-C8	2.77	108.65	105.74
3	B	2002	COA	O4B-C1B-C2B	-2.76	100.72	106.62
3	B	2002	COA	C6A-C5A-N7A	2.74	137.36	132.09
3	B	2002	COA	C2A-N1A-C6A	2.73	123.21	118.73
3	B	2002	COA	C4A-C5A-N7A	-2.65	107.55	110.58
3	B	2002	COA	O2A-P1A-O3A	2.54	114.13	107.27
2	B	2001	ADP	C5-N7-C8	2.51	107.40	103.45
3	B	2002	COA	C3P-N4P-C5P	-2.44	118.29	122.82
3	B	2002	COA	N9A-C8A-N7A	-2.30	110.67	113.94
3	B	2002	COA	C6P-C7P-N8P	-2.15	107.43	112.00
3	B	2002	COA	C5A-N7A-C8A	2.15	106.82	103.45
2	B	2001	ADP	C6-C5-N7	2.12	136.18	132.09
2	B	2001	ADP	C3'-C2'-C1'	2.11	105.45	101.46
2	B	2001	ADP	N9-C8-N7	-2.09	110.96	113.94
2	B	2001	ADP	O3B-PB-O2B	2.04	115.46	107.80

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O2A
2	B	2001	ADP	C5'-O5'-PA-O3A
3	B	2002	COA	C5B-O5B-P1A-O1A
3	B	2002	COA	O9P-C9P-CAP-CBP
3	B	2002	COA	N8P-C9P-CAP-CBP
3	B	2002	COA	N8P-C9P-CAP-OAP
3	B	2002	COA	C2P-C3P-N4P-C5P
4	B	2003	Y2A	OHB-CB-CG-CGC
4	B	2003	Y2A	CA-CB-CG-CGC
3	B	2002	COA	C6P-C5P-N4P-C3P
3	B	2002	COA	O5P-C5P-N4P-C3P
4	B	2003	Y2A	CAC-CA-CB-CBC
3	B	2002	COA	O9P-C9P-CAP-OAP
4	B	2003	Y2A	CAC-CA-CB-OHB
3	B	2002	COA	P2A-O3A-P1A-O2A
3	B	2002	COA	C4B-C3B-O3B-P3B
3	B	2002	COA	S1P-C2P-C3P-N4P
4	B	2003	Y2A	CBC-CB-CG-CGC
3	B	2002	COA	C5B-O5B-P1A-O2A
3	B	2002	COA	C5B-O5B-P1A-O3A
4	B	2003	Y2A	CA-CB-CBC-OB2
4	B	2003	Y2A	CG-CB-CBC-OB2
4	B	2003	Y2A	CAC-CA-CB-CG
3	B	2002	COA	P2A-O3A-P1A-O1A
2	B	2001	ADP	PA-O3A-PB-O1B
2	B	2001	ADP	PA-O3A-PB-O3B
3	B	2002	COA	P1A-O3A-P2A-O5A
4	B	2003	Y2A	OHB-CB-CBC-OB2
4	B	2003	Y2A	CG-CB-CBC-OB1
3	B	2002	COA	CDP-CBP-CCP-O6A

There are no ring outliers.

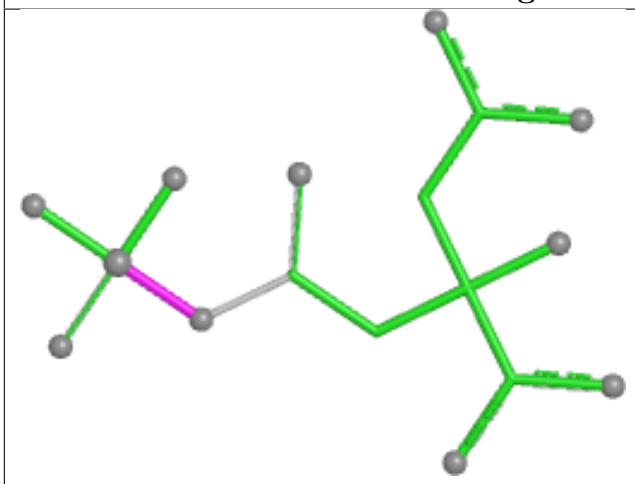
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2003	Y2A	3	0
2	B	2001	ADP	1	0
3	B	2002	COA	2	0

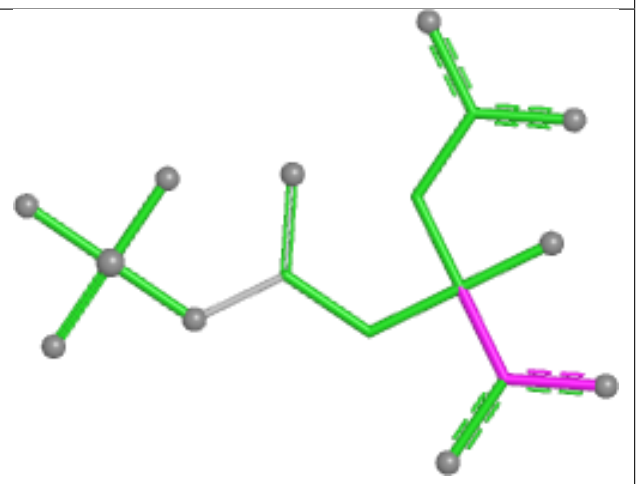
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

