



Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 02:02 PM EDT

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.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

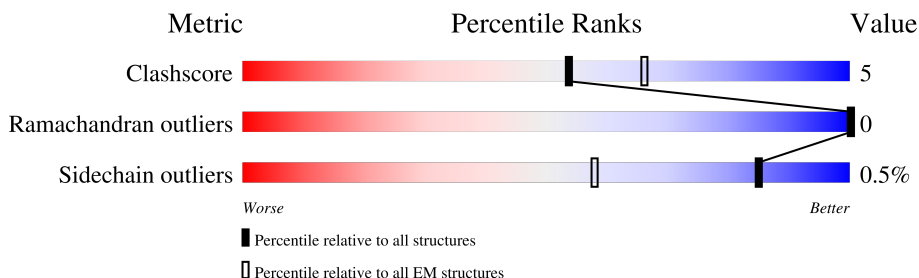
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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)
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 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.

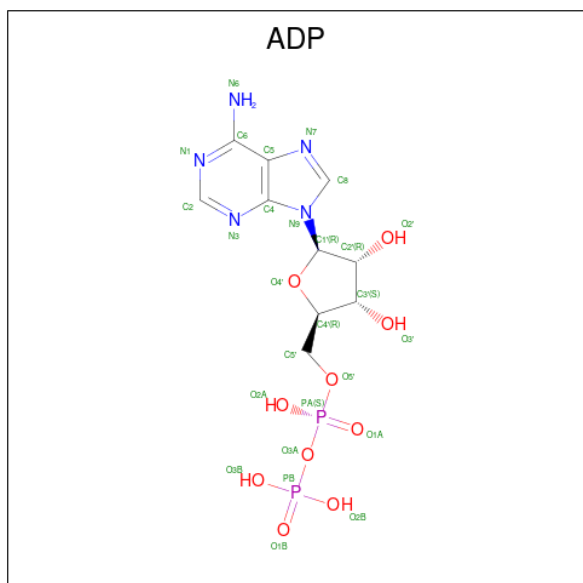
- Molecule 1 is a protein called ATP-citrate synthase.

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:

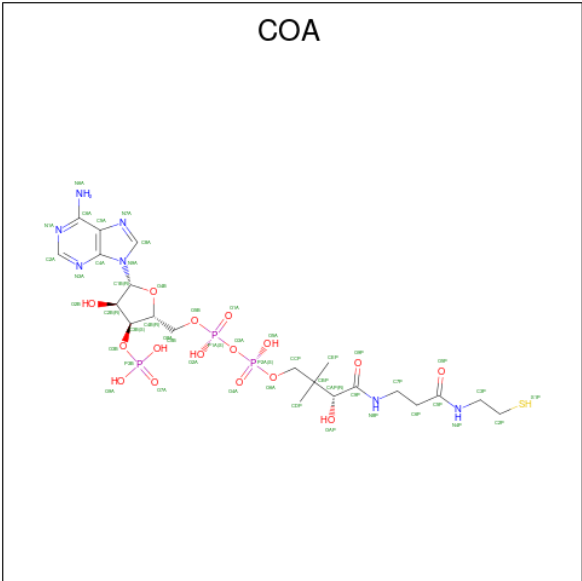
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	GLN	GLU	engineered mutation	UNP P53396
B	599	GLN	GLU	engineered mutation	UNP P53396
C	599	GLN	GLU	engineered mutation	UNP P53396
D	599	GLN	GLU	engineered mutation	UNP P53396

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



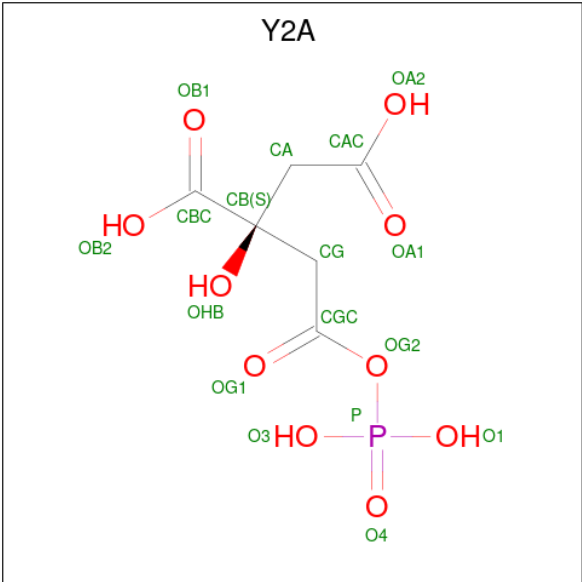
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

