



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:38 AM UTC

PDB ID : 7L1S / pdb_00007l1s
EMDB ID : EMD-23117
Title : PS3 F1-ATPase Pi-bound Dwell
Authors : Sobti, M.; Ueno, H.; Noji, H.; Stewart, A.G.
Deposited on : 2020-12-15
Resolution : 3.60 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:

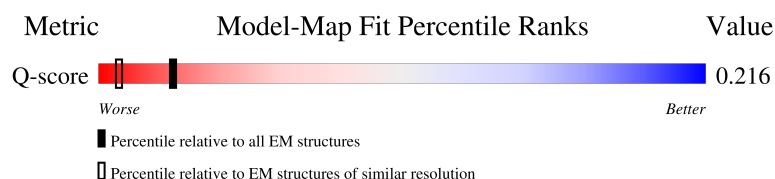
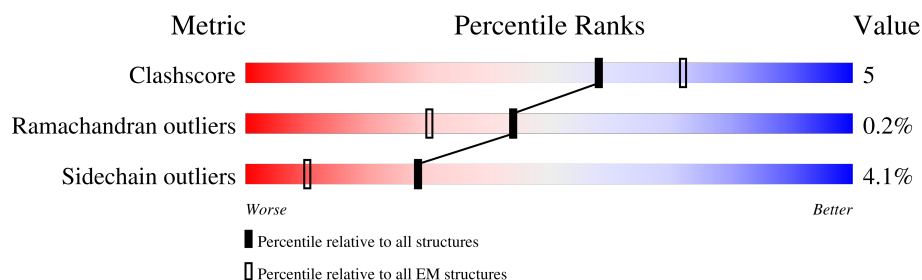
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

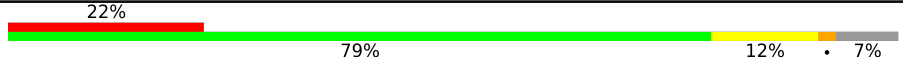
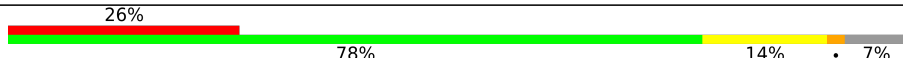
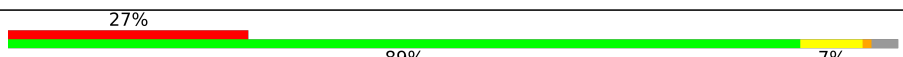
The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	510	
1	B	510	
1	C	510	
2	D	484	

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Mol	Chain	Length	Quality of chain
2	E	484	22% 84% 12% ..
2	F	484	25% 87% 8% ..
3	G	285	54% 89% 8% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24176 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 synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	474	Total	C	N	O	S	0	0
			3636	2303	637	687	9		
1	B	475	Total	C	N	O	S	0	0
			3643	2308	638	688	9		
1	C	476	Total	C	N	O	S	0	0
			3649	2311	639	690	9		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0M3VGF9
A	-6	SER	-	expression tag	UNP A0A0M3VGF9
A	-5	HIS	-	expression tag	UNP A0A0M3VGF9
A	-4	HIS	-	expression tag	UNP A0A0M3VGF9
A	-3	HIS	-	expression tag	UNP A0A0M3VGF9
A	-2	HIS	-	expression tag	UNP A0A0M3VGF9
A	-1	HIS	-	expression tag	UNP A0A0M3VGF9
A	0	HIS	-	expression tag	UNP A0A0M3VGF9
A	1	GLY	-	expression tag	UNP A0A0M3VGF9
A	193	SER	CYS	conflict	UNP A0A0M3VGF9
A	463	PHE	TRP	conflict	UNP A0A0M3VGF9
B	-7	MET	-	expression tag	UNP A0A0M3VGF9
B	-6	SER	-	expression tag	UNP A0A0M3VGF9
B	-5	HIS	-	expression tag	UNP A0A0M3VGF9
B	-4	HIS	-	expression tag	UNP A0A0M3VGF9
B	-3	HIS	-	expression tag	UNP A0A0M3VGF9
B	-2	HIS	-	expression tag	UNP A0A0M3VGF9
B	-1	HIS	-	expression tag	UNP A0A0M3VGF9
B	0	HIS	-	expression tag	UNP A0A0M3VGF9
B	1	GLY	-	expression tag	UNP A0A0M3VGF9
B	193	SER	CYS	conflict	UNP A0A0M3VGF9
B	463	PHE	TRP	conflict	UNP A0A0M3VGF9
C	-7	MET	-	expression tag	UNP A0A0M3VGF9
C	-6	SER	-	expression tag	UNP A0A0M3VGF9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP A0A0M3VGF9
C	-4	HIS	-	expression tag	UNP A0A0M3VGF9
C	-3	HIS	-	expression tag	UNP A0A0M3VGF9
C	-2	HIS	-	expression tag	UNP A0A0M3VGF9
C	-1	HIS	-	expression tag	UNP A0A0M3VGF9
C	0	HIS	-	expression tag	UNP A0A0M3VGF9
C	1	GLY	-	expression tag	UNP A0A0M3VGF9
C	193	SER	CYS	conflict	UNP A0A0M3VGF9
C	463	PHE	TRP	conflict	UNP A0A0M3VGF9

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	470	Total	C	N	O	S	0	0
			3621	2285	627	696	13		
2	E	470	Total	C	N	O	S	0	0
			3622	2285	627	696	14		
2	F	471	Total	C	N	O	S	0	0
			3629	2290	628	697	14		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	MET	-	expression tag	UNP A0A0M4U1P9
D	-9	HIS	-	expression tag	UNP A0A0M4U1P9
D	-8	HIS	-	expression tag	UNP A0A0M4U1P9
D	-7	HIS	-	expression tag	UNP A0A0M4U1P9
D	-6	HIS	-	expression tag	UNP A0A0M4U1P9
D	-5	HIS	-	expression tag	UNP A0A0M4U1P9
D	-4	HIS	-	expression tag	UNP A0A0M4U1P9
D	-3	HIS	-	expression tag	UNP A0A0M4U1P9
D	-2	HIS	-	expression tag	UNP A0A0M4U1P9
D	-1	HIS	-	expression tag	UNP A0A0M4U1P9
D	0	HIS	-	expression tag	UNP A0A0M4U1P9
D	190	ASP	GLU	conflict	UNP A0A0M4U1P9
E	-10	MET	-	expression tag	UNP A0A0M4U1P9
E	-9	HIS	-	expression tag	UNP A0A0M4U1P9
E	-8	HIS	-	expression tag	UNP A0A0M4U1P9
E	-7	HIS	-	expression tag	UNP A0A0M4U1P9
E	-6	HIS	-	expression tag	UNP A0A0M4U1P9
E	-5	HIS	-	expression tag	UNP A0A0M4U1P9
E	-4	HIS	-	expression tag	UNP A0A0M4U1P9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	HIS	-	expression tag	UNP A0A0M4U1P9
E	-2	HIS	-	expression tag	UNP A0A0M4U1P9
E	-1	HIS	-	expression tag	UNP A0A0M4U1P9
E	0	HIS	-	expression tag	UNP A0A0M4U1P9
E	190	ASP	GLU	conflict	UNP A0A0M4U1P9
F	-10	MET	-	expression tag	UNP A0A0M4U1P9
F	-9	HIS	-	expression tag	UNP A0A0M4U1P9
F	-8	HIS	-	expression tag	UNP A0A0M4U1P9
F	-7	HIS	-	expression tag	UNP A0A0M4U1P9
F	-6	HIS	-	expression tag	UNP A0A0M4U1P9
F	-5	HIS	-	expression tag	UNP A0A0M4U1P9
F	-4	HIS	-	expression tag	UNP A0A0M4U1P9
F	-3	HIS	-	expression tag	UNP A0A0M4U1P9
F	-2	HIS	-	expression tag	UNP A0A0M4U1P9
F	-1	HIS	-	expression tag	UNP A0A0M4U1P9
F	0	HIS	-	expression tag	UNP A0A0M4U1P9
F	190	ASP	GLU	conflict	UNP A0A0M4U1P9

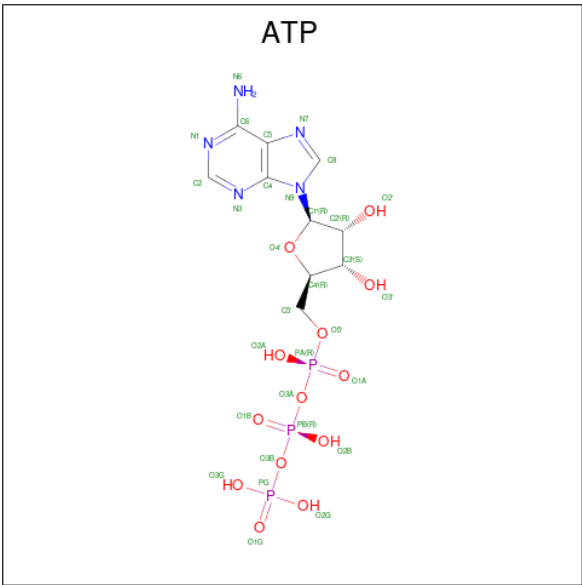
- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	282	Total	C	N	O	S	0	0
			2211	1393	388	420	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	112	CYS	SER	conflict	UNP A0A0M4TPJ7
G	215	CYS	ILE	conflict	UNP A0A0M4TPJ7