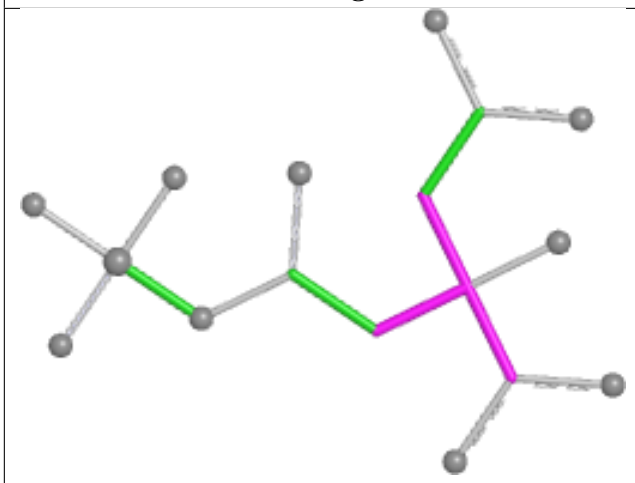
Ligand Y2A B 2003



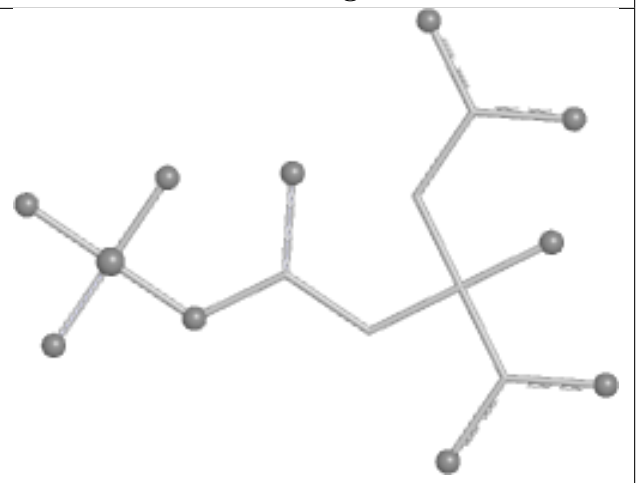
Bond lengths



Bond angles

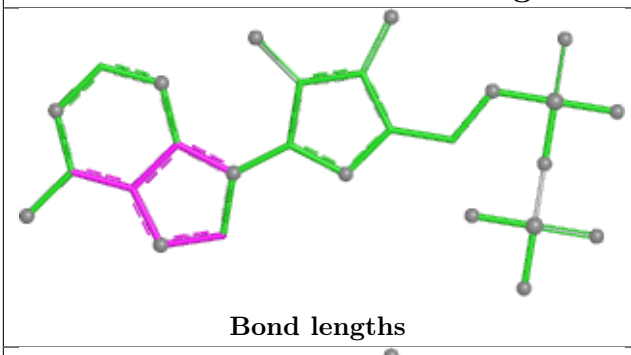


Torsions

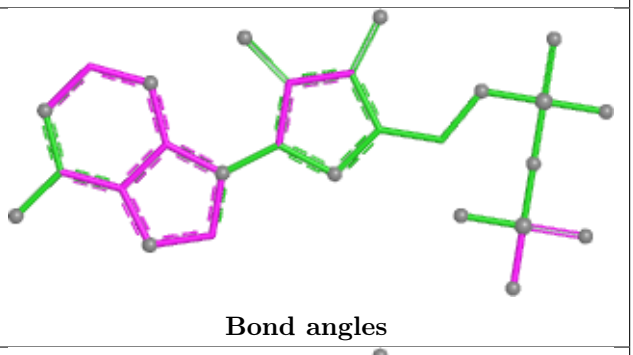


Rings

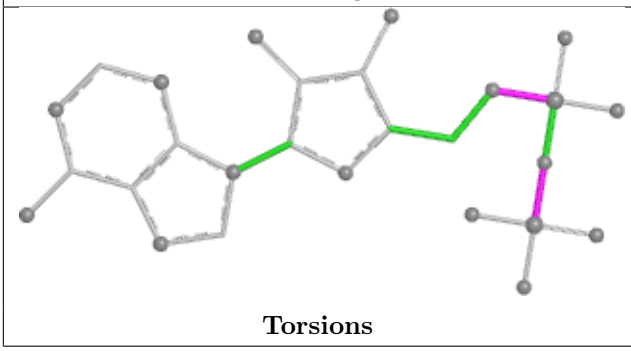
Ligand ADP B 2001



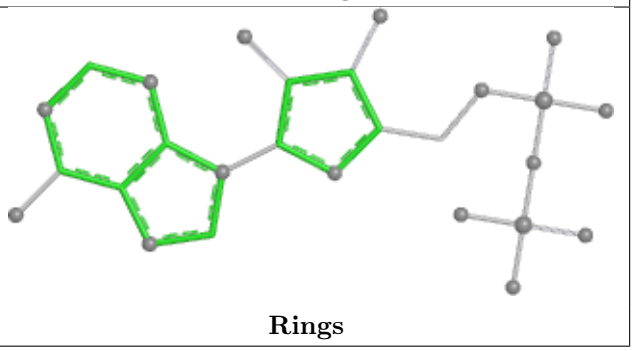
Bond lengths



Bond angles

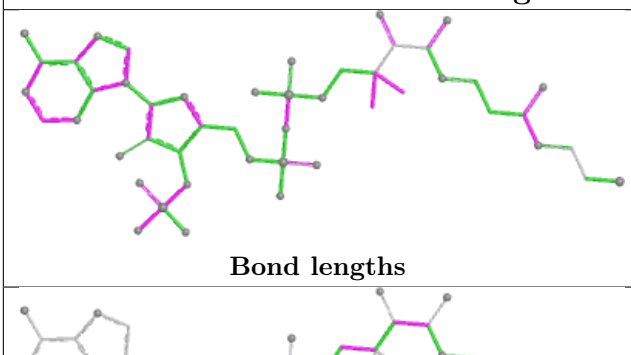


Torsions

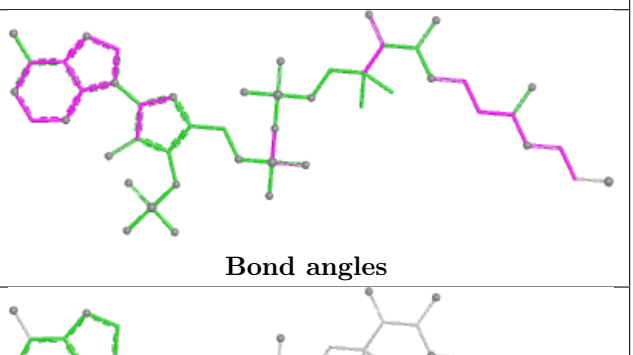


Rings

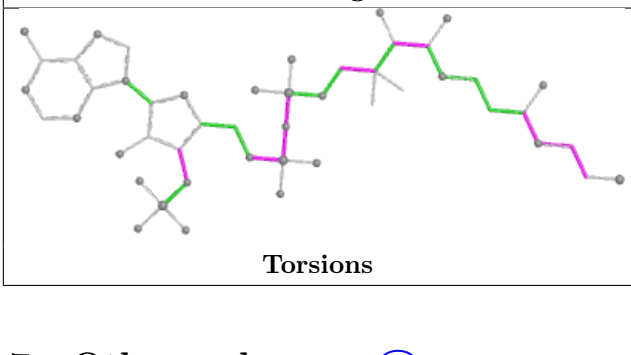
Ligand COA B 2002



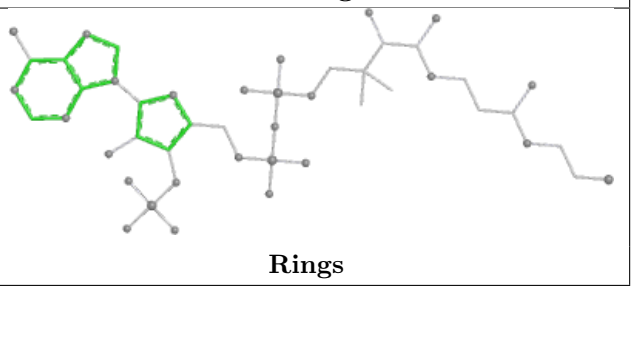
Bond lengths



Bond angles



