



## Full wwPDB EM Validation Report ⓘ

Jul 28, 2025 – 10:20 AM EDT

PDB ID : 9BXU / pdb\_00009bxu  
EMDB ID : EMD-45012  
Title : Cryo-EM structure of ATP synthase DP state  
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.  
Deposited on : 2024-05-22  
Resolution : 3.00 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

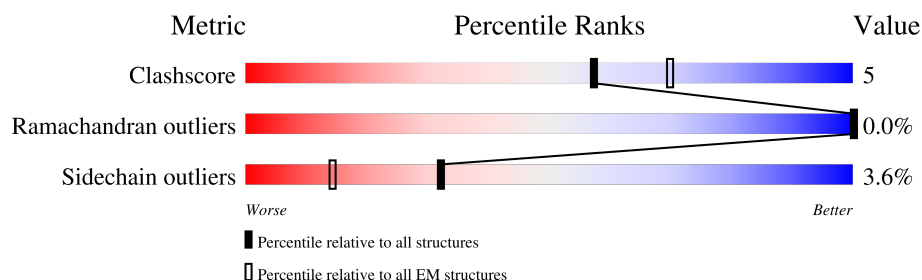
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



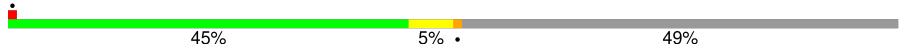
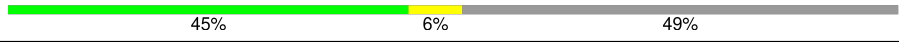
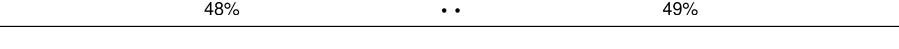


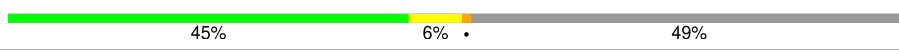

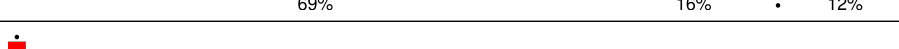



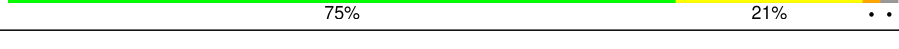
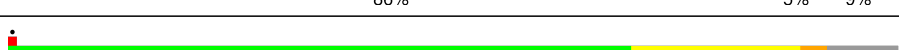
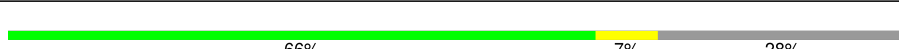


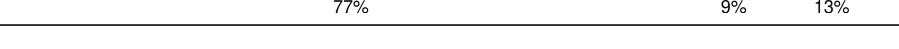
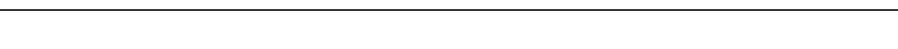



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	8	67	
2	D	570	
2	E	570	
2	F	570	
3	G	273	
4	H	168	
5	I	136	
6	J	108	

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Mol	Chain	Length	Quality of chain
7	K	141	
7	L	141	
7	M	141	
7	N	141	
7	O	141	
7	P	141	
7	Q	141	
7	R	141	
8	S	213	
9	T	103	
10	U	71	
11	V	238	
12	W	88	
13	a	226	
14	c	76	
15	d	166	
16	i	58	
17	k	29	
18	A	550	
18	B	550	
18	C	550	

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 38469 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 protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	31	Total	C	N	O	S	0	0
			247	165	35	45	2		

- 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
			3543	2246	601	684	12		
2	E	467	Total	C	N	O	S	0	0
			3532	2240	599	681	12		
2	F	467	Total	C	N	O	S	0	0
			3532	2240	599	681	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	272	Total	C	N	O	S	0	0
			2093	1320	363	403	7		

- Molecule 4 is a protein called ATP synthase F1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	130	Total	C	N	O	S	0	0
			961	602	163	194	2		

- Molecule 5 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	48	Total	C	N	O	S	0	0
			373	238	68	66	1		

- Molecule 6 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	48	Total	C	N	O	0	0
			365	221	77	67		

- Molecule 7 is a protein called ATP synthase lipid-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	L	72	Total	C	N	O	S	0	0
			509	338	79	89	3		
7	M	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	N	72	Total	C	N	O	S	0	0
			510	339	80	89	2		
7	O	72	Total	C	N	O	S	0	0
			510	339	80	89	2		
7	P	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	Q	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
7	R	72	Total	C	N	O	S	0	0
			510	338	80	89	3		

- Molecule 8 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	187	Total	C	N	O	S	0	0
			1423	905	244	265	9		

- Molecule 9 is a protein called ATP synthase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	81	Total	C	N	O	S	0	0
			587	382	94	110	1		

- Molecule 10 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	43	Total	C	N	O	0	0
			301	200	50	51		

- Molecule 11 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	212	Total	C	N	O	S	0	0
			1710	1102	295	308	5		

- Molecule 12 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	81	Total	C	N	O	S	0	0
			641	418	109	111	3		

- Molecule 13 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	221	Total	C	N	O	S	0	0
			1685	1120	267	287	11		

- Molecule 14 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	c	69	Total	C	N	O	0	0
			402	243	80	79		

- Molecule 15 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	d	153	Total	C	N	O	S	0	0
			1160	747	188	222	3		

- Molecule 16 is a protein called ATP synthase membrane subunit K, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	42	Total	C	N	O	S	0	0
			303	199	49	53	2		

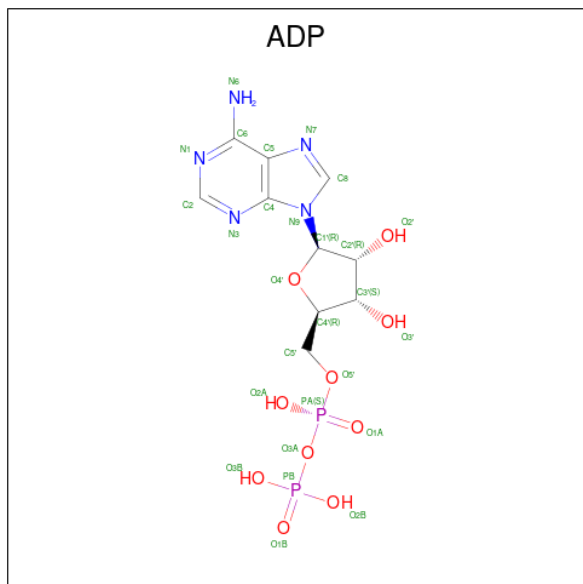
- Molecule 17 is a protein called unknow peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	k	29	Total	C	N	O	0	0
			145	87	29	29		

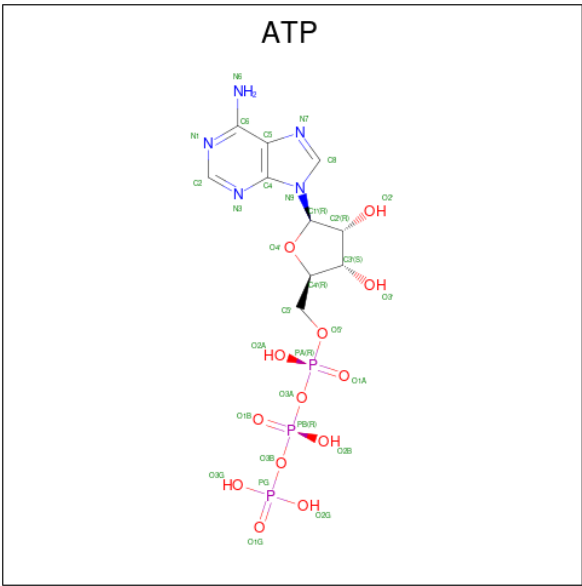
- Molecule 18 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	507	Total	C	N	O	S	0	0
			3832	2415	675	730	12		
18	C	495	Total	C	N	O	S	0	0
			3756	2366	665	713	12		
18	B	480	Total	C	N	O	S	0	0
			3635	2291	643	689	12		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).