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

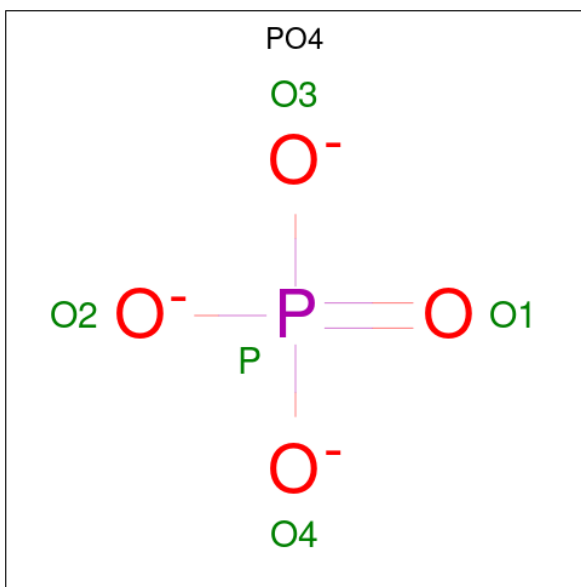


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

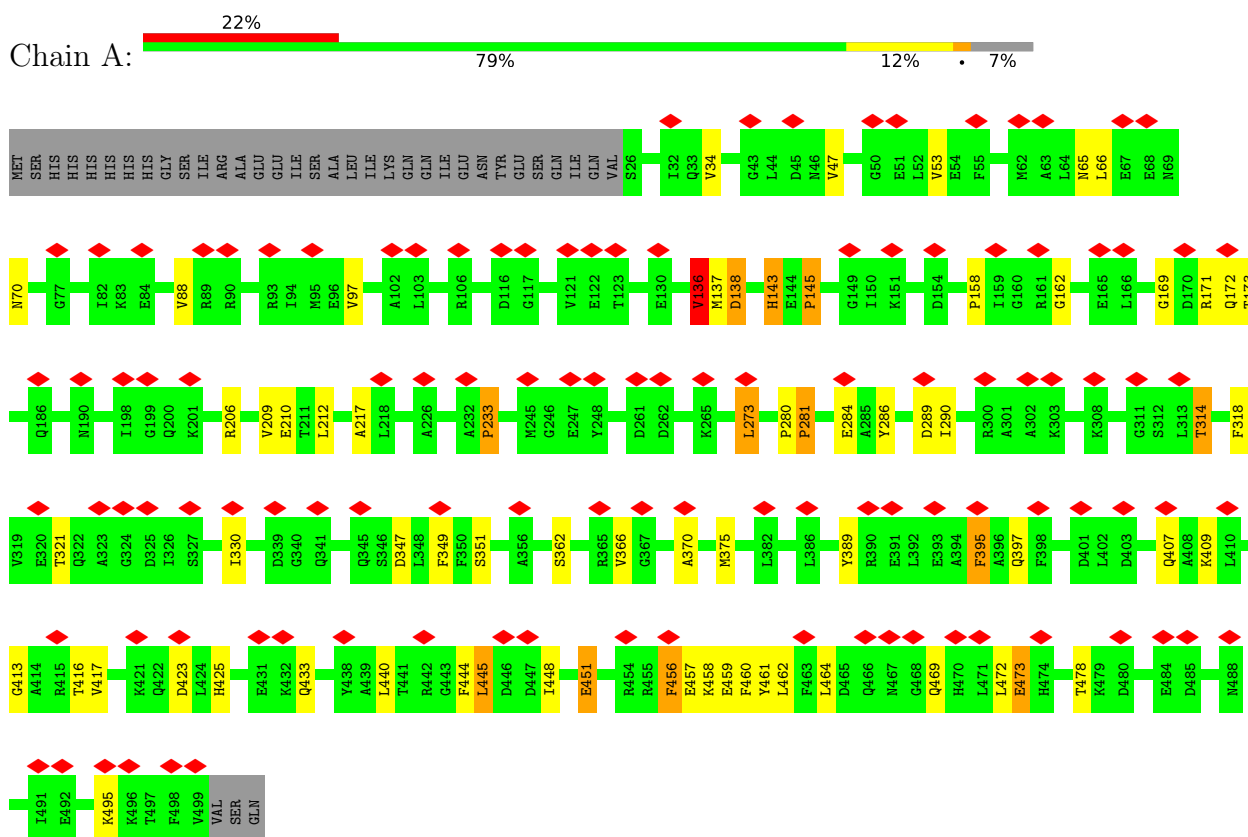


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
6	A	1	5	4	1	0

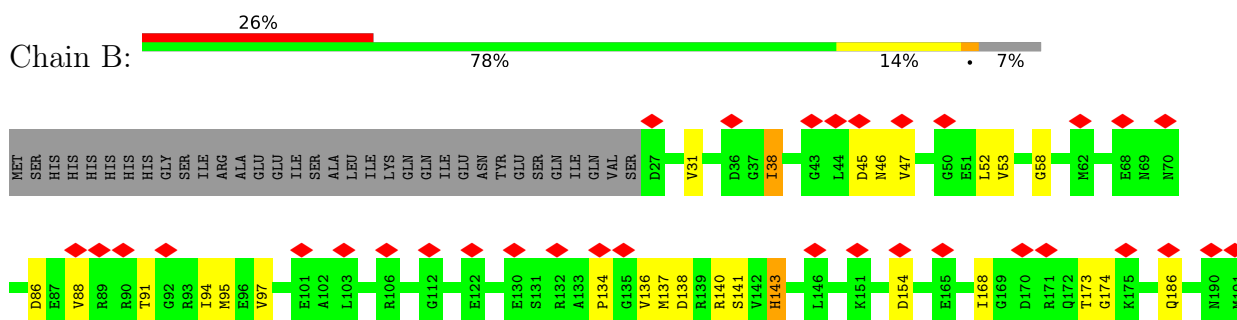
3 Residue-property plots

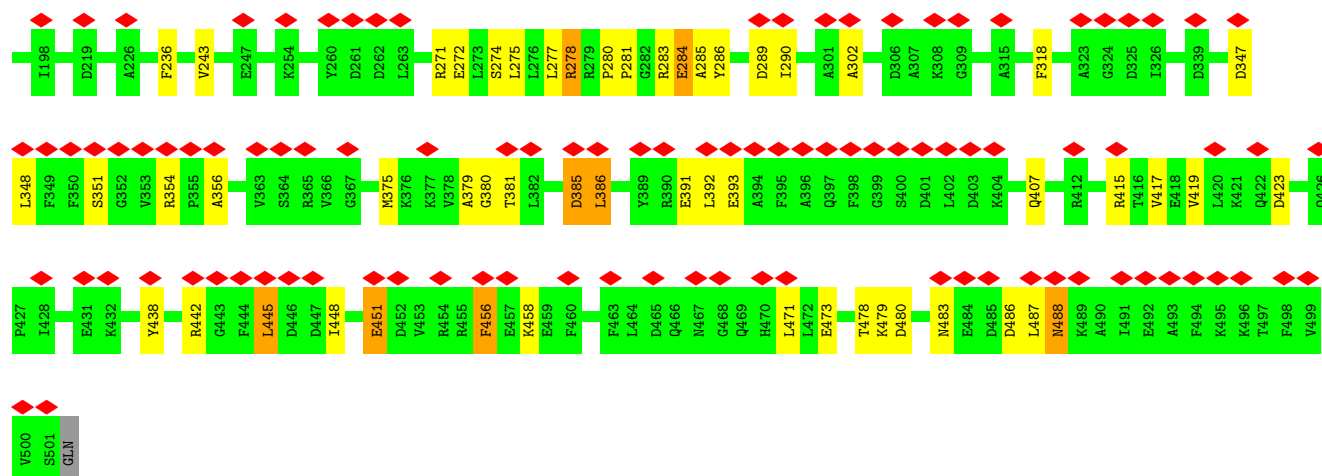
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: ATP synthase subunit alpha

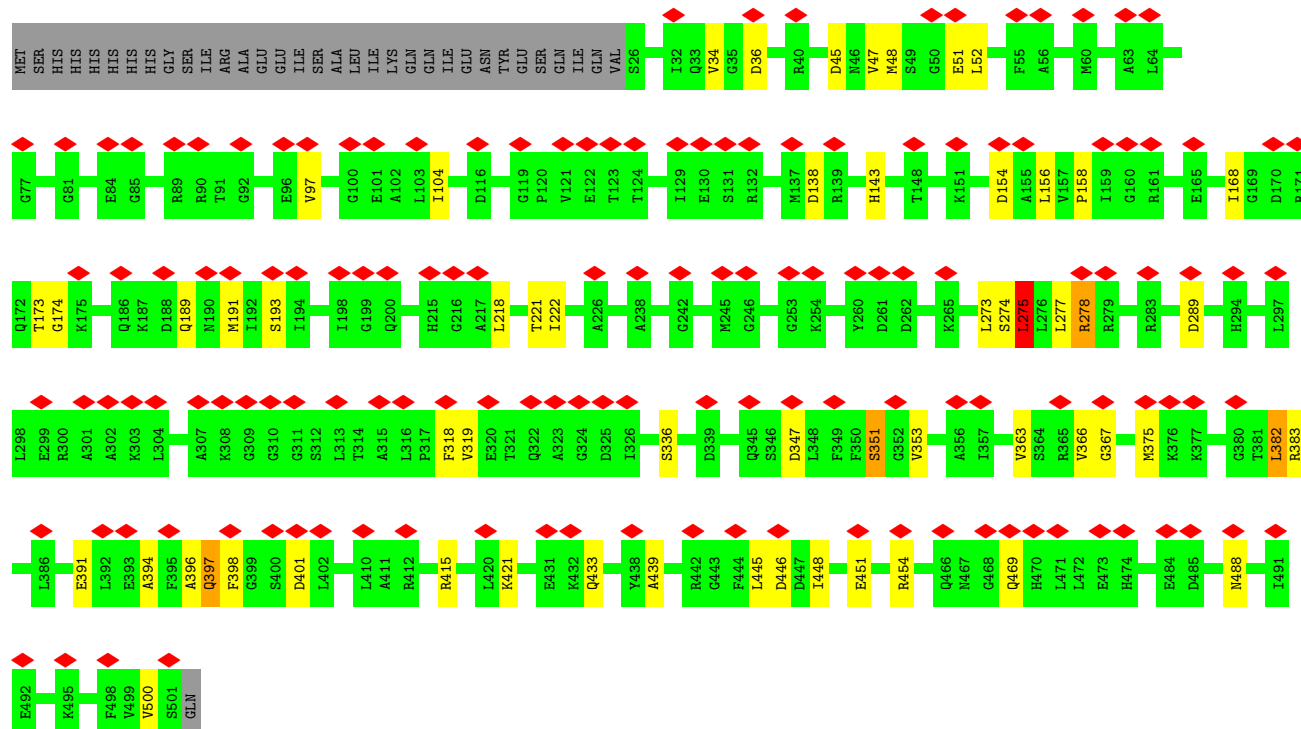
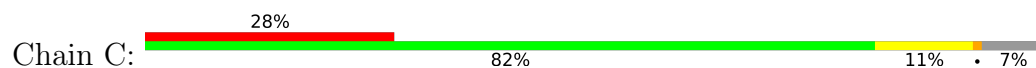


• Molecule 1: ATP synthase subunit alpha

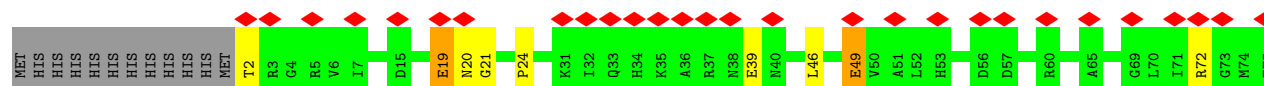
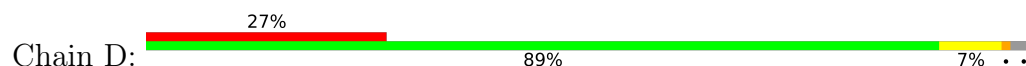


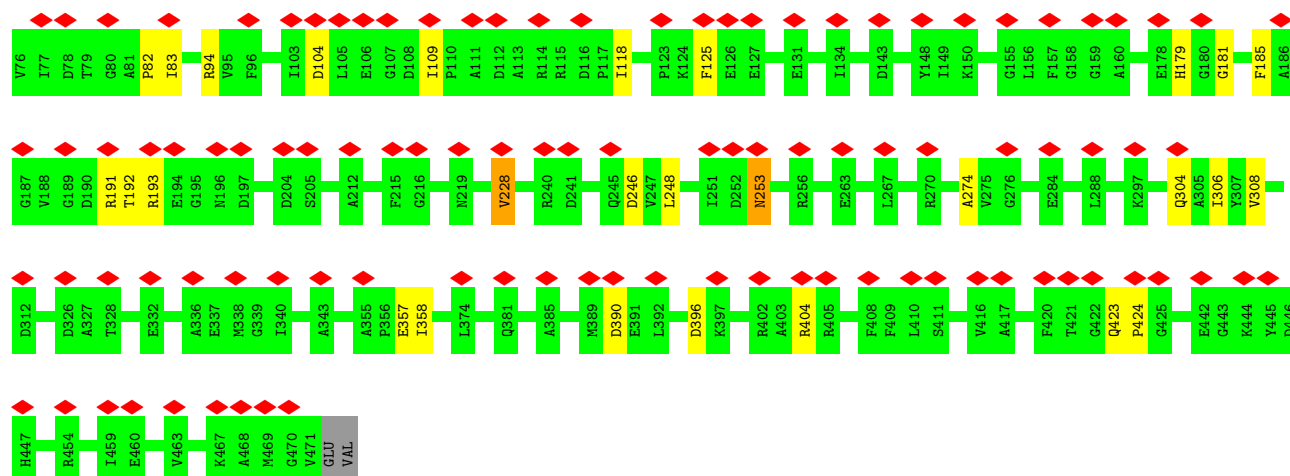


- Molecule 1: ATP synthase subunit alpha

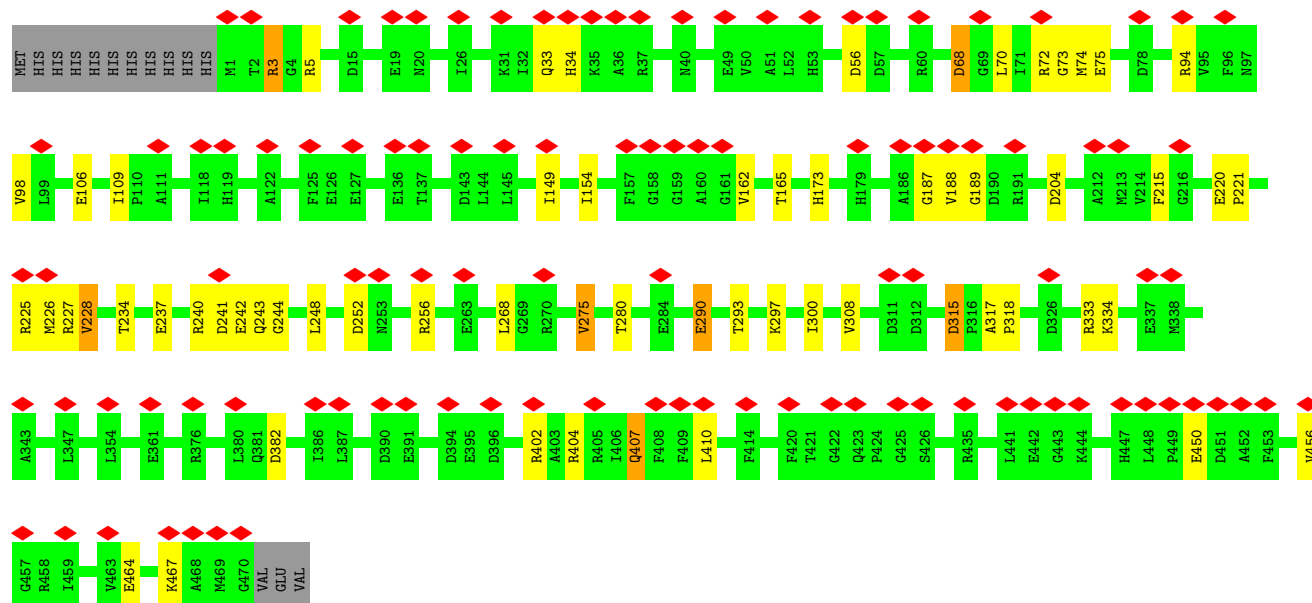
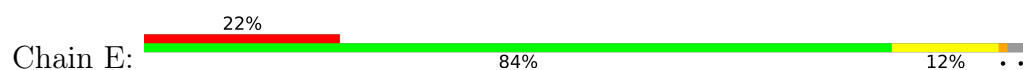


- Molecule 2: ATP synthase subunit beta

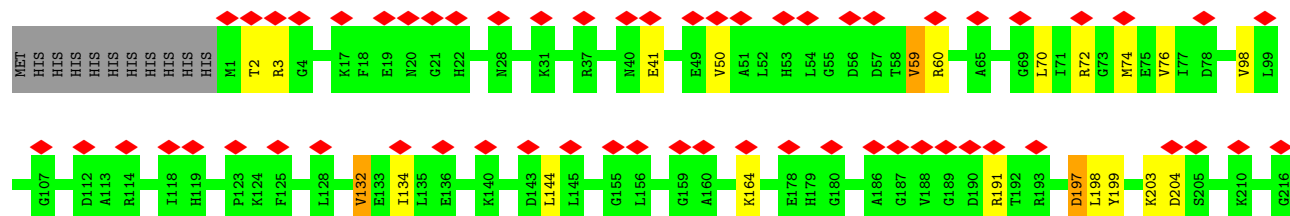
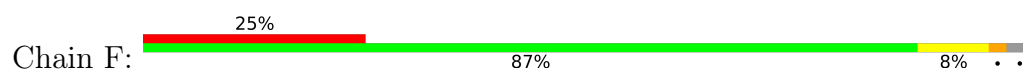


