



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:31 AM UTC

PDB ID : 6TMH / pdb_00006tmh
EMDB ID : EMD-10521
Title : Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase dimer, OSCP/F1/c-ring model
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2019-12-04
Resolution : 3.10 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

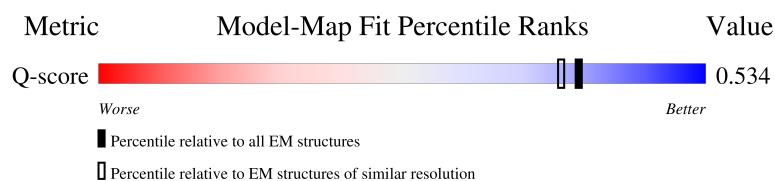
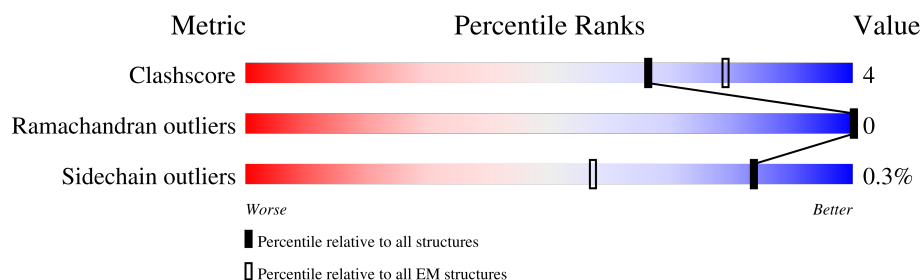
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

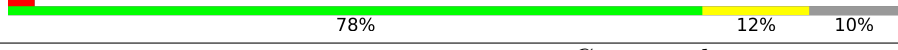
The reported resolution of this entry is 3.10 Å.

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.



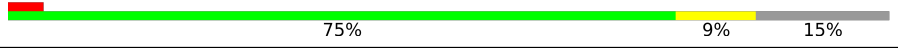
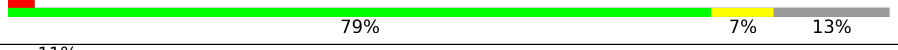
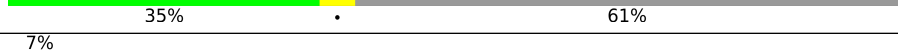
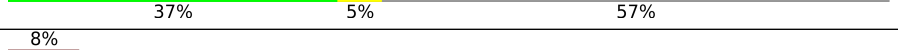
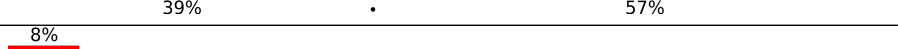
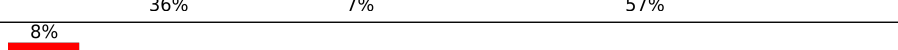
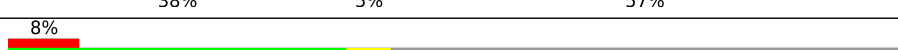
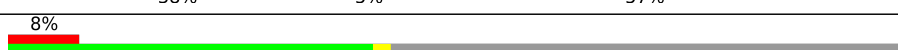
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	i	145	
2	A	565	
2	C	565	
2	E	565	

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Mol	Chain	Length	Quality of chain
3	B	560	
3	D	560	
3	F	560	
4	g	314	
5	d	183	
6	e	73	
7	G	252	
8	H	166	
8	I	166	
8	J	166	
8	K	166	
8	L	166	
8	M	166	
8	N	166	
8	O	166	
8	P	166	
8	Q	166	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 65413 atoms, of which 33003 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 Inhibitor of F1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	i	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		

- Molecule 2 is a protein called ATP synthase subunit alpha,subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	512	Total	C	H	N	O	S	0	0
			7924	2464	4002	688	751	19		
2	E	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
2	C	487	Total	C	H	N	O	S	0	0
			7521	2341	3799	653	710	18		

- Molecule 3 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
3	F	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
3	D	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		

- Molecule 4 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	g	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		

- Molecule 5 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	d	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		

- Molecule 6 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	e	65	Total	C	H	N	O	S	0	0
			1077	337	539	99	98	4		

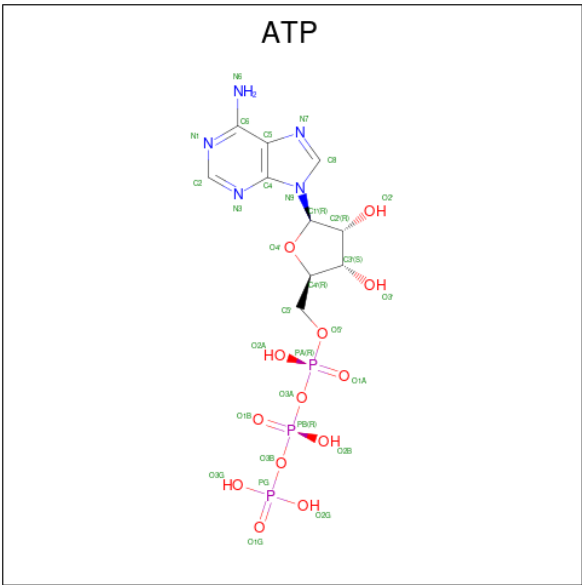
- Molecule 7 is a protein called Oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	99	Total	C	H	N	O	S	0	0
			1618	507	821	141	147	2		

- Molecule 8 is a protein called subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	I	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	J	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	K	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	L	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	M	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	N	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	O	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	P	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
8	Q	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

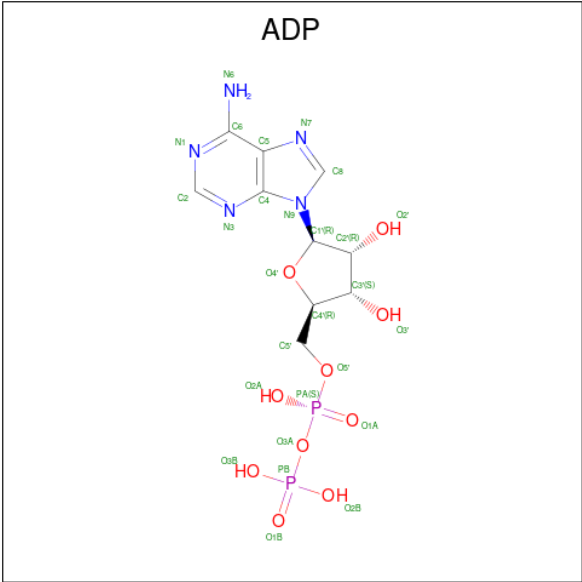


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	H	N	O	P
			42	10	11	5	13	3
9	E	1	Total	C	H	N	O	P
			42	10	11	5	13	3
9	C	1	Total	C	H	N	O	P
			42	10	11	5	13	3

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

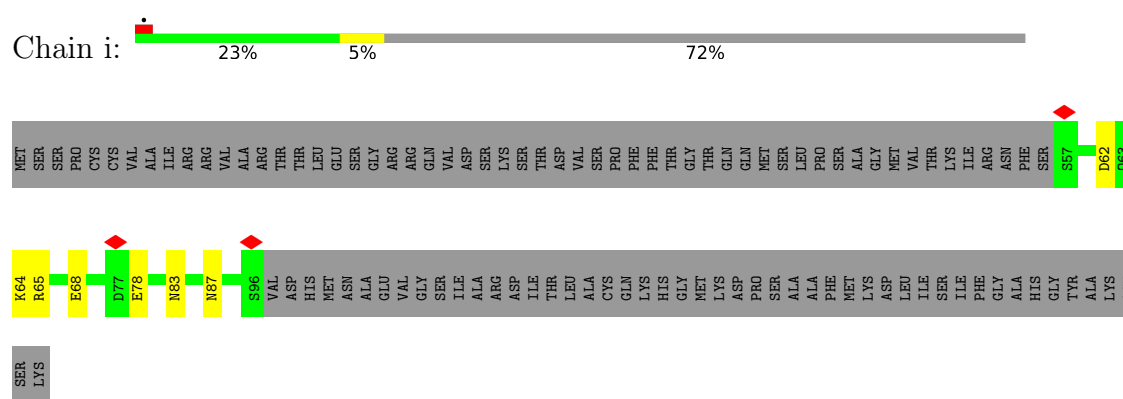


Mol	Chain	Residues	Atoms						AltConf
11	B	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
11	D	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

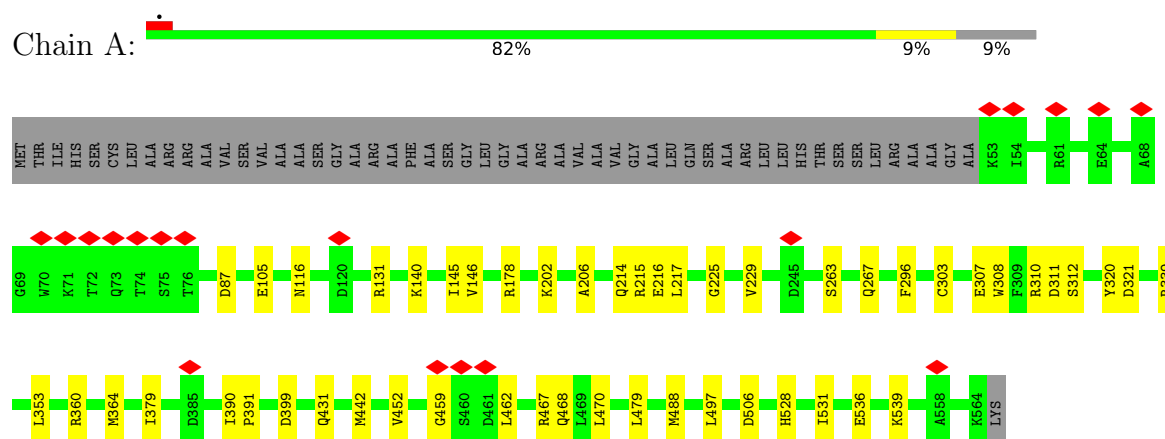
3 Residue-property plots

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.

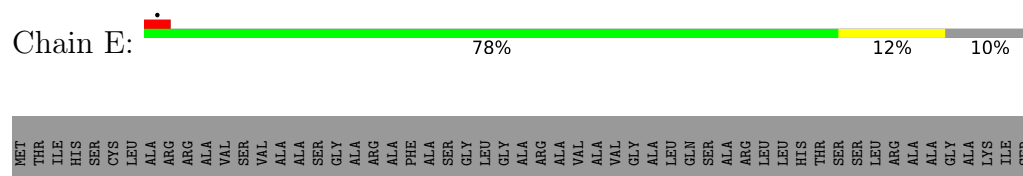
- Molecule 1: Inhibitor of F1



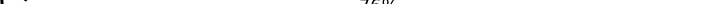
- Molecule 2: ATP synthase subunit alpha,subunit alpha



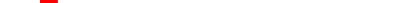
- Molecule 2: ATP synthase subunit alpha,subunit alpha



- Molecule 2: ATP synthase subunit alpha,subunit alpha

Chain C:  76% 10% 14%

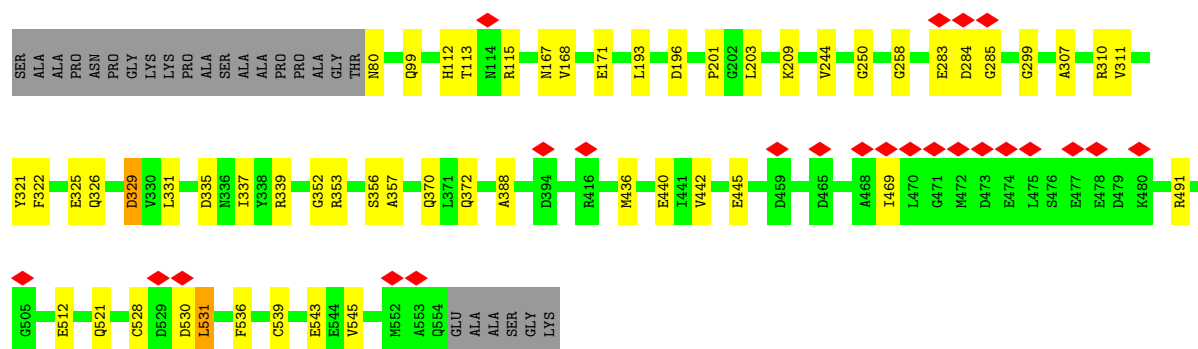
- Molecule 3: ATP synthase subunit beta

Chain B:  78% 8% 14%

- Molecule 3: ATP synthase subunit beta

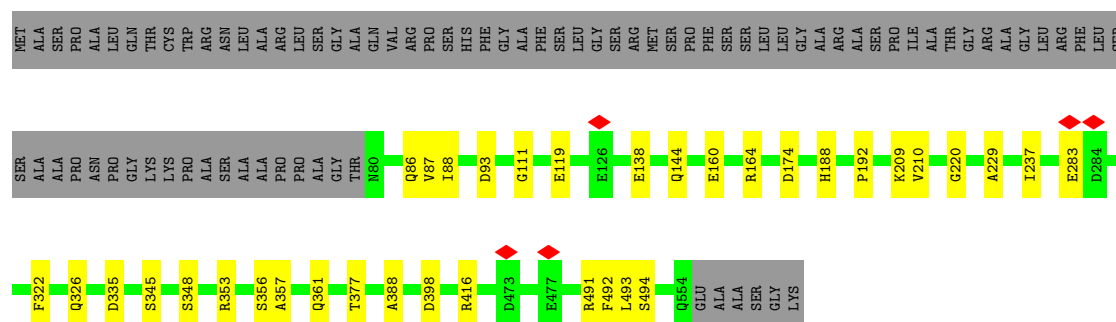
Chain F:  75% 9% 15%





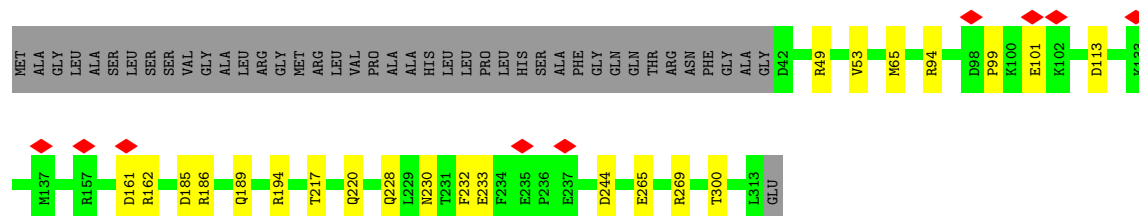
• Molecule 3: ATP synthase subunit beta

Chain D: 78% 7% 15%



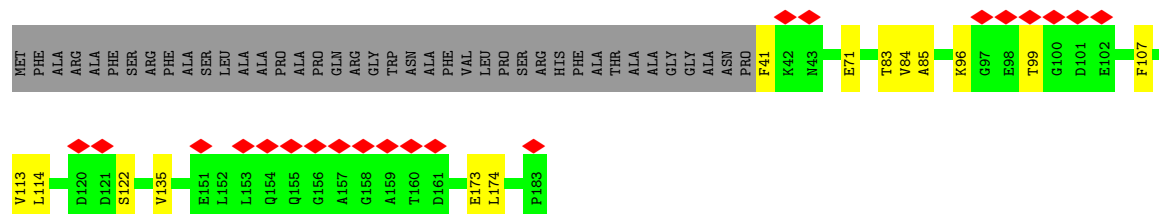
• Molecule 4: ATP synthase subunit gamma

Chain g: 79% 7% 13%



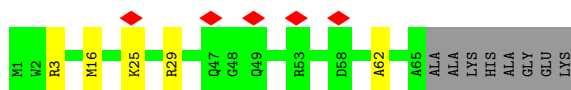
• Molecule 5: ATP synthase subunit delta