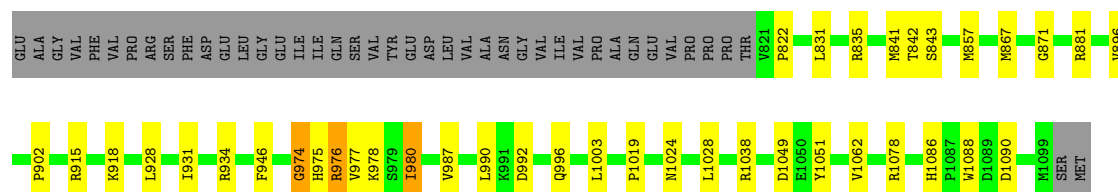


Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			48	21	7	16	3	

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

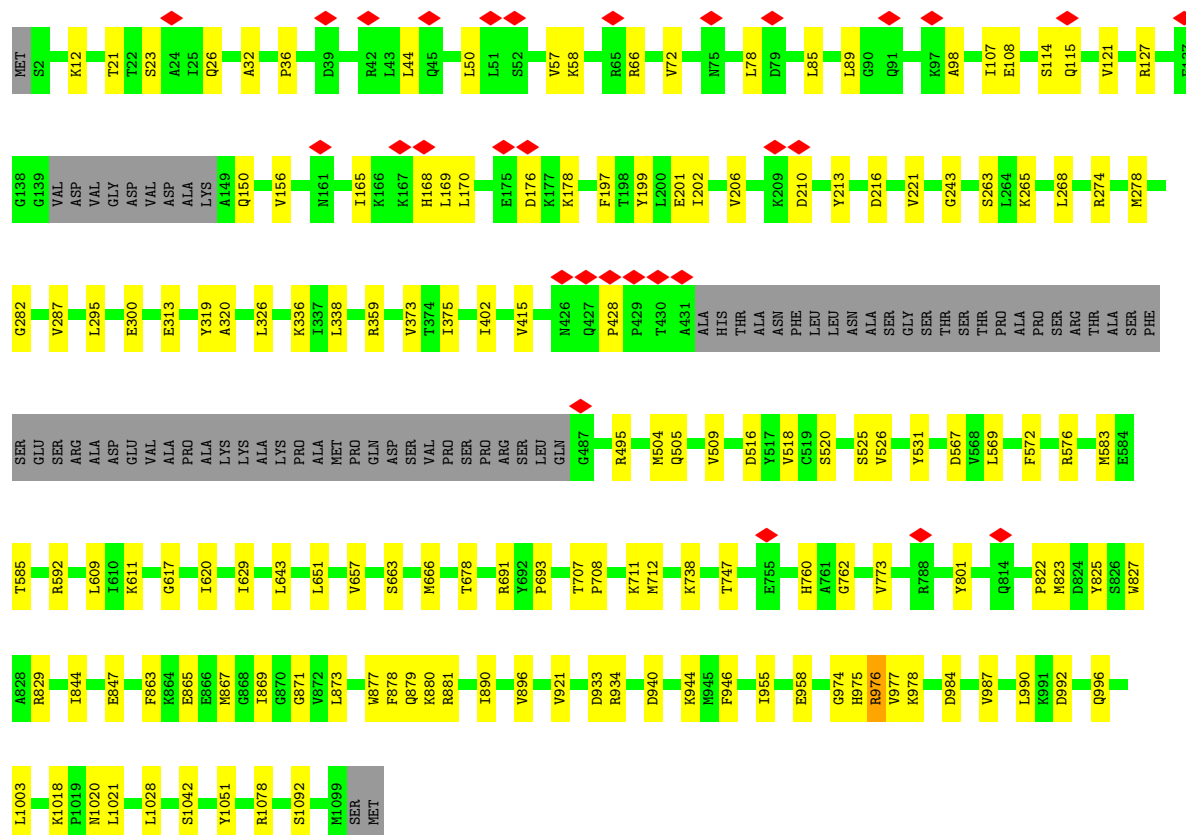


Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	O	P	0
			17	6	10	1	



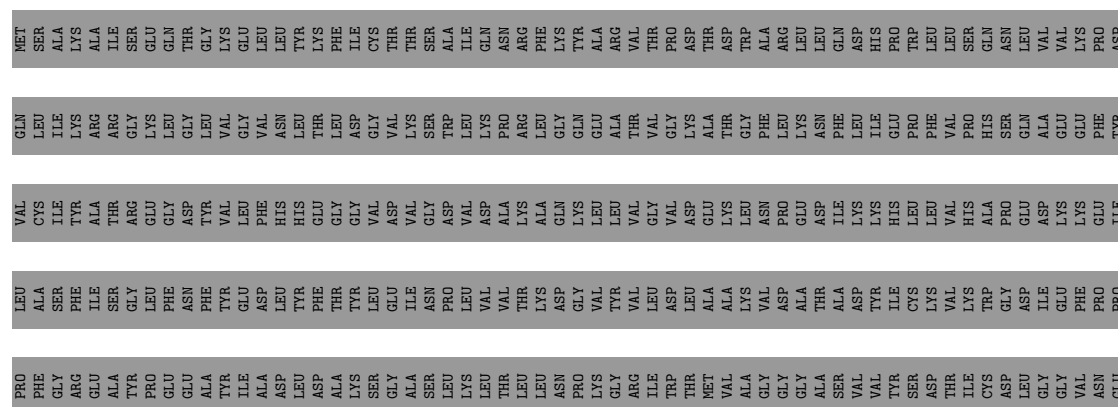
• Molecule 1: ATP-citrate synthase

Chain B: 80% 13% 6%



• Molecule 1: ATP-citrate synthase

Chain C: 23% 75%



M1067	Y872	GLU	GLY	THR	SER	ILE	PRO	PHE	SER
L1074	L873	ALA	ARG	THR	ARG	PRO	PRO	TYR	THR
R1078	Q879	VAL	GLY	GLU	GLY	ALA	GLY	TRP	GLY
M1099	I890	VAL	MET	LYS	THR	THR	LYS	HIS	LEU
SER	E591	PRO	SER	ILE	ARG	GLY	GLY	GLU	GLN
MET	M892	ARG	ASN	CYS	LYS	LEU	LYS	ILE	GLY
	V896	SER	GLU	ARG	LEU	SER	LEU	ILE	LYS
		PHE	ASN	GLY	LEU	THR	PRO	THR	THR
	R915	GLU	ASN	LYS	ASN	LYS	VAL	VAL	PHE
	L928	LEU	ILE	GLY	ILE	ALA	PHE	LYS	SER
	L929	GLY	ARG	GLY	SER	ASP	SER	LYS	SER
		GLU	GLN	ARG	GLN	GLY	ASN	ASN	ARG
	G932	ILE	THR	LEU	THR	GLY	ALA	ALA	HIS
	D933	GLN	THR	LYS	THR	VAL	VAL	THR	THR
	R934	SER	ASP	PRO	ASP	THR	ALA	ASP	LYS
		VAL	GLY	ILE	GLY	ILE	ALA	ALA	LYS
	L939	TYR	VAL	VAL	VAL	ILE	ILE	MET	ILE
	D940	GLU	THR	VAL	VAL	ILE	ILE	ARG	VAL
		ASP	CYS	CYS	TYR	GLY	GLY	LYS	TRP
	K944	LEU	GLY	ILE	GLY	ALA	ALA	HIS	GLY
	K945	VAL	VAL	THR	VAL	ILE	VAL	PRO	MET
	F946	ALA	ALA	THR	ALA	GLY	GLY	VAL	GLY
		ASN	ILE	CYS	ILE	GLY	ILE	ASP	ASP
	T955	VAL	ILE	THR	ASP	GLY	LYS	ILE	LEU
	E958	VAL	MET	THR	ARG	GLY	GLN	ASN	GLN
	G974	PRO	PHE	GLY	TYR	GLY	PRO	PHE	THR
	H975	ALA	SER	SER	PRO	CYS	ALA	ALA	LEU
	R976	GLN	GLY	SER	GLY	PHE	LEU	SER	ASP
	V977	GLU	GLY	GLU	SER	LYS	LEU	LEU	PHE
		VAL	THR	VAL	THR	ILE	ASP	ARG	ASP
	I980	PRO	GLN	GLN	PHE	GLY	SER	TYR	VAL
	K981	PRO	PHE	THR	MET	THR	ALA	VAL	VAL
		PRO	GLY	THR	ASP	GLY	TYR	CYS	VAL
	V987	THR	HIS	THR	HIS	GLY	ASP	SER	THR
		V821	ALA	GLY	VAL	GLY	SER	ARG	ASP
	L990	P822	GLY	ALA	LEU	MET	THR	THR	GLU
	K991	M823	ALA	ALA	ARG	LEU	GLU	ASP	PRO
	D992	D824	CYS	CYS	TYR	ASP	MET	GLY	PRO
	Q996	Y825	ALA	ALA	GLN	ASN	THR	SER	SER
		S826	ASN	ASN	THR	ILE	VAL	VAL	VAL
		W827	THR	GLN	THR	ALA	TYR	ALA	MET
		A828	ALA	SER	GLY	ALA	ALA	ALA	VAL
	L1003	R829	GLU	THR	VAL	LYS	GLN	ILE	THR
	P1019								
	M1020	R835	THR	LYS	MET	LEU	ILE	TYR	PRO
	L1021	I844	ALA	ALA	THR	VAL	PHE	ARG	ARG
			VAL	ILE	ILE	VAL	THR	THR	THR
	L1028	E847	LYS	LYS	VAL	VAL	GLY	ALA	GLY
		R848	ASN	ASN	LEU	SER	ILE	ASP	ASP
	Y1051		GLN	GLN	GLY	VAL	ILE	HIS	HIS
	F1061	M867	ALA	LEU	GLU	ALA	ALA	LYS	LYS
	V1062	G871	ILE	ILE	TYR	ILE	GLN	GLN	GLN
			LYS	LYS	VAL	VAL	GLY	LYS	LYS