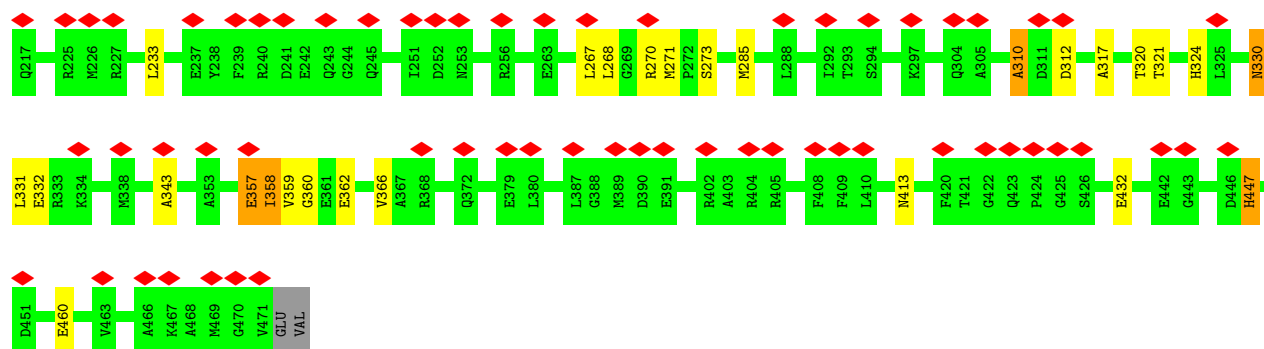


• Molecule 2: ATP synthase subunit beta

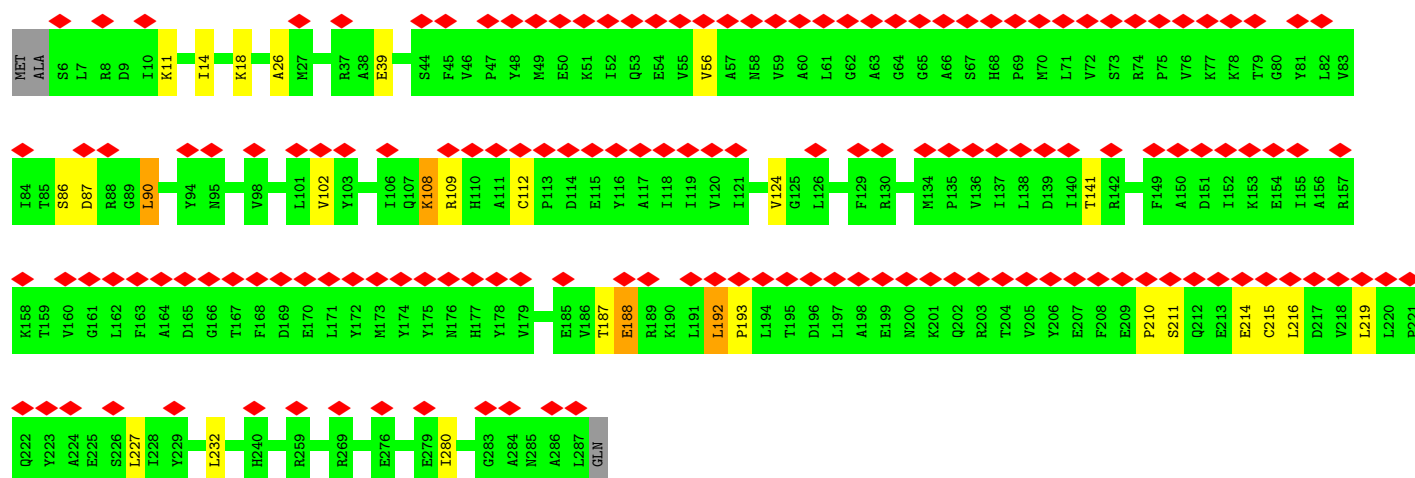
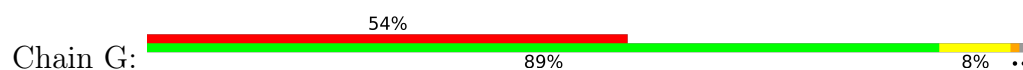


• Molecule 2: ATP synthase subunit beta





• Molecule 3: ATP synthase gamma chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	367412	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.963	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	215.04, 215.04, 215.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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	0.74	1/3695 (0.0%)	1.38	17/5004 (0.3%)
1	B	0.77	0/3702	1.40	21/5014 (0.4%)
1	C	0.69	0/3708	1.23	7/5022 (0.1%)
2	D	0.68	0/3684	1.17	7/4991 (0.1%)
2	E	0.70	0/3685	1.24	15/4991 (0.3%)
2	F	0.67	0/3692	1.20	3/5001 (0.1%)
3	G	0.67	0/2244	1.21	1/3036 (0.0%)
All	All	0.71	1/24410 (0.0%)	1.27	71/33059 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	PRO	C-O	-5.30	1.20	1.24

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	PRO	N-CA-C	8.20	124.04	111.57
1	C	275	LEU	N-CA-C	-7.94	102.62	111.28
1	A	395	PHE	CA-CB-CG	7.36	121.16	113.80
1	A	145	PRO	N-CA-C	7.25	122.58	111.57
1	B	138	ASP	N-CA-C	-6.81	104.09	112.88
1	B	380	GLY	N-CA-C	-6.80	106.85	114.40
2	E	73	GLY	N-CA-C	-6.79	105.70	115.27
1	A	145	PRO	CB-CA-C	-6.77	101.25	110.60
2	E	382	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	351	SER	N-CA-C	-6.56	105.27	113.20
1	A	158	PRO	N-CA-C	6.50	121.04	111.03
1	A	318	PHE	CA-CB-CG	6.35	120.15	113.80
1	B	318	PHE	CA-CB-CG	6.35	120.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ASN	OD1-CG-ND2	-6.26	116.34	122.60
2	F	310	ALA	N-CA-C	-6.13	97.73	110.80
1	C	397	GLN	N-CA-C	-6.12	105.66	113.01
2	D	82	PRO	CB-CA-C	-6.08	101.74	110.75
2	F	413	ASN	CA-CB-CG	6.08	118.68	112.60
1	A	289	ASP	CA-CB-CG	5.96	118.56	112.60
2	E	243	GLN	N-CA-C	-5.96	105.71	112.87
1	A	173	THR	N-CA-C	-5.96	102.84	110.53
2	E	173	HIS	CB-CG-CD2	-5.95	123.47	131.20
2	E	221	PRO	N-CA-CB	5.90	106.50	103.19
2	E	204	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	423	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	58	GLY	CA-C-N	5.68	129.04	120.75
1	B	58	GLY	C-N-CA	5.68	129.04	120.75
1	B	407	GLN	OE1-CD-NE2	-5.58	117.02	122.60
2	E	215	PHE	CA-CB-CG	5.54	119.34	113.80
3	G	39	GLU	N-CA-C	-5.54	105.24	111.28
2	E	56	ASP	CA-C-N	5.52	129.98	122.19
2	E	56	ASP	C-N-CA	5.52	129.98	122.19
1	B	272	GLU	CB-CA-C	-5.52	102.21	110.88
1	A	136	VAL	CA-C-O	-5.47	116.11	121.58
1	A	233	PRO	CA-C-N	-5.47	112.00	120.31
1	A	233	PRO	C-N-CA	-5.47	112.00	120.31
1	B	236	PHE	CA-CB-CG	5.45	119.25	113.80
2	D	21	GLY	N-CA-C	-5.45	107.80	115.32
1	B	143	HIS	CB-CG-CD2	-5.43	124.15	131.20
2	D	104	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	284	GLU	N-CA-C	-5.41	99.28	110.80
2	E	33	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	C	439	ALA	N-CA-C	-5.37	105.51	111.36
2	D	396	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	451	GLU	N-CA-C	5.25	117.41	111.11
1	B	280	PRO	N-CA-C	5.22	117.08	110.70
1	C	318	PHE	CA-CB-CG	5.21	119.02	113.80
1	A	425	HIS	CB-CG-CD2	-5.20	124.43	131.20
2	E	68	ASP	CA-CB-CG	5.17	117.77	112.60
2	F	360	GLY	CA-C-O	-5.16	118.11	122.29
1	B	479	LYS	CA-C-N	-5.16	112.19	121.62
1	B	479	LYS	C-N-CA	-5.16	112.19	121.62
1	B	423	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	289	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	433	GLN	OE1-CD-NE2	-5.14	117.46	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	34	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	A	209	VAL	N-CA-C	-5.12	105.40	110.62
1	B	154	ASP	CA-CB-CG	5.12	117.72	112.60
2	D	308	VAL	CA-C-N	5.12	125.41	119.47
2	D	308	VAL	C-N-CA	5.12	125.41	119.47
1	A	407	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	433	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	281	PRO	N-CA-CB	-5.10	97.89	103.25
2	E	280	THR	CA-C-O	-5.10	116.06	122.63
2	E	293	THR	CB-CA-C	-5.07	99.37	110.67
1	C	347	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	154	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	347	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	186	GLN	CA-C-N	5.02	131.13	121.54
1	B	186	GLN	C-N-CA	5.02	131.13	121.54
2	E	280	THR	CB-CA-C	-5.01	104.60	112.12

There are no chirality outliers.

There are no planarity outliers.