Torsions



Rings

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.

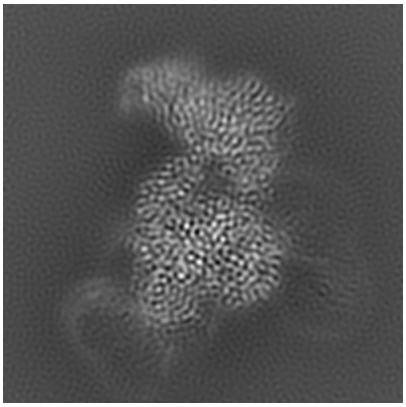
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23387. These allow visual inspection of the internal detail of the map and identification of artifacts.

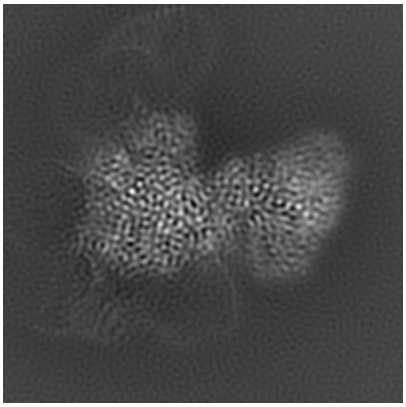
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

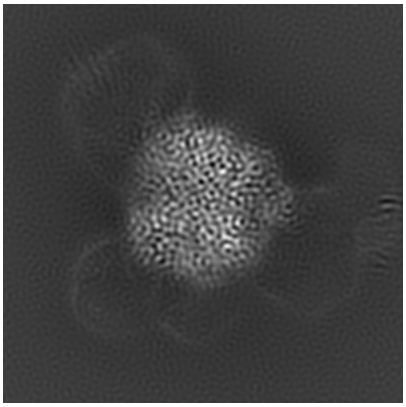
6.1.1 Primary map



X



Y

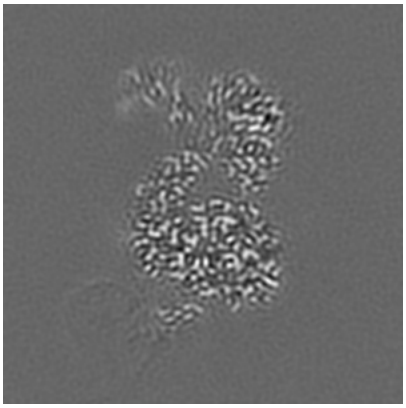


Z

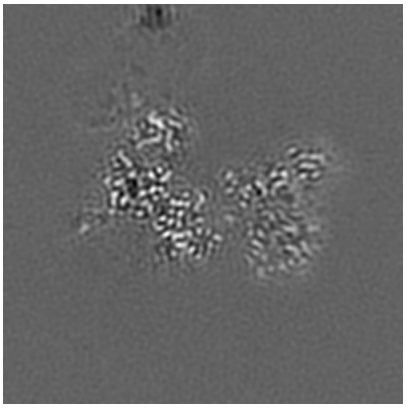
The images above show the map projected in three orthogonal directions.