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	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 (\AA)	191.4, 191.4, 191.4	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: ADP, COA, Y2A

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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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 ⓘ

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%)	89	95
1	B	858/909 (94%)	855 (100%)	3 (0%)	91	96
1	C	230/909 (25%)	227 (99%)	3 (1%)	65	83
1	D	230/909 (25%)	228 (99%)	2 (1%)	75	88
All	All	1547/3636 (42%)	1538 (99%)	9 (1%)	85	92

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 [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](#)

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
2	ADP	B	2001	-	24,29,29	0.87	0	29,45,45	1.21	3 (10%)
4	Y2A	B	2003	-	15,16,16	1.33	1 (6%)	21,24,24	1.32	1 (4%)
3	COA	B	2002	-	43,50,50	1.87	15 (34%)	56,75,75	1.64	7 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	2001	-	-	5/12/32/32	0/3/3/3
4	Y2A	B	2003	-	-	10/19/21/21	-
3	COA	B	2002	-	-	16/44/64/64	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	COA	P3B-O8A	-3.72	1.41	1.54
3	B	2002	COA	P3B-O9A	-3.51	1.41	1.54
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	C5P-N4P	-2.47	1.27	1.33
3	B	2002	COA	CDP-CBP	-2.45	1.48	1.53
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
3	B	2002	COA	C5A-N7A	-2.19	1.32	1.39
3	B	2002	COA	P1A-O2A	-2.18	1.45	1.55
3	B	2002	COA	C6A-N1A	-2.03	1.28	1.36
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 (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	COA	N3A-C2A-N1A	-5.37	121.38	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
4	B	2003	Y2A	OB2-CBC-CB	3.84	120.51	113.14
2	B	2001	ADP	N3-C2-N1	-3.63	123.75	128.67
3	B	2002	COA	C2P-C3P-N4P	-2.89	105.74	112.31
3	B	2002	COA	O2A-P1A-O3A	2.54	114.13	107.27
2	B	2001	ADP	C4-C5-N7	-2.52	106.68	109.34
3	B	2002	COA	C3P-N4P-C5P	-2.44	118.29	122.82
3	B	2002	COA	C6P-C7P-N8P	-2.15	107.43	112.00
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

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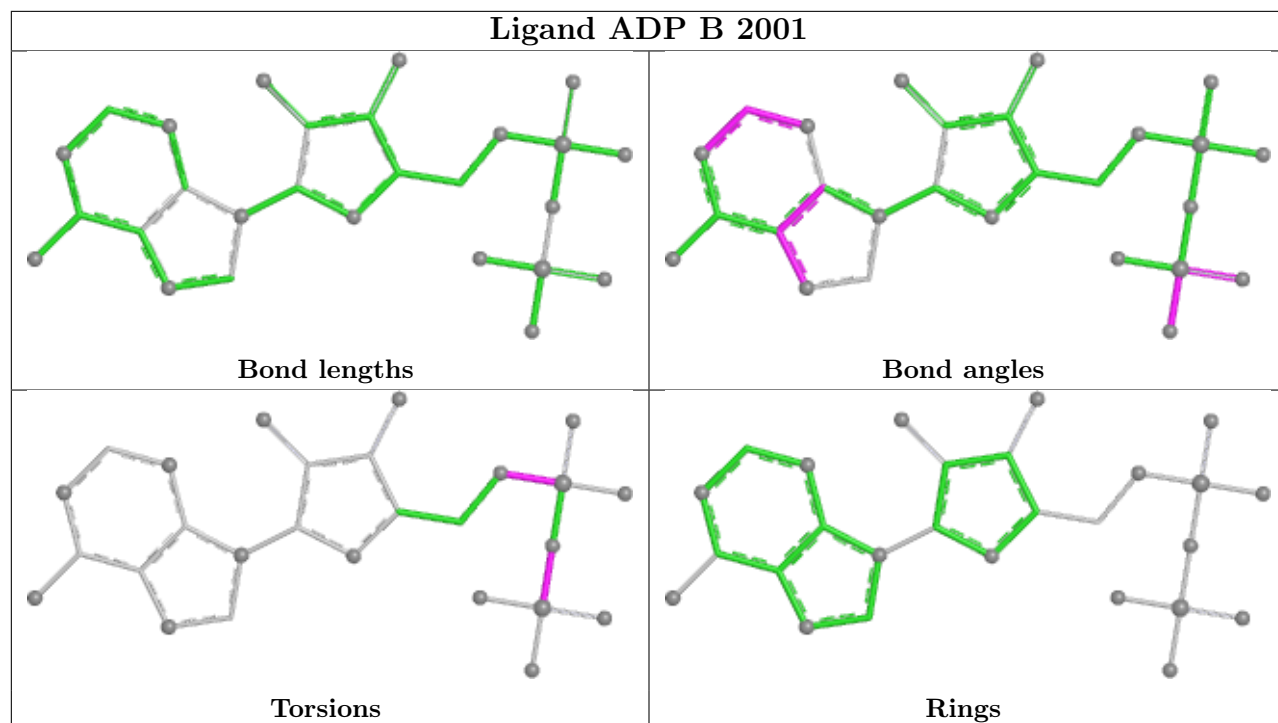
Mol	Chain	Res	Type	Atoms
3	B	2002	COA	P1A-O3A-P2A-O5A
4	B	2003	Y2A	OHB-CB-CBC-OB2
4	B	2003	Y2A	CG-CB-CBC-OB1
3	B	2002	COA	CDP-CBP-CCP-O6A