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

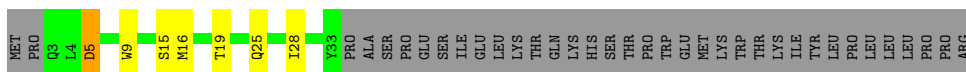


### 3 Residue-property plots


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.

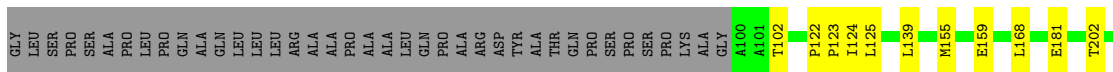
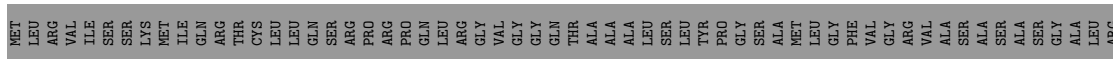
#### • Molecule 1: ATP synthase protein 8

Chain 8: 



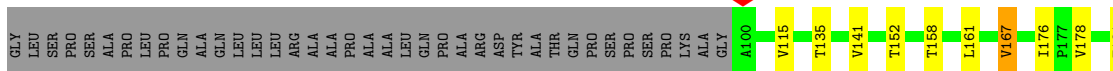
#### • Molecule 2: ATP synthase subunit beta

Chain D: 



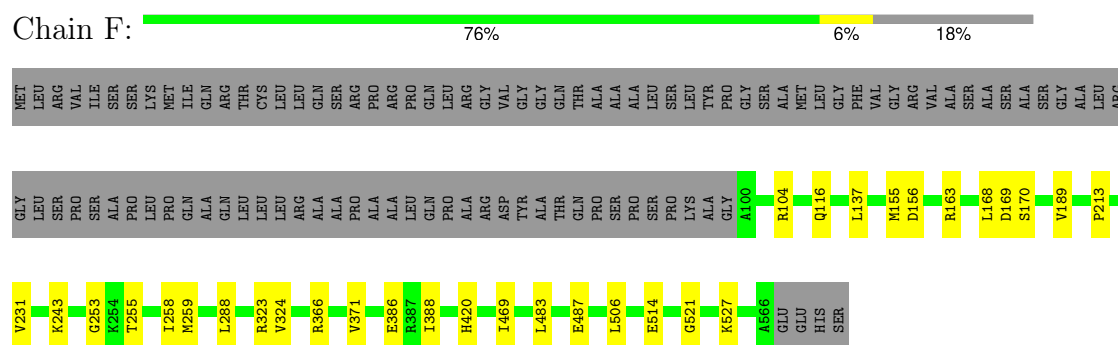
#### • Molecule 2: ATP synthase subunit beta

Chain E: 



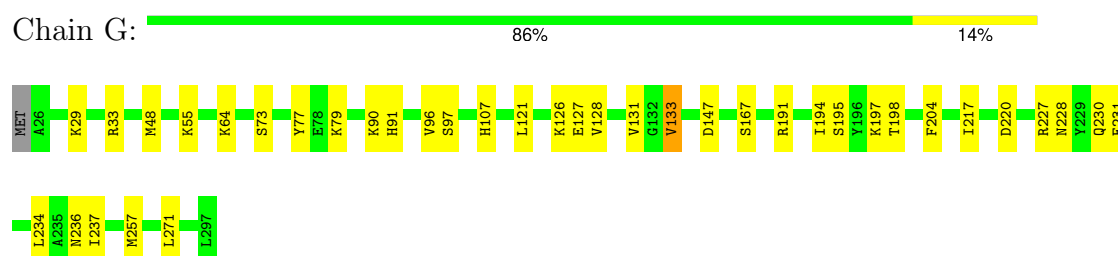
#### • Molecule 2: ATP synthase subunit beta

## Chain F:



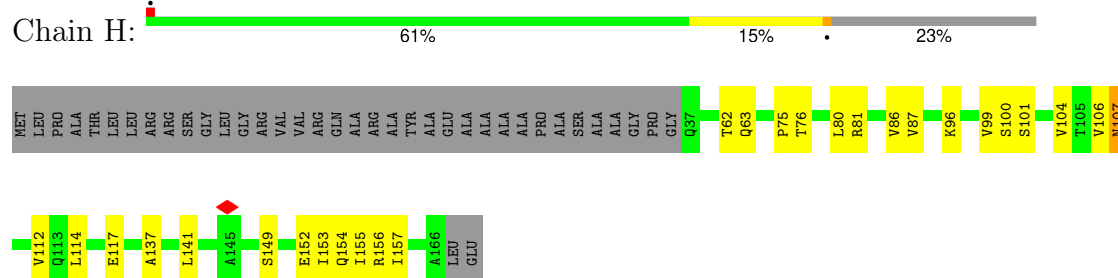
- Molecule 3: ATP synthase subunit gamma

## Chain G:



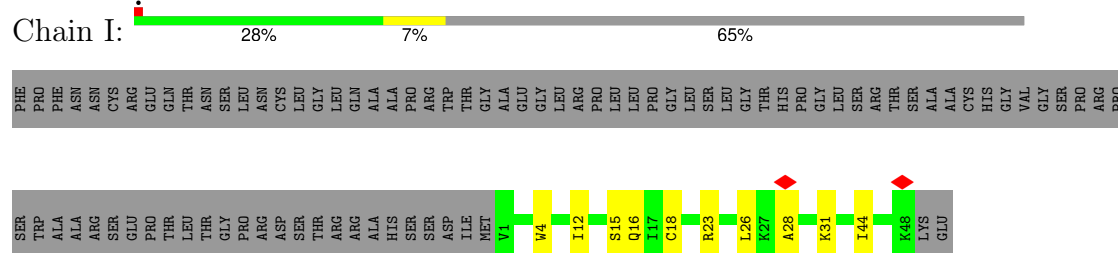
- Molecule 4: ATP synthase F1 subunit delta