Chain d: 11% 70% 8% 22%

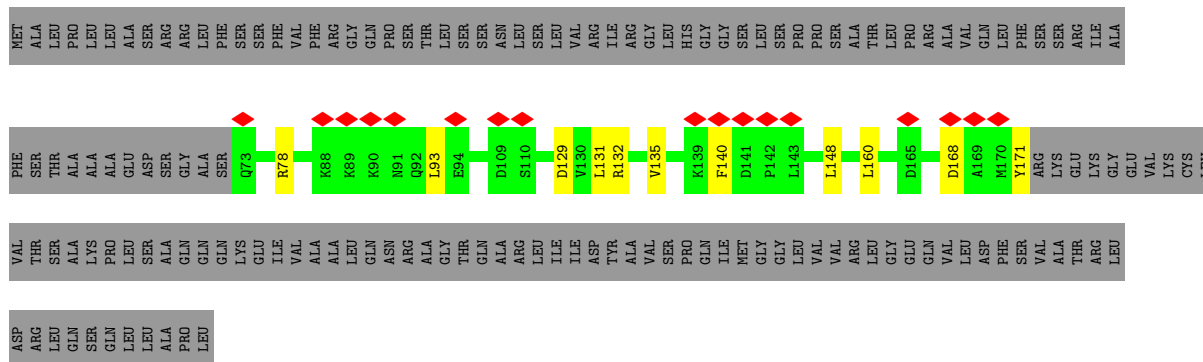


• Molecule 6: ATP synthase subunit epsilon

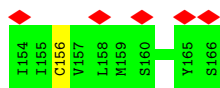
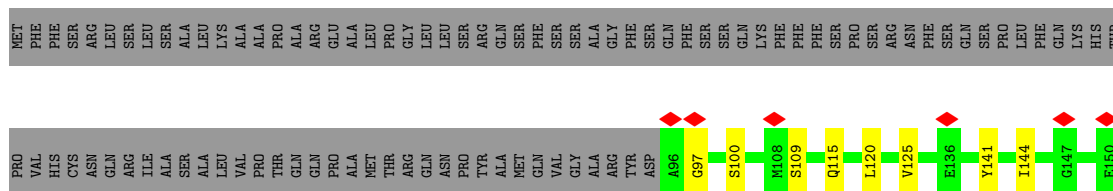
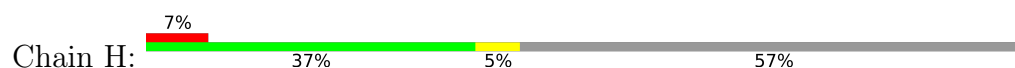
Chain e: 7% 82% 7% 11%



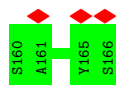
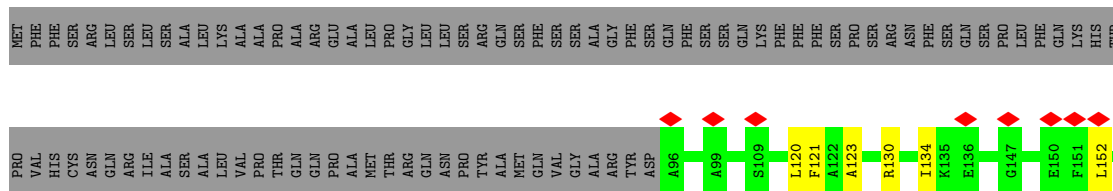
- Molecule 7: Oligomycin sensitivity conferring protein (OSCP)



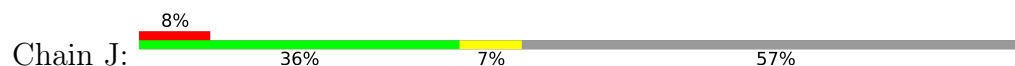
- Molecule 8: subunit c

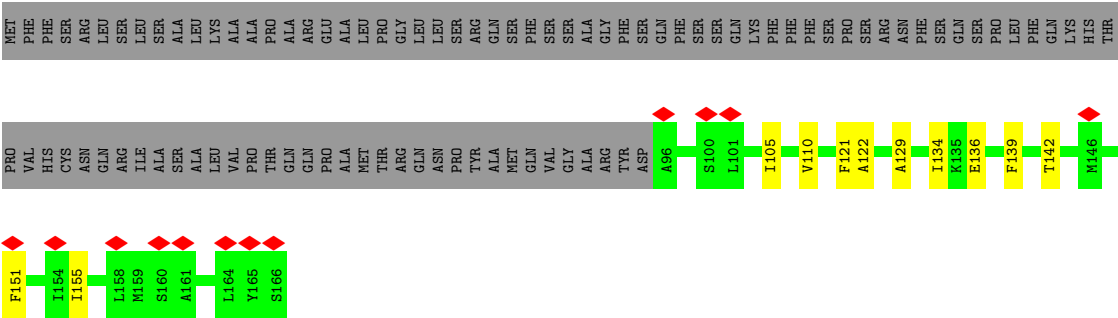


- Molecule 8: subunit c

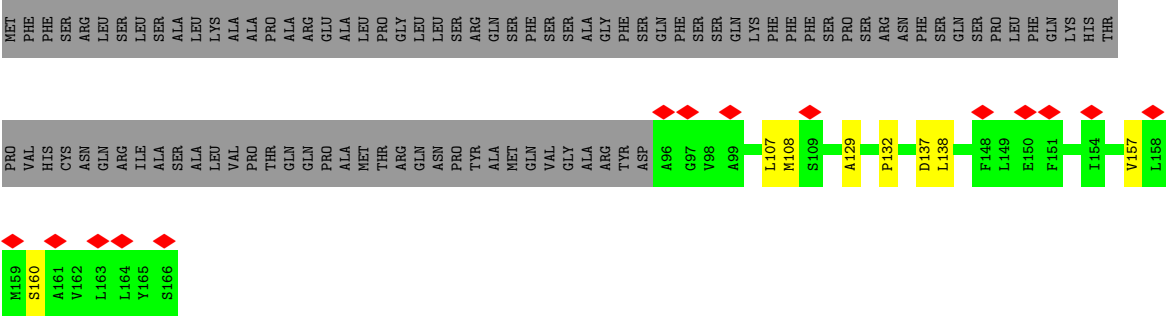
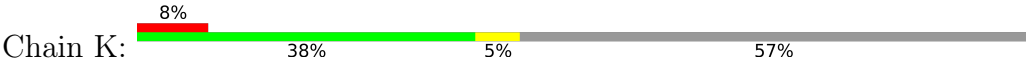


- Molecule 8: subunit c

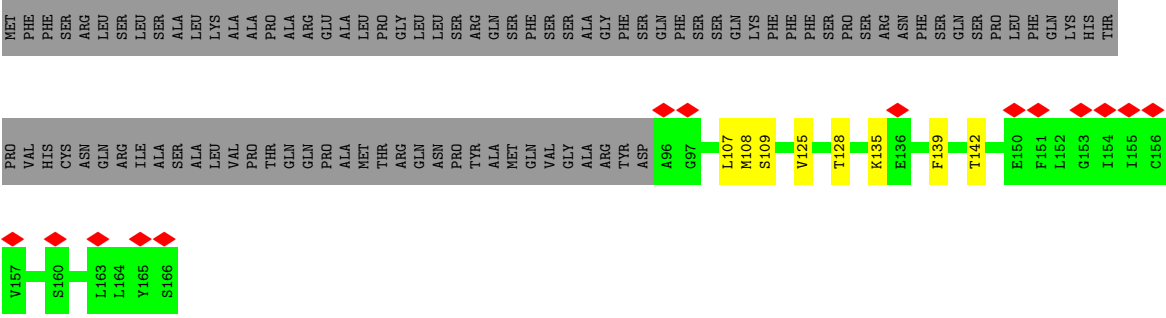
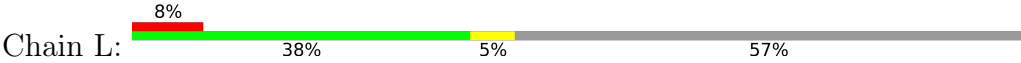




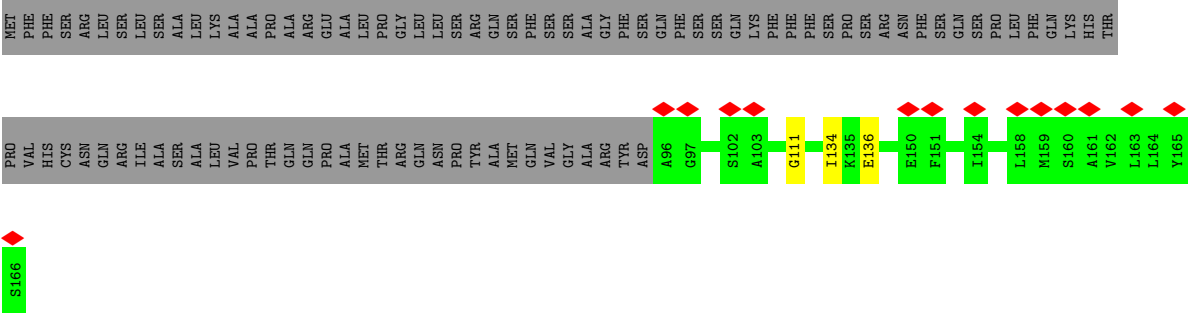
• Molecule 8: subunit c



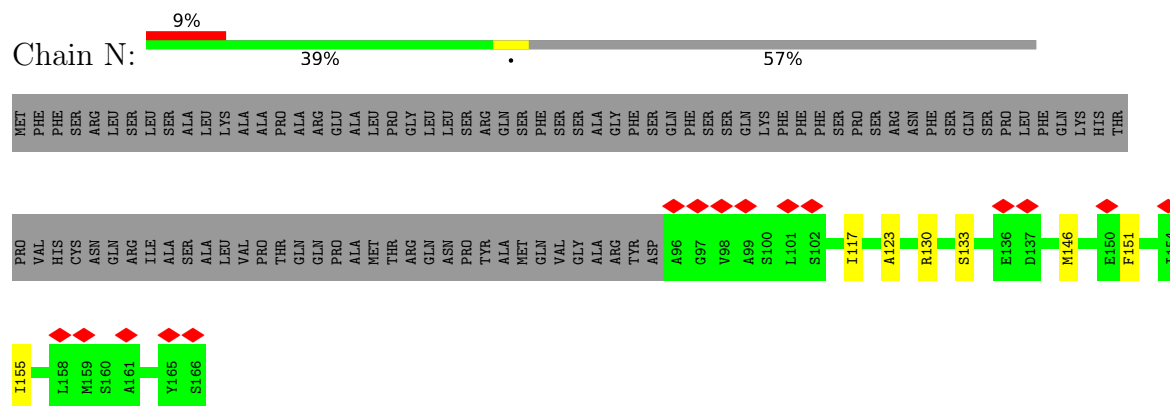
• Molecule 8: subunit c



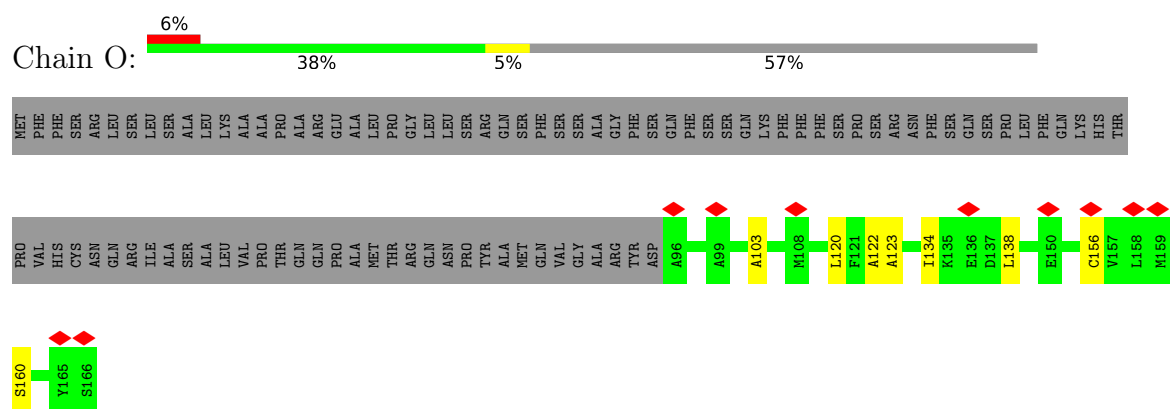
• Molecule 8: subunit c



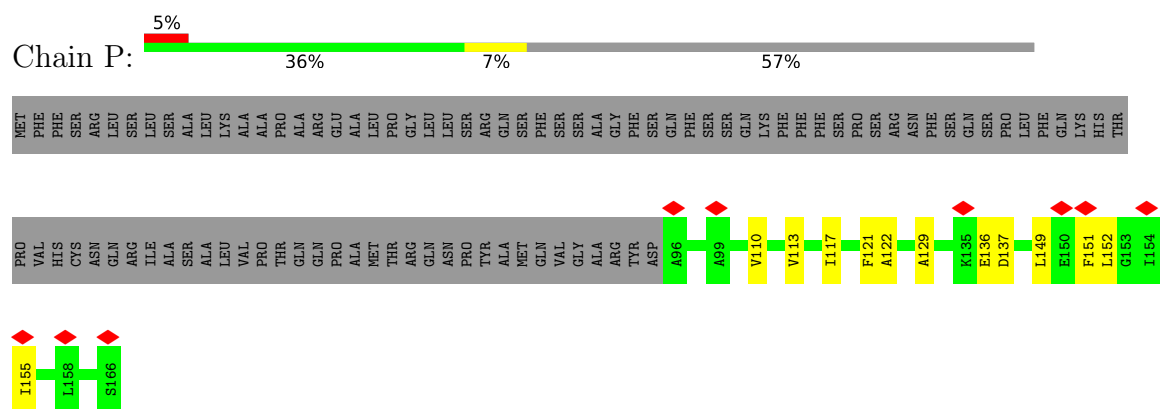
● Molecule 8: subunit c



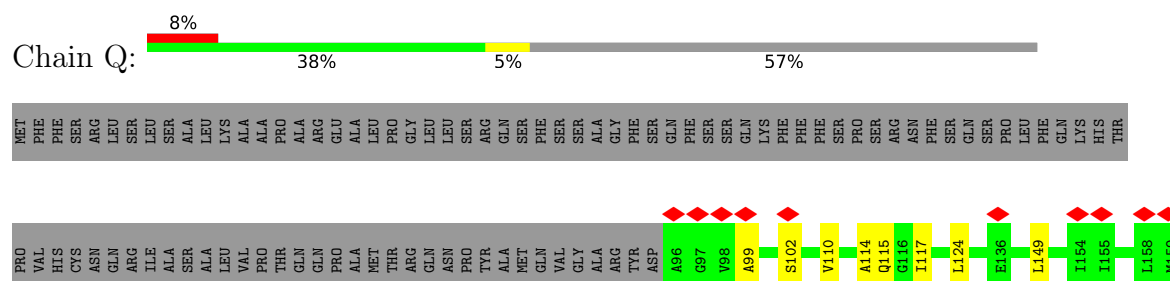
● Molecule 8: subunit c

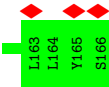


● Molecule 8: subunit c



● Molecule 8: subunit c





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	203010	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.329	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	i	0.22	0/343	0.29	0/459
2	A	0.33	0/3979	0.34	0/5372
2	C	0.35	0/3776	0.38	0/5099
2	E	0.33	0/3942	0.35	0/5322
3	B	0.34	0/3698	0.35	0/5016
3	D	0.35	0/3672	0.35	0/4980
3	F	0.31	0/3672	0.35	0/4980
4	g	0.28	0/2145	0.31	0/2890
5	d	0.21	0/1083	0.31	0/1466
6	e	0.19	0/547	0.30	0/733
7	G	0.17	0/807	0.29	0/1085
8	H	0.18	0/507	0.27	0/686
8	I	0.19	0/507	0.30	0/686
8	J	0.19	0/507	0.28	0/686
8	K	0.21	0/507	0.32	0/686
8	L	0.18	0/507	0.30	0/686
8	M	0.21	0/507	0.31	0/686
8	N	0.19	0/507	0.24	0/686
8	O	0.20	0/507	0.28	0/686
8	P	0.19	0/507	0.31	0/686
8	Q	0.21	0/507	0.35	0/686
All	All	0.30	0/32734	0.34	0/44262

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
2	A	0	1
2	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
3	B	0	1
3	D	0	1
3	F	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	321	ASP	Peptide
3	B	335	ASP	Peptide
2	C	321	ASP	Peptide
3	D	335	ASP	Peptide
2	E	321	ASP	Peptide
3	F	335	ASP	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	i	336	324	324	5	0
2	A	3922	4002	4002	30	0
2	C	3722	3799	3799	32	0
2	E	3886	3962	3961	40	0
3	B	3638	3676	3675	29	0
3	D	3612	3653	3653	22	0
3	F	3612	3653	3653	34	0
4	g	2116	2173	2173	16	0
5	d	1069	1076	1076	10	0
6	e	538	539	539	4	0
7	G	797	821	821	8	0
8	H	501	527	527	6	0
8	I	501	527	527	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	501	527	527	11	0
8	K	501	527	527	7	0
8	L	501	527	527	7	0
8	M	501	527	527	2	0
8	N	501	527	527	6	0
8	O	501	527	527	8	0
8	P	501	527	527	10	0
8	Q	501	527	527	6	0
9	A	31	11	11	0	0
9	C	31	11	11	0	0
9	E	31	11	11	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
11	B	27	11	11	1	0
11	D	27	11	11	0	0
All	All	32410	33003	33001	254	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 4.