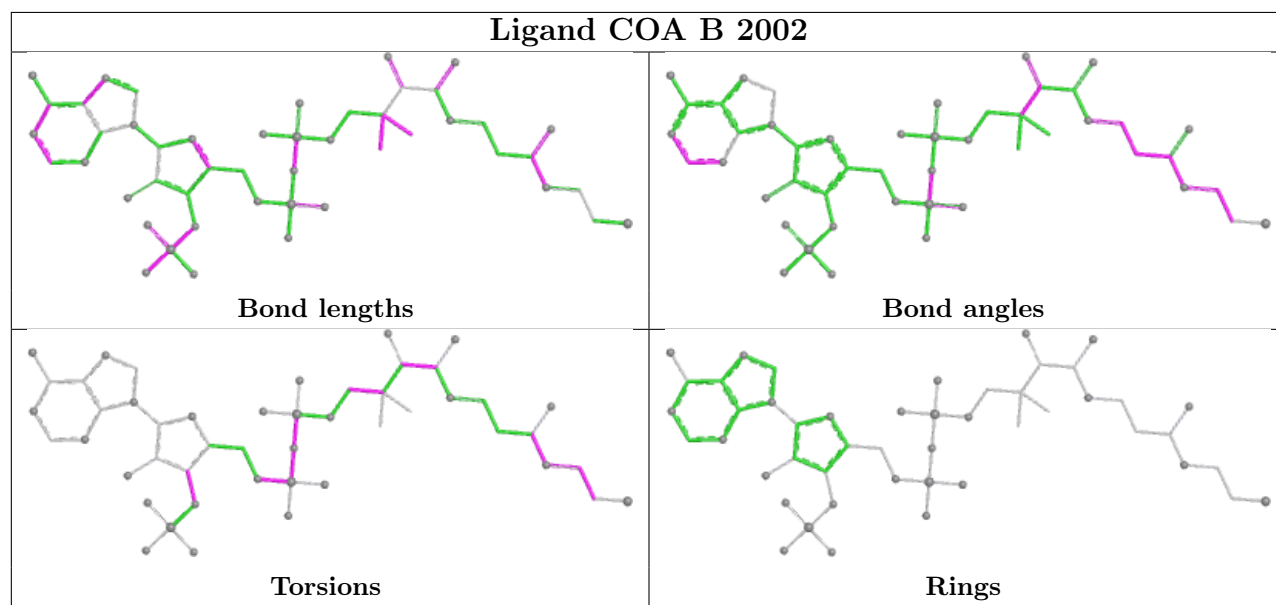
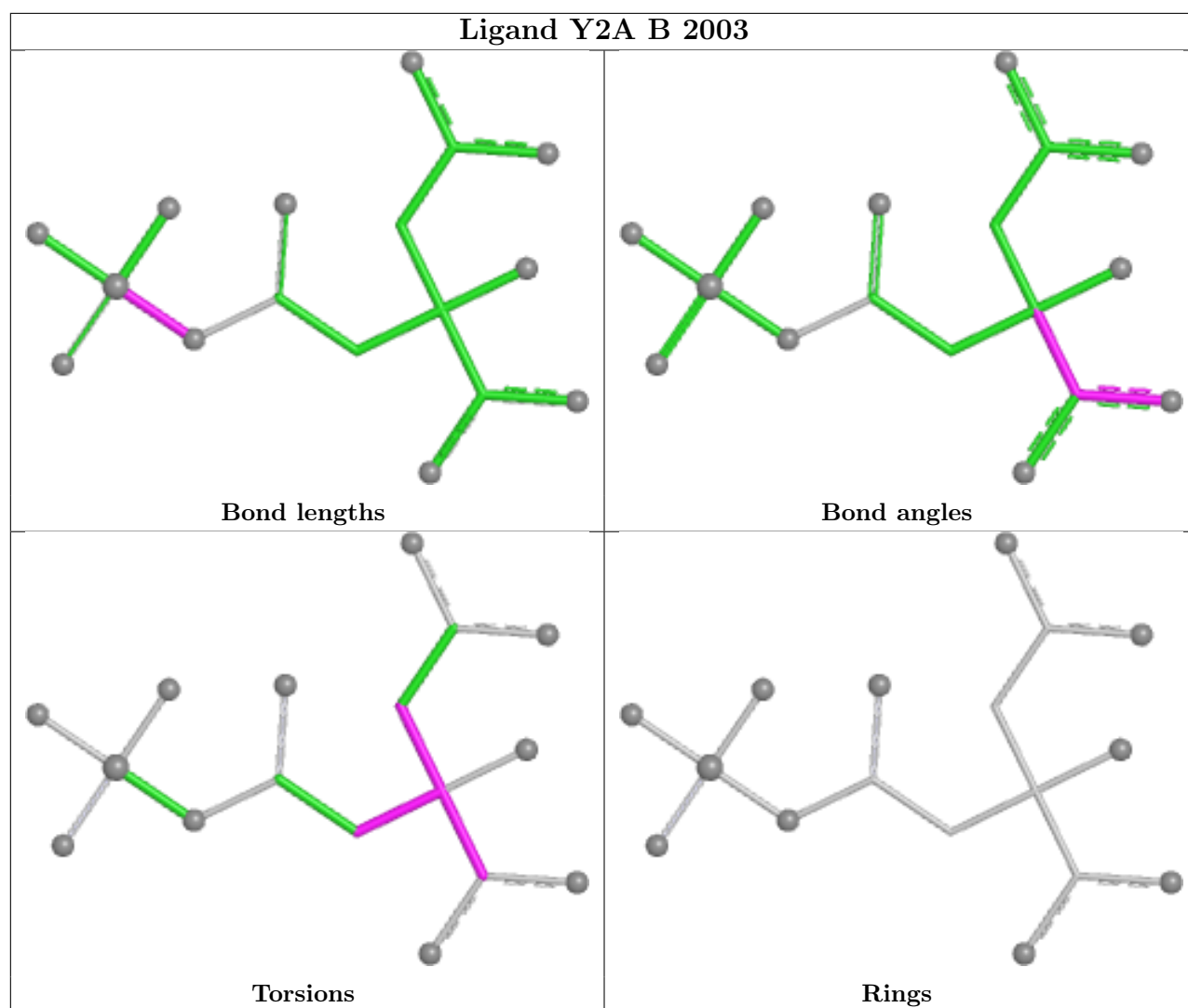
There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

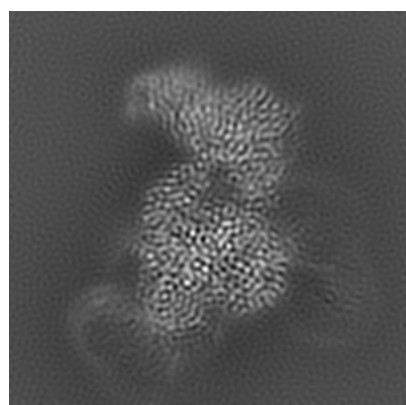
6 Map visualisation [i](#)

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

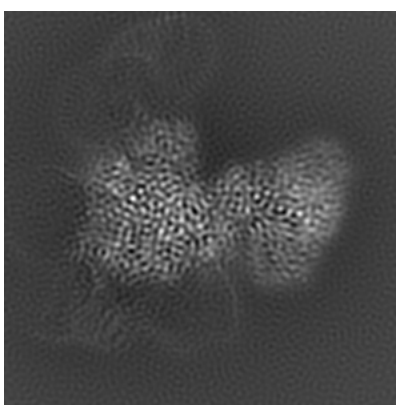
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