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	3636	0	3710	40	0
1	B	3643	0	3718	47	0
1	C	3649	0	3723	41	0
2	D	3621	0	3630	22	0
2	E	3622	0	3634	37	0
2	F	3629	0	3643	31	0
3	G	2211	0	2257	17	0
4	A	31	0	12	2	0
4	B	31	0	12	3	0
4	C	31	0	12	2	0
4	D	31	0	12	1	0
4	F	31	0	12	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	5	0	0	0	0
All	All	24176	0	24375	228	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 (228) 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)
4:A:601:ATP:H5'1	4:A:601:ATP:H8	1.37	0.88
1:B:451:GLU:CD	1:B:451:GLU:H	1.88	0.82
4:A:601:ATP:H5'1	4:A:601:ATP:C8	2.15	0.81
1:A:172:GLN:HA	1:A:172:GLN:NE2	1.94	0.80
2:D:274:ALA:O	3:G:280:ILE:HD11	1.82	0.79
1:A:273:LEU:O	1:A:273:LEU:HD23	1.83	0.78
2:E:94:ARG:HH21	2:E:109:ILE:HG13	1.48	0.78
1:B:271:ARG:HD2	1:B:285:ALA:HB3	1.67	0.76
1:A:273:LEU:HD23	1:A:273:LEU:C	2.12	0.75
2:E:402:ARG:HG2	2:E:402:ARG:HH21	1.52	0.72
1:B:448:ILE:N	1:B:448:ILE:HD12	2.07	0.70
1:B:448:ILE:HD12	1:B:448:ILE:H	1.57	0.69
1:C:415:ARG:HE	1:C:446:ASP:HA	1.57	0.69
1:C:448:ILE:HD12	1:C:448:ILE:H	1.59	0.67
1:B:348:LEU:HB3	1:B:356:ALA:HB1	1.76	0.66
2:E:98:VAL:HG22	2:E:228:VAL:HG23	1.78	0.66
1:A:458:LYS:O	1:A:461:TYR:HB2	1.95	0.66
1:A:445:LEU:HA	1:A:448:ILE:HD13	1.78	0.65
1:C:173:THR:N	4:C:600:ATP:O2B	2.27	0.65
1:C:363:VAL:HG12	1:C:383:ARG:HE	1.60	0.64
2:D:39:GLU:CD	2:D:39:GLU:H	2.05	0.64
2:D:2:THR:HB	2:D:20:ASN:HD22	1.63	0.64
2:E:189:GLY:O	2:E:256:ARG:NH2	2.29	0.64
1:C:363:VAL:HG12	1:C:383:ARG:NE	2.13	0.64
2:E:275:VAL:HG23	2:E:275:VAL:O	1.98	0.63
1:C:174:GLY:H	4:C:600:ATP:PB	2.21	0.63
2:E:187:GLY:HA2	2:E:252:ASP:HB2	1.81	0.63
1:B:53:VAL:HG22	1:B:88:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:402:ARG:HG2	2:E:402:ARG:NH2	2.13	0.63
2:E:290:GLU:HA	2:E:290:GLU:OE1	1.98	0.62
2:F:330:ASN:OD1	2:F:330:ASN:N	2.32	0.62
1:C:451:GLU:N	1:C:451:GLU:OE1	2.33	0.61
1:A:143:HIS:CG	1:A:143:HIS:O	2.53	0.61
1:C:193:SER:HB2	1:C:221:THR:HG22	1.82	0.61
1:B:438:TYR:CE2	1:B:442:ARG:HG3	2.37	0.60
1:B:483:ASN:HB3	1:B:486:ASP:HB2	1.84	0.60
1:C:448:ILE:HD12	1:C:448:ILE:N	2.17	0.59
1:B:45:ASP:HA	2:F:72:ARG:HH21	1.67	0.59
2:E:450:GLU:CD	2:E:450:GLU:H	2.10	0.59
1:B:386:LEU:HD12	1:B:386:LEU:O	2.03	0.59
1:C:366:VAL:HG12	1:C:366:VAL:O	2.03	0.58
2:F:199:TYR:CZ	2:F:203:LYS:HD2	2.38	0.58
1:C:189:GLN:N	1:C:189:GLN:OE1	2.31	0.58
3:G:216:LEU:HA	3:G:219:LEU:HG	1.86	0.58
1:B:451:GLU:OE1	1:B:451:GLU:N	2.34	0.57
3:G:211:SER:HB2	3:G:214:GLU:HB2	1.85	0.57
1:A:172:GLN:HA	1:A:172:GLN:HE21	1.67	0.57
1:A:456:PHE:C	1:A:456:PHE:CD2	2.83	0.57
2:F:358:ILE:N	2:F:358:ILE:HD13	2.19	0.57
1:A:451:GLU:H	1:A:451:GLU:CD	2.12	0.56
2:E:464:GLU:HA	2:E:467:LYS:HD3	1.87	0.56
2:F:362:GLU:OE2	2:F:362:GLU:HA	2.05	0.56
2:E:187:GLY:HA2	2:E:252:ASP:CB	2.36	0.56
2:D:49:GLU:O	2:D:49:GLU:HG3	2.06	0.56
1:B:385:ASP:OD1	1:B:385:ASP:N	2.37	0.56
1:B:438:TYR:CZ	1:B:442:ARG:HG3	2.41	0.56
1:B:354:ARG:HB3	4:B:600:ATP:N6	2.21	0.55
1:C:48:MET:HE3	1:C:51:GLU:HG3	1.87	0.55
1:C:469:GLN:OE1	1:C:469:GLN:HA	2.07	0.55
2:D:94:ARG:HH11	2:D:94:ARG:HG3	1.71	0.54
1:A:469:GLN:OE1	1:A:469:GLN:HA	2.07	0.54
3:G:109:ARG:O	3:G:109:ARG:HG3	2.06	0.54
1:A:233:PRO:HG3	1:A:273:LEU:HD12	1.88	0.54
1:B:448:ILE:H	1:B:448:ILE:CD1	2.22	0.53
3:G:192:LEU:HD12	3:G:193:PRO:HA	1.88	0.53
1:A:416:THR:HA	1:A:440:LEU:HD21	1.91	0.53
1:A:53:VAL:HG22	1:A:88:VAL:HG22	1.90	0.53
1:B:379:ALA:C	1:B:381:THR:H	2.16	0.53
2:F:197:ASP:OD2	2:F:197:ASP:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLU:OE1	1:A:451:GLU:N	2.24	0.53
1:C:391:GLU:OE2	2:D:404:ARG:NH1	2.38	0.52
2:F:310:ALA:C	2:F:312:ASP:H	2.17	0.52
1:C:143:HIS:CG	1:C:143:HIS:O	2.62	0.52
1:C:104:ILE:HA	1:C:222:ILE:HG12	1.91	0.52
2:E:240:ARG:HE	2:E:300:ILE:HG13	1.74	0.51
1:A:66:LEU:HB3	2:E:72:ARG:HD3	1.92	0.51
1:A:448:ILE:HD12	1:A:448:ILE:H	1.75	0.51
2:D:19:GLU:C	2:D:19:GLU:CD	2.78	0.51
1:A:389:TYR:CD1	1:A:413:GLY:HA3	2.46	0.51
1:B:445:LEU:HD23	1:B:445:LEU:O	2.10	0.51
3:G:11:LYS:HD2	3:G:11:LYS:O	2.11	0.51
1:C:448:ILE:H	1:C:448:ILE:CD1	2.23	0.51
2:E:315:ASP:O	2:E:318:PRO:HD2	2.11	0.51
1:A:145:PRO:HB3	1:A:370:ALA:O	2.11	0.51
1:B:174:GLY:H	4:B:600:ATP:PB	2.33	0.51
1:C:218:LEU:HA	1:C:221:THR:OG1	2.10	0.51
1:C:156:LEU:CD2	1:C:382:LEU:HB3	2.41	0.50
1:B:456:PHE:C	1:B:456:PHE:CD2	2.88	0.50
1:C:351:SER:O	1:C:351:SER:OG	2.27	0.50
1:B:168:ILE:HG23	1:B:168:ILE:O	2.12	0.50
2:F:331:LEU:HA	2:F:343:ALA:O	2.11	0.50
3:G:108:LYS:HE2	3:G:108:LYS:N	2.27	0.50
2:D:423:GLN:HG2	2:D:424:PRO:HD2	1.93	0.50
2:F:60:ARG:HG2	2:F:268:LEU:HD23	1.93	0.50
1:C:353:VAL:HA	1:C:421:LYS:HE3	1.94	0.49
1:B:473:GLU:OE1	1:B:473:GLU:HA	2.10	0.49
1:A:286:TYR:HB3	1:A:290:ILE:HG13	1.94	0.49
2:F:460:GLU:OE1	2:F:460:GLU:N	2.27	0.49
3:G:90:LEU:O	3:G:90:LEU:HD12	2.13	0.49
2:D:191:ARG:NH1	4:D:500:ATP:O1A	2.46	0.49
2:E:241:ASP:HA	2:E:297:LYS:HD3	1.94	0.49
2:D:83:ILE:HB	2:D:118:ILE:HD12	1.94	0.48
1:A:290:ILE:HG21	1:A:330:ILE:HD12	1.95	0.48
2:E:3:ARG:CB	2:E:3:ARG:CZ	2.91	0.48
1:A:162:GLY:H	1:A:314:THR:HB	1.78	0.48
1:A:212:LEU:HB3	1:A:217:ALA:HB3	1.95	0.48
1:C:396:ALA:C	1:C:398:PHE:N	2.71	0.48
2:F:357:GLU:CD	2:F:357:GLU:N	2.70	0.48
2:D:193:ARG:O	2:D:193:ARG:HG2	2.14	0.47
1:B:379:ALA:C	1:B:381:THR:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ALA:O	1:C:397:GLN:HG2	2.15	0.47
2:D:49:GLU:O	2:D:49:GLU:CG	2.62	0.47
1:A:444:PHE:HB3	1:A:495:LYS:HD2	1.95	0.47
1:C:158:PRO:HG2	1:C:367:GLY:HA2	1.96	0.47
1:C:289:ASP:N	1:C:289:ASP:OD1	2.47	0.47
2:D:358:ILE:HG22	2:D:358:ILE:O	2.14	0.47
2:F:271:MET:HE2	2:F:271:MET:HB3	1.78	0.47
2:E:154:ILE:N	2:E:154:ILE:HD12	2.30	0.47
1:C:396:ALA:C	1:C:398:PHE:H	2.23	0.46
1:A:389:TYR:CG	1:A:413:GLY:HA3	2.51	0.46
2:E:242:GLU:C	2:E:244:GLY:N	2.72	0.46
1:C:273:LEU:C	1:C:273:LEU:HD23	2.40	0.46
2:E:75:GLU:CD	2:E:75:GLU:O	2.58	0.46
1:B:415:ARG:O	1:B:419:VAL:N	2.45	0.46
1:B:451:GLU:CD	1:B:451:GLU:N	2.66	0.46
1:C:45:ASP:HA	2:D:72:ARG:HH21	1.81	0.46
1:B:354:ARG:HB3	4:B:600:ATP:C6	2.51	0.46
1:A:210:GLU:OE1	1:A:210:GLU:HA	2.15	0.46
2:E:5:ARG:HH11	2:E:5:ARG:HB2	1.81	0.45
2:F:3:ARG:HA	2:F:76:VAL:O	2.16	0.45
1:C:191:MET:HB2	1:C:191:MET:HE2	1.62	0.45
1:C:451:GLU:N	1:C:451:GLU:CD	2.73	0.45
2:F:310:ALA:C	2:F:312:ASP:N	2.74	0.45
1:C:415:ARG:NH2	1:C:446:ASP:O	2.36	0.45
1:C:421:LYS:HB2	1:C:454:ARG:HD3	1.97	0.45
3:G:188:GLU:C	3:G:188:GLU:CD	2.84	0.45
1:C:277:LEU:O	1:C:278:ARG:HB2	2.17	0.45
1:A:171:ARG:O	1:A:171:ARG:HG3	2.16	0.45
1:A:349:PHE:C	1:A:351:SER:H	2.25	0.45
1:A:460:PHE:CE2	1:A:464:LEU:HD11	2.52	0.45
2:F:267:LEU:N	2:F:267:LEU:HD23	2.31	0.45
2:E:220:GLU:O	2:E:225:ARG:NH1	2.50	0.45
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.83	0.44
1:A:472:LEU:O	1:A:473:GLU:C	2.57	0.44
1:B:286:TYR:HB3	1:B:290:ILE:HG13	2.00	0.44
2:E:226:MET:HG2	2:E:227:ARG:HD3	2.00	0.44
2:F:164:LYS:HB2	2:F:164:LYS:HE3	1.83	0.44
2:F:460:GLU:H	2:F:460:GLU:CD	2.18	0.44
1:B:488:ASN:N	1:B:488:ASN:HD22	2.16	0.44
2:D:185:PHE:CD2	2:D:185:PHE:C	2.95	0.44
1:A:448:ILE:H	1:A:448:ILE:CD1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASP:OD2	2:F:270:ARG:NE	2.49	0.44
1:A:409:LYS:HA	1:A:409:LYS:HD2	1.73	0.44
2:F:70:LEU:HD23	2:F:70:LEU:HA	1.78	0.44
2:F:324:HIS:CD2	2:F:324:HIS:N	2.86	0.44
1:B:386:LEU:HD12	1:B:386:LEU:C	2.40	0.44
1:B:448:ILE:N	1:B:448:ILE:CD1	2.76	0.44
2:E:315:ASP:OD1	2:E:315:ASP:C	2.60	0.43
1:A:448:ILE:HD12	1:A:448:ILE:N	2.33	0.43
1:B:52:LEU:HB3	1:B:91:THR:HG21	2.00	0.43
1:C:415:ARG:NE	1:C:446:ASP:HA	2.28	0.43
2:D:228:VAL:O	2:D:228:VAL:CG1	2.65	0.43
1:A:469:GLN:HE21	1:A:473:GLU:HG2	1.84	0.43
1:B:94:ILE:O	1:B:95:MET:C	2.60	0.43
1:B:283:ARG:O	1:B:284:GLU:C	2.59	0.43
2:E:404:ARG:HG2	2:E:404:ARG:HH21	1.84	0.43
1:B:38:ILE:HD13	1:B:38:ILE:N	2.33	0.43
2:E:189:GLY:HA3	2:E:256:ARG:HE	1.84	0.43
2:E:275:VAL:O	2:E:275:VAL:CG2	2.65	0.43
2:E:188:VAL:HG22	2:E:228:VAL:HG12	2.01	0.43
1:A:347:ASP:OD2	1:A:347:ASP:N	2.41	0.43
1:B:391:GLU:C	1:B:391:GLU:CD	2.85	0.43
3:G:192:LEU:HD13	3:G:192:LEU:HA	1.93	0.43
1:A:395:PHE:HB2	3:G:26:ALA:HB2	2.01	0.43
2:E:242:GLU:C	2:E:244:GLY:H	2.27	0.43
2:E:450:GLU:CD	2:E:450:GLU:N	2.76	0.43
1:A:206:ARG:NH2	2:D:125:PHE:O	2.51	0.43
2:F:198:LEU:O	2:F:199:TYR:C	2.61	0.43
1:A:459:GLU:O	1:A:462:LEU:N	2.51	0.42
2:F:310:ALA:O	2:F:312:ASP:N	2.51	0.42
1:B:134:PRO:HG2	1:B:302:ALA:HB3	1.99	0.42
3:G:210:PRO:HB2	3:G:215:CYS:HB2	2.00	0.42
2:E:317:ALA:HB3	2:E:318:PRO:HD3	2.02	0.42
2:F:50:VAL:HG13	2:F:59:VAL:HG22	2.01	0.42
1:A:136:VAL:O	1:A:137:MET:HB2	2.19	0.42
2:E:3:ARG:HB2	2:E:3:ARG:NH2	2.35	0.42
1:B:393:GLU:O	1:B:393:GLU:CD	2.63	0.42
2:F:144:LEU:HD11	2:F:366:VAL:HG12	2.01	0.42
3:G:56:VAL:HB	3:G:219:LEU:HD13	2.02	0.42
1:B:471:LEU:HD13	1:B:487:LEU:HD13	2.02	0.42
1:C:382:LEU:HA	1:C:382:LEU:HD12	1.72	0.42
2:F:191:ARG:NH1	4:F:500:ATP:O2G	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:285:MET:HE2	2:F:285:MET:HB3	1.81	0.42
1:C:336:SER:O	2:D:191:ARG:NH2	2.52	0.42
2:E:407:GLN:O	2:E:410:LEU:HB2	2.19	0.42
2:F:132:VAL:HG21	2:F:358:ILE:HG13	2.02	0.42
2:F:317:ALA:O	2:F:320:THR:HG22	2.19	0.42
2:D:179:HIS:CG	2:D:248:LEU:HD11	2.54	0.41
3:G:86:SER:O	3:G:124:VAL:HG22	2.20	0.41
1:B:274:SER:O	1:B:275:LEU:C	2.63	0.41
1:B:442:ARG:HD3	1:B:442:ARG:HA	1.94	0.41
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.88	0.41
2:E:5:ARG:NH1	2:E:5:ARG:CB	2.82	0.41
1:B:391:GLU:CD	1:B:391:GLU:O	2.63	0.41
1:B:478:THR:O	1:B:478:THR:HG22	2.20	0.41
1:C:488:ASN:N	1:C:488:ASN:HD22	2.19	0.41
2:F:447:HIS:ND1	2:F:447:HIS:N	2.63	0.41
3:G:232:LEU:HD23	3:G:232:LEU:HA	1.87	0.41
1:A:169:GLY:O	1:A:321:THR:HG22	2.21	0.41
1:C:45:ASP:OD2	1:C:45:ASP:N	2.53	0.41
2:E:162:VAL:HG12	2:E:333:ARG:HA	2.02	0.41
3:G:108:LYS:HD3	3:G:108:LYS:HA	1.72	0.41
2:E:290:GLU:OE1	2:E:290:GLU:CA	2.66	0.41
2:F:134:ILE:HD13	2:F:359:VAL:HG12	2.02	0.41
1:A:138:ASP:OD1	1:A:138:ASP:N	2.53	0.41
1:B:136:VAL:O	1:B:137:MET:HB2	2.20	0.41
1:B:173:THR:HG22	1:B:173:THR:O	2.21	0.41
2:D:357:GLU:H	2:D:357:GLU:HG2	1.66	0.41
2:E:70:LEU:HD23	2:E:70:LEU:HA	1.88	0.41
1:C:274:SER:O	1:C:275:LEU:C	2.64	0.40
2:D:181:GLY:HA3	2:D:246:ASP:O	2.21	0.40
2:F:41:GLU:H	2:F:41:GLU:HG3	1.69	0.40
3:G:14:ILE:HG22	3:G:18:LYS:HE2	2.02	0.40
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.86	0.40
2:E:94:ARG:HH11	2:E:106:GLU:HB2	1.86	0.40
1:B:46:ASN:N	1:B:46:ASN:ND2	2.69	0.40
1:B:275:LEU:O	1:B:278:ARG:N	2.54	0.40
2:D:390:ASP:OD2	2:D:390:ASP:N	2.55	0.40