6.2 Central slices

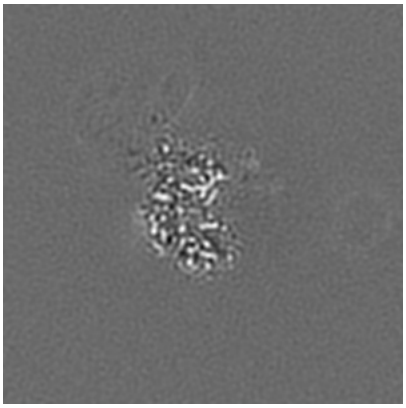
6.2.1 Primary map



X Index: 110



Y Index: 110

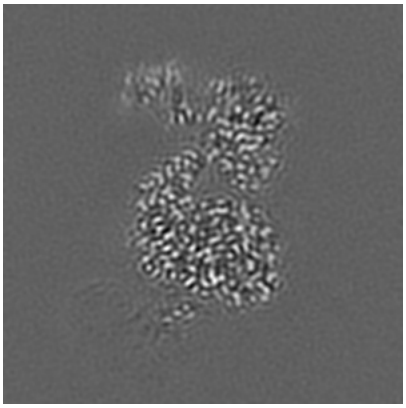


Z Index: 110

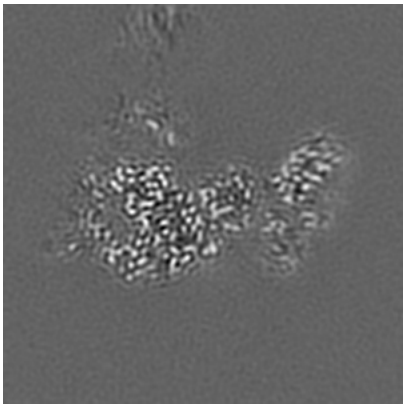
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

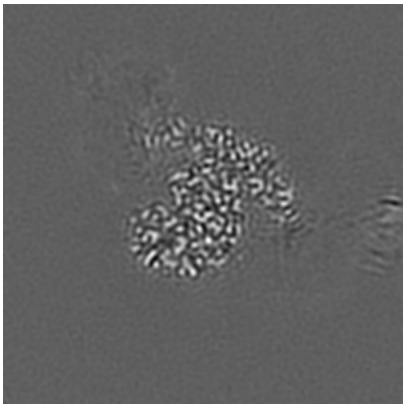
6.3.1 Primary map



X Index: 112



Y Index: 98

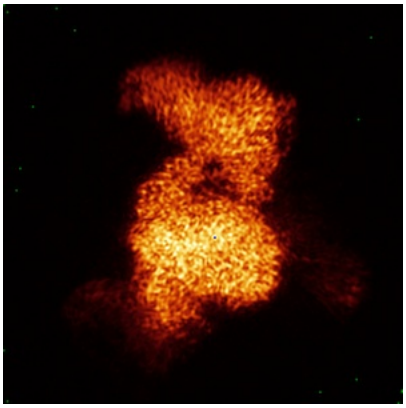


Z Index: 85

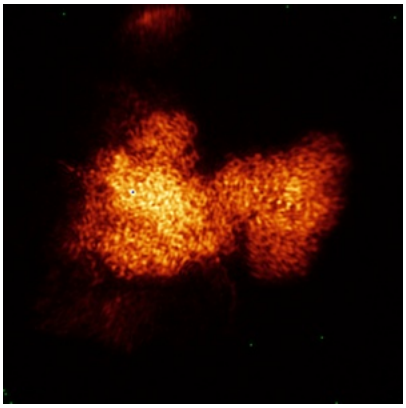
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