All (254) 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)
2:C:260:GLN:NE2	2:C:321:ASP:OD2	2.00	0.95
4:g:186:ARG:NH2	6:e:62:ALA:O	2.12	0.82
2:C:303:CYS:SG	2:C:320:TYR:OH	2.37	0.81
2:E:343:ARG:NH2	3:D:398:ASP:OD2	2.15	0.79
3:B:194:PHE:O	3:B:197:GLN:NE2	2.16	0.78
2:E:318:ILE:HD11	2:E:373:LEU:HD11	1.67	0.77
2:A:303:CYS:SG	2:A:320:TYR:OH	2.42	0.76
2:E:445:GLU:OE2	2:E:472:ARG:NH1	2.19	0.76
4:g:101:GLU:O	4:g:194:ARG:NH1	2.19	0.75
5:d:173:GLU:OE2	8:N:133:SER:OG	2.05	0.75
2:A:87:ASP:OD1	3:B:353:ARG:NH2	2.19	0.74
3:D:283:GLU:OE2	3:D:283:GLU:N	2.22	0.72
3:D:348:SER:OG	3:D:353:ARG:NH2	2.22	0.72
8:H:115:GLN:NE2	8:Q:115:GLN:OE1	2.22	0.72
2:C:247:GLU:OE1	2:C:252:TYR:OH	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:210:VAL:HG22	2:C:216:GLU:OE1	1.90	0.71
7:G:129:ASP:OD1	7:G:132:ARG:NH2	2.24	0.71
3:F:543:GLU:OE1	3:F:543:GLU:N	2.23	0.71
4:g:217:THR:OG1	4:g:220:GLN:OE1	2.06	0.70
2:C:217:LEU:HD11	2:C:379:ILE:HD12	1.73	0.69
2:E:157:ARG:NH2	2:E:170:GLY:O	2.25	0.69
4:g:265:GLU:OE2	4:g:269:ARG:NH2	2.25	0.69
2:A:442:MET:HE1	2:A:497:LEU:HD22	1.75	0.68
4:g:99:PRO:O	4:g:194:ARG:NH2	2.27	0.68
5:d:41:PHE:N	5:d:122:SER:O	2.26	0.68
2:A:462:LEU:O	2:A:467:ARG:NH2	2.28	0.67
7:G:135:VAL:HG22	7:G:140:PHE:CE2	2.31	0.66
3:F:258:GLY:O	3:F:339:ARG:NE	2.29	0.65
4:g:94:ARG:NH2	4:g:228:GLN:O	2.30	0.65
5:d:71:GLU:OE1	8:N:130:ARG:NH2	2.30	0.65
2:A:214:GLN:NE2	2:A:216:GLU:OE1	2.30	0.64
2:C:178:ARG:NH1	2:C:307:GLU:OE1	2.30	0.64
2:A:296:PHE:CE1	2:A:353:LEU:HD11	2.33	0.64
2:A:308:TRP:O	2:A:312:SER:OG	2.11	0.64
2:A:536:GLU:O	2:A:539:LYS:NZ	2.21	0.64
8:J:134:ILE:HD13	8:K:132:PRO:HG3	1.80	0.63
8:H:109:SER:OG	8:H:156:CYS:SG	2.48	0.63
2:E:405:GLU:OE2	2:E:418:ASN:ND2	2.30	0.63
2:A:178:ARG:NH1	2:A:307:GLU:OE1	2.33	0.61
2:A:215:ARG:NH2	2:A:399:ASP:OD1	2.32	0.61
3:D:345:SER:N	3:D:361:GLN:OE1	2.32	0.61
2:E:253:CYS:SG	2:E:254:ILE:N	2.74	0.61
7:G:148:LEU:HD23	7:G:160:LEU:HD21	1.82	0.60
3:B:491:ARG:O	3:B:494:SER:OG	2.19	0.60
3:D:491:ARG:O	3:D:494:SER:OG	2.20	0.60
2:C:202:LYS:NZ	2:C:517:GLU:OE2	2.35	0.60
3:F:112:HIS:ND1	3:F:113:THR:O	2.35	0.59
8:P:151:PHE:CZ	8:P:155:ILE:HD11	2.37	0.59
8:K:107:LEU:C	8:K:108:MET:HE2	2.27	0.59
8:J:134:ILE:HD11	8:K:129:ALA:HA	1.83	0.59
8:J:139:PHE:O	8:J:142:THR:OG1	2.17	0.59
3:B:185:TYR:OH	3:B:325:GLU:OE2	2.18	0.59
2:E:202:LYS:NZ	2:E:517:GLU:OE2	2.33	0.58
5:d:174:LEU:HD13	6:e:16:MET:HE3	1.86	0.58
4:g:232:PHE:O	8:I:130:ARG:NH2	2.37	0.57
8:K:137:ASP:OD2	8:L:135:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:ARG:NH1	3:D:192:PRO:O	2.38	0.57
2:C:225:GLY:O	2:C:229:VAL:HG23	2.05	0.57
2:E:78:GLU:OE2	2:E:141:ARG:NH1	2.38	0.57
8:I:134:ILE:HD11	8:J:129:ALA:HA	1.87	0.57
4:g:161:ASP:OD1	4:g:162:ARG:NH1	2.37	0.57
2:A:468:GLN:NE2	2:A:506:ASP:OD2	2.37	0.56
8:J:105:ILE:O	8:K:108:MET:HE1	2.05	0.56
2:A:310:ARG:NH1	2:A:360:ARG:O	2.37	0.56
2:A:178:ARG:NH2	2:A:311:ASP:OD2	2.38	0.56
2:C:388:ALA:O	2:C:392:THR:OG1	2.17	0.56
5:d:85:ALA:HB3	5:d:113:VAL:CG1	2.36	0.56
2:E:217:LEU:HD11	2:E:379:ILE:HD12	1.87	0.56
2:E:289:SER:O	3:F:370:GLN:NE2	2.39	0.56
8:N:151:PHE:CZ	8:N:155:ILE:HD11	2.41	0.56
2:C:442:MET:HE1	2:C:497:LEU:HD22	1.88	0.55
3:F:528:CYS:SG	3:F:531:LEU:HD23	2.47	0.55
3:D:138:GLU:N	3:D:138:GLU:OE1	2.39	0.55
5:d:85:ALA:HB3	5:d:113:VAL:HG12	1.88	0.55
3:B:160:GLU:N	3:B:160:GLU:OE1	2.40	0.54
2:C:307:GLU:OE2	2:C:360:ARG:NE	2.35	0.54
3:F:115:ARG:NE	3:F:171:GLU:OE2	2.33	0.54
7:G:168:ASP:O	7:G:171:TYR:N	2.41	0.54
2:E:198:MET:O	2:E:237:GLN:NE2	2.40	0.54
3:F:283:GLU:N	3:F:283:GLU:OE1	2.41	0.54
4:g:185:ASP:OD1	4:g:189:GLN:NE2	2.40	0.54
2:E:355:SER:HB2	3:D:301:MET:HB3	1.90	0.53
2:C:390:ILE:HB	2:C:391:PRO:HD3	1.90	0.53
3:F:357:ALA:O	4:g:300:THR:OG1	2.20	0.52
2:E:87:ASP:OD1	3:F:353:ARG:NH2	2.42	0.52
2:C:452:VAL:HG12	2:C:452:VAL:O	2.09	0.52
1:i:64:LYS:NZ	3:B:468:ALA:O	2.37	0.52
3:B:283:GLU:OE1	3:B:283:GLU:N	2.38	0.52
8:N:151:PHE:CE2	8:N:155:ILE:HD11	2.44	0.52
2:E:318:ILE:HD11	2:E:373:LEU:CD1	2.37	0.52
2:C:399:ASP:OD1	3:B:262:ARG:NH2	2.39	0.52
2:C:310:ARG:NH1	2:C:360:ARG:O	2.43	0.52
4:g:233:GLU:O	5:d:83:THR:OG1	2.17	0.52
2:E:69:GLY:O	2:E:73:GLN:NE2	2.43	0.52
3:F:244:VAL:HG21	3:F:331:LEU:HD11	1.91	0.52
7:G:135:VAL:HG22	7:G:140:PHE:CD2	2.44	0.52
8:Q:117:ILE:HG13	8:Q:149:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:338:ARG:NH1	3:F:352:GLY:O	2.41	0.51
2:A:263:SER:O	2:A:267:GLN:NE2	2.44	0.51
8:L:107:LEU:C	8:L:108:MET:HE2	2.36	0.51
2:E:215:ARG:NH2	2:E:399:ASP:OD1	2.42	0.51
3:F:445:GLU:OE2	3:F:521:GLN:NE2	2.42	0.51
3:F:491:ARG:HB3	3:F:536:PHE:O	2.11	0.51
2:A:116:ASN:OD1	2:A:339:ARG:NH2	2.37	0.51
2:E:278:MET:SD	2:E:281:THR:OG1	2.69	0.51
2:C:116:ASN:OD1	2:C:339:ARG:NH2	2.39	0.51
8:N:117:ILE:HD13	8:N:146:MET:HE1	1.93	0.50
4:g:230:ASN:O	8:I:130:ARG:NH2	2.44	0.50
2:E:386:VAL:HG11	2:E:403:PHE:HE1	1.76	0.50
2:C:97:GLY:O	2:C:141:ARG:NH1	2.44	0.50
2:E:510:PRO:HA	2:E:513:ILE:HD12	1.93	0.50
8:H:141:TYR:HA	8:H:144:ILE:HD12	1.93	0.50
8:P:152:LEU:HD22	8:Q:110:VAL:HG13	1.94	0.50
8:H:120:LEU:HD21	8:I:121:PHE:HB2	1.93	0.50
3:F:528:CYS:HG	3:F:536:PHE:HZ	1.60	0.50
3:B:491:ARG:HB3	3:B:536:PHE:O	2.11	0.49
8:M:134:ILE:HG22	8:M:136:GLU:H	1.78	0.49
2:C:342:GLY:N	2:C:346:TYR:O	2.44	0.49
8:L:139:PHE:O	8:L:142:THR:OG1	2.26	0.49
3:B:228:GLY:O	3:B:233:LYS:NZ	2.46	0.48
3:B:297:VAL:HG12	3:B:311:VAL:CG2	2.42	0.48
1:i:64:LYS:HD2	2:C:458:PHE:HE1	1.78	0.48
8:I:152:LEU:HD22	8:J:110:VAL:HG21	1.96	0.48
2:E:379:ILE:HD11	2:E:394:VAL:HG21	1.96	0.48
2:E:512:GLU:OE1	2:E:515:ARG:NH2	2.44	0.48
3:F:80:ASN:ND2	3:F:99:GLN:O	2.47	0.48
3:D:111:GLY:O	3:D:144:GLN:NE2	2.47	0.48
2:E:297:LEU:O	2:E:300:TYR:N	2.44	0.48
3:B:126:GLU:OE1	7:G:78:ARG:NH2	2.47	0.48
3:F:512:GLU:OE1	3:F:512:GLU:N	2.47	0.48
2:E:178:ARG:NE	2:E:307:GLU:OE1	2.45	0.48
3:F:322:PHE:O	3:F:326:GLN:HB2	2.14	0.47
8:J:136:GLU:OE1	8:J:136:GLU:N	2.46	0.47
3:B:183:LYS:NZ	3:B:325:GLU:OE2	2.47	0.47
3:D:160:GLU:N	3:D:160:GLU:OE1	2.46	0.47
5:d:84:VAL:HG22	5:d:114:LEU:HD23	1.96	0.47
3:F:209:LYS:NZ	3:F:539:CYS:O	2.48	0.47
8:O:134:ILE:HD12	8:O:138:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:119:GLU:OE1	3:B:310:ARG:NE	2.47	0.47
3:B:399:PRO:O	3:B:403:THR:HG23	2.14	0.47
8:K:157:VAL:O	8:K:160:SER:OG	2.25	0.47
3:B:238:MET:SD	3:B:267:LEU:HD13	2.55	0.46
2:E:261:LYS:O	2:E:264:THR:OG1	2.31	0.46
2:E:528:HIS:HB3	2:E:531:ILE:HD12	1.97	0.46
3:B:168:VAL:HG13	3:B:169:ILE:HG23	1.98	0.46
7:G:131:LEU:O	7:G:135:VAL:HG23	2.16	0.46
8:O:134:ILE:HD11	8:P:129:ALA:HA	1.96	0.46
3:D:322:PHE:O	3:D:326:GLN:HB2	2.14	0.46
8:H:97:GLY:O	8:H:100:SER:OG	2.28	0.46
2:C:158:VAL:N	2:C:167:ASP:OD2	2.43	0.46
8:O:120:LEU:HD21	8:P:121:PHE:HB3	1.98	0.45
3:F:203:LEU:HD11	3:F:442:VAL:HG12	1.99	0.45
3:F:337:ILE:HG22	3:F:388:ALA:O	2.16	0.45
3:B:209:LYS:NZ	3:B:492:PHE:O	2.49	0.45
3:D:210:VAL:HG22	3:D:493:LEU:HB3	1.98	0.45
2:A:87:ASP:OD2	3:B:353:ARG:NE	2.49	0.45
1:i:62:ASP:OD2	1:i:65:ARG:NH2	2.49	0.45
2:A:202:LYS:HE2	2:A:488:MET:HE2	1.97	0.45
3:F:193:LEU:N	3:F:196:ASP:OD2	2.50	0.45
3:D:345:SER:CA	3:D:361:GLN:OE1	2.65	0.45
3:B:119:GLU:OE2	3:B:188:HIS:NE2	2.43	0.45
2:E:175:LYS:HG2	2:E:176:GLU:H	1.82	0.45
2:E:145:ILE:HG22	2:E:146:VAL:N	2.32	0.44
4:g:113:ASP:OD1	4:g:113:ASP:N	2.49	0.44
3:B:487:ARG:NE	3:B:533:GLU:OE1	2.49	0.44
2:A:225:GLY:O	2:A:229:VAL:HG23	2.17	0.44
2:C:96:GLU:OE1	2:C:96:GLU:N	2.48	0.44
2:C:472:ARG:NH1	2:C:501:VAL:O	2.50	0.44
1:i:68:GLU:OE2	3:B:472:MET:N	2.38	0.44
8:P:117:ILE:HG12	8:P:149:LEU:HD22	1.98	0.44
2:C:120:ASP:OD2	2:C:121:ASN:N	2.50	0.44
2:C:221:ASP:O	2:C:226:LYS:NZ	2.51	0.44
4:g:49:ARG:O	4:g:53:VAL:HG23	2.17	0.44
2:E:438:VAL:HG11	2:E:497:LEU:HB2	2.00	0.44
2:E:531:ILE:HD11	2:E:548:LYS:HB3	2.00	0.44
3:B:202:GLY:O	3:B:219:LYS:N	2.44	0.44
3:F:299:GLY:HA3	3:F:311:VAL:HG21	2.00	0.44
3:F:307:ALA:O	3:F:311:VAL:HG23	2.17	0.44
2:C:160:ASP:OD1	2:C:164:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:237:ILE:HD11	3:D:388:ALA:HB2	2.00	0.43
2:C:316:CYS:SG	2:C:317:VAL:N	2.91	0.43
8:L:108:MET:HE2	8:L:108:MET:HA	2.00	0.43
2:A:390:ILE:HB	2:A:391:PRO:HD3	2.00	0.43
2:E:390:ILE:HB	2:E:391:PRO:HD3	2.00	0.43
1:i:83:ASN:O	1:i:87:ASN:ND2	2.51	0.43
3:D:229:ALA:O	3:D:416:ARG:NH2	2.48	0.43
8:O:156:CYS:SG	8:P:110:VAL:HG11	2.59	0.43
8:L:128:THR:HG23	8:L:135:LYS:HG2	2.01	0.43
8:Q:99:ALA:O	8:Q:102:SER:OG	2.28	0.43
2:A:105:GLU:OE1	2:A:140:LYS:NZ	2.44	0.43
3:B:235:VAL:HG23	11:B:601:ADP:O1A	2.19	0.43
2:A:442:MET:HE1	2:A:497:LEU:CD2	2.47	0.43
2:A:364:MET:N	2:A:364:MET:SD	2.92	0.42
3:F:201:PRO:HB2	3:F:436:MET:HE1	2.01	0.42
3:D:209:LYS:NZ	3:D:492:PHE:O	2.44	0.42
8:J:151:PHE:CE2	8:J:155:ILE:HD11	2.54	0.42
2:A:206:ALA:O	2:A:431:GLN:NE2	2.52	0.42
2:C:445:GLU:OE2	2:C:472:ARG:NH1	2.52	0.42
3:F:284:ASP:OD1	3:F:285:GLY:N	2.52	0.42
3:D:356:SER:OG	3:D:357:ALA:N	2.51	0.42
5:d:96:LYS:N	5:d:99:THR:OG1	2.53	0.42
2:A:459:GLY:O	2:A:467:ARG:NE	2.52	0.42
3:F:469:ILE:HD13	4:g:65:MET:HE3	2.00	0.42
8:I:120:LEU:HD21	8:J:121:PHE:HB2	2.00	0.42
2:E:468:GLN:NE2	2:E:506:ASP:OD2	2.44	0.42
3:B:222:LYS:NZ	3:B:375:ILE:O	2.45	0.42
8:P:113:VAL:HG22	8:Q:114:ALA:CB	2.49	0.42
2:E:316:CYS:SG	2:E:317:VAL:N	2.92	0.42
2:C:206:ALA:O	2:C:431:GLN:NE2	2.53	0.42
3:F:321:TYR:CE1	3:F:325:GLU:OE1	2.72	0.42
2:A:528:HIS:HB3	2:A:531:ILE:HD12	2.02	0.42
8:J:151:PHE:CZ	8:J:155:ILE:HD11	2.54	0.42
8:N:123:ALA:HB2	8:O:122:ALA:HB1	2.01	0.42
2:A:131:ARG:NH1	3:B:105:ASN:OD1	2.48	0.42
2:A:217:LEU:HD11	2:A:379:ILE:HD12	2.02	0.42
8:I:123:ALA:HB2	8:J:122:ALA:HB1	2.02	0.42
2:E:310:ARG:NH1	2:E:360:ARG:O	2.53	0.42
3:D:164:ARG:NH1	3:D:174:ASP:OD2	2.52	0.42
2:E:172:ILE:HG22	2:E:173:PRO:O	2.20	0.42
3:D:220:GLY:O	3:D:377:THR:OG1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:201:PRO:O	3:B:436:MET:HE3	2.20	0.41
3:B:487:ARG:NH2	3:B:533:GLU:OE2	2.52	0.41
8:P:136:GLU:O	8:P:137:ASP:HB2	2.19	0.41
2:E:244:THR:HG21	2:E:249:LYS:HB2	2.02	0.41
2:E:298:ALA:HB3	2:E:299:PRO:HD3	2.02	0.41
3:F:528:CYS:SG	3:F:536:PHE:HZ	2.44	0.41
6:e:25:LYS:O	6:e:29:ARG:N	2.45	0.41
8:O:120:LEU:HD21	8:P:121:PHE:CB	2.50	0.41
2:A:452:VAL:O	2:A:470:LEU:HD21	2.21	0.41
3:F:168:VAL:HG23	3:F:310:ARG:O	2.20	0.41
2:C:89:ILE:HD12	2:C:336:LEU:CB	2.50	0.41
7:G:93:LEU:HD11	7:G:171:TYR:OH	2.21	0.41
8:L:109:SER:OG	8:M:111:GLY:N	2.54	0.41
2:E:120:ASP:OD1	2:E:120:ASP:N	2.54	0.41
8:O:123:ALA:HB2	8:P:122:ALA:HB1	2.02	0.41
3:F:356:SER:OG	3:F:357:ALA:N	2.49	0.41
2:A:202:LYS:NZ	2:A:479:LEU:O	2.49	0.41
2:E:483:ARG:NH2	3:F:440:GLU:OE2	2.52	0.41
3:B:487:ARG:O	3:B:491:ARG:HG2	2.21	0.41
3:F:167:ASN:OD1	3:F:171:GLU:N	2.54	0.41
8:K:138:LEU:HD22	8:L:125:VAL:HG13	2.03	0.41
8:O:103:ALA:O	8:O:160:SER:OG	2.39	0.41
3:F:250:GLY:HA3	3:F:329:ASP:O	2.20	0.41
3:D:86:GLN:HB3	3:D:93:ASP:HB2	2.03	0.41
2:E:178:ARG:NH2	2:E:307:GLU:OE1	2.55	0.40
2:C:95:LEU:HB3	2:C:98:VAL:HG23	2.03	0.40
3:F:530:ASP:OD1	3:F:531:LEU:N	2.54	0.40
4:g:244:ASP:OD1	6:e:3:ARG:NH1	2.53	0.40
2:C:386:VAL:HG11	2:C:403:PHE:HE2	1.86	0.40
3:D:87:VAL:O	3:D:88:ILE:HD13	2.21	0.40
3:D:119:GLU:OE2	3:D:188:HIS:NE2	2.49	0.40
5:d:107:PHE:N	5:d:135:VAL:O	2.54	0.40
2:A:145:ILE:HG22	2:A:146:VAL:N	2.37	0.40
8:H:125:VAL:HG11	8:Q:124:LEU:HA	2.03	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	i	38/145 (26%)	37 (97%)	1 (3%)	0	100	100
2	A	510/565 (90%)	485 (95%)	25 (5%)	0	100	100
2	C	485/565 (86%)	466 (96%)	19 (4%)	0	100	100
2	E	505/565 (89%)	470 (93%)	35 (7%)	0	100	100
3	B	477/560 (85%)	450 (94%)	27 (6%)	0	100	100
3	D	473/560 (84%)	451 (95%)	22 (5%)	0	100	100
3	F	473/560 (84%)	447 (94%)	26 (6%)	0	100	100
4	g	270/314 (86%)	266 (98%)	4 (2%)	0	100	100
5	d	141/183 (77%)	134 (95%)	7 (5%)	0	100	100
6	e	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
7	G	96/252 (38%)	91 (95%)	5 (5%)	0	100	100
8	H	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
8	I	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
8	J	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
8	K	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
8	L	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
8	M	69/166 (42%)	65 (94%)	4 (6%)	0	100	100
8	N	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
8	O	69/166 (42%)	69 (100%)	0	0	100	100
8	P	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
8	Q	69/166 (42%)	69 (100%)	0	0	100	100
All	All	4221/6002 (70%)	4029 (96%)	192 (4%)	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	i	37/125 (30%)	36 (97%)	1 (3%)	39	67
2	A	421/454 (93%)	421 (100%)	0	100	100
2	C	398/454 (88%)	396 (100%)	2 (0%)	81	85
2	E	416/454 (92%)	414 (100%)	2 (0%)	81	85
3	B	390/447 (87%)	389 (100%)	1 (0%)	86	87
3	D	388/447 (87%)	388 (100%)	0	100	100
3	F	388/447 (87%)	384 (99%)	4 (1%)	68	79
4	g	228/257 (89%)	228 (100%)	0	100	100
5	d	118/144 (82%)	118 (100%)	0	100	100
6	e	57/61 (93%)	57 (100%)	0	100	100
7	G	87/212 (41%)	87 (100%)	0	100	100
8	H	52/133 (39%)	52 (100%)	0	100	100
8	I	52/133 (39%)	52 (100%)	0	100	100
8	J	52/133 (39%)	52 (100%)	0	100	100
8	K	52/133 (39%)	52 (100%)	0	100	100
8	L	52/133 (39%)	52 (100%)	0	100	100
8	M	52/133 (39%)	52 (100%)	0	100	100
8	N	52/133 (39%)	52 (100%)	0	100	100
8	O	52/133 (39%)	52 (100%)	0	100	100
8	P	52/133 (39%)	52 (100%)	0	100	100
8	Q	52/133 (39%)	52 (100%)	0	100	100
All	All	3448/4832 (71%)	3438 (100%)	10 (0%)	84	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	i	78	GLU