## Chain H:



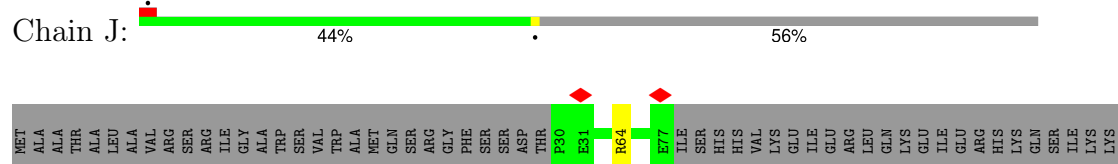
- Molecule 5: ATP synthase F1 subunit epsilon

## Chain I:



- Molecule 6: ATPase inhibitor, mitochondrial

## Chain J:



LYS  
ASN  
ASP  
ASP  
ASP

• Molecule 7: ATP synthase lipid-binding protein

Chain K:  45% 5% 49%

MET PHE ALA ALA CYS THR LYS LEU ALA CYS THR PRO PRO ALA LEU ILE ARG GLY SER ARG VAL ALA ALA TYR ARG PRO PRO ILE SER ALA ALA VAL SER LEU LEU ARG ARG PRO PRO GLY GLY GLY THR THR VAL PHE ASN GLY ALA GLN ASN GLY VAL SER GLN PRO PRO ILE ILE ARG GLU PHE GLN

THR SER ALA VAL SER ARG ASP I2 A6 I25 I33 A37 L46 F47 F54 A55 L56 I62 F73 MET

• Molecule 7: ATP synthase lipid-binding protein

Chain L:  45% 6% 49%

MET PHE ALA ALA CYS THR LYS LEU ALA CYS THR PRO PRO ALA LEU ILE ARG GLY SER ARG VAL ALA ALA TYR ARG PRO PRO ILE SER ALA ALA VAL SER LEU LEU ARG ARG PRO PRO GLY GLY GLY THR THR VAL PHE ASN GLY ALA GLN ASN GLY VAL SER GLN PRO PRO ILE ILE ARG GLU PHE GLN

THR SER ALA VAL SER ARG ASP I2 I25 F29 N39 L46 F54 A55 L56 A68 F69 L70 I71 L72 F73 MET

• Molecule 7: ATP synthase lipid-binding protein

Chain M:  48% 2% 49%

MET PHE ALA ALA CYS THR LYS LEU ALA CYS THR PRO PRO ALA LEU ILE ARG GLY SER ARG VAL ALA ALA TYR ARG PRO PRO ILE SER ALA ALA VAL SER LEU LEU ARG ARG PRO PRO GLY GLY GLY THR THR VAL PHE ASN GLY ALA GLN ASN GLY VAL SER GLN PRO PRO ILE ILE ARG GLU PHE GLN

THR SER ALA VAL SER ARG ASP I2 I9 I33 L56 M60 F73 MET

• Molecule 7: ATP synthase lipid-binding protein

Chain N:  41% 10% 49%

MET PHE ALA ALA CYS THR LYS LEU ALA CYS THR PRO PRO ALA LEU ILE ARG GLY SER ARG VAL ALA ALA TYR ARG PRO PRO ILE SER ALA ALA VAL SER LEU LEU ARG ARG PRO PRO GLY GLY GLY THR THR VAL PHE ASN GLY ALA GLN ASN GLY VAL SER GLN PRO PRO ILE ILE ARG GLU PHE GLN

THR SER ALA VAL SER ARG ASP I2 S21 I25 V28 F29 G30 S31 L32 I33 Q45 L46 Y49 G61 L62 I71 L72 F73 MET

• Molecule 7: ATP synthase lipid-binding protein

Chain O:  43% 6% 49%

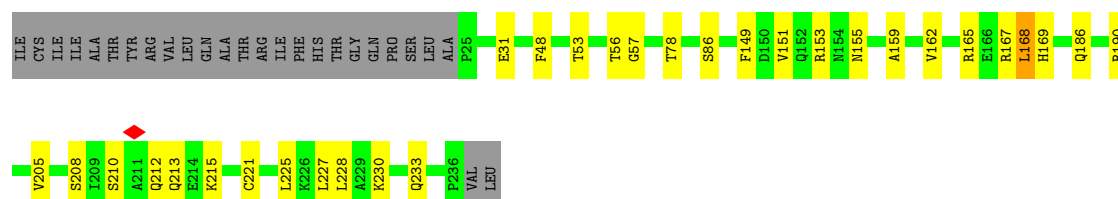
MET PHE ALA ALA CYS THR LYS LEU ALA CYS THR PRO PRO ALA LEU ILE ARG GLY SER ARG VAL ALA ALA TYR ARG PRO PRO ILE SER ALA ALA VAL SER LEU LEU ARG ARG PRO PRO GLY GLY GLY THR THR VAL PHE ASN GLY ALA GLN ASN GLY VAL SER GLN PRO PRO ILE ILE ARG GLU PHE GLN

THR SER ALA VAL SER ARG ASP I2 A5 I9 L32 Y36 P40 K43 L46 Y49 F54 A55 L56 F63 F69 F73 MET

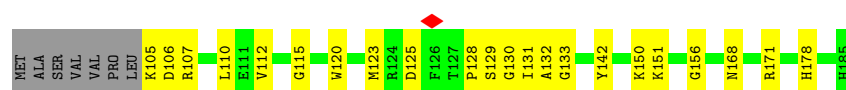


MET	VAL	P3	A45	GIU	GIU	LYS	LYS	LYS	GLN	ASP	GLU	LEU	LYS	ARG	ILE	GIU	ARG	GIU	LEU	ALA	ALA	GIU	GLN	GLU	ASP	SER	ILE	LEU	LYS
-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

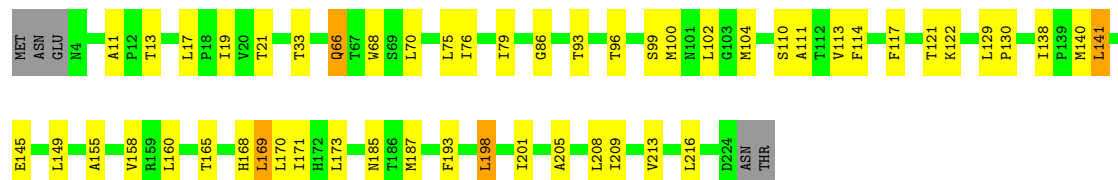
- Chain V:  76% 13% 11%



- Chain W:  67% 25% 8%



- Chain a:  75% 21% ..

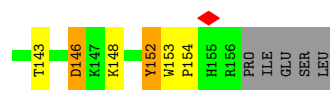


- Chain c: 



- Chain d:  70% 19% 8%





- Molecule 16: ATP synthase membrane subunit K, mitochondrial

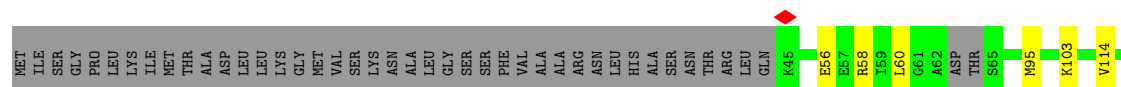
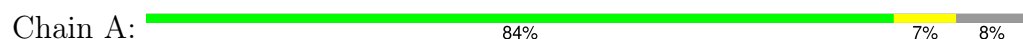


- Molecule 17: unknown peptide

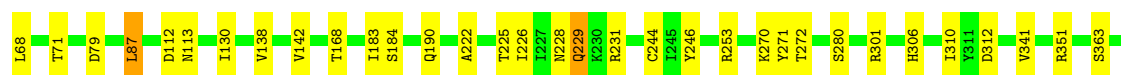
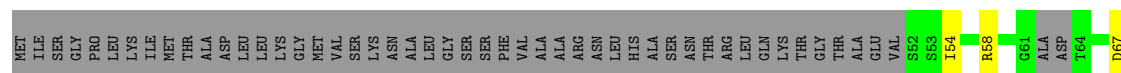
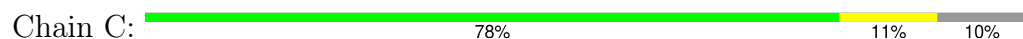


There are no outlier residues recorded for this chain.