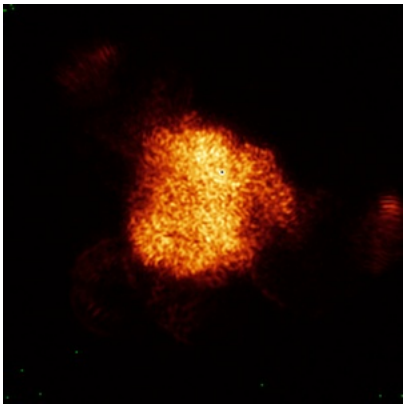
6.4.1 Primary map



X



Y

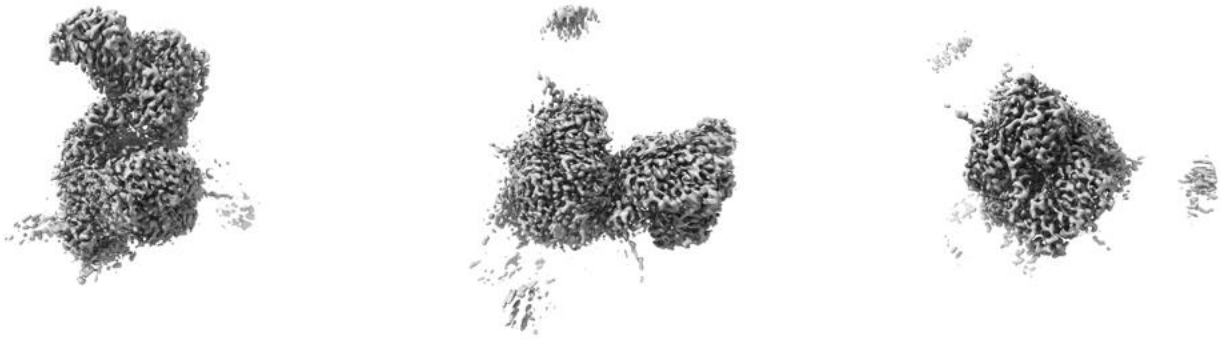


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

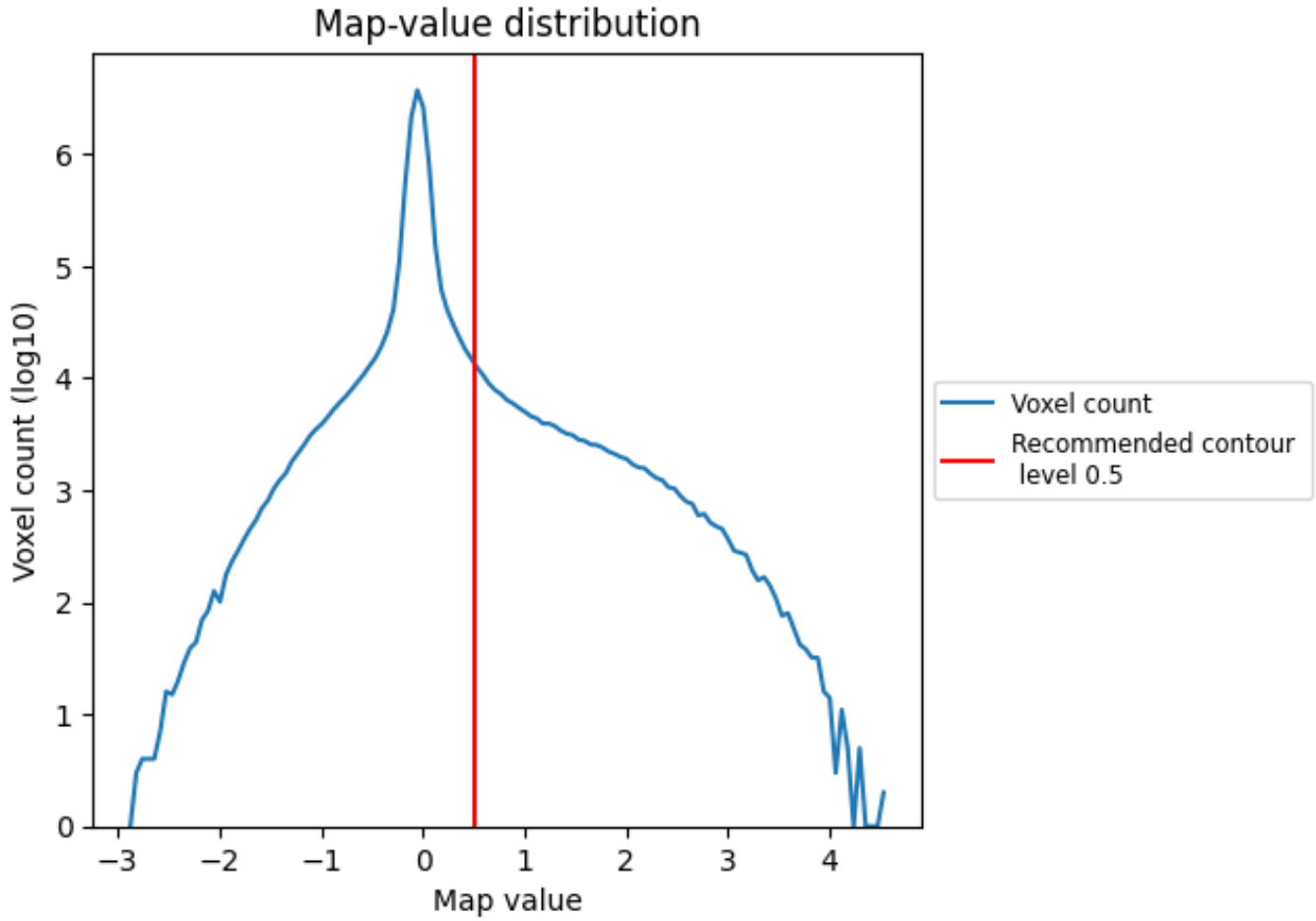
6.6 Mask visualisation (i)