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	472/510 (92%)	458 (97%)	13 (3%)	1 (0%)	43	72
1	B	473/510 (93%)	453 (96%)	18 (4%)	2 (0%)	30	61
1	C	474/510 (93%)	456 (96%)	17 (4%)	1 (0%)	43	72
2	D	468/484 (97%)	448 (96%)	19 (4%)	1 (0%)	43	72
2	E	468/484 (97%)	455 (97%)	13 (3%)	0	100	100
2	F	469/484 (97%)	456 (97%)	13 (3%)	0	100	100
3	G	280/285 (98%)	271 (97%)	9 (3%)	0	100	100
All	All	3104/3267 (95%)	2997 (97%)	102 (3%)	5 (0%)	44	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	HIS
1	C	278	ARG
1	B	278	ARG
1	A	281	PRO
2	D	24	PRO

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	386/419 (92%)	365 (95%)	21 (5%)	20	47
1	B	387/419 (92%)	369 (95%)	18 (5%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	388/419 (93%)	375 (97%)	13 (3%)	32	57
2	D	386/400 (96%)	377 (98%)	9 (2%)	44	64
2	E	386/400 (96%)	369 (96%)	17 (4%)	25	52
2	F	387/400 (97%)	371 (96%)	16 (4%)	27	53
3	G	238/240 (99%)	228 (96%)	10 (4%)	26	53
All	All	2558/2697 (95%)	2454 (96%)	104 (4%)	28	53

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	47	VAL
1	A	65	ASN
1	A	70	ASN
1	A	97	VAL
1	A	136	VAL
1	A	138	ASP
1	A	143	HIS
1	A	273	LEU
1	A	284	GLU
1	A	314	THR
1	A	362	SER
1	A	366	VAL
1	A	375	MET
1	A	397	GLN
1	A	417	VAL
1	A	445	LEU
1	A	456	PHE
1	A	457	GLU
1	A	473	GLU
1	A	478	THR
1	B	31	VAL
1	B	38	ILE
1	B	47	VAL
1	B	86	ASP
1	B	97	VAL
1	B	140	ARG
1	B	141	SER
1	B	243	VAL
1	B	375	MET

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Mol	Chain	Res	Type
1	B	385	ASP
1	B	386	LEU
1	B	417	VAL
1	B	445	LEU
1	B	451	GLU
1	B	456	PHE
1	B	458	LYS
1	B	480	ASP
1	B	488	ASN
1	C	34	VAL
1	C	47	VAL
1	C	97	VAL
1	C	138	ASP
1	C	168	ILE
1	C	275	LEU
1	C	319	VAL
1	C	351	SER
1	C	375	MET
1	C	382	LEU
1	C	401	ASP
1	C	445	LEU
1	C	500	VAL
2	D	19	GLU
2	D	46	LEU
2	D	49	GLU
2	D	109	ILE
2	D	192	THR
2	D	228	VAL
2	D	253	ASN
2	D	304	GLN
2	D	306	ILE
2	E	3	ARG
2	E	68	ASP
2	E	74	MET
2	E	149	ILE
2	E	165	THR
2	E	228	VAL
2	E	234	THR
2	E	237	GLU
2	E	248	LEU
2	E	268	LEU
2	E	275	VAL

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Mol	Chain	Res	Type
2	E	290	GLU
2	E	308	VAL
2	E	315	ASP
2	E	334	LYS
2	E	407	GLN
2	E	456	VAL
2	F	2	THR
2	F	59	VAL
2	F	74	MET
2	F	98	VAL
2	F	132	VAL
2	F	197	ASP
2	F	204	ASP
2	F	233	LEU
2	F	273	SER
2	F	321	THR
2	F	330	ASN
2	F	332	GLU
2	F	357	GLU
2	F	358	ILE
2	F	432	GLU
2	F	447	HIS
3	G	87	ASP
3	G	90	LEU
3	G	102	VAL
3	G	108	LYS
3	G	112	CYS
3	G	141	THR
3	G	187	THR
3	G	188	GLU
3	G	192	LEU
3	G	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	255	HIS
1	A	488	ASN
1	B	46	ASN
1	B	65	ASN
1	B	143	HIS

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Mol	Chain	Res	Type
1	B	397	GLN
1	B	488	ASN
1	C	46	ASN
1	C	397	GLN
1	C	488	ASN
2	D	33	GLN
2	D	245	GLN
2	D	324	HIS
2	D	365	GLN
2	D	401	HIS
2	E	33	GLN
2	E	169	GLN
2	E	200	HIS
2	E	381	GLN
2	E	407	GLN
2	F	28	ASN
2	F	34	HIS
2	F	217	GLN
2	F	407	GLN
3	G	110	HIS
3	G	183	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	F	500	-	32,33,33	0.88	1 (3%)	48,52,52	1.31	7 (14%)
4	ATP	A	601	5	32,33,33	0.50	0	48,52,52	0.70	0
4	ATP	B	600	5	32,33,33	0.87	0	48,52,52	1.29	5 (10%)
6	PO4	A	603	-	4,4,4	0.77	0	6,6,6	0.47	0
4	ATP	C	600	5	32,33,33	0.53	0	48,52,52	0.68	0
4	ATP	D	500	5	32,33,33	0.52	0	48,52,52	0.56	0

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	ATP	F	500	-	-	2/22/38/38	0/3/3/3
4	ATP	A	601	5	-	1/22/38/38	0/3/3/3
4	ATP	B	600	5	-	3/22/38/38	0/3/3/3
4	ATP	C	600	5	-	1/22/38/38	0/3/3/3
4	ATP	D	500	5	-	1/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	500	ATP	C5-C4	-2.12	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ATP	O2G-PG-O3B	3.32	115.75	104.64
4	F	500	ATP	O3G-PG-O3B	3.00	114.71	104.64
4	B	600	ATP	C5-C4-N3	-2.94	122.66	126.72
4	B	600	ATP	C4-C5-N7	2.83	113.81	110.58
4	F	500	ATP	C4-C5-N7	2.81	113.80	110.58
4	F	500	ATP	C5-C4-N3	-2.75	122.93	126.72
4	B	600	ATP	O2A-PA-O3A	2.63	114.38	107.27
4	F	500	ATP	O2A-PA-O3A	2.63	114.37	107.27
4	F	500	ATP	O2B-PB-O3A	2.62	114.36	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ATP	N3-C4-N9	2.34	131.14	127.17
4	F	500	ATP	C2-N1-C6	-2.19	115.14	118.73
4	F	500	ATP	C5-C6-N1	2.18	123.05	117.51

There are no chirality outliers.

All (8) torsion outliers are listed below:

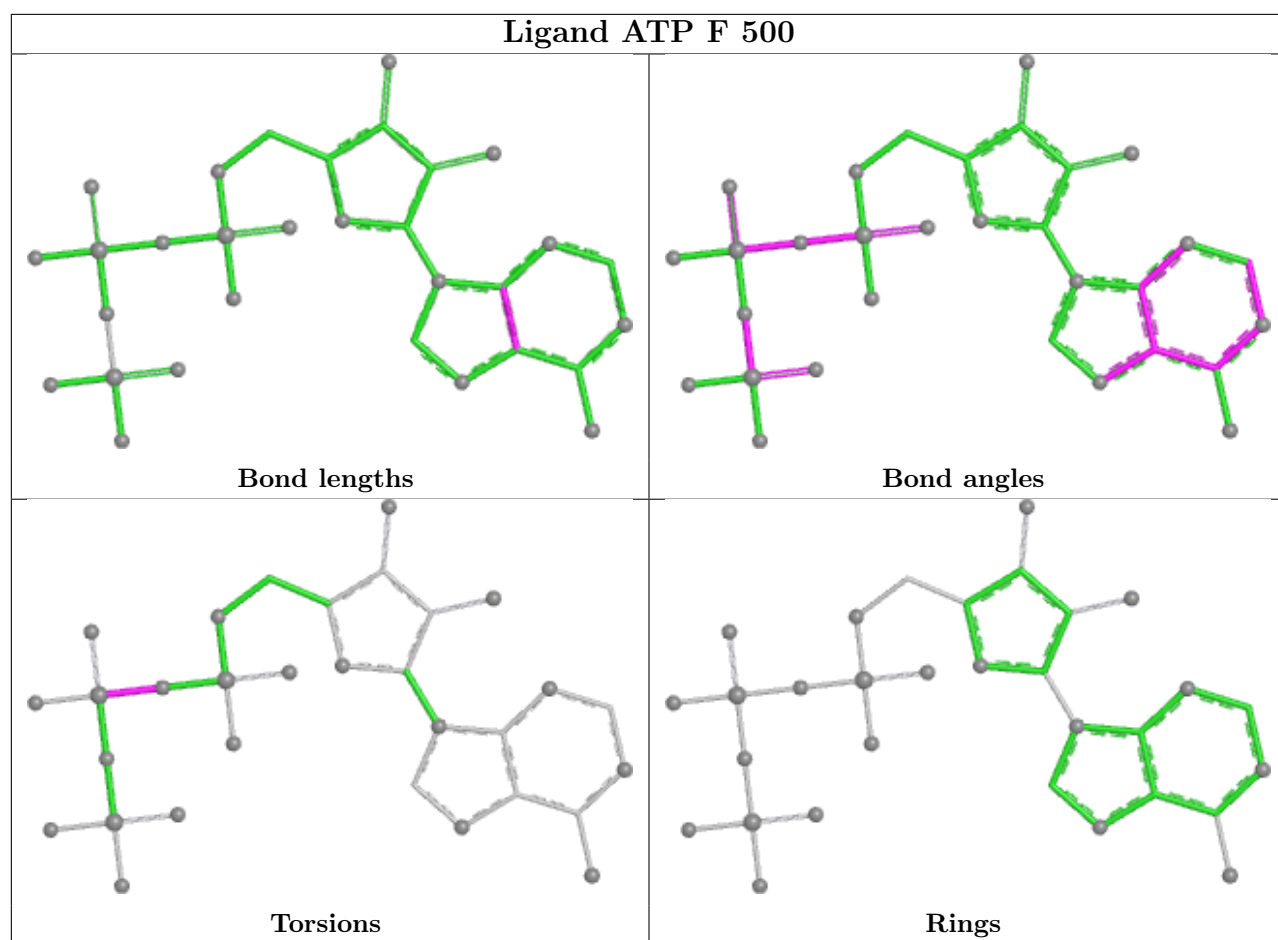
Mol	Chain	Res	Type	Atoms
4	B	600	ATP	C5'-O5'-PA-O1A
4	F	500	ATP	PA-O3A-PB-O2B
4	A	601	ATP	O4'-C4'-C5'-O5'
4	B	600	ATP	PB-O3B-PG-O1G
4	F	500	ATP	PA-O3A-PB-O1B
4	B	600	ATP	O4'-C4'-C5'-O5'
4	C	600	ATP	O4'-C4'-C5'-O5'
4	D	500	ATP	O4'-C4'-C5'-O5'