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Mol	Chain	Res	Type
2	E	316	CYS
2	E	322	ASP
2	C	457	GLN
2	C	462	LEU
3	B	341	THR
3	F	329	ASP
3	F	372	GLN
3	F	531	LEU
3	F	545	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	194	HIS
2	A	528	HIS
2	E	354	HIS
2	C	354	HIS
3	B	99	GLN
3	B	265	ASN
3	B	336	ASN
3	B	458	GLN
3	F	86	GLN
3	F	248	HIS
3	D	205	GLN
3	D	269	HIS
3	D	336	ASN
3	D	342	GLN
4	g	143	GLN
8	M	115	GLN
8	P	131	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
9	ATP	A	601	10	32,33,33	3.13	13 (40%)	48,52,52	1.91	11 (22%)
9	ATP	C	601	10	32,33,33	3.14	13 (40%)	48,52,52	1.94	11 (22%)
11	ADP	D	601	10	28,29,29	3.06	10 (35%)	43,45,45	2.08	10 (23%)
9	ATP	E	601	10	32,33,33	3.14	12 (37%)	48,52,52	1.96	11 (22%)
11	ADP	B	601	10	28,29,29	3.09	10 (35%)	43,45,45	1.98	9 (20%)

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
9	ATP	A	601	10	-	3/22/38/38	0/3/3/3
9	ATP	C	601	10	-	4/22/38/38	0/3/3/3
11	ADP	D	601	10	-	2/16/32/32	0/3/3/3
9	ATP	E	601	10	-	3/22/38/38	0/3/3/3
11	ADP	B	601	10	-	4/16/32/32	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	ATP	O4'-C1'	8.68	1.62	1.42
11	B	601	ADP	O4'-C1'	8.65	1.62	1.42
9	E	601	ATP	O4'-C1'	8.59	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	601	ADP	O4'-C1'	8.59	1.61	1.42
9	C	601	ATP	O4'-C1'	8.55	1.61	1.42
9	A	601	ATP	C2'-C1'	-7.36	1.30	1.53
9	E	601	ATP	C2'-C1'	-7.30	1.30	1.53
9	C	601	ATP	C2'-C1'	-7.29	1.30	1.53
11	B	601	ADP	C2'-C1'	-7.29	1.30	1.53
11	D	601	ADP	C2'-C1'	-7.21	1.30	1.53
9	C	601	ATP	O4'-C4'	-6.46	1.30	1.45
9	A	601	ATP	O4'-C4'	-6.41	1.30	1.45
9	E	601	ATP	O4'-C4'	-6.38	1.30	1.45
11	D	601	ADP	O4'-C4'	-6.34	1.30	1.45
11	B	601	ADP	O4'-C4'	-6.20	1.31	1.45
9	E	601	ATP	PA-O3A	4.98	1.64	1.59
9	C	601	ATP	PB-O3A	4.93	1.64	1.59
9	C	601	ATP	PA-O3A	4.90	1.64	1.59
9	E	601	ATP	PB-O3B	4.88	1.64	1.59
11	B	601	ADP	PA-O3A	4.87	1.64	1.59
9	E	601	ATP	PB-O3A	4.84	1.64	1.59
9	A	601	ATP	PA-O3A	4.79	1.64	1.59
9	A	601	ATP	PB-O3A	4.76	1.64	1.59
11	D	601	ADP	PA-O3A	4.71	1.64	1.59
9	C	601	ATP	PB-O3B	4.58	1.64	1.59
9	A	601	ATP	PB-O3B	4.40	1.64	1.59
9	E	601	ATP	C6-N6	4.20	1.44	1.34
9	A	601	ATP	C6-N6	4.18	1.44	1.34
11	B	601	ADP	C6-N6	4.17	1.44	1.34
11	D	601	ADP	C6-N6	4.16	1.44	1.34
9	C	601	ATP	C6-N6	4.10	1.44	1.34
11	B	601	ADP	C5-C4	-3.33	1.33	1.39
9	C	601	ATP	C5-C4	-3.24	1.33	1.39
11	D	601	ADP	C5-C4	-3.23	1.33	1.39
9	E	601	ATP	C5-C4	-3.16	1.33	1.39
9	A	601	ATP	C5-C4	-3.13	1.33	1.39
9	C	601	ATP	O3'-C3'	-2.91	1.35	1.43
11	D	601	ADP	O3'-C3'	-2.88	1.35	1.43
9	A	601	ATP	O3'-C3'	-2.87	1.35	1.43
11	B	601	ADP	O3'-C3'	-2.87	1.35	1.43
9	E	601	ATP	O3'-C3'	-2.85	1.35	1.43
11	B	601	ADP	C5-N7	-2.83	1.33	1.39
11	D	601	ADP	C5-N7	-2.80	1.34	1.39
9	A	601	ATP	C8-N9	-2.78	1.32	1.37
9	A	601	ATP	C5-N7	-2.77	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	601	ATP	O2'-C2'	2.76	1.49	1.43
9	C	601	ATP	C5-N7	-2.71	1.34	1.39
9	C	601	ATP	O2'-C2'	2.70	1.49	1.43
9	C	601	ATP	C8-N9	-2.69	1.33	1.37
11	B	601	ADP	O2'-C2'	2.67	1.49	1.43
9	A	601	ATP	O2'-C2'	2.64	1.49	1.43
9	E	601	ATP	C5-N7	-2.63	1.34	1.39
11	D	601	ADP	O2'-C2'	2.63	1.49	1.43
11	B	601	ADP	C8-N9	-2.46	1.33	1.37
9	E	601	ATP	C8-N9	-2.44	1.33	1.37
11	D	601	ADP	C8-N9	-2.36	1.33	1.37
9	C	601	ATP	C4-N9	-2.06	1.33	1.37
9	A	601	ATP	C4-N9	-2.01	1.33	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	601	ATP	N3-C2-N1	-5.62	120.08	128.58
11	B	601	ADP	N3-C2-N1	-5.58	120.13	128.58
11	D	601	ADP	N3-C2-N1	-5.52	120.22	128.58
9	C	601	ATP	N3-C2-N1	-5.47	120.31	128.58
9	A	601	ATP	N3-C2-N1	-5.28	120.58	128.58
11	D	601	ADP	N6-C6-N1	-5.28	106.62	118.38
11	B	601	ADP	N6-C6-N1	-4.95	107.36	118.38
9	A	601	ATP	C5-C4-N3	-4.81	120.10	126.72
9	C	601	ATP	C5-C4-N3	-4.70	120.24	126.72
9	E	601	ATP	N9-C8-N7	-4.69	107.28	113.94
11	D	601	ADP	C5-C4-N3	-4.69	120.26	126.72
11	B	601	ADP	C5-C4-N3	-4.66	120.30	126.72
9	E	601	ATP	C5-C4-N3	-4.59	120.39	126.72
9	C	601	ATP	N9-C8-N7	-4.52	107.52	113.94
9	A	601	ATP	N9-C8-N7	-4.44	107.64	113.94
9	C	601	ATP	N6-C6-N1	-3.99	109.48	118.38
9	A	601	ATP	N6-C6-N1	-3.97	109.53	118.38
11	D	601	ADP	C5-C6-N6	3.97	133.11	123.29
11	B	601	ADP	N9-C8-N7	-3.94	108.34	113.94
11	D	601	ADP	N9-C8-N7	-3.89	108.41	113.94
9	E	601	ATP	N6-C6-N1	-3.77	109.99	118.38
11	B	601	ADP	C5-C6-N6	3.67	132.37	123.29
9	E	601	ATP	C4-N9-C1'	-3.56	118.30	126.63
9	E	601	ATP	C4-N9-C8	3.54	109.45	105.74
9	A	601	ATP	N3-C4-N9	3.51	133.14	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	601	ATP	C4-N9-C8	3.45	109.36	105.74
9	C	601	ATP	N3-C4-N9	3.43	133.00	127.17
9	A	601	ATP	C4-N9-C8	3.36	109.27	105.74
9	E	601	ATP	N3-C4-N9	3.36	132.88	127.17
11	D	601	ADP	C3'-C2'-C1'	3.31	107.73	101.46
9	C	601	ATP	C4-N9-C1'	-3.25	119.03	126.63
9	A	601	ATP	C4-N9-C1'	-3.24	119.05	126.63
9	E	601	ATP	C2-N3-C4	3.24	119.74	111.83
11	D	601	ADP	C2-N3-C4	3.23	119.71	111.83
11	B	601	ADP	C2-N3-C4	3.22	119.71	111.83
9	C	601	ATP	C2-N3-C4	3.21	119.67	111.83
9	A	601	ATP	C2-N3-C4	3.14	119.50	111.83
11	B	601	ADP	N3-C4-N9	2.86	132.03	127.17
9	E	601	ATP	C5-N7-C8	2.80	107.85	103.45
9	C	601	ATP	C5-C6-N6	2.79	130.20	123.29
9	A	601	ATP	C5-C6-N6	2.77	130.14	123.29
11	D	601	ADP	N3-C4-N9	2.75	131.84	127.17
9	A	601	ATP	C5-N7-C8	2.72	107.73	103.45
9	C	601	ATP	C5-N7-C8	2.67	107.65	103.45
11	D	601	ADP	C5-N7-C8	2.59	107.52	103.45
9	E	601	ATP	C5-C6-N6	2.57	129.65	123.29
11	B	601	ADP	C5-N7-C8	2.55	107.46	103.45
9	E	601	ATP	C1'-N9-C8	2.32	132.25	127.09
11	B	601	ADP	C4-N9-C8	2.18	108.03	105.74
9	A	601	ATP	C1'-N9-C8	2.06	131.67	127.09
9	C	601	ATP	C1'-N9-C8	2.03	131.61	127.09
11	D	601	ADP	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	601	ATP	C5'-O5'-PA-O1A
9	C	601	ATP	C5'-O5'-PA-O1A
9	C	601	ATP	C5'-O5'-PA-O2A
9	C	601	ATP	C5'-O5'-PA-O3A
11	B	601	ADP	C5'-O5'-PA-O1A
9	E	601	ATP	PB-O3B-PG-O1G
11	D	601	ADP	PB-O3A-PA-O1A
11	B	601	ADP	O4'-C4'-C5'-O5'
9	A	601	ATP	C5'-O5'-PA-O1A
9	A	601	ATP	C5'-O5'-PA-O2A