- Molecule 18: ATP synthase subunit alpha

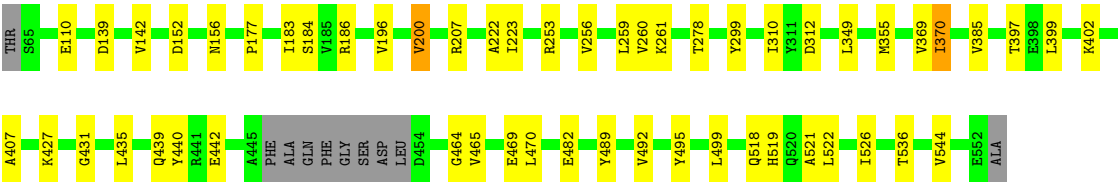


- Molecule 18: ATP synthase subunit alpha



- Molecule 18: ATP synthase subunit alpha





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38186	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)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.338	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	8	0.15	0/252	0.36	0/342
2	D	0.14	0/3600	0.28	0/4885
2	E	0.15	0/3589	0.30	0/4868
2	F	0.15	0/3589	0.30	0/4868
3	G	0.21	0/2119	0.34	0/2853
4	H	0.11	0/974	0.25	0/1326
5	I	0.09	0/378	0.22	0/507
6	J	0.16	0/370	0.30	0/490
7	K	0.49	0/522	0.68	0/704
7	L	0.50	0/518	0.63	0/700
7	M	0.39	0/522	0.52	0/704
7	N	0.39	0/519	0.54	0/701
7	O	0.39	0/519	0.53	0/701
7	P	0.38	0/522	0.54	0/704
7	Q	0.51	0/522	0.63	0/704
7	R	0.56	0/519	0.68	0/700
8	S	0.24	0/1440	0.38	0/1937
9	T	0.13	0/598	0.30	0/822
10	U	0.18	0/309	0.30	0/423
11	V	0.22	0/1741	0.36	0/2347
12	W	0.33	0/656	0.45	0/885
13	a	0.13	0/1723	0.32	0/2359
14	c	0.08	0/403	0.20	0/550
15	d	0.13	0/1185	0.28	0/1617
16	i	0.08	0/308	0.22	0/417
18	A	0.15	0/3882	0.29	0/5241
18	B	0.17	0/3683	0.34	2/4973 (0.0%)
18	C	0.14	0/3803	0.29	0/5131
All	All	0.22	0/38765	0.35	2/52459 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	518	GLN	CA-C-N	-5.54	115.85	122.44
18	B	518	GLN	C-N-CA	-5.54	115.85	122.44