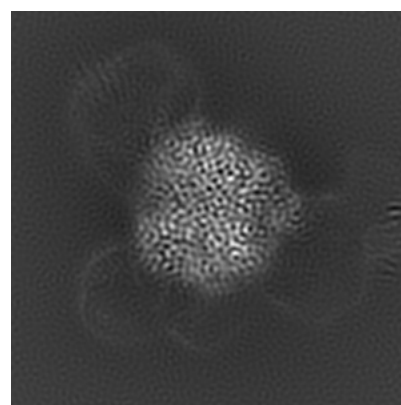
6.1.1 Primary map



X



Y

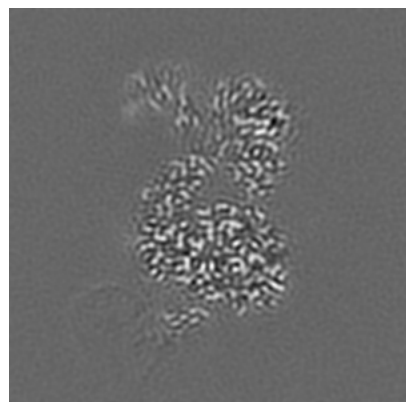


Z

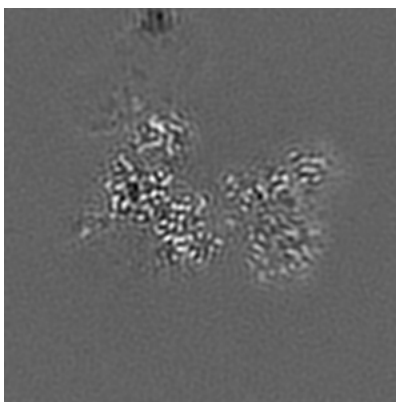
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

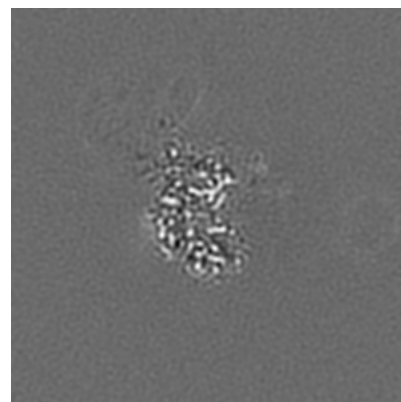
6.2.1 Primary map



X Index: 110



Y Index: 110

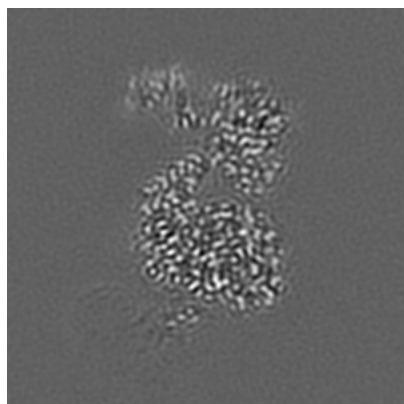


Z Index: 110

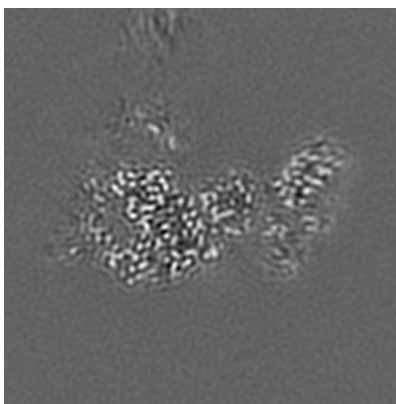
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

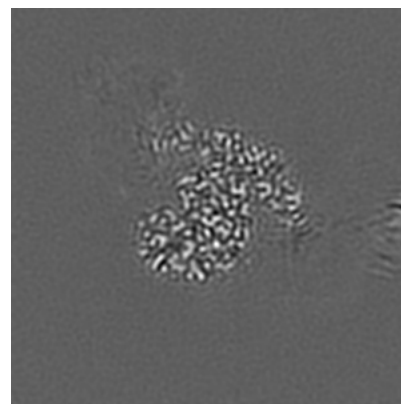
6.3.1 Primary map



X Index: 112



Y Index: 98

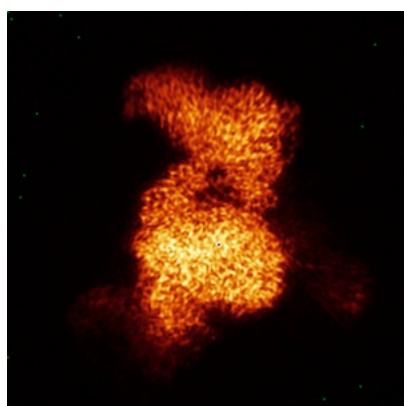


Z Index: 85

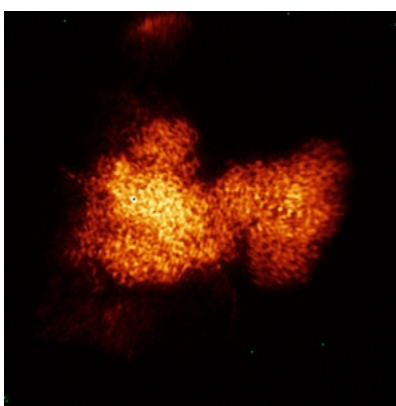
The images above show the largest variance slices of the map in three orthogonal directions.

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

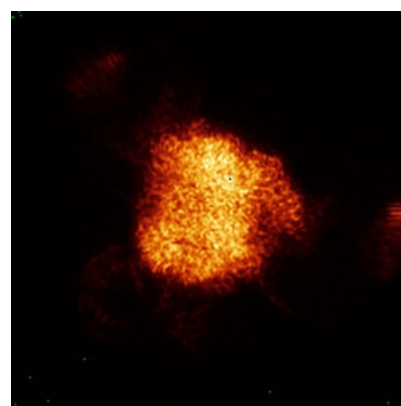
6.4.1 Primary map



X



Y

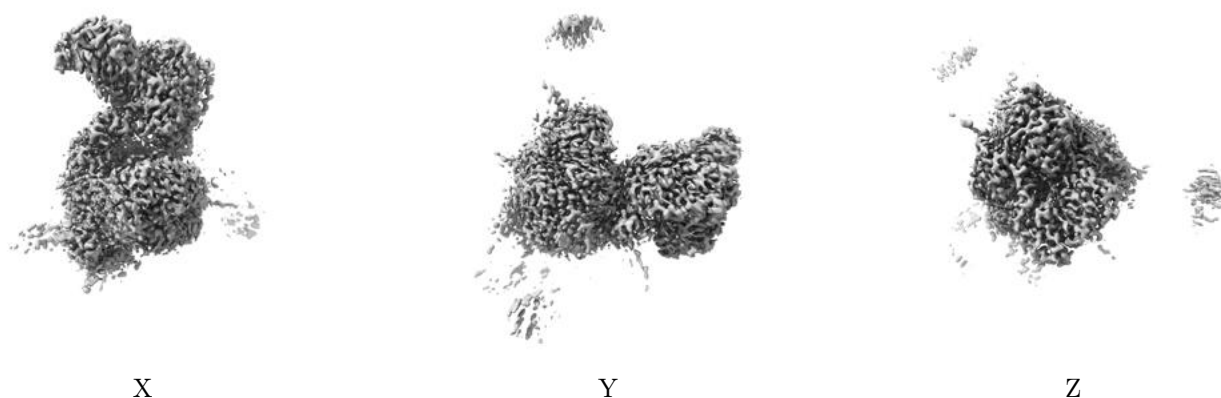


Z

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



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.