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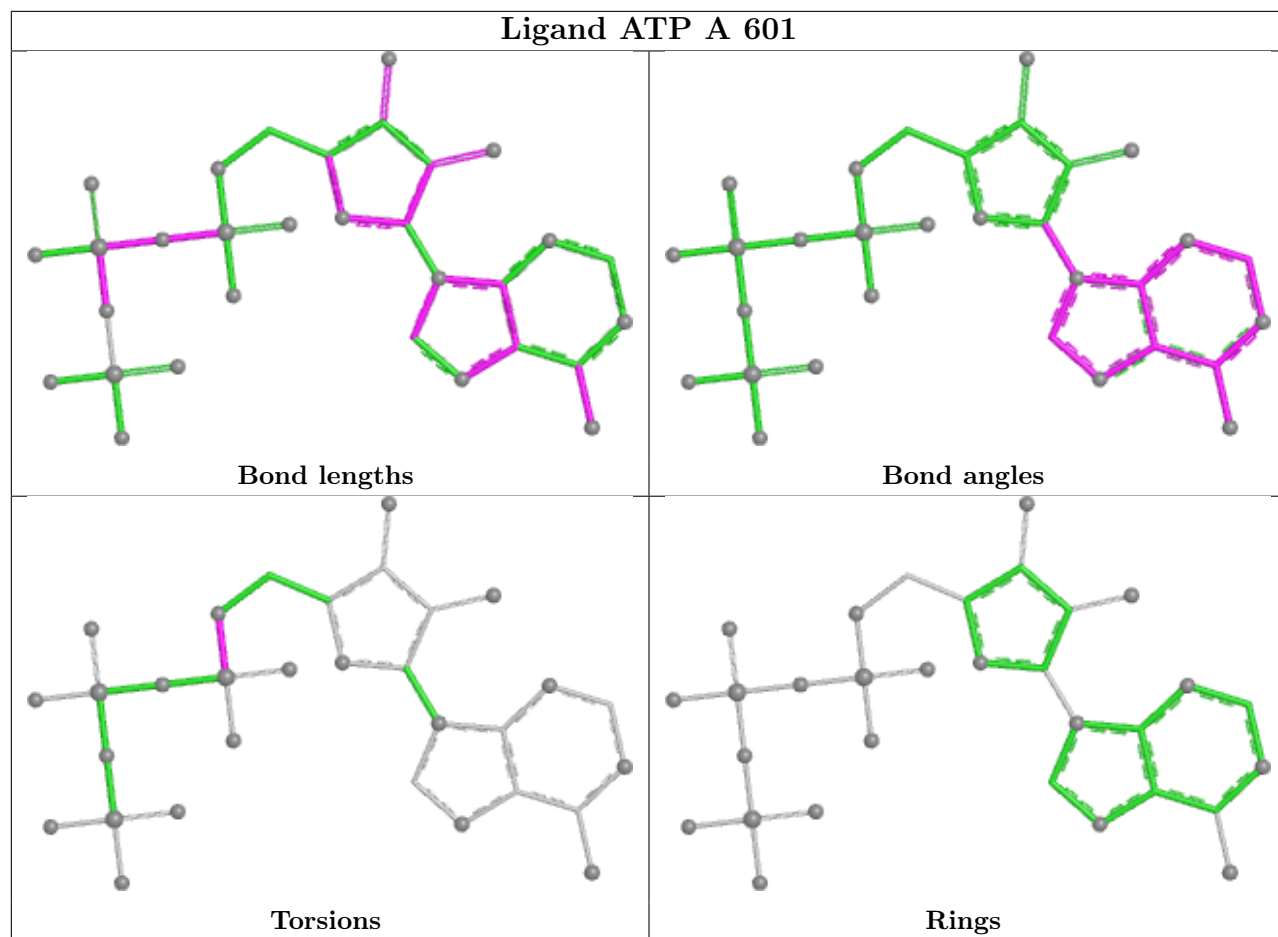
Mol	Chain	Res	Type	Atoms
9	A	601	ATP	C5'-O5'-PA-O3A
9	E	601	ATP	C5'-O5'-PA-O3A
11	B	601	ADP	C5'-O5'-PA-O3A
11	D	601	ADP	C5'-O5'-PA-O1A
11	B	601	ADP	PB-O3A-PA-O1A
9	C	601	ATP	PB-O3B-PG-O3G

There are no ring outliers.

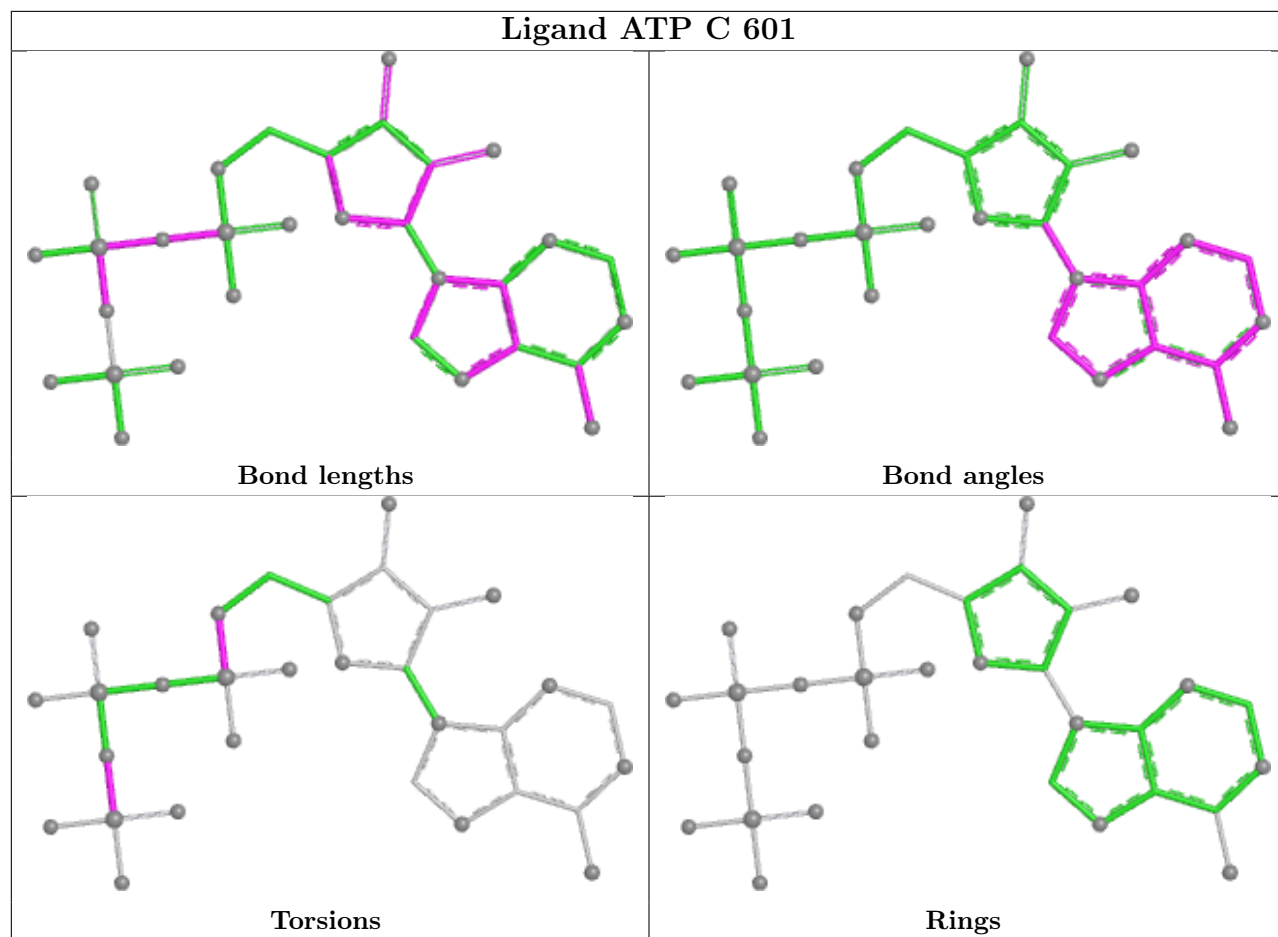
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	601	ADP	1	0

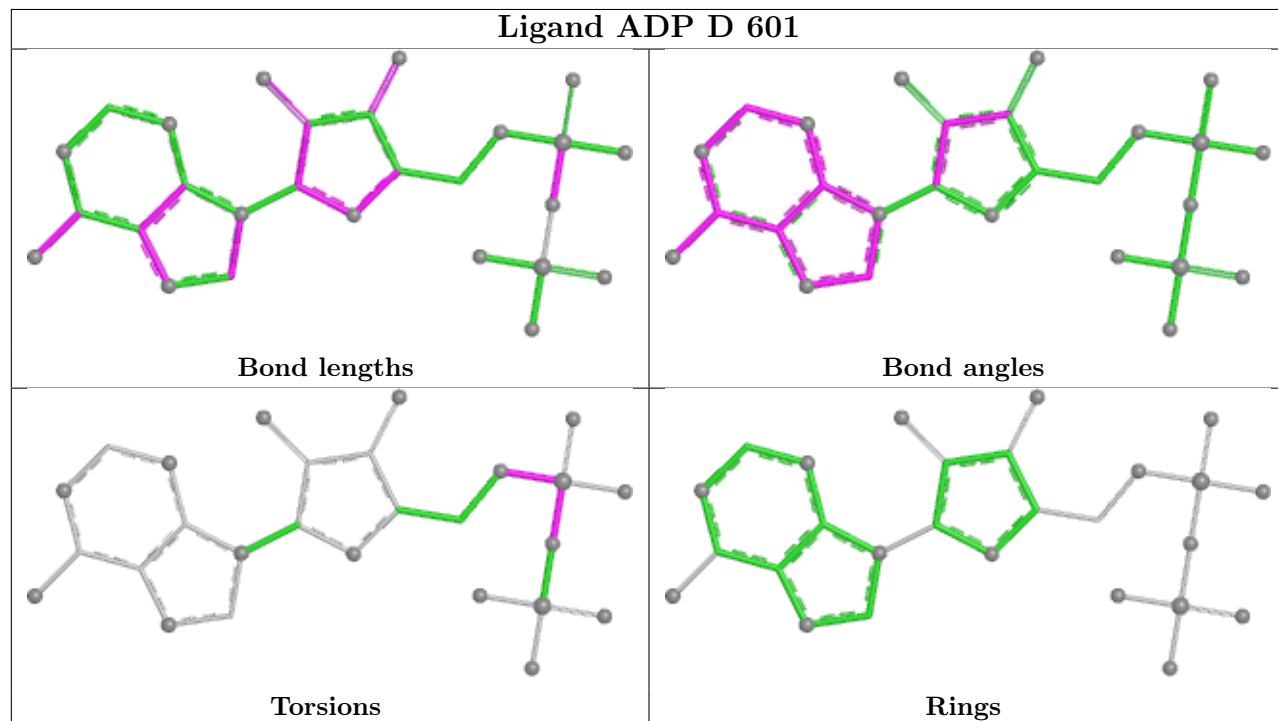
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