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	247	0	243	8	0
2	D	3543	0	3585	20	0
2	E	3532	0	3590	21	0
2	F	3532	0	3590	19	0
3	G	2093	0	2147	23	0
4	H	961	0	957	17	0
5	I	373	0	389	7	0
6	J	365	0	350	2	0
7	K	513	0	532	6	0
7	L	509	0	521	7	0
7	M	513	0	532	5	0
7	N	510	0	525	11	0
7	O	510	0	525	10	0
7	P	513	0	532	5	0
7	Q	513	0	532	8	0
7	R	510	0	523	10	0
8	S	1423	0	1530	24	0
9	T	587	0	591	20	0
10	U	301	0	286	0	0
11	V	1710	0	1779	30	0
12	W	641	0	626	16	0
13	a	1685	0	1767	35	0
14	c	402	0	271	3	0
15	d	1160	0	1109	31	0
16	i	303	0	284	3	0
17	k	145	0	33	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	A	3832	0	3921	21	0
18	B	3635	0	3726	31	0
18	C	3756	0	3862	33	0
19	D	27	0	12	0	0
19	F	27	0	12	1	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	1	0	0	0	0
21	A	31	0	12	0	0
21	B	31	0	12	0	0
21	C	31	0	12	0	0
All	All	38469	0	38918	354	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 (354) 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)
12:W:168:ASN:HD22	12:W:171:ARG:HH12	1.35	0.73
15:d:53:ASP:N	15:d:53:ASP:OD1	2.24	0.69
11:V:162:VAL:HG13	11:V:165:ARG:HH21	1.58	0.69
15:d:126:ILE:HB	15:d:131:MET:HE2	1.75	0.68
4:H:137:ALA:HB1	4:H:157:ILE:HG22	1.74	0.68
4:H:86:VAL:HG12	4:H:96:LYS:HG2	1.78	0.65
11:V:31:GLU:HG2	12:W:150:LYS:HD2	1.79	0.64
18:A:222:ALA:HB1	18:A:310:ILE:HD13	1.79	0.64
15:d:69:ASP:OD1	15:d:69:ASP:N	2.31	0.64
9:T:26:ARG:HA	9:T:30:PHE:HB3	1.80	0.64
18:A:522:LEU:HD11	18:A:536:THR:HG23	1.80	0.63
18:C:228:ASN:OD1	18:C:231:ARG:NH1	2.32	0.63
11:V:162:VAL:HA	11:V:165:ARG:HE	1.63	0.63
8:S:78:PHE:HB2	8:S:80:PRO:HD3	1.80	0.62
15:d:133:ILE:O	15:d:137:ASN:ND2	2.31	0.62
2:D:386:GLU:HG3	18:A:280:SER:HB2	1.81	0.62
7:O:5:ALA:HB1	7:P:6:ALA:HB3	1.83	0.61
3:G:191:ARG:HH21	3:G:195:SER:HB2	1.66	0.61
13:a:155:ALA:HA	13:a:158:VAL:HG12	1.82	0.61
1:8:9:TRP:CG	13:a:99:SER:HG	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:76:ILE:HB	13:a:213:VAL:HG21	1.82	0.60
4:H:100:SER:OG	5:I:18:CYS:SG	2.58	0.60
8:S:158:ILE:HG21	8:S:174:SER:HB3	1.83	0.60
11:V:53:THR:HB	11:V:57:GLY:HA3	1.84	0.60
2:E:336:ARG:HD3	2:E:396:ILE:HG13	1.83	0.59
18:C:396:GLU:OE2	18:C:409:ASN:ND2	2.36	0.58
3:G:227:ARG:NH1	3:G:228:ASN:OD1	2.36	0.58
8:S:120:VAL:HG21	8:S:134:LEU:HD21	1.85	0.58
3:G:127:GLU:OE1	3:G:127:GLU:N	2.33	0.58
9:T:67:GLN:HA	12:W:115:GLY:H	1.68	0.58
18:B:222:ALA:HB1	18:B:310:ILE:HD13	1.86	0.58
2:E:316:GLU:O	2:E:321:ARG:NH1	2.37	0.58
3:G:217:ILE:HG12	4:H:75:PRO:HG2	1.86	0.58
2:E:483:LEU:HD23	2:E:487:GLU:HG2	1.86	0.58
4:H:117:GLU:OE1	5:I:15:SER:OG	2.22	0.58
2:F:255:THR:O	2:F:259:MET:HG2	2.04	0.57
12:W:129:SER:HB3	12:W:133:GLY:HA3	1.85	0.57
3:G:90:LYS:H	3:G:126:LYS:HE2	1.68	0.57
1:8:5:ASP:OD1	1:8:5:ASP:N	2.35	0.57
11:V:155:ASN:HD21	15:d:34:TRP:HB3	1.69	0.57
3:G:77:TYR:OH	3:G:230:GLN:OE1	2.23	0.57
2:D:213:PRO:O	18:A:253:ARG:NH1	2.38	0.57
2:D:369:SER:OG	2:D:370:ALA:N	2.36	0.57
3:G:79:LYS:HD2	4:H:107:ASN:HD22	1.69	0.57
18:B:196:VAL:HA	18:B:200:VAL:HG23	1.86	0.56
9:T:42:THR:HG22	9:T:44:ALA:H	1.70	0.56
3:G:73:SER:OG	3:G:236:ASN:ND2	2.35	0.56
8:S:76:GLU:OE1	8:S:77:LYS:N	2.38	0.56
3:G:121:LEU:HD23	3:G:128:VAL:HG11	1.87	0.56
18:B:526:ILE:HD11	18:B:536:THR:HG21	1.87	0.56
11:V:169:HIS:HA	15:d:50:PRO:HG3	1.88	0.56
2:D:181:GLU:HB2	2:D:202:THR:HG22	1.88	0.55
11:V:205:VAL:HG21	14:c:14:LYS:HG2	1.86	0.55
2:E:115:VAL:HG11	2:E:167:VAL:HG11	1.88	0.55
12:W:107:ARG:H	12:W:107:ARG:HD2	1.71	0.55
9:T:34:ALA:O	9:T:38:LEU:N	2.39	0.55
18:A:228:ASN:OD1	18:A:231:ARG:NH1	2.31	0.55
18:C:112:ASP:OD1	18:C:113:ASN:ND2	2.40	0.55
9:T:67:GLN:HG2	12:W:115:GLY:HA3	1.89	0.55
18:A:450:GLY:HA2	18:A:453:LEU:HD23	1.88	0.55
5:I:28:ALA:HA	5:I:31:LYS:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:153:ARG:NH2	15:d:94:GLU:OE2	2.40	0.54
18:B:223:ILE:HD11	18:B:259:LEU:HD11	1.88	0.54
15:d:13:TRP:HZ3	15:d:32:LYS:HG2	1.71	0.54
12:W:142:TYR:OH	12:W:156:GLY:O	2.24	0.54
2:D:292:MET:HE1	2:D:309:LEU:HD21	1.89	0.54
8:S:180:GLN:O	8:S:183:SER:OG	2.25	0.54
2:D:436:ILE:HG23	2:D:507:SER:HB3	1.89	0.54
18:C:222:ALA:HB1	18:C:310:ILE:HD13	1.90	0.54
13:a:205:ALA:O	13:a:209:ILE:HG12	2.08	0.53
18:A:220:SER:HA	18:A:223:ILE:HG22	1.89	0.53
2:D:231:VAL:HG13	2:D:506:LEU:HD22	1.89	0.53
18:B:465:VAL:O	18:B:469:GLU:HG2	2.07	0.53
2:D:124:ILE:HG22	2:D:125:LEU:HG	1.90	0.53
2:F:259:MET:HE1	2:F:288:LEU:HD13	1.91	0.53