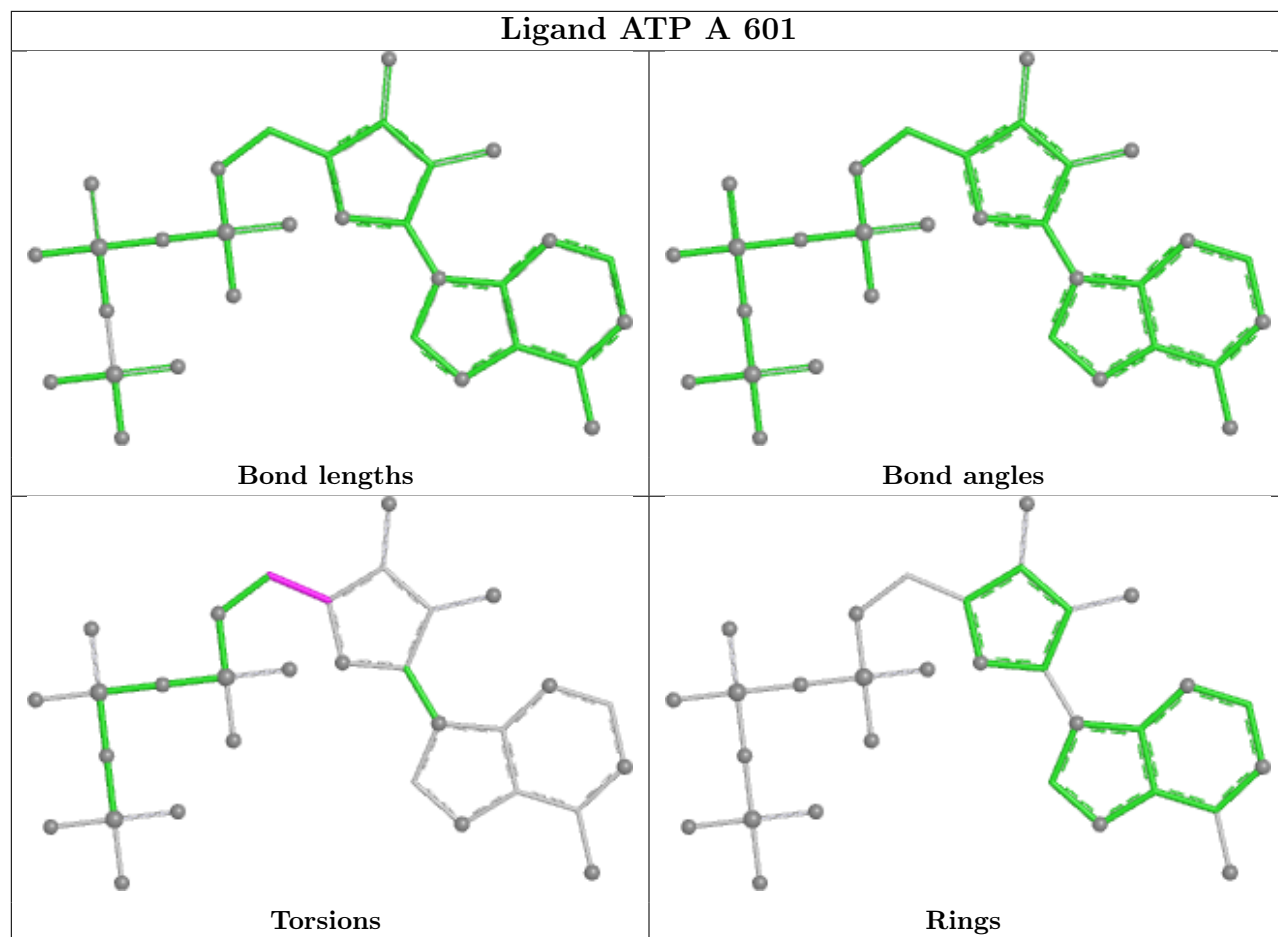
There are no ring outliers.

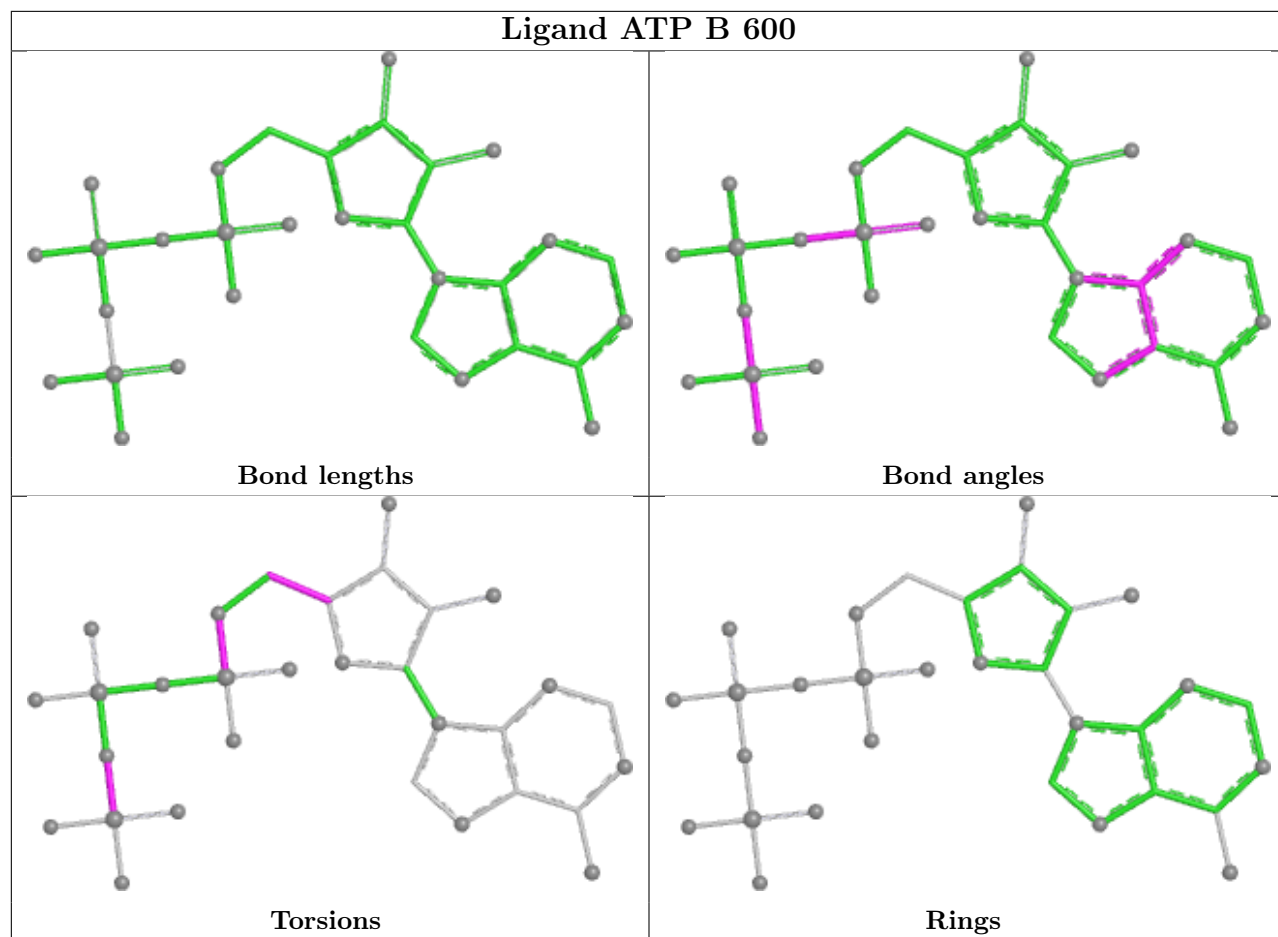
5 monomers are involved in 9 short contacts:

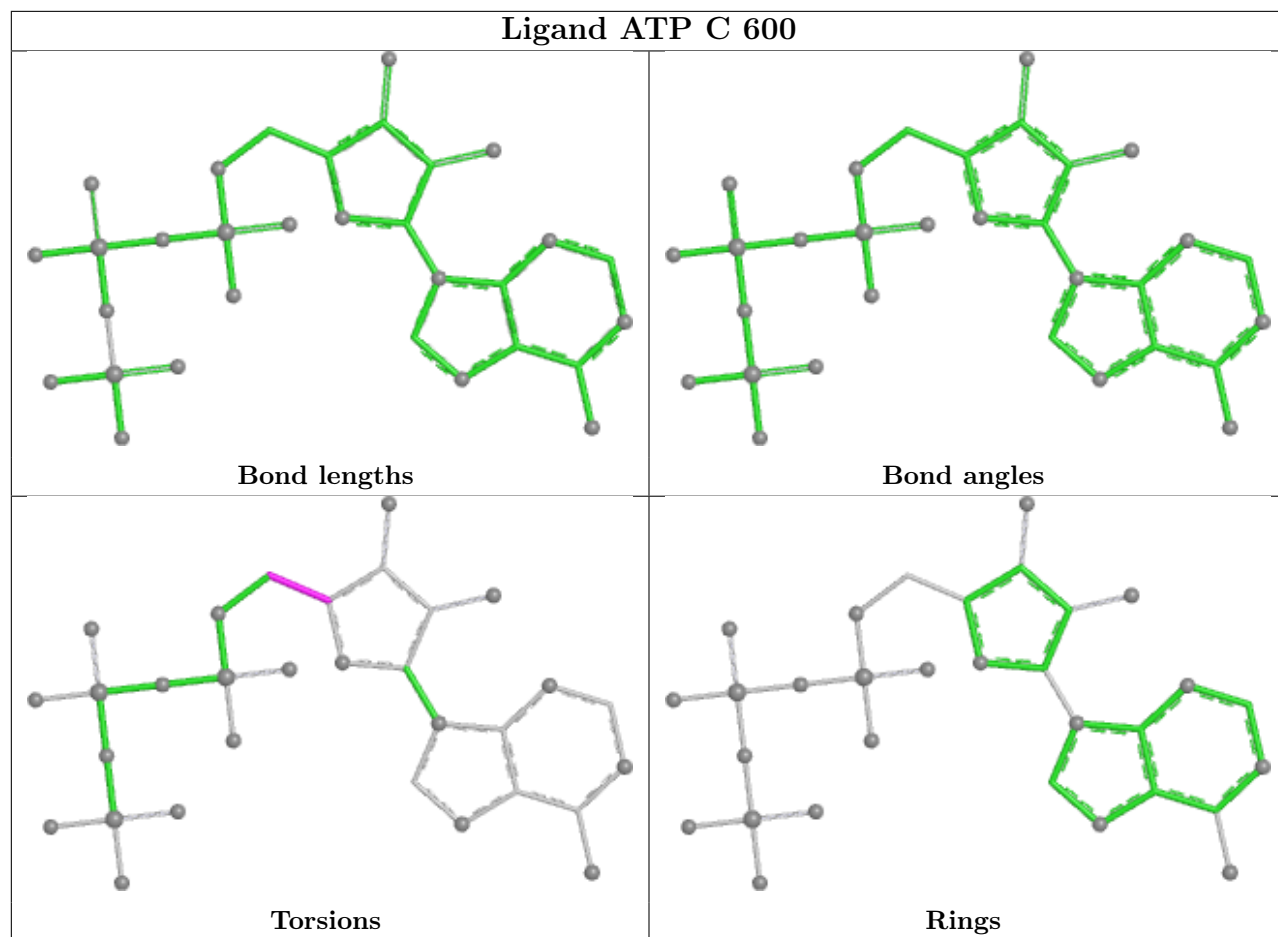
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	500	ATP	1	0
4	A	601	ATP	2	0
4	B	600	ATP	3	0
4	C	600	ATP	2	0
4	D	500	ATP	1	0

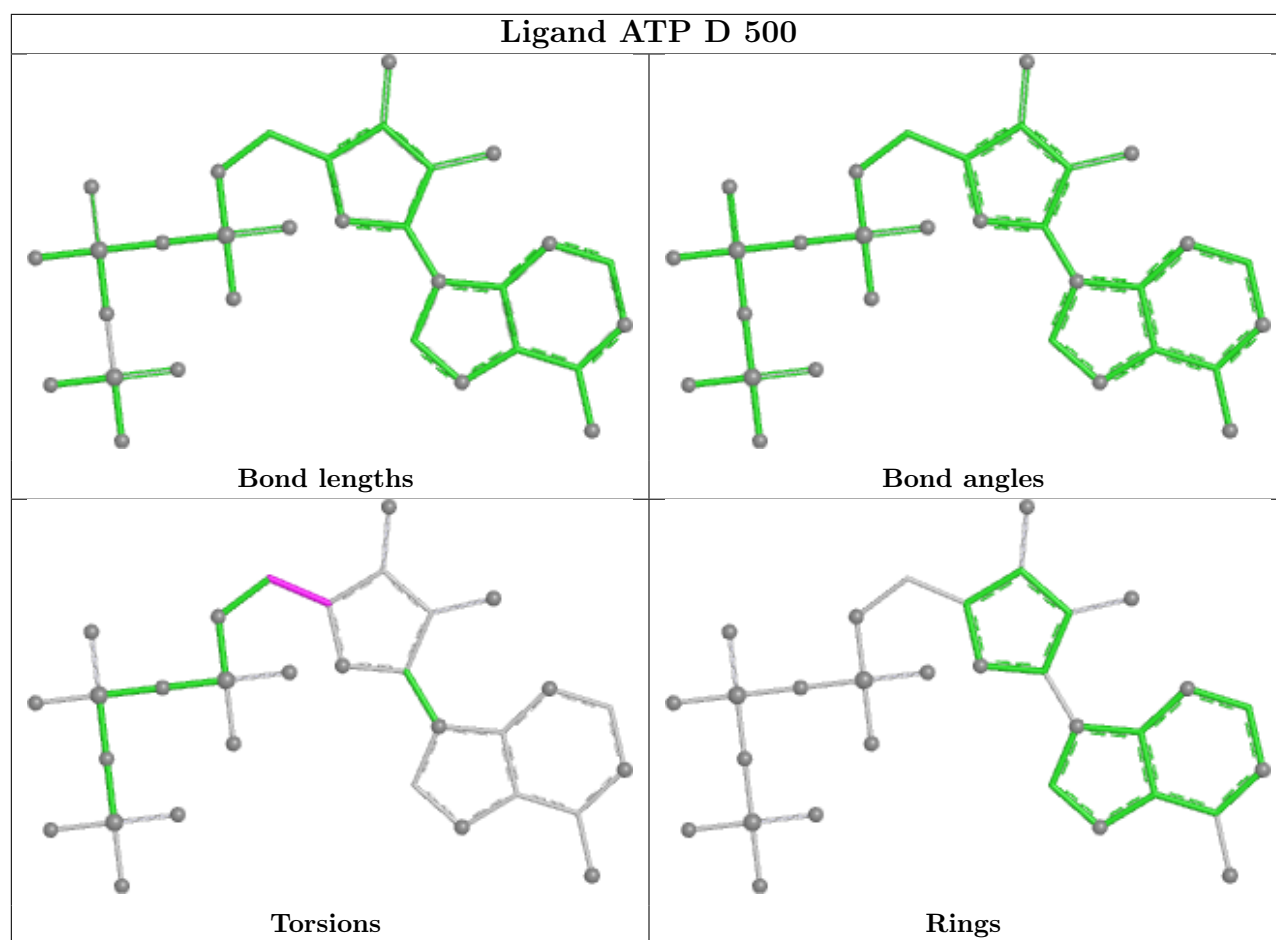
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

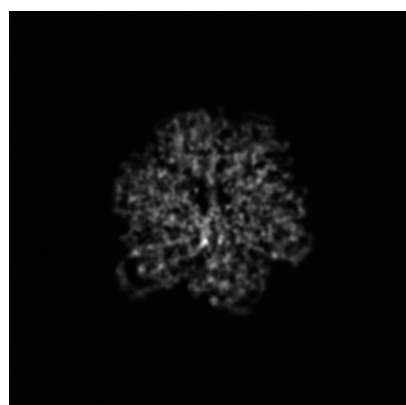
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23117. These allow visual inspection of the internal detail of the map and identification of artifacts.