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

7 Map analysis

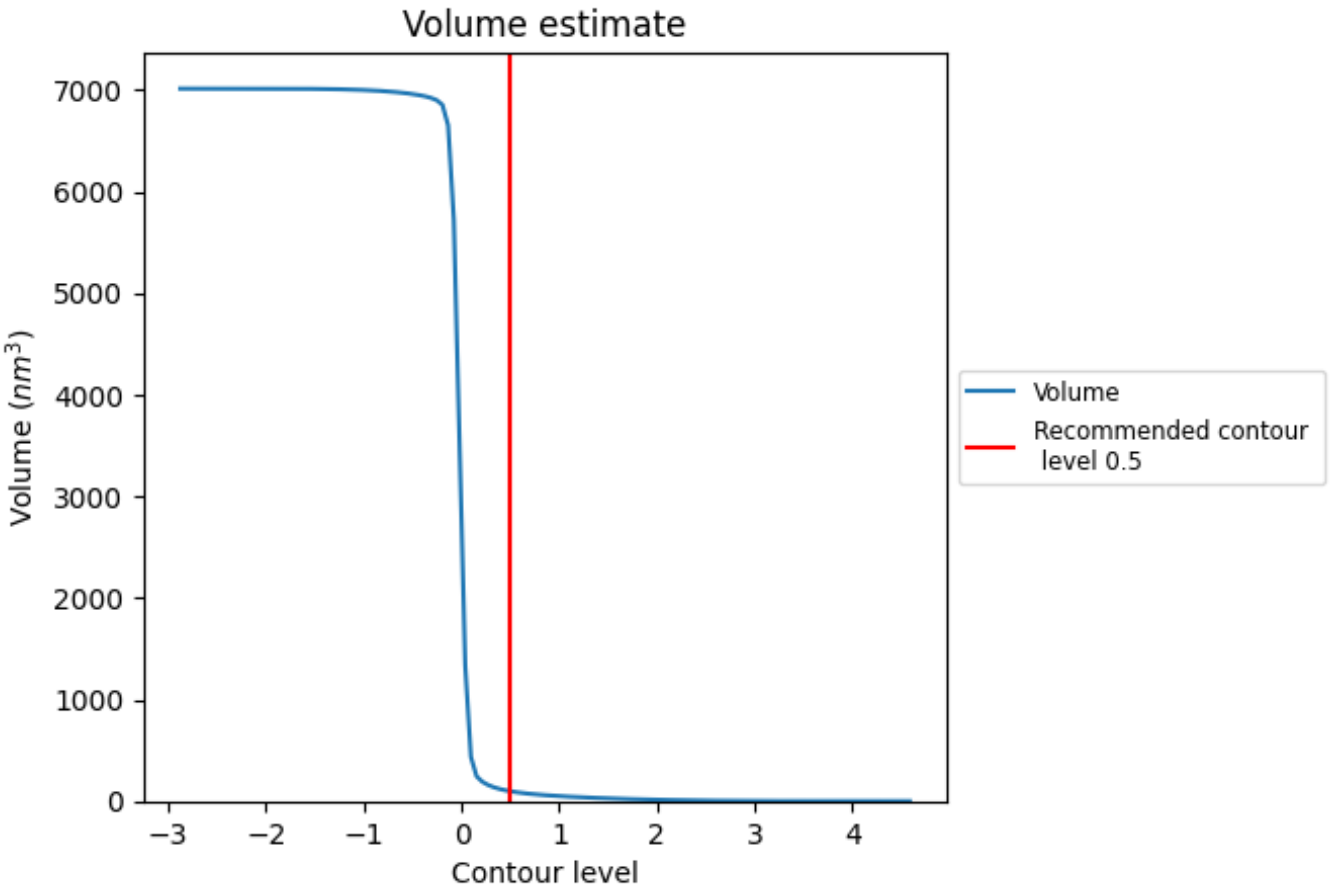
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