8:S:44:GLN:HA	8:S:47:LYS:HE3	1.91	0.53
4:H:107:ASN:N	4:H:107:ASN:OD1	2.41	0.53
8:S:55:ILE:HD11	8:S:95:LEU:HB3	1.90	0.53
3:G:220:ASP:HB3	4:H:76:THR:HG23	1.91	0.53
2:F:213:PRO:O	18:C:253:ARG:NH1	2.41	0.52
4:H:141:LEU:HD21	4:H:157:ILE:HD13	1.91	0.52
15:d:55:ALA:HA	15:d:58:LYS:HD2	1.91	0.52
18:A:95:MET:O	18:A:134:THR:OG1	2.25	0.52
18:B:522:LEU:HD11	18:B:536:THR:HG23	1.91	0.52
13:a:93:THR:OG1	13:a:96:THR:OG1	2.25	0.52
18:B:253:ARG:HG2	18:B:278:THR:HG21	1.91	0.52
18:C:517:SER:OG	18:C:518:GLN:OE1	2.16	0.52
7:K:46:LEU:HD22	7:R:33:ILE:HG23	1.91	0.52
13:a:110:SER:HA	13:a:113:VAL:HG22	1.91	0.52
18:B:152:ASP:OD1	18:B:156:ASN:N	2.43	0.52
18:B:312:ASP:O	18:B:369:VAL:HB	2.10	0.52
8:S:141:PHE:HB2	11:V:233:GLN:HG2	1.90	0.52
15:d:152:TYR:CD1	15:d:154:PRO:HD3	2.44	0.52
8:S:88:LEU:HD13	18:A:58:ARG:HE	1.75	0.51
18:B:399:LEU:HB2	18:B:407:ALA:HB1	1.92	0.51
7:O:63:PHE:CE1	13:a:170:LEU:HD21	2.45	0.51
12:W:112:VAL:HG11	12:W:120:TRP:HB2	1.93	0.51
7:Q:18:VAL:HG21	7:R:64:CYS:HB2	1.93	0.51
18:B:519:HIS:C	18:B:521:ALA:H	2.19	0.51
9:T:29:THR:HA	9:T:32:HIS:CD2	2.46	0.51
18:C:301:ARG:NH1	18:C:351:ARG:O	2.44	0.51
2:D:155:MET:HE1	2:D:323:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:15:GLU:CD	8:S:15:GLU:H	2.19	0.51
2:E:544:LEU:H	2:E:544:LEU:HD12	1.75	0.50
9:T:50:ILE:HG22	9:T:54:LYS:HE3	1.93	0.50
1:8:15:SER:O	1:8:19:THR:HG22	2.11	0.50
2:D:288:LEU:HG	2:D:292:MET:HE2	1.94	0.50
7:N:33:ILE:HD13	7:O:49:TYR:HD2	1.75	0.50
9:T:22:TYR:O	9:T:26:ARG:N	2.43	0.50
7:K:37:ALA:O	7:L:39:ASN:ND2	2.45	0.50
11:V:168:LEU:HD13	15:d:49:PRO:HB3	1.94	0.50
11:V:151:VAL:HG22	15:d:11:ILE:HD13	1.94	0.50
16:i:17:TYR:HB3	16:i:21:TYR:HE1	1.77	0.50
9:T:42:THR:O	9:T:45:GLU:HG3	2.12	0.50
4:H:80:LEU:HD22	4:H:99:VAL:HG11	1.93	0.50
1:8:9:TRP:CD1	13:a:99:SER:HG	2.29	0.49
18:B:183:ILE:HG12	18:B:186:ARG:HH21	1.77	0.49
7:K:54:PHE:CE1	7:L:56:LEU:HD21	2.47	0.49
18:C:500:GLU:HG3	18:C:502:SER:H	1.77	0.49
2:E:450:MET:HE3	2:E:460:TYR:HD1	1.77	0.49
15:d:153:TRP:N	15:d:154:PRO:HD3	2.27	0.49
9:T:49:ALA:O	9:T:53:LEU:HG	2.11	0.49
11:V:149:PHE:O	11:V:153:ARG:HG3	2.12	0.49
11:V:225:LEU:HD23	11:V:228:LEU:HD12	1.95	0.49
2:E:390:THR:HG23	2:E:395:SER:HB3	1.95	0.49
13:a:86:GLY:HA3	13:a:93:THR:HG22	1.94	0.49
7:N:29:PHE:HE2	7:O:56:LEU:HD23	1.77	0.48
18:C:54:ILE:O	18:C:58:ARG:HG2	2.12	0.48
18:C:225:THR:O	18:C:229:GLN:NE2	2.46	0.48
5:I:23:ARG:HA	5:I:26:LEU:HD13	1.95	0.48
7:M:60:MET:SD	7:M:60:MET:N	2.86	0.48
8:S:173:MET:SD	11:V:225:LEU:HD22	2.53	0.48
12:W:110:LEU:H	12:W:110:LEU:HD23	1.78	0.48
2:F:104:ARG:NH2	2:F:116:GLN:OE1	2.47	0.48
13:a:111:ALA:HA	13:a:114:PHE:CE1	2.48	0.48
15:d:152:TYR:HB2	15:d:154:PRO:HG3	1.96	0.48
2:F:366:ARG:NH2	18:C:79:ASP:OD2	2.46	0.48
3:G:197:LYS:NZ	3:G:198:THR:O	2.46	0.48
18:C:484:GLN:HA	18:C:487:VAL:HG12	1.96	0.48
4:H:153:ILE:O	4:H:157:ILE:HG23	2.14	0.48
4:H:154:GLN:HA	4:H:157:ILE:HG12	1.96	0.47
11:V:208:SER:O	11:V:213:GLN:NE2	2.46	0.47
13:a:11:ALA:O	13:a:13:THR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:256:VAL:O	18:A:260:VAL:HG13	2.13	0.47
13:a:168:HIS:HA	13:a:171:ILE:HD12	1.95	0.47
18:B:499:LEU:HD12	18:B:499:LEU:H	1.79	0.47
2:D:349:ASN:HD21	2:D:403:TYR:HB2	1.80	0.47
2:E:450:MET:HE3	2:E:460:TYR:CD1	2.49	0.47
4:H:63:GLN:OE1	4:H:81:ARG:NH2	2.48	0.47
7:Q:65:LEU:HG	7:R:63:PHE:HE1	1.80	0.47
7:N:29:PHE:CE2	7:O:56:LEU:HD23	2.50	0.47
8:S:64:ILE:O	8:S:67:LYS:HG3	2.15	0.47
2:E:482:ILE:HG22	2:E:483:LEU:HD12	1.97	0.47
13:a:129:LEU:HD12	13:a:130:PRO:HD2	1.96	0.47
15:d:152:TYR:HD1	15:d:154:PRO:HD3	1.80	0.47
18:C:370:ILE:HG13	18:C:385:VAL:HG11	1.97	0.47
2:D:486:ASP:OD1	2:D:486:ASP:N	2.48	0.47
2:F:137:LEU:HD13	2:F:156:ASP:HB3	1.96	0.47
13:a:140:MET:HE3	13:a:140:MET:HB3	1.75	0.47
14:c:19:ARG:O	14:c:23:GLN:HG2	2.15	0.47
2:D:260:GLU:OE2	2:D:264:ASN:ND2	2.48	0.46
2:D:249:GLY:O	2:D:254:LYS:NZ	2.48	0.46
7:O:40:PRO:HB3	7:P:42:LEU:HD11	1.96	0.46
7:N:33:ILE:HD11	7:O:46:LEU:HA	1.98	0.46
18:C:244:CYS:HB2	18:C:272:THR:HG22	1.98	0.46
18:B:370:ILE:HD11	18:B:385:VAL:HG21	1.97	0.46
3:G:55:LYS:HG3	18:A:452:ASP:OD2	2.15	0.46
15:d:13:TRP:HA	15:d:16:PHE:HB3	1.96	0.46
18:C:246:TYR:OH	18:C:312:ASP:OD2	2.22	0.46
8:S:38:GLU:CD	8:S:80:PRO:HG3	2.40	0.46
7:M:33:ILE:HD13	7:N:32:LEU:HA	1.98	0.46
12:W:105:LYS:HD2	12:W:105:LYS:HA	1.77	0.46
7:K:56:LEU:HD11	7:R:54:PHE:HE1	1.80	0.46