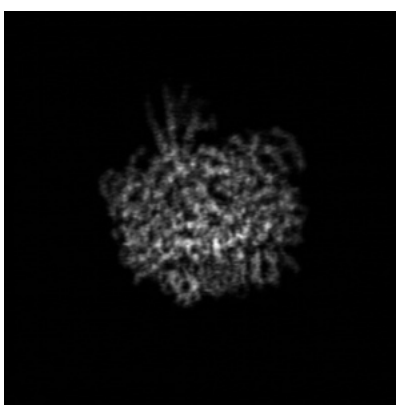
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

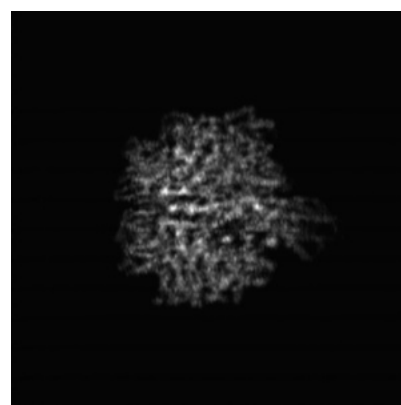
6.1.1 Primary map



X



Y

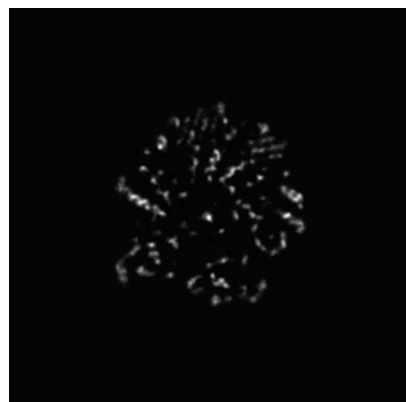


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

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

6.3 Largest variance slices [i](#)

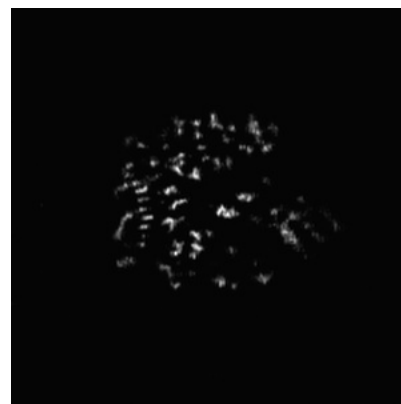
6.3.1 Primary map



X Index: 106



Y Index: 129

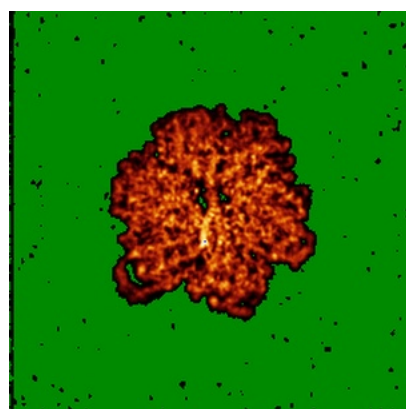


Z Index: 118

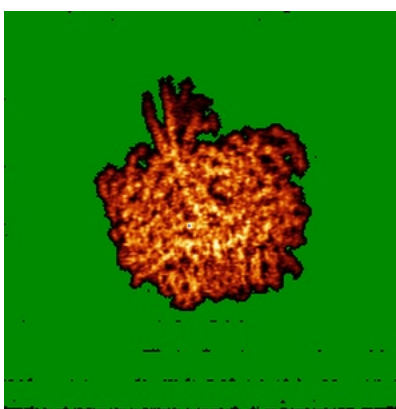
The images above show the largest variance slices of the map in three orthogonal directions.

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

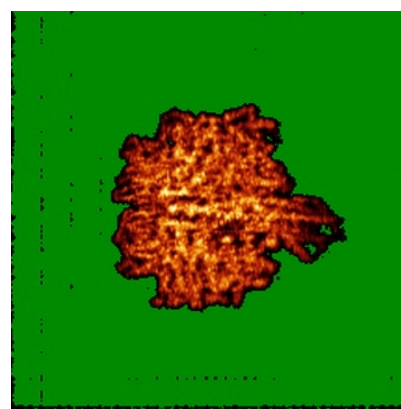
6.4.1 Primary map



X



Y

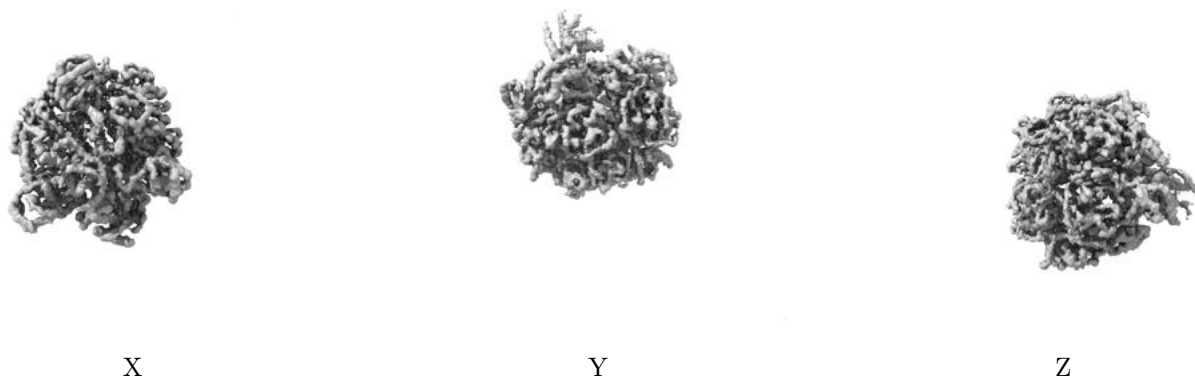


Z

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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

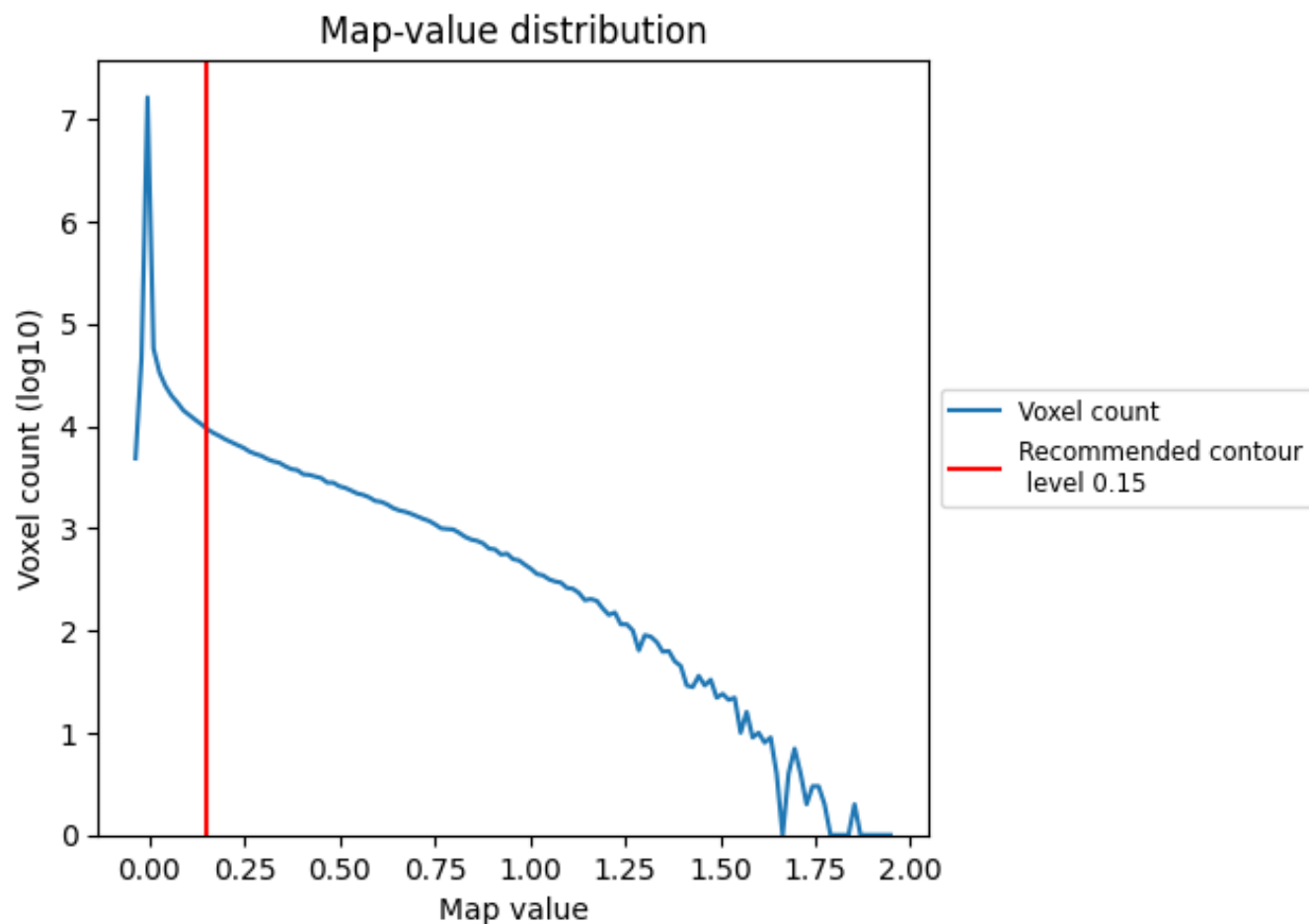
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

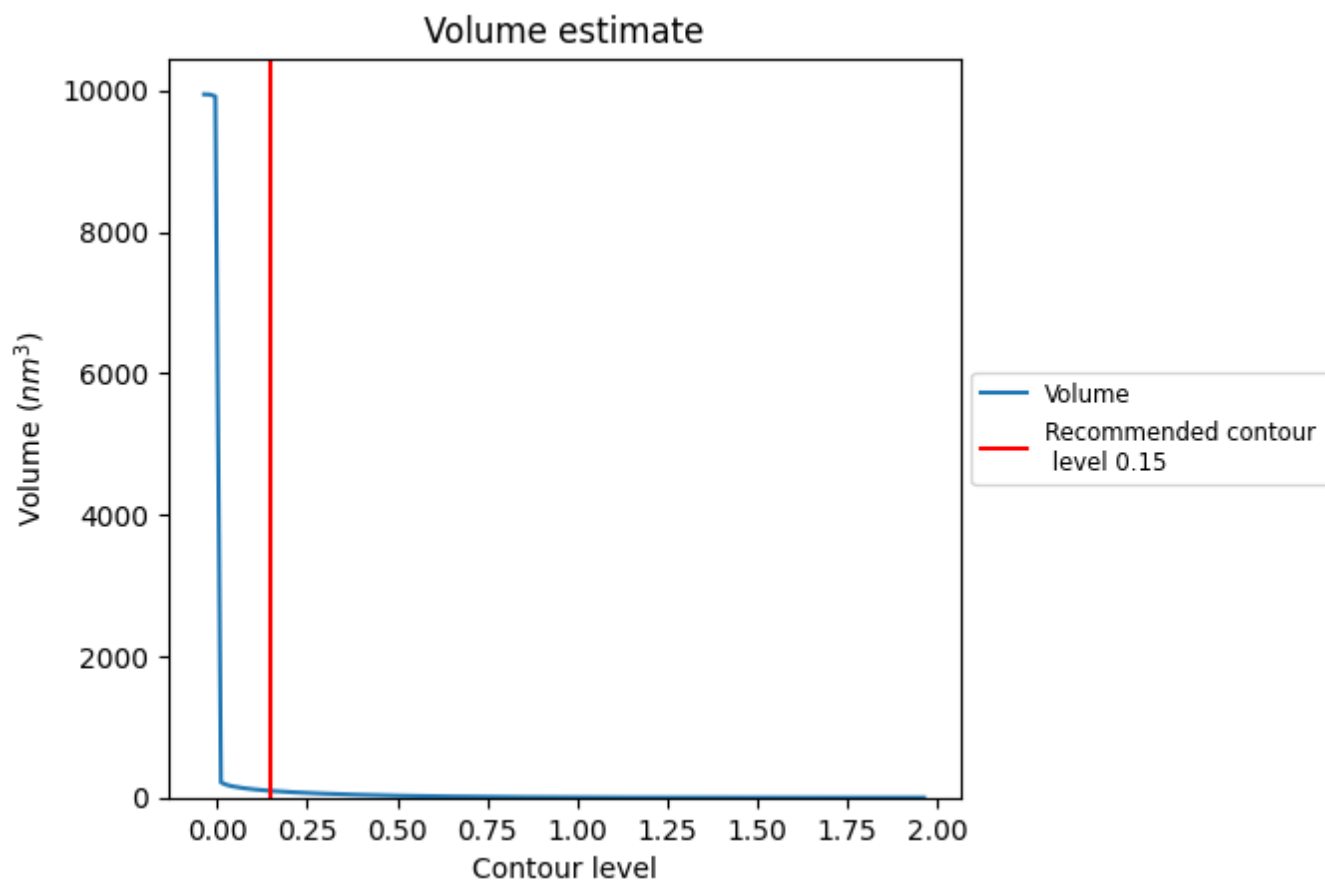
This section contains the results of statistical analysis of the map.