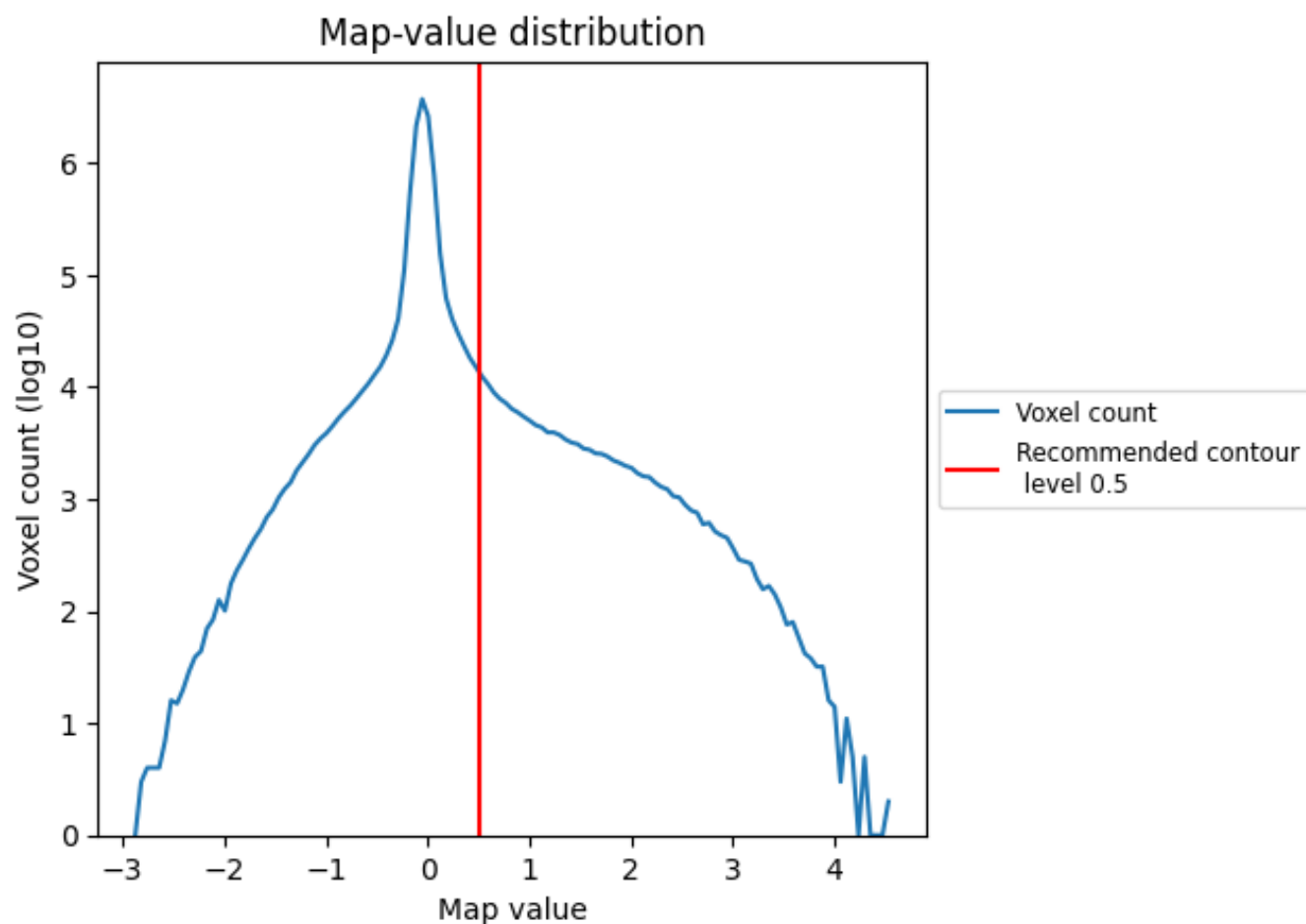
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

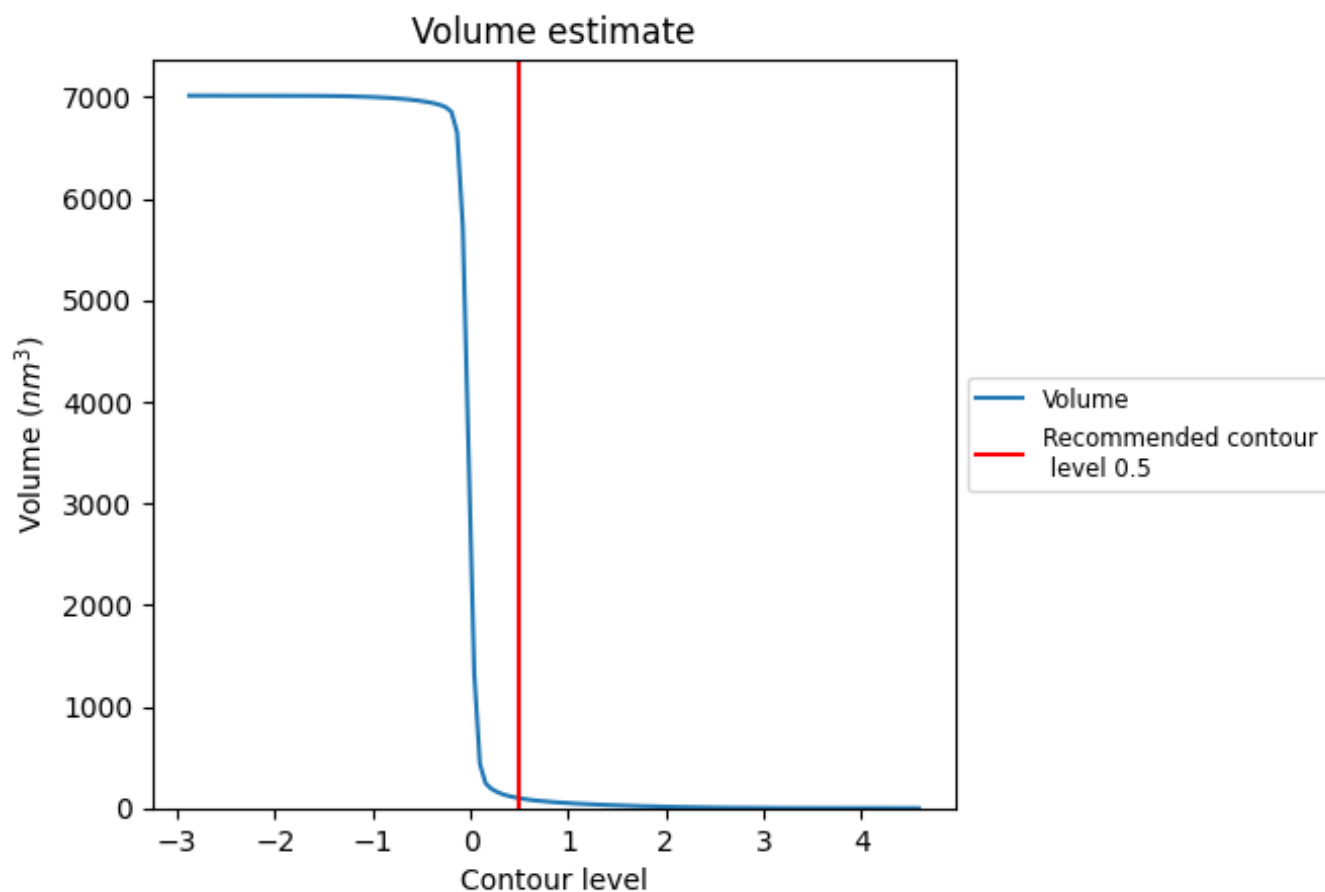
This section contains the results of statistical analysis of the map.