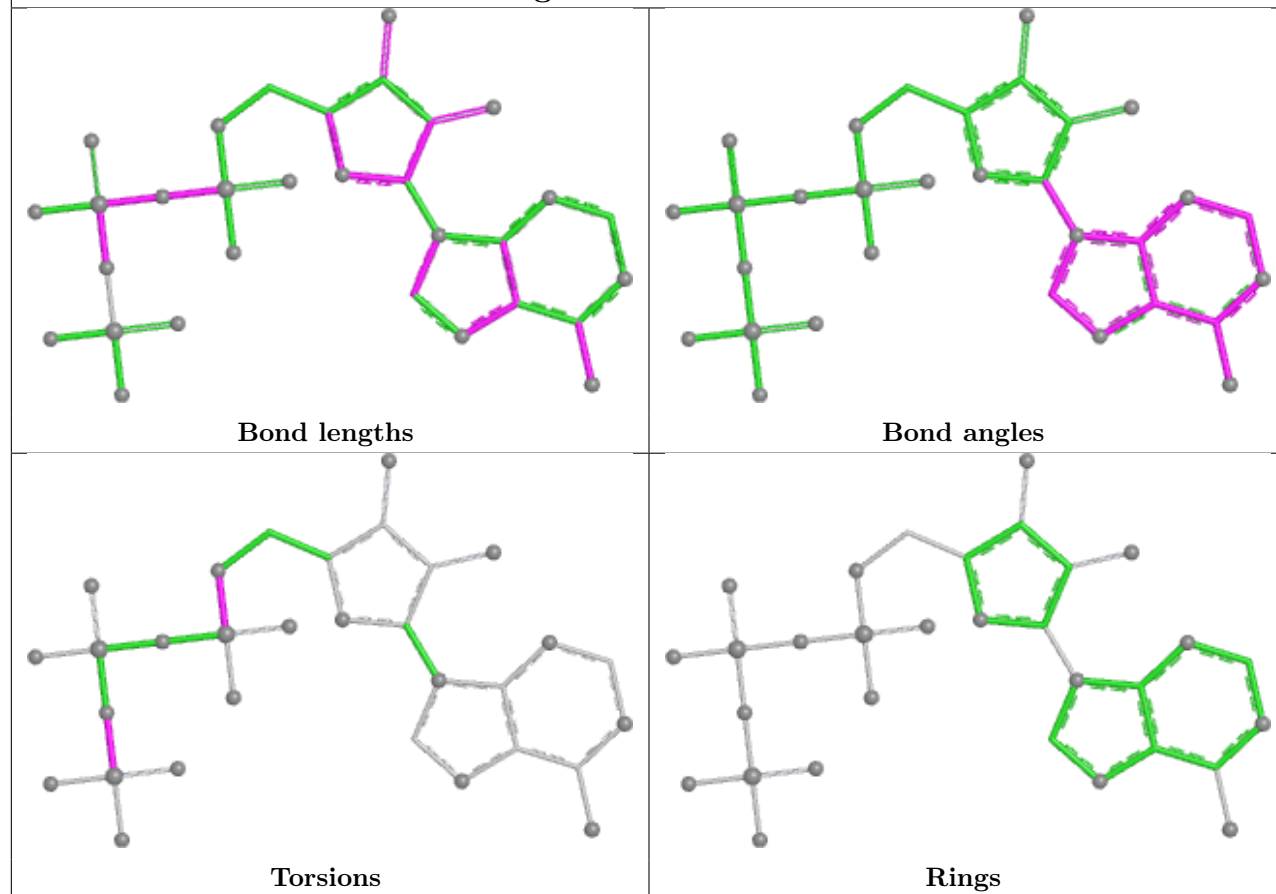
Ligand ATP C 601



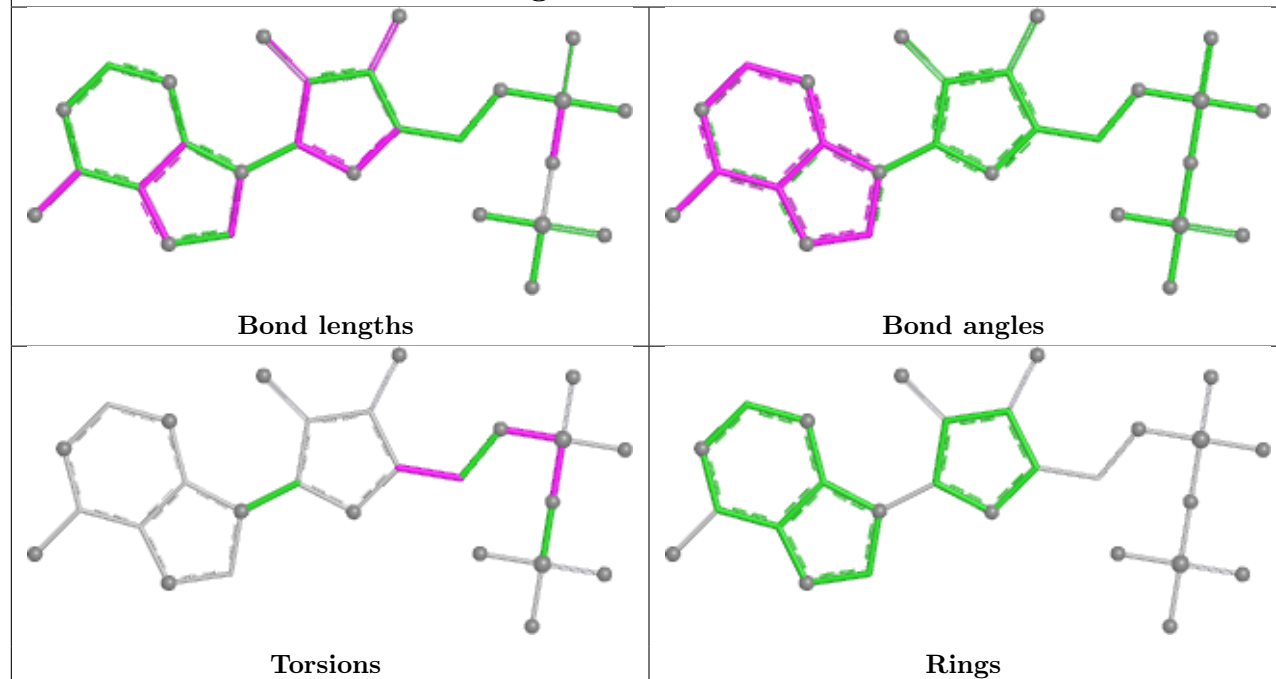
Ligand ADP D 601



Ligand ATP E 601



Ligand ADP B 601



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	170:MET	C	171:TYR	N	3.30

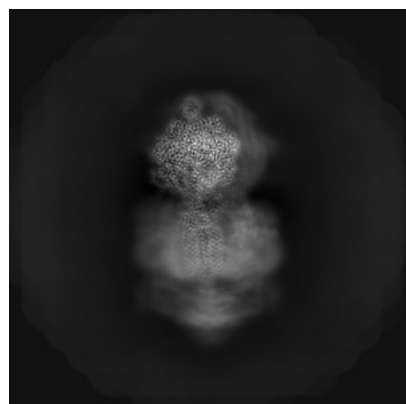
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10521. These allow visual inspection of the internal detail of the map and identification of artifacts.

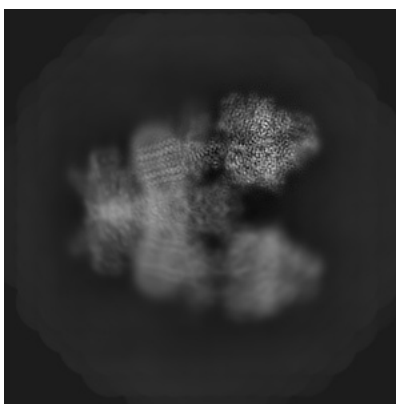
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

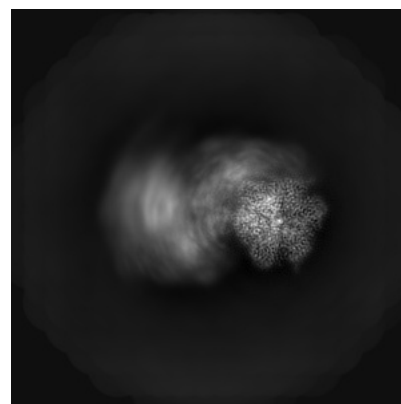
6.1.1 Primary map



X

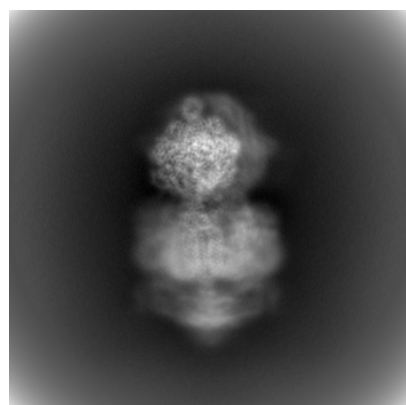


Y

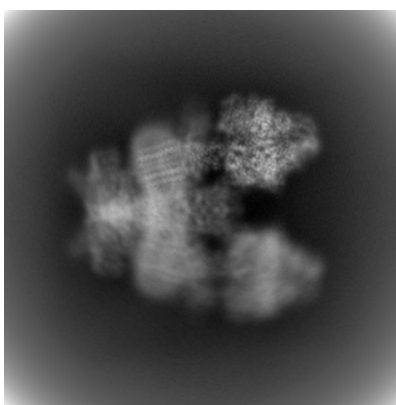


Z

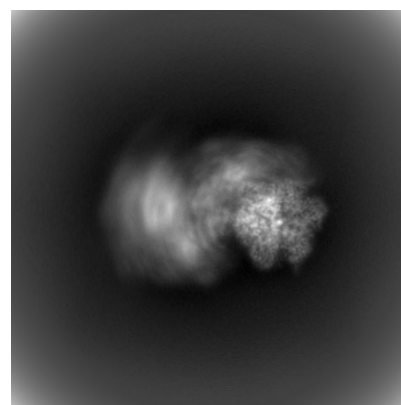
6.1.2 Raw map



X



Y

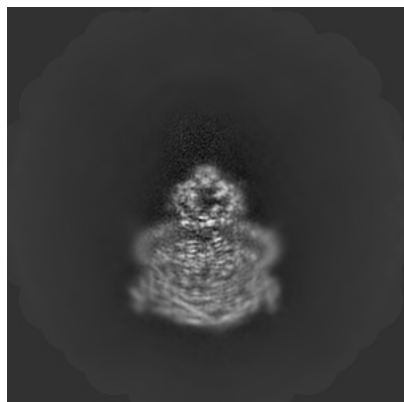


Z

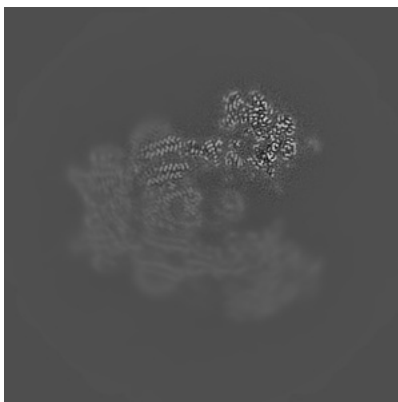
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

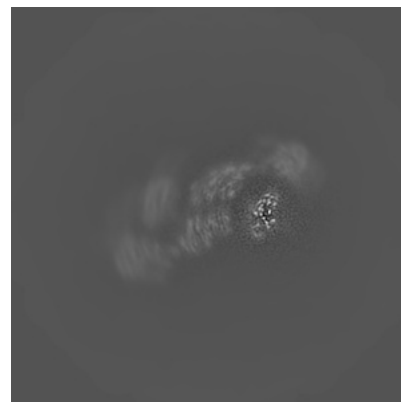
6.2.1 Primary map



X Index: 280

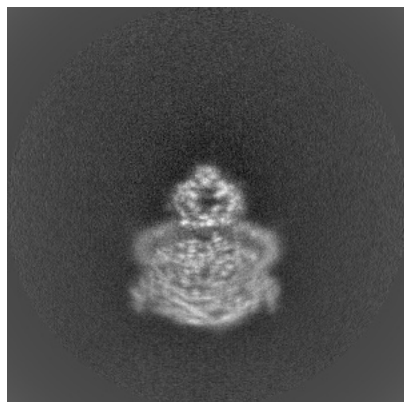


Y Index: 280

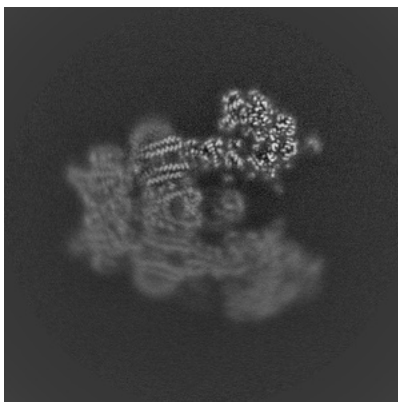


Z Index: 280

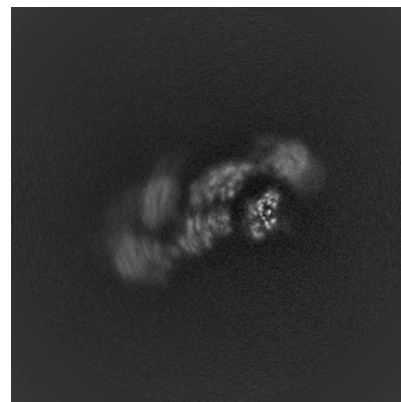
6.2.2 Raw map



X Index: 280



Y Index: 280

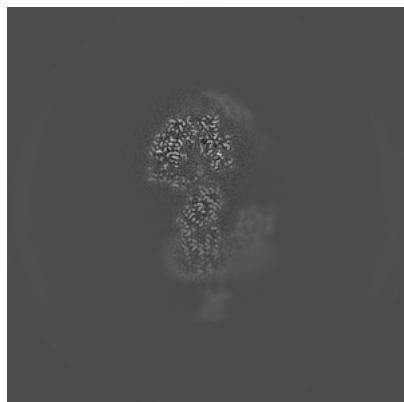


Z Index: 280

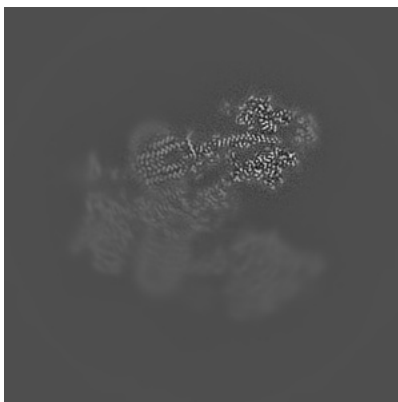
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

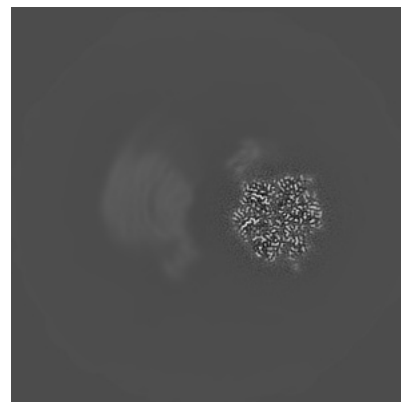
6.3.1 Primary map



X Index: 360

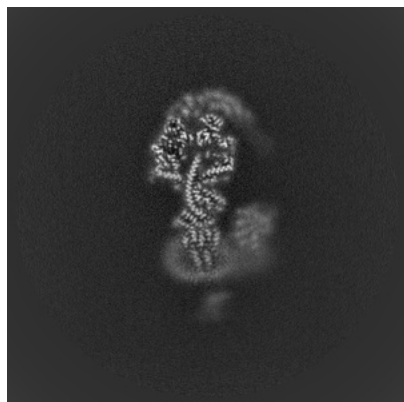


Y Index: 262

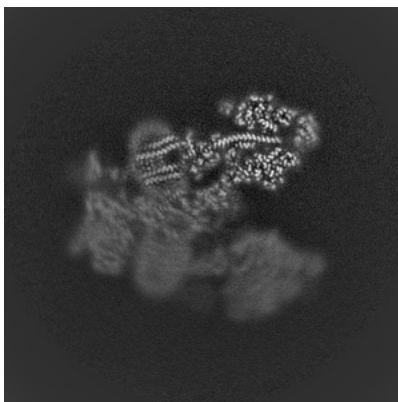


Z Index: 366

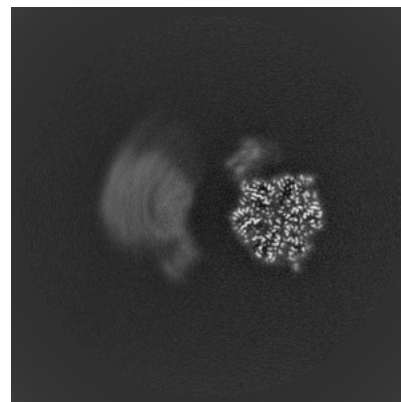
6.3.2 Raw map



X Index: 366



Y Index: 263

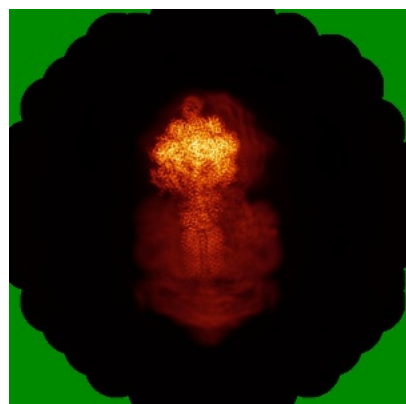


Z Index: 366

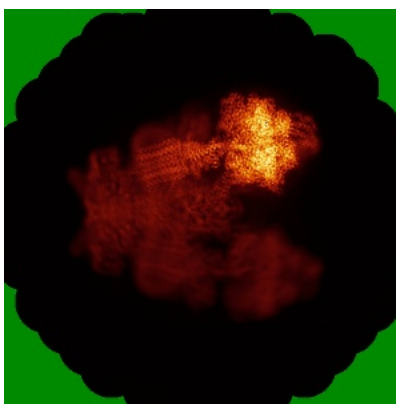
The images above show the largest variance slices of the map in three orthogonal directions.