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.

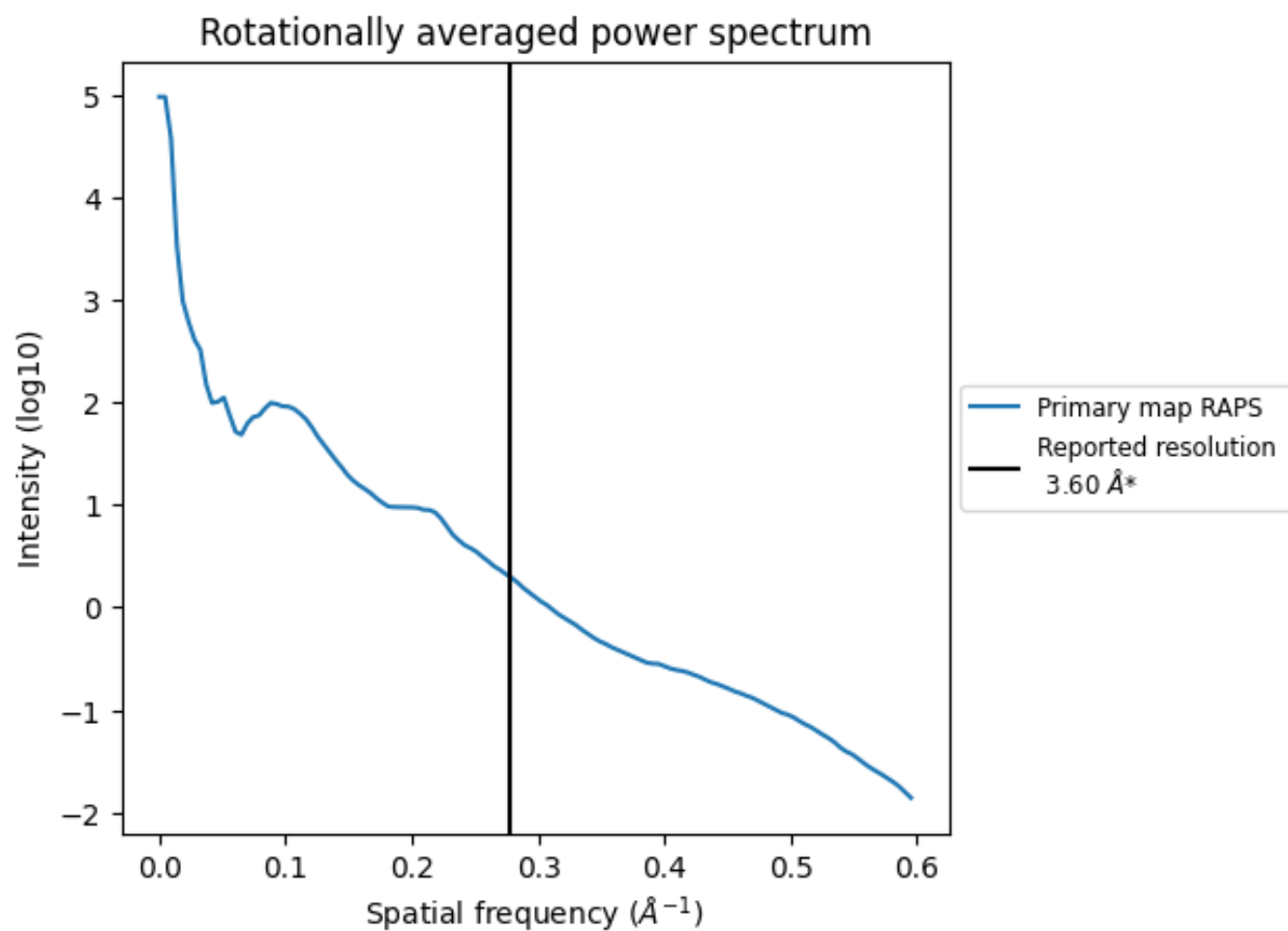
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm^3 ; this corresponds to an approximate mass of 86 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 0.278 Å⁻¹

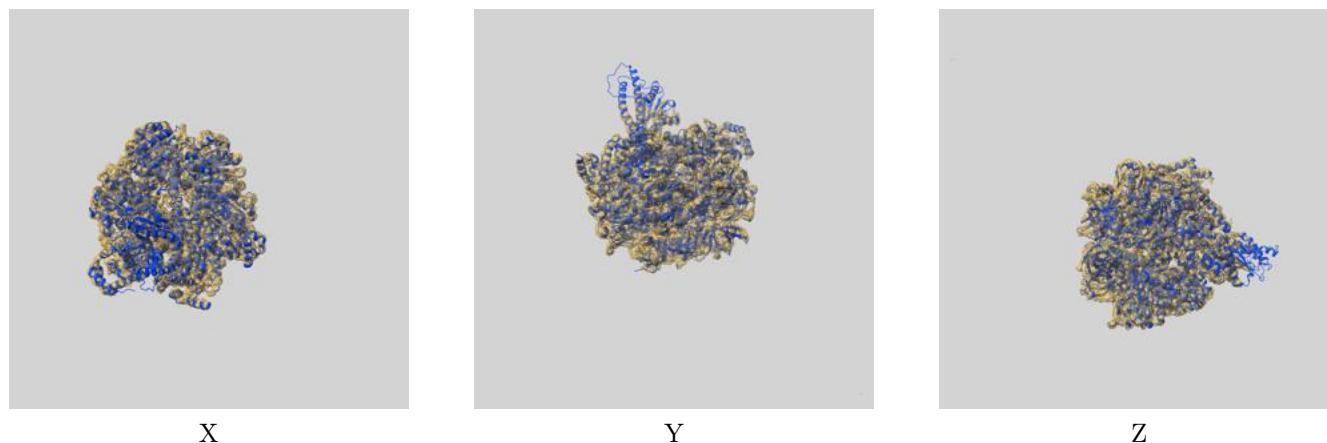
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

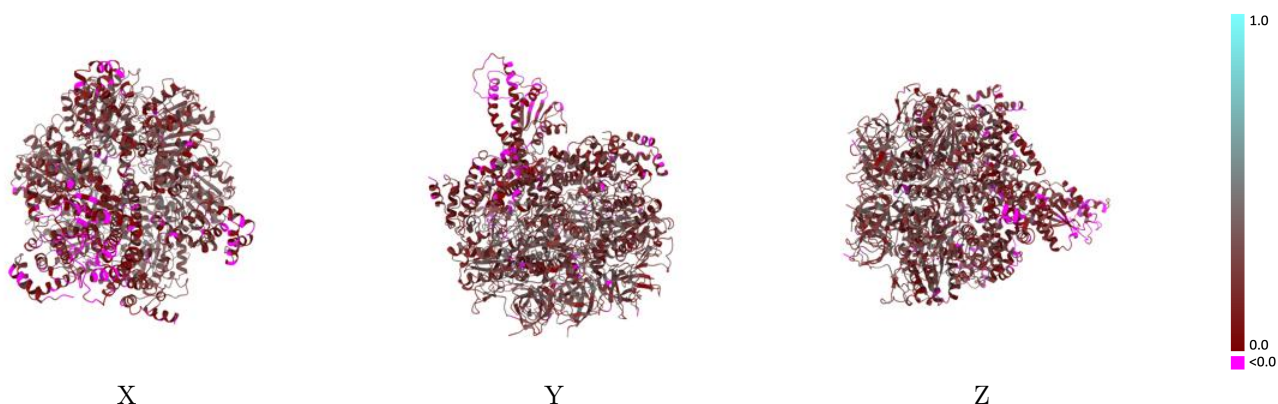
This section contains information regarding the fit between EMDB map EMD-23117 and PDB model 7L1S. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



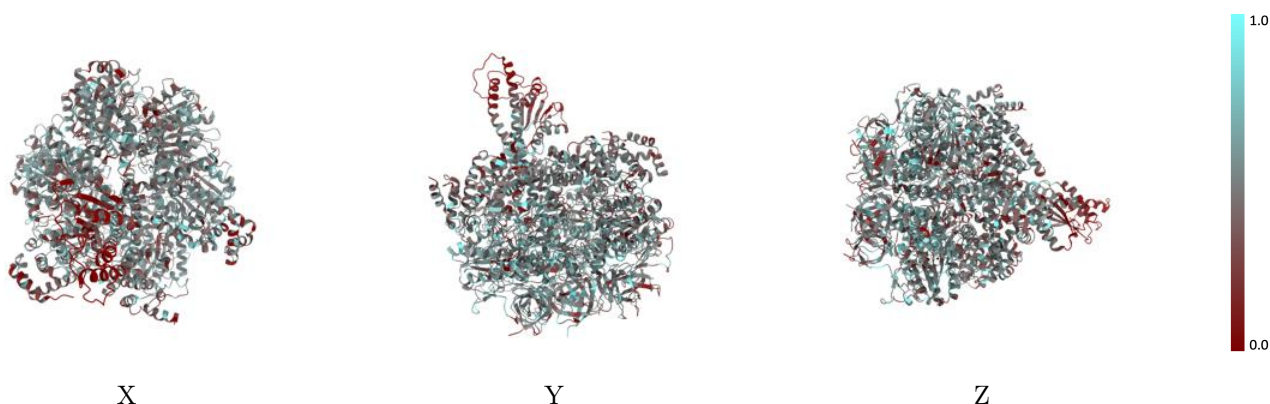
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



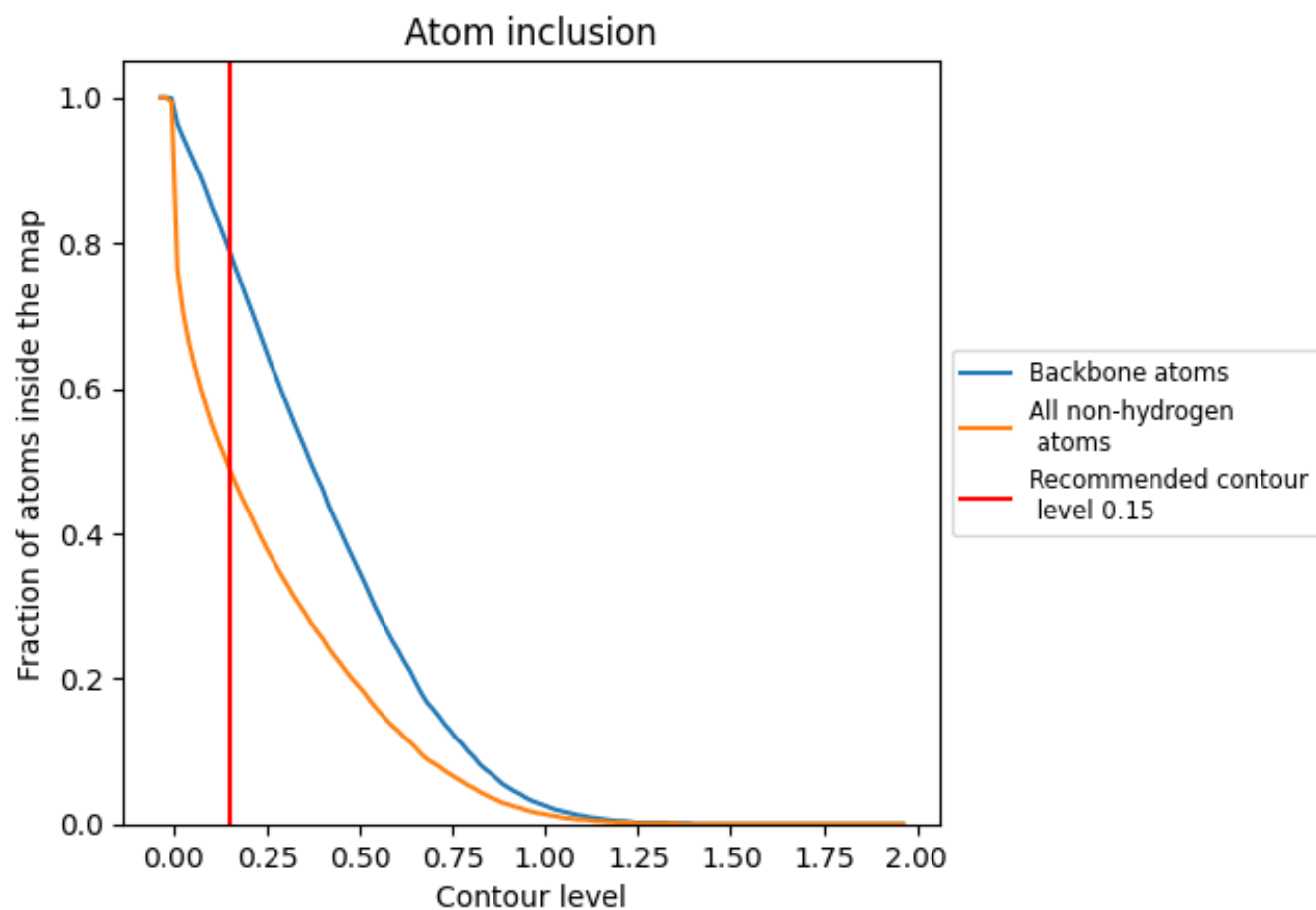
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 49% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4880	0.2160
A	0.5240	0.2280
B	0.4910	0.2120
C	0.4870	0.2170
D	0.4920	0.2320
E	0.5160	0.2370
F	0.5080	0.2320
G	0.3410	0.1080

1.0

0.0

<0.0