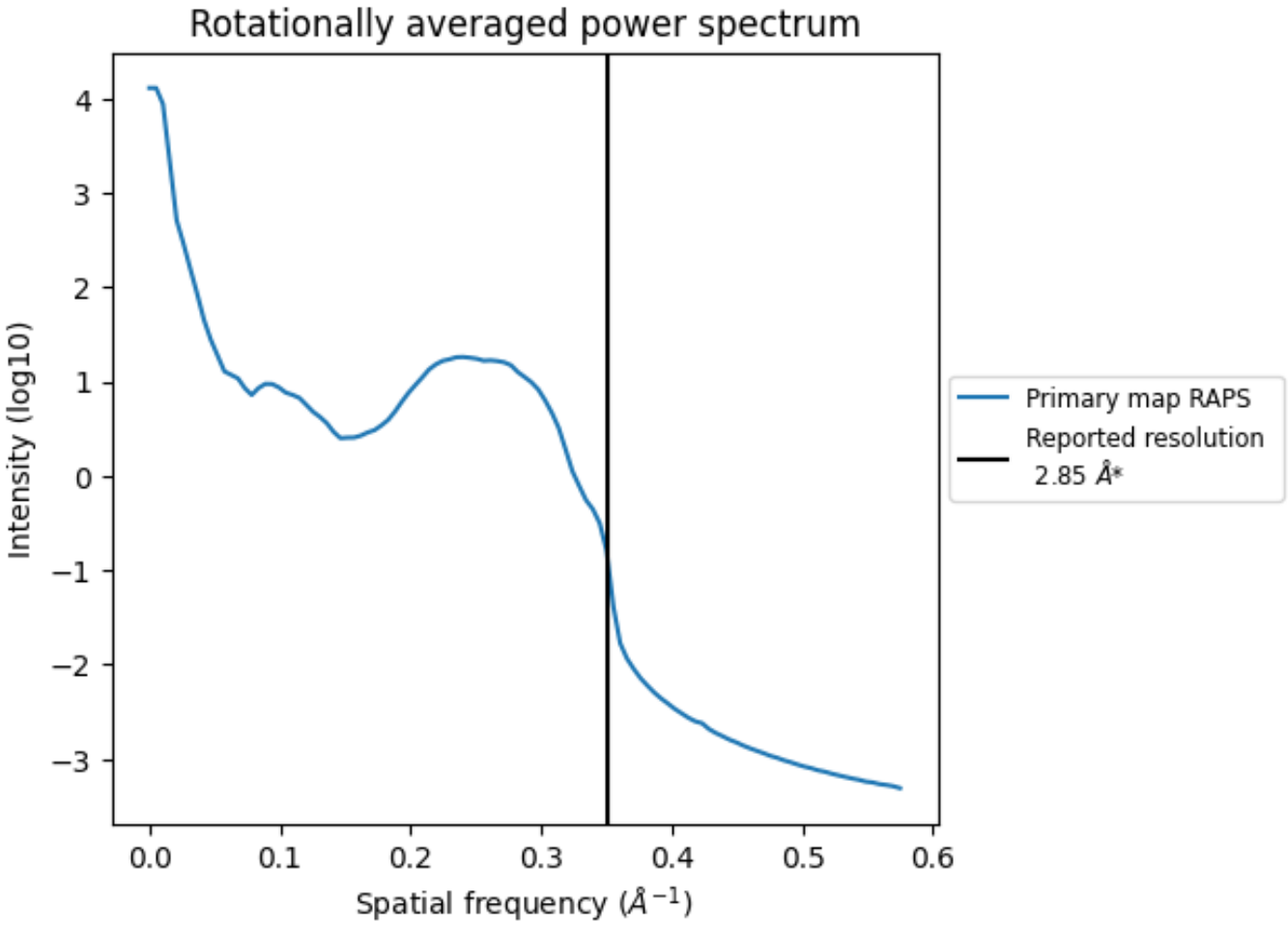
7.2 Volume estimate



The volume at the recommended contour level is 97 nm^3; this corresponds to an approximate mass of 88 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 (i)



*Reported resolution corresponds to spatial frequency of 0.351 Å^{-1}

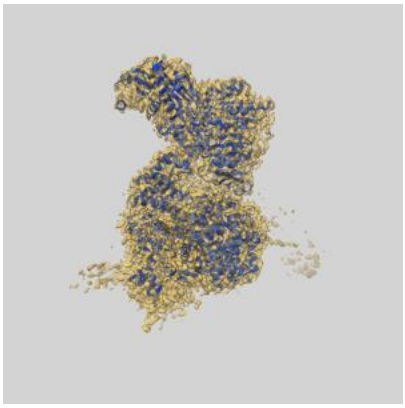
8 Fourier-Shell correlation (i)

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

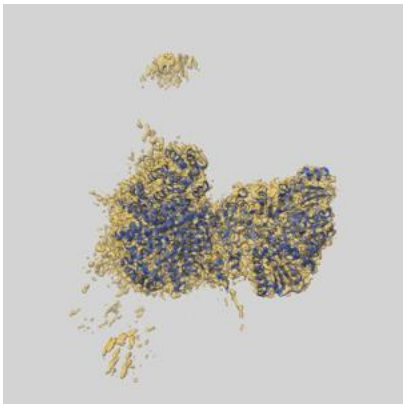
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23387 and PDB model 7LIW. Per-residue inclusion information can be found in section 3 on page 6.

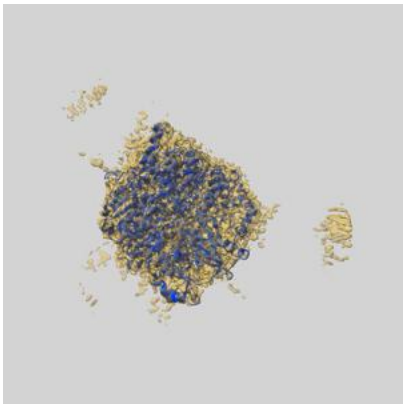
9.1 Map-model overlay



X



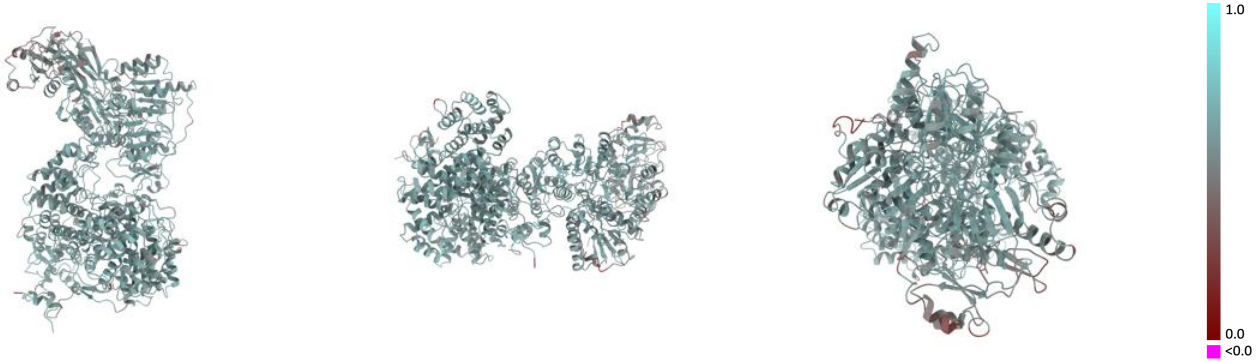
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