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.

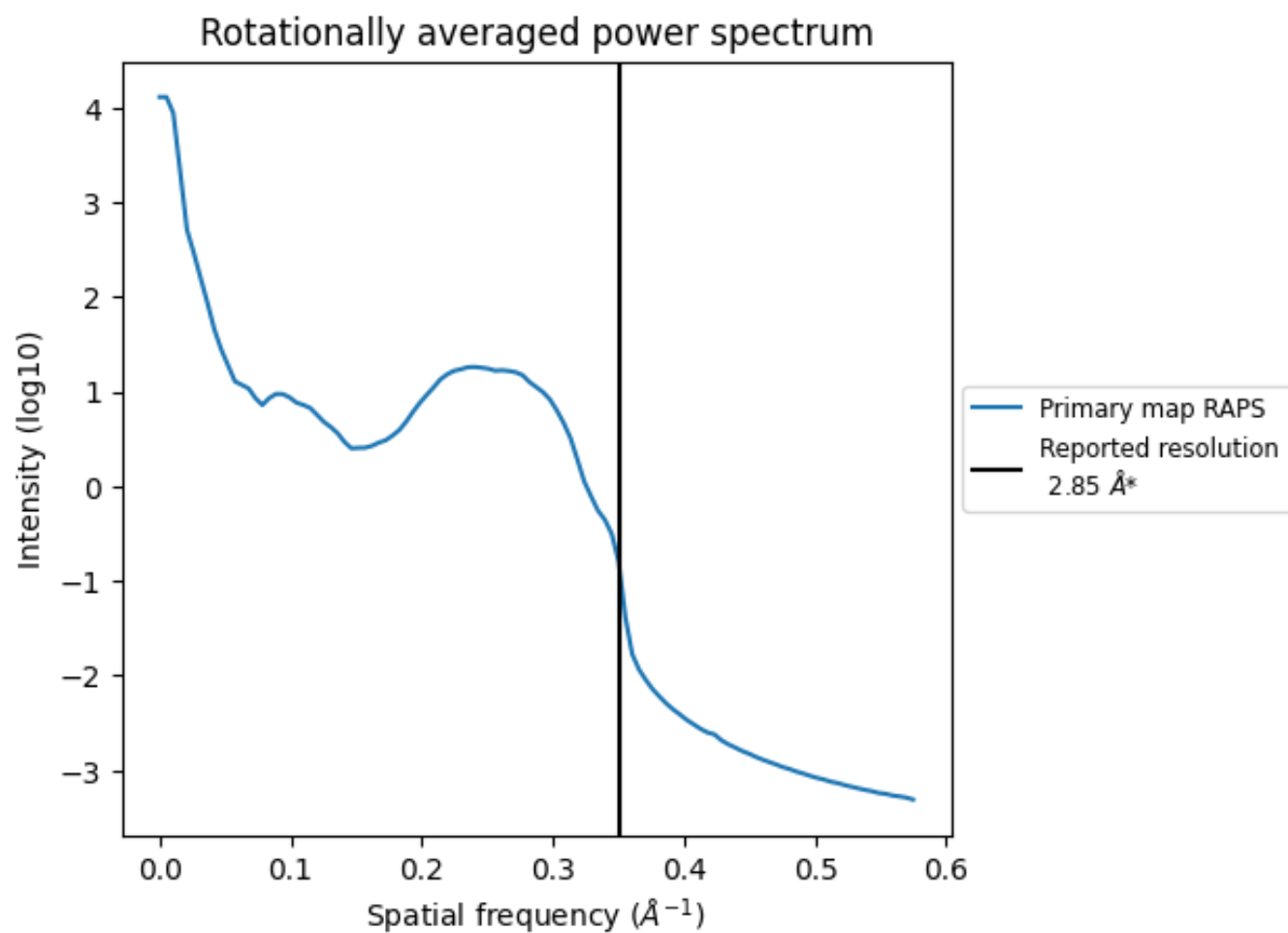
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

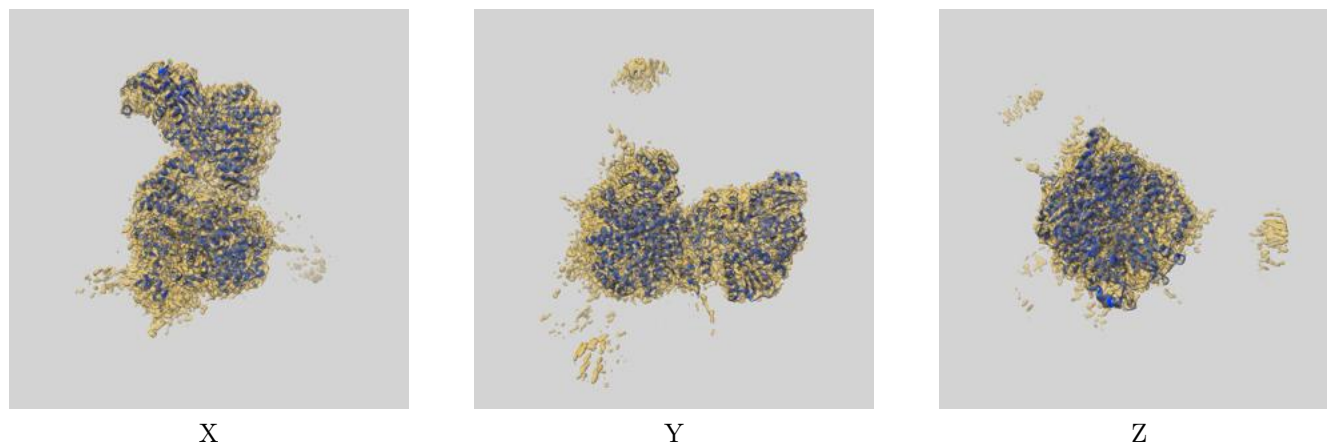
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