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

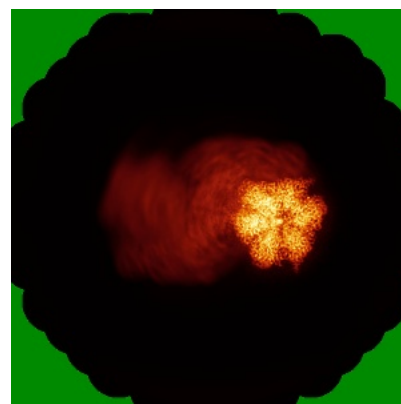
6.4.1 Primary map



X

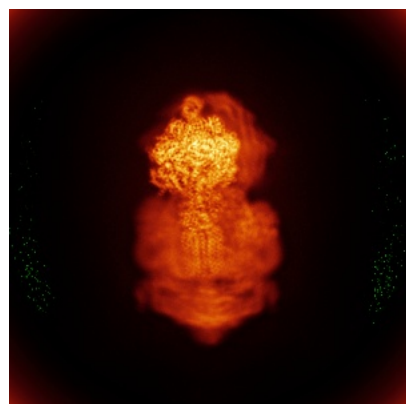


Y

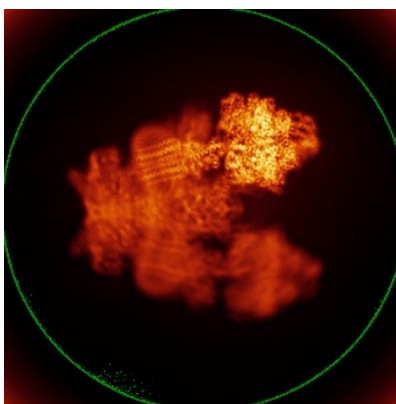


Z

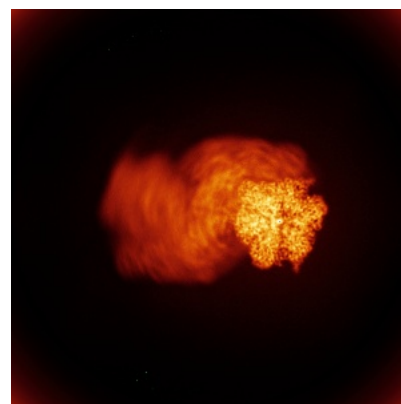
6.4.2 Raw map



X



Y

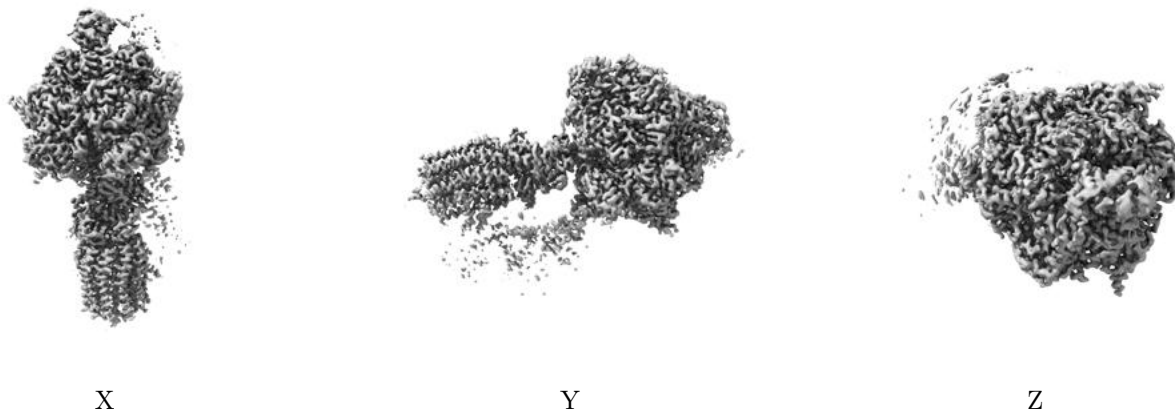


Z

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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

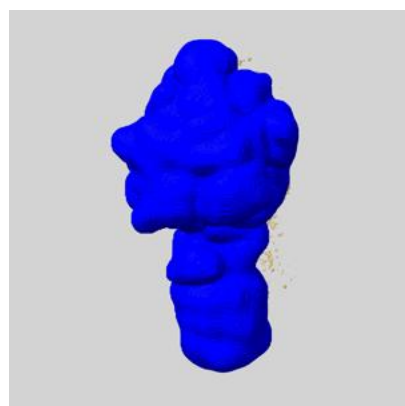
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

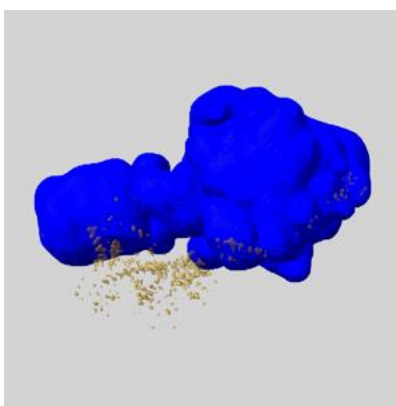
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

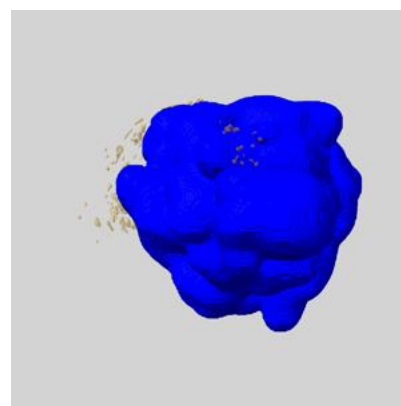
6.6.1 emd_10521_msk_1.map [i](#)



X



Y

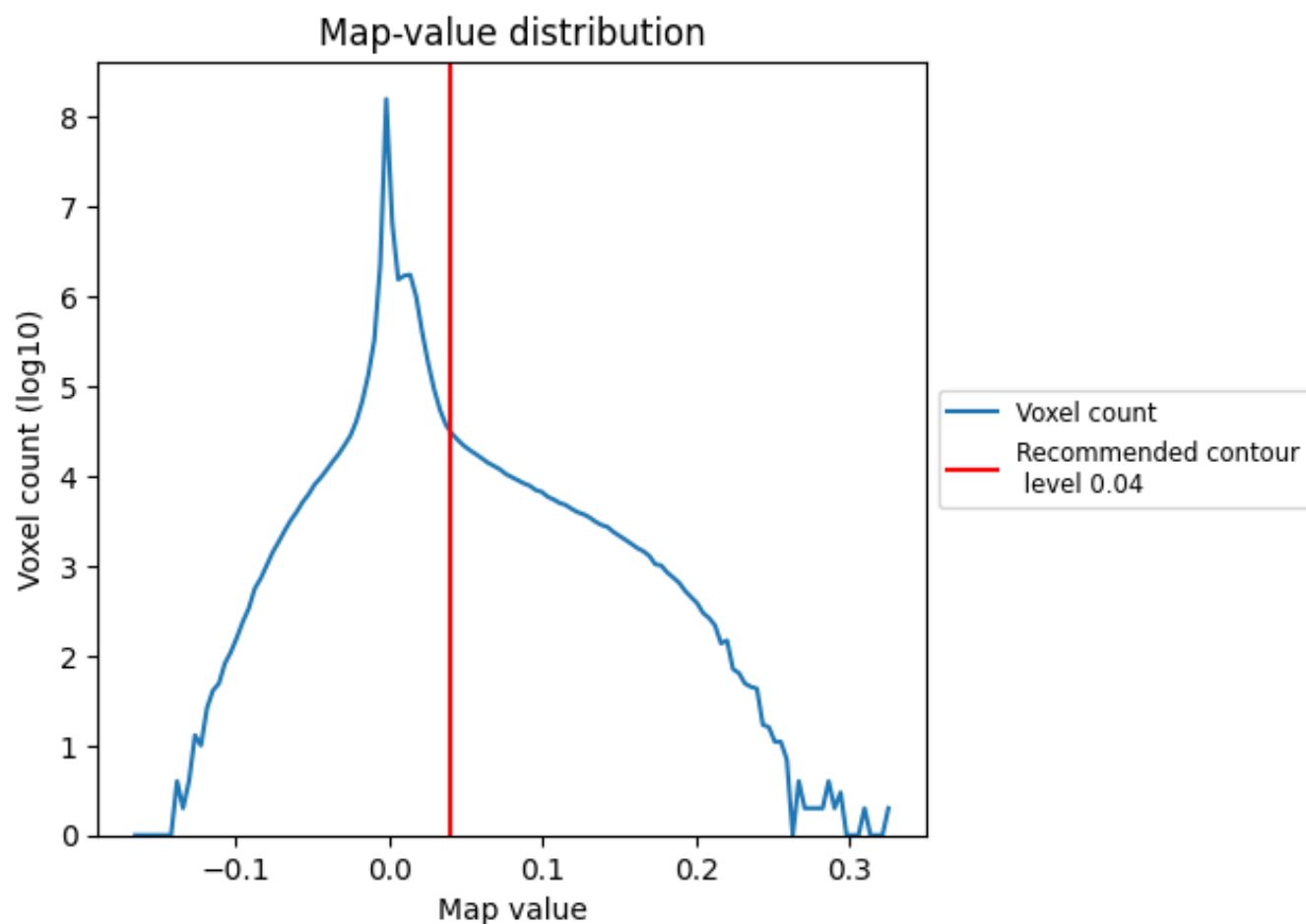


Z

7 Map analysis [i](#)

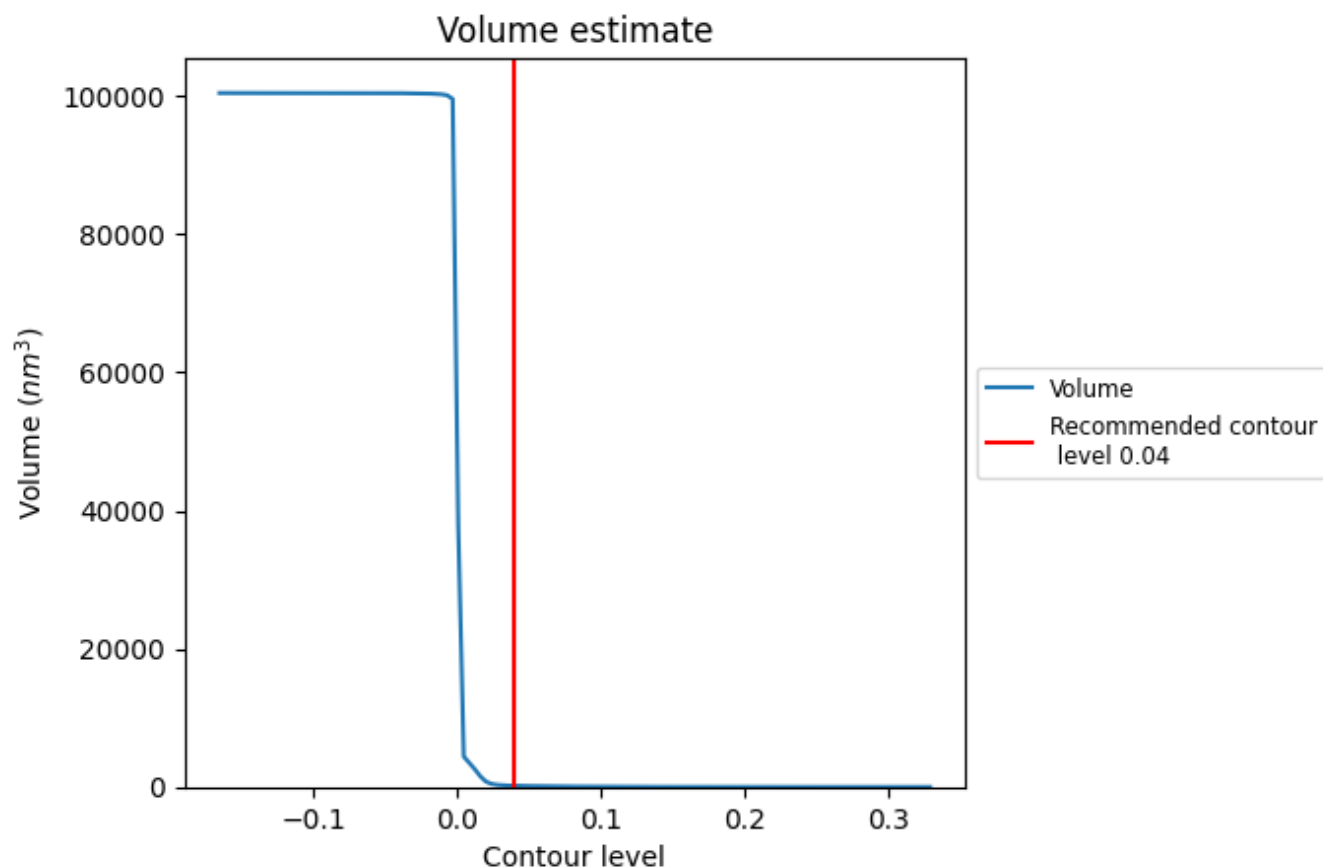
This section contains the results of statistical analysis of the map.

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.