15:d:13:TRP:CZ3	15:d:32:LYS:HG2	2.50	0.46
18:A:520:GLN:HE21	18:A:520:GLN:HB2	1.63	0.46
1:8:16:MET:SD	13:a:100:MET:HB2	2.55	0.46
2:F:514:GLU:OE2	2:F:521:GLY:N	2.41	0.46
12:W:105:LYS:HD2	12:W:123:MET:HE3	1.98	0.45
2:E:220:VAL:HB	18:B:261:LYS:HD2	1.98	0.45
7:N:45:GLN:HG3	7:N:49:TYR:CE2	2.51	0.45
1:8:25:GLN:HB3	13:a:70:LEU:HD21	1.98	0.45
13:a:75:LEU:O	13:a:79:ILE:HG13	2.16	0.45
8:S:33:GLU:CD	8:S:33:GLU:H	2.24	0.45
13:a:66:GLN:O	15:d:152:TYR:OH	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:243:LYS:HE2	2:F:388:ILE:O	2.17	0.45
2:F:386:GLU:HG3	18:C:280:SER:HB2	1.99	0.45
7:P:54:PHE:CE1	7:Q:56:LEU:HD11	2.51	0.45
8:S:52:ALA:HA	8:S:55:ILE:HG22	1.99	0.45
8:S:165:ARG:HH12	18:C:71:THR:HG21	1.81	0.45
8:S:141:PHE:CD1	11:V:233:GLN:HG2	2.51	0.45
4:H:104:VAL:HG22	4:H:114:LEU:HD13	1.99	0.45
7:N:21:SER:OG	7:N:61:GLY:HA3	2.17	0.45
7:Q:8:PHE:HD1	7:R:71:ILE:HD11	1.82	0.45
18:A:370:ILE:HD11	18:A:385:VAL:HG21	1.98	0.45
18:B:495:TYR:HD2	18:B:544:VAL:HG11	1.82	0.45
18:A:144:GLU:OE2	18:A:305:LYS:NZ	2.49	0.45
3:G:234:LEU:O	3:G:237:ILE:HG22	2.17	0.44
7:R:38:ARG:O	7:R:39:ASN:C	2.60	0.44
12:W:128:PRO:HB2	12:W:131:ILE:H	1.82	0.44
18:A:56:GLU:HG2	18:A:60:LEU:HD23	1.99	0.44
11:V:159:ALA:HB2	15:d:38:LEU:HD13	1.98	0.44
18:B:183:ILE:HG12	18:B:184:SER:H	1.82	0.44
2:D:407:ASP:OD1	2:D:407:ASP:N	2.50	0.44
18:A:314:LEU:HD23	18:A:314:LEU:HA	1.85	0.44
18:C:270:LYS:HG3	18:C:271:TYR:HD1	1.82	0.44
2:F:163:ARG:NH1	18:B:110:GLU:O	2.50	0.44
15:d:31:LEU:O	15:d:35:ASN:ND2	2.50	0.44
18:B:470:LEU:HD23	18:B:470:LEU:HA	1.86	0.44
8:S:127:ASP:OD1	8:S:128:GLU:N	2.50	0.44
11:V:86:SER:OG	13:a:198:LEU:HD22	2.17	0.44
18:A:183:ILE:HG12	18:A:184:SER:H	1.83	0.44
18:B:439:GLN:O	18:B:442:GLU:HG2	2.17	0.44
18:B:177:PRO:HG3	18:B:355:MET:HE1	2.00	0.44
18:B:256:VAL:O	18:B:260:VAL:HG13	2.18	0.44
7:N:25:ILE:HA	7:N:28:VAL:HG12	1.98	0.44
9:T:37:GLU:HG3	9:T:38:LEU:HG	2.00	0.44
13:a:117:PHE:O	13:a:121:THR:OG1	2.27	0.44
18:C:87:LEU:H	18:C:87:LEU:HG	1.67	0.44
7:L:68:ALA:O	7:L:71:ILE:HG22	2.17	0.44
12:W:130:GLY:O	12:W:132:ALA:N	2.44	0.44
18:A:301:ARG:NH1	18:A:351:ARG:O	2.51	0.44
3:G:231:GLU:OE2	5:I:12:ILE:HB	2.18	0.43
8:S:32:LEU:O	8:S:35:VAL:HG12	2.18	0.43
11:V:186:GLN:O	11:V:190:ARG:HG3	2.18	0.43
18:C:71:THR:HG23	18:C:130:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:C:443:VAL:HG11	18:C:460:LEU:HD23	2.00	0.43
18:C:466:ARG:NH2	18:C:499:LEU:O	2.50	0.43
3:G:77:TYR:HD2	3:G:204:PHE:HD2	1.65	0.43
7:N:33:ILE:CG1	7:O:46:LEU:HD12	2.48	0.43
15:d:28:ALA:O	15:d:32:LYS:HG3	2.17	0.43
15:d:30:SER:O	15:d:34:TRP:HD1	2.01	0.43
15:d:146:ASP:OD1	15:d:146:ASP:N	2.51	0.43
18:C:458:GLN:O	18:C:462:SER:OG	2.31	0.43
18:B:142:VAL:HG11	18:B:299:TYR:HB2	2.00	0.43
2:D:336:ARG:HD3	2:D:396:ILE:HG13	1.99	0.43
9:T:19:ALA:O	9:T:23:SER:OG	2.28	0.43
9:T:21:THR:O	9:T:25:PRO:HG2	2.17	0.43
9:T:71:LYS:HG3	11:V:48:PHE:HE1	1.83	0.43
11:V:227:LEU:HD23	11:V:230:LYS:HD2	2.00	0.43
13:a:198:LEU:HA	13:a:201:ILE:HG12	2.00	0.43
2:F:231:VAL:HG12	2:F:506:LEU:HD22	1.99	0.43
3:G:29:LYS:O	3:G:33:ARG:HG3	2.19	0.43
13:a:93:THR:HG1	13:a:96:THR:HG1	1.62	0.43
16:i:21:TYR:CZ	16:i:22:THR:HG23	2.54	0.43
9:T:37:GLU:OE2	11:V:56:THR:OG1	2.28	0.43
18:B:399:LEU:HA	18:B:402:LYS:HG2	2.01	0.43
18:B:427:LYS:HE3	18:B:427:LYS:HB2	1.87	0.43
7:L:25:ILE:HG13	7:L:54:PHE:HD1	1.84	0.43
8:S:141:PHE:HD1	11:V:233:GLN:HG2	1.83	0.43
2:D:122:PRO:HA	2:D:123:PRO:HD3	1.94	0.43
2:E:564:LYS:HD3	2:E:564:LYS:HA	1.64	0.43
7:K:6:ALA:HB1	7:R:8:PHE:HB2	2.00	0.43
9:T:50:ILE:O	9:T:54:LYS:HG3	2.18	0.43
2:E:302:ASP:N	2:E:302:ASP:OD1	2.50	0.43
13:a:185:ASN:HB3	13:a:187:MET:HE2	2.01	0.43
13:a:198:LEU:O	13:a:201:ILE:HG12	2.19	0.43
4:H:152:GLU:O	4:H:156:ARG:HG3	2.19	0.42
11:V:149:PHE:HB2	11:V:153:ARG:HH21	1.84	0.42
1:8:16:MET:SD	13:a:104:MET:HG3	2.58	0.42
11:V:212:GLN:HA	11:V:215:LYS:HD2	2.01	0.42
2:F:253:GLY:HA2	19:F:601:ADP:O1A	2.19	0.42
3:G:147:ASP:OD1	3:G:147:ASP:N	2.42	0.42
15:d:37:THR:HB	15:d:41:ARG:CZ	2.50	0.42
7:O:54:PHE:CE1	7:P:56:LEU:HD21	2.54	0.42
8:S:165:ARG:HG2	8:S:170:TYR:HD1	1.83	0.42
9:T:34:ALA:HB1	9:T:38:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:d:57:TYR:O	15:d:61:VAL:N	2.45	0.42
18:C:183:ILE:HG12	18:C:184:SER:H	1.84	0.42
18:C:222:ALA:O	18:C:226:ILE:HG12	2.19	0.42
11:V:210:SER:HB3	11:V:213:GLN:HG3	2.02	0.42
2:F:243:LYS:HD2	2:F:420:HIS:O	2.20	0.42