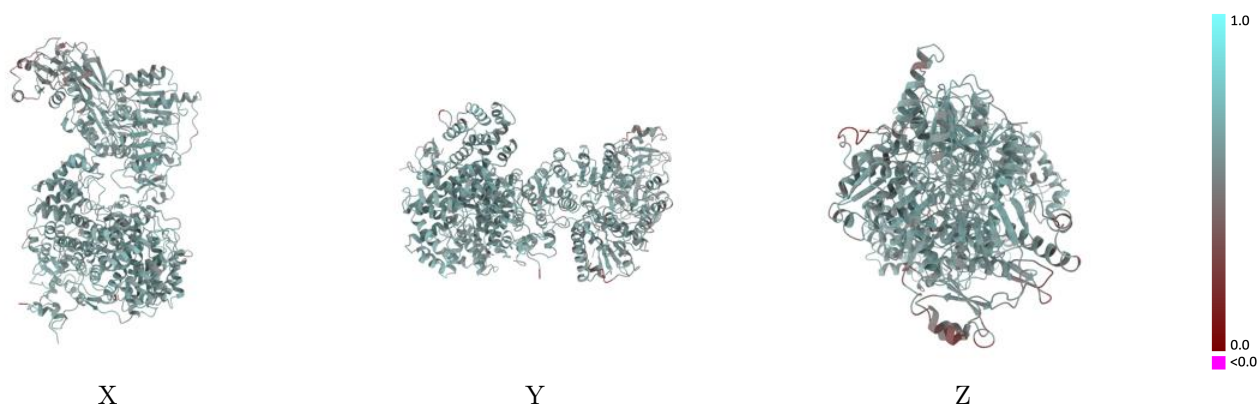
This section contains information regarding the fit between EMDB map EMD-23387 and PDB model 7LIW. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



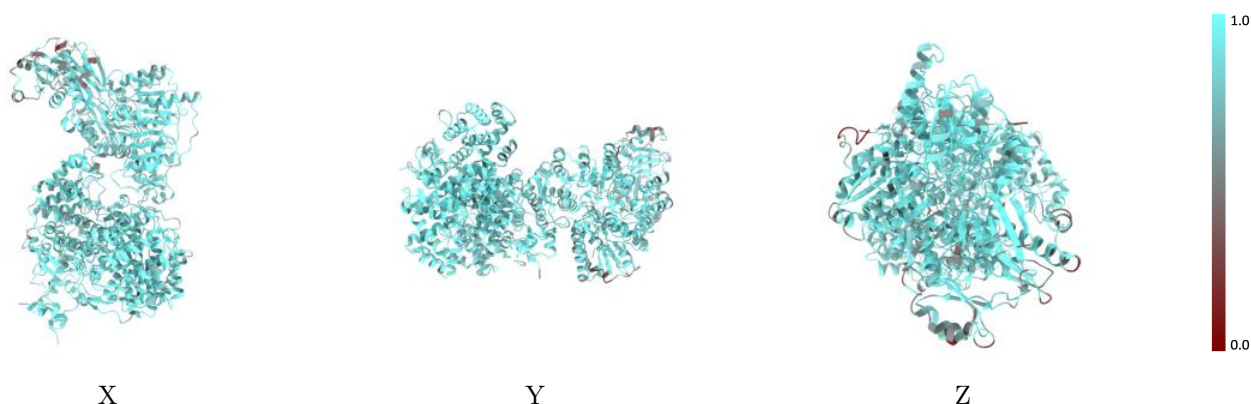
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



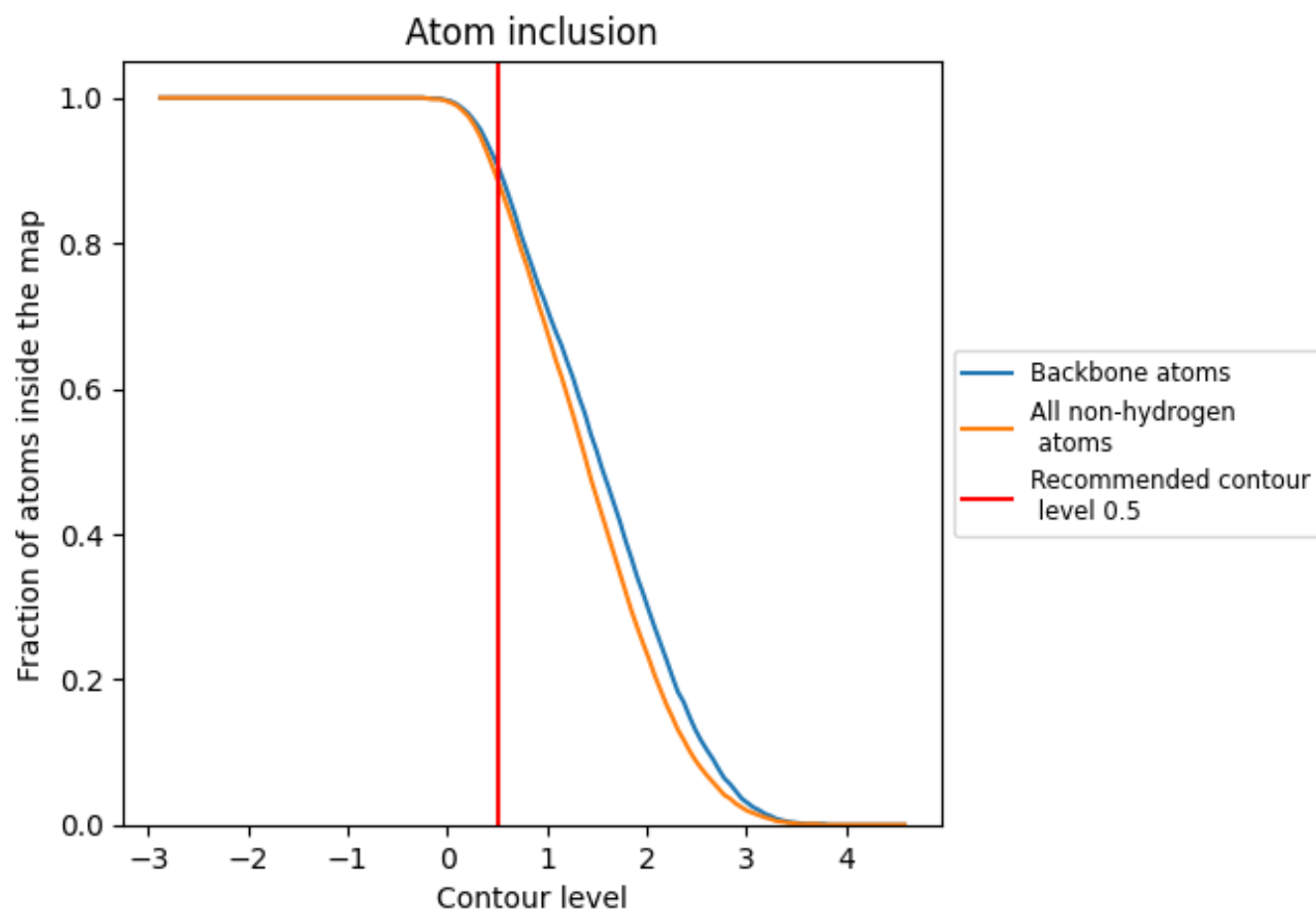
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

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	<div><div></div></div> 0.8890	<div><div></div></div> 0.5870
A	<div><div></div></div> 0.9180	<div><div></div></div> 0.6030
B	<div><div></div></div> 0.8680	<div><div></div></div> 0.5750
C	<div><div></div></div> 0.9130	<div><div></div></div> 0.6000
D	<div><div></div></div> 0.9140	<div><div></div></div> 0.6030