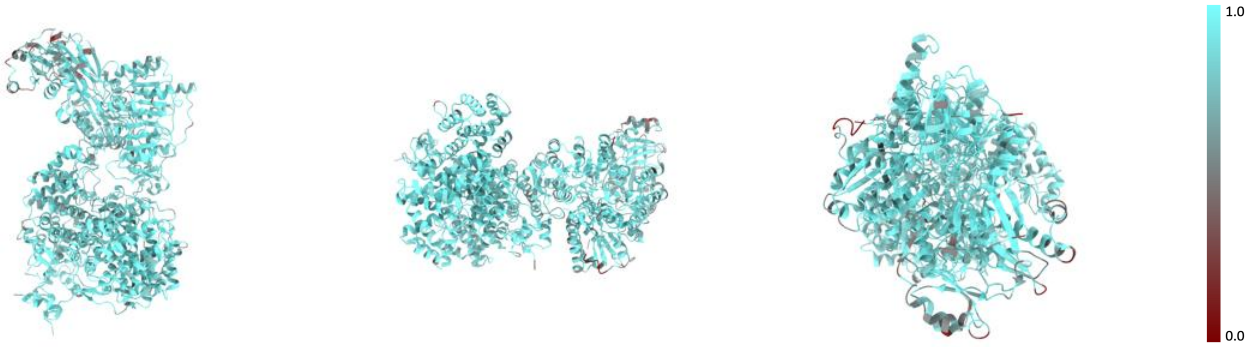
9.2 Q-score mapped to coordinate model



X Y Z

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.

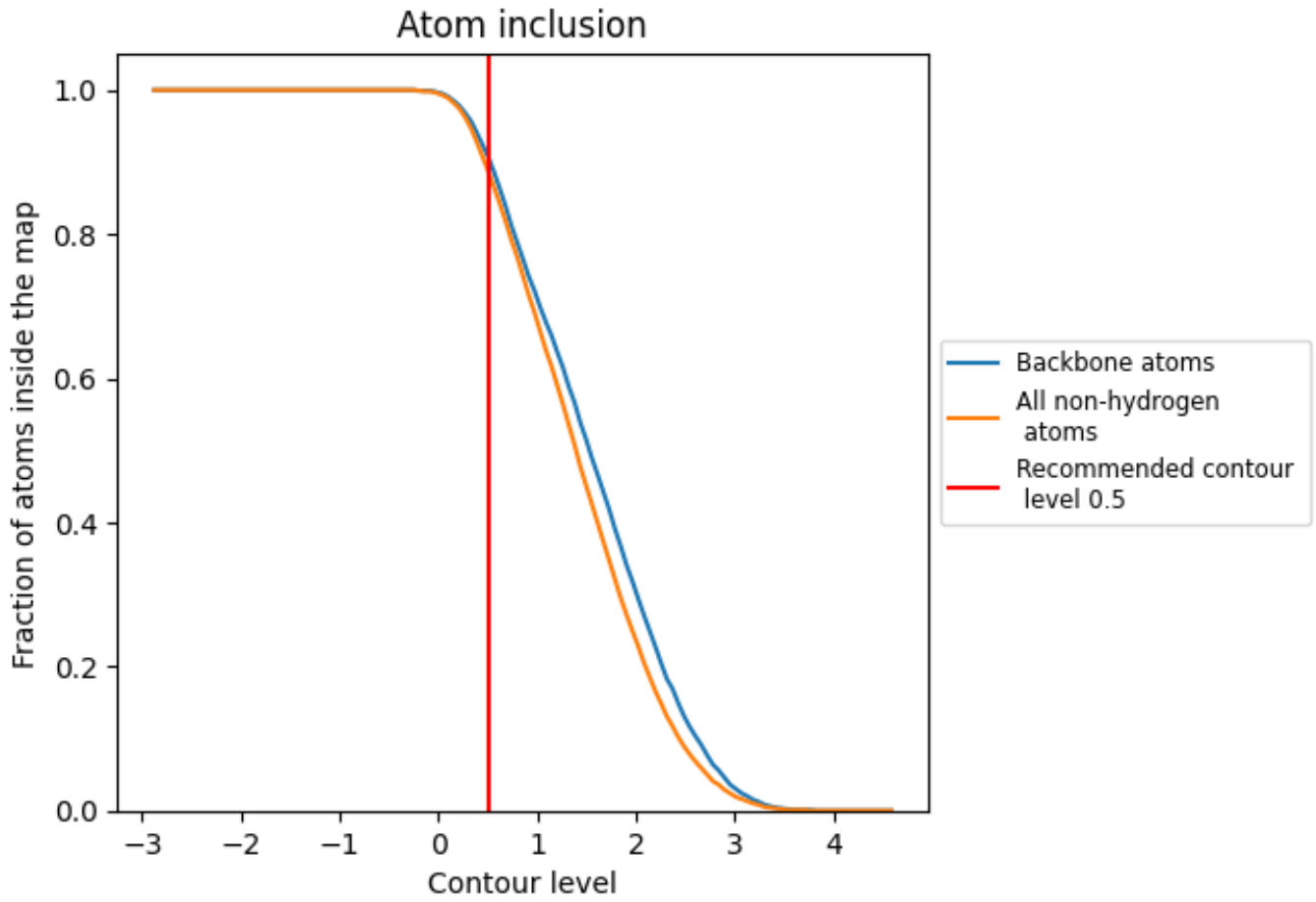
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8890	0.5870
A	0.9180	0.6030
B	0.8680	0.5750
C	0.9130	0.6000
D	0.9140	0.6030