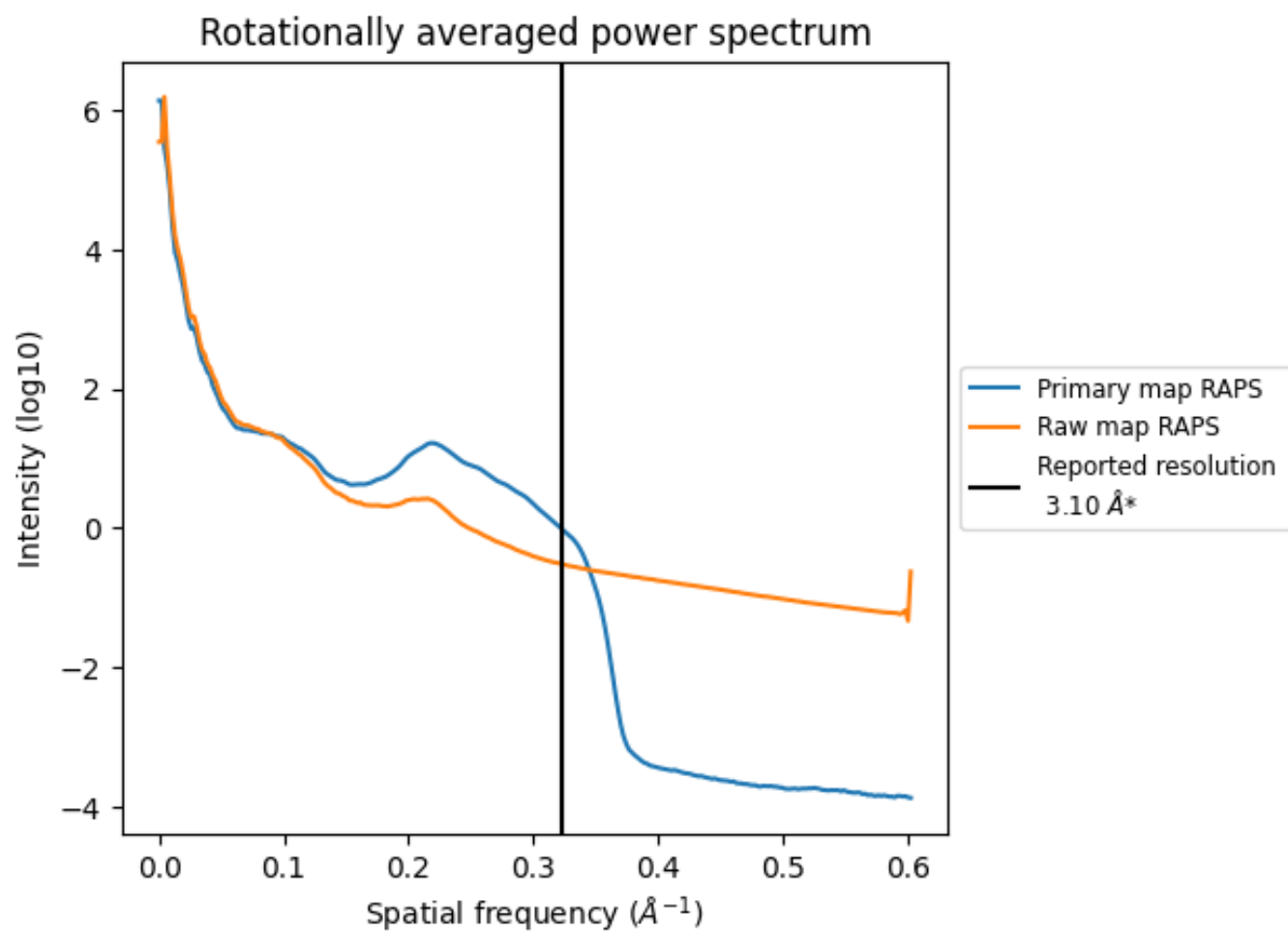
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 155 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 ⓘ

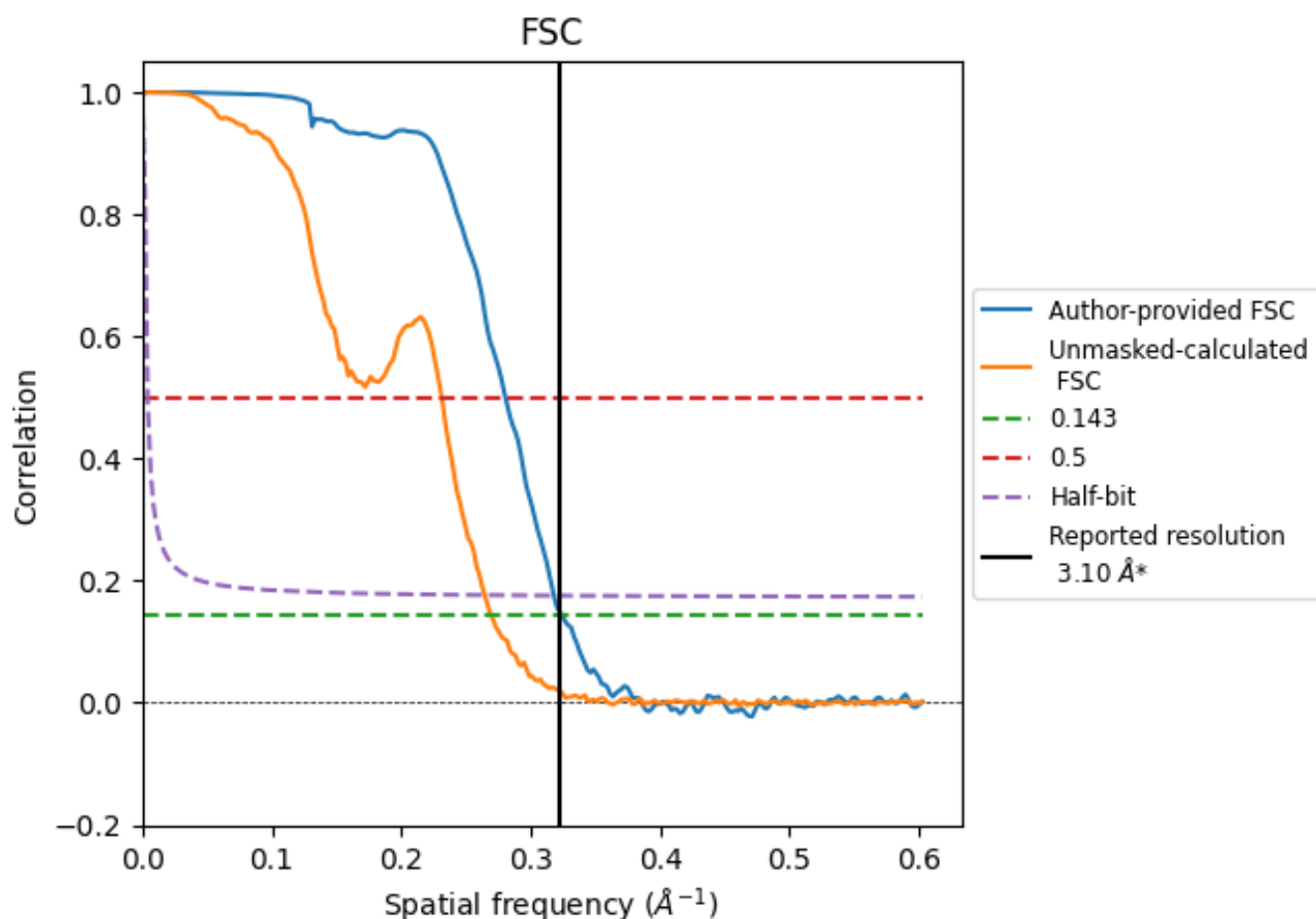


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

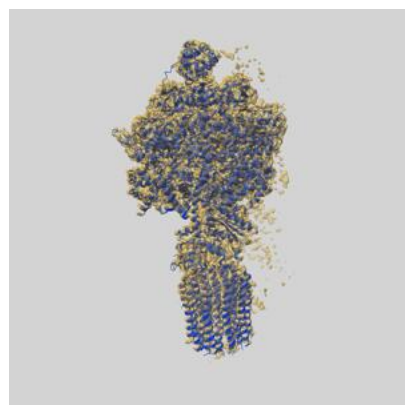
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.56	3.14
Unmasked-calculated*	3.71	4.32	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 3.1 by more than 10 %

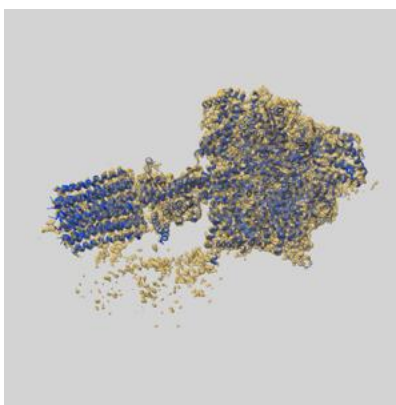
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10521 and PDB model 6TMH. Per-residue inclusion information can be found in section [3](#) on page [8](#).

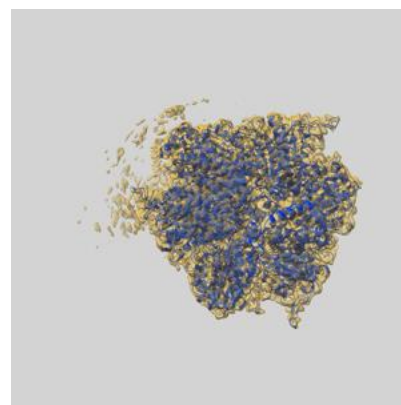
9.1 Map-model overlay [i](#)



X



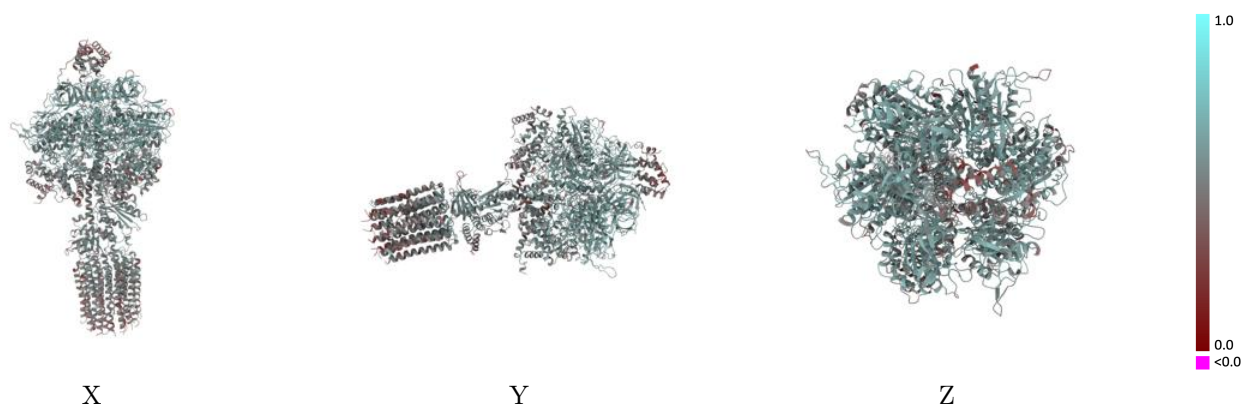
Y



Z

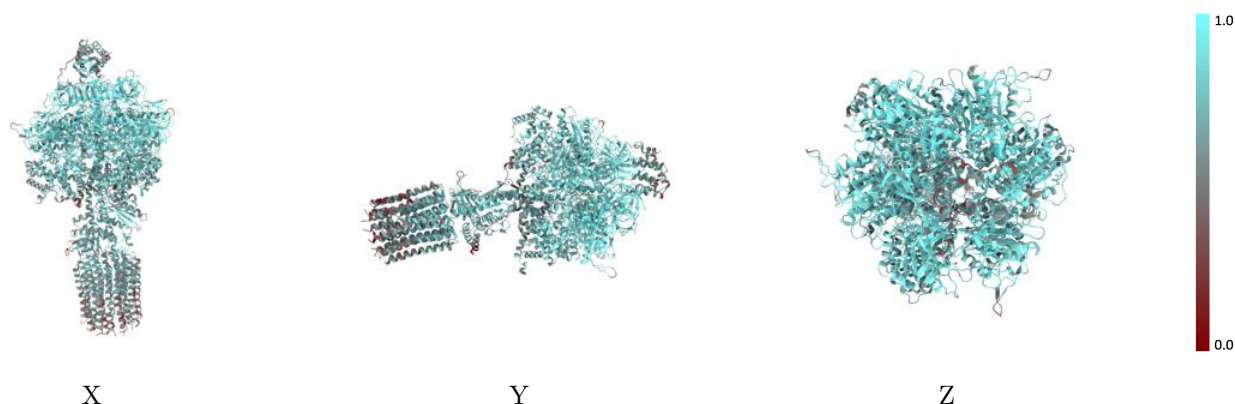
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



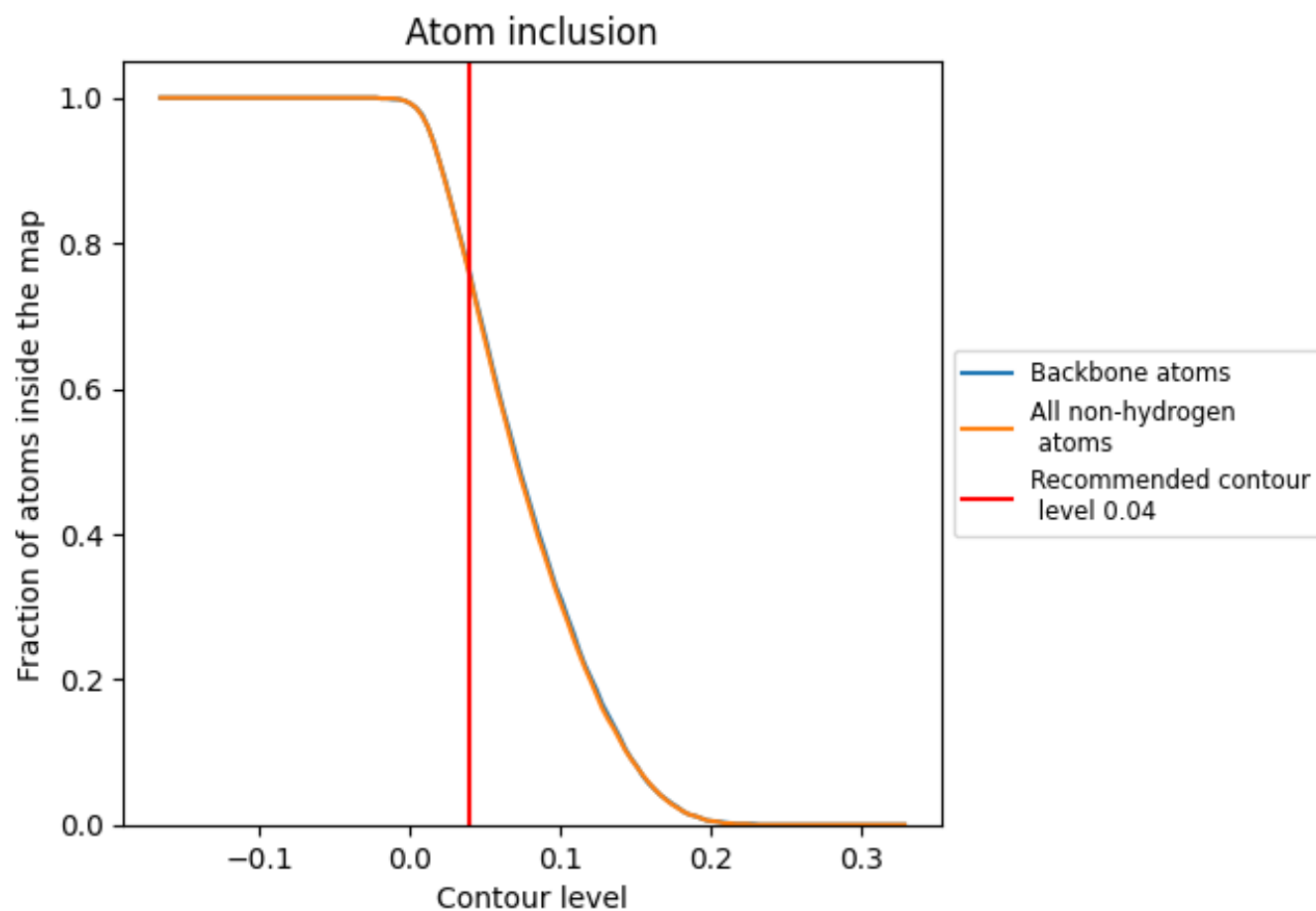
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.5340
A	 0.7900	 0.5490
B	 0.8430	 0.5780
C	 0.8400	 0.5700
D	 0.8400	 0.5680
E	 0.8020	 0.5470
F	 0.7950	 0.5420
G	 0.5950	 0.4150
H	 0.5710	 0.4700
I	 0.5490	 0.4480
J	 0.5510	 0.4510
K	 0.5730	 0.4560
L	 0.5650	 0.4380
M	 0.5670	 0.4450
N	 0.5670	 0.4580
O	 0.6020	 0.4790
P	 0.5840	 0.4480
Q	 0.5840	 0.4630
d	 0.6250	 0.4850
e	 0.6880	 0.5080
g	 0.7550	 0.5340
i	 0.6440	 0.4830