2:F:527:LYS:HE3	2:F:527:LYS:HB3	1.86	0.42
7:N:30:GLY:O	7:N:33:ILE:HG22	2.19	0.42
7:R:50:ALA:O	7:R:51:ILE:C	2.63	0.42
13:a:170:LEU:HD23	13:a:170:LEU:HA	1.80	0.42
2:E:480:ILE:HD11	2:E:485:MET:HG3	2.00	0.42
9:T:16:VAL:O	9:T:20:VAL:HG23	2.19	0.42
18:A:223:ILE:HD12	18:A:223:ILE:HA	1.87	0.42
2:E:411:ASP:HB3	2:E:414:PRO:HD2	2.02	0.42
4:H:155:ILE:HD11	5:I:4:TRP:HB3	2.00	0.42
12:W:105:LYS:HG3	12:W:106:ASP:H	1.84	0.42
18:C:67:ASP:OD1	18:C:68:LEU:N	2.51	0.42
18:C:306:HIS:HD2	18:C:363:SER:HB3	1.84	0.42
3:G:91:HIS:H	3:G:128:VAL:HG12	1.84	0.42
7:K:33:ILE:HG13	7:L:46:LEU:HG	2.02	0.42
11:V:221:CYS:O	11:V:225:LEU:HG	2.20	0.42
13:a:198:LEU:HG	13:a:201:ILE:HD11	2.02	0.42
15:d:124:ASN:OD1	15:d:124:ASN:N	2.50	0.42
2:F:527:LYS:H	2:F:527:LYS:HG2	1.60	0.41
11:V:31:GLU:HA	12:W:150:LYS:HB2	2.02	0.41
18:A:480:ALA:O	18:A:484:GLN:HG3	2.20	0.41
2:E:537:LEU:HD23	2:E:537:LEU:HA	1.85	0.41
7:P:25:ILE:HG21	7:Q:56:LEU:HD22	2.02	0.41
9:T:51:GLN:O	9:T:55:LYS:HG3	2.20	0.41
18:B:489:TYR:HA	18:B:492:VAL:HG22	2.01	0.41
2:E:176:ILE:HD13	2:E:327:THR:HG23	2.02	0.41
2:E:275:PHE:HB3	2:E:309:LEU:HD23	2.02	0.41
3:G:167:SER:HB3	5:I:16:GLN:HE21	1.84	0.41
7:Q:65:LEU:HD13	7:Q:65:LEU:HA	1.85	0.41
8:S:22:LEU:HD22	8:S:85:LEU:HD22	2.01	0.41
18:C:462:SER:O	18:C:466:ARG:HD3	2.20	0.41
3:G:96:VAL:HA	3:G:133:VAL:HG13	2.02	0.41
4:H:149:SER:O	4:H:153:ILE:HG12	2.19	0.41
7:Q:3:ASP:OD1	7:Q:3:ASP:N	2.44	0.41
18:C:424:ARG:HG2	18:C:531:LYS:HE2	2.03	0.41
18:B:431:GLY:O	18:B:435:LEU:HG	2.19	0.41
18:B:440:TYR:CG	18:B:464:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:THR:HG23	2:E:161:LEU:HD12	2.01	0.41
7:L:29:PHE:CZ	7:M:56:LEU:HD12	2.56	0.41
7:R:45:GLN:HA	7:R:45:GLN:NE2	2.36	0.41
18:C:537:ASP:O	18:C:541:LYS:HG3	2.21	0.41
13:a:96:THR:HG23	13:a:165:THR:HG22	2.03	0.41
15:d:126:ILE:HG23	15:d:127:PRO:HD2	2.03	0.41
3:G:97:SER:HB3	3:G:107:HIS:CD2	2.56	0.41
9:T:71:LYS:HG3	11:V:48:PHE:CE1	2.55	0.41
1:8:15:SER:HB2	13:a:21:THR:HG22	2.03	0.41
2:D:336:ARG:NH1	2:D:389:THR:O	2.53	0.41
2:D:453:ASN:OD1	2:D:453:ASN:N	2.53	0.41
2:F:155:MET:HE1	2:F:323:ARG:HG3	2.03	0.41
7:O:43:LYS:HE3	7:O:43:LYS:HB2	1.79	0.41
8:S:76:GLU:O	8:S:77:LYS:HB2	2.20	0.41
13:a:141:LEU:H	13:a:141:LEU:HG	1.69	0.41
13:a:208:LEU:HD13	13:a:208:LEU:HA	1.93	0.41
15:d:58:LYS:HA	15:d:61:VAL:HB	2.03	0.41
15:d:134:GLU:HA	15:d:137:ASN:HD22	1.85	0.41
18:C:467:LEU:HD23	18:C:467:LEU:HA	1.83	0.41
18:B:207:ARG:NH1	18:B:349:LEU:O	2.54	0.41
2:F:189:VAL:HG22	2:F:324:VAL:HG22	2.03	0.41
7:L:29:PHE:HZ	7:M:56:LEU:HD12	1.86	0.41
7:M:33:ILE:CD1	7:N:32:LEU:HA	2.51	0.41
7:Q:55:ALA:O	7:Q:58:GLU:HG3	2.21	0.41
8:S:81:LEU:H	8:S:81:LEU:HG	1.64	0.41
13:a:114:PHE:HE1	16:i:24:THR:HB	1.86	0.41
2:E:141:VAL:HA	2:E:152:THR:HG22	2.02	0.40
7:R:21:SER:O	7:R:25:ILE:HG12	2.21	0.40
13:a:13:THR:HB	13:a:19:ILE:HG13	2.03	0.40
2:E:527:LYS:HE3	2:E:527:LYS:HB3	1.84	0.40
6:J:64:ARG:HH21	18:C:456:ALA:HB2	1.87	0.40
11:V:167:ARG:NH1	15:d:80:PRO:HG2	2.36	0.40
12:W:125:ASP:OD1	12:W:125:ASP:N	2.53	0.40
15:d:148:LYS:HA	15:d:153:TRP:CZ3	2.57	0.40
18:B:139:ASP:OD1	18:B:139:ASP:N	2.54	0.40
18:B:440:TYR:CD1	18:B:464:GLY:HA3	2.57	0.40
2:E:469:ILE:HA	2:E:472:ASP:OD2	2.22	0.40
6:J:64:ARG:NH1	18:C:455:ALA:HB1	2.36	0.40
13:a:169:LEU:HD13	13:a:169:LEU:HA	1.89	0.40
18:A:95:MET:HE3	18:A:103:LYS:HD3	2.04	0.40
2:F:169:ASP:OD1	2:F:170:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:48:MET:SD	3:G:257:MET:HE3	2.62	0.40
2:D:527:LYS:HE3	2:D:527:LYS:HB3	1.94	0.40
2:F:483:LEU:HB3	2:F:487:GLU:HG3	2.03	0.40
3:G:271:LEU:HD23	3:G:271:LEU:HA	1.81	0.40
13:a:138:ILE:H	13:a:138:ILE:HG12	1.70	0.40
14:c:10:LEU:O	14:c:14:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	29/67 (43%)	29 (100%)	0	0	100	100
2	D	468/570 (82%)	450 (96%)	18 (4%)	0	100	100
2	E	465/570 (82%)	451 (97%)	14 (3%)	0	100	100
2	F	465/570 (82%)	453 (97%)	12 (3%)	0	100	100
3	G	270/273 (99%)	266 (98%)	4 (2%)	0	100	100
4	H	128/168 (76%)	126 (98%)	2 (2%)	0	100	100
5	I	46/136 (34%)	43 (94%)	3 (6%)	0	100	100
6	J	46/108 (43%)	46 (100%)	0	0	100	100
7	K	70/141 (50%)	68 (97%)	2 (3%)	0	100	100
7	L	70/141 (50%)	70 (100%)	0	0	100	100
7	M	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
7	N	70/141 (50%)	68 (97%)	2 (3%)	0	100	100
7	O	70/141 (50%)	70 (100%)	0	0	100	100
7	P	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
7	Q	70/141 (50%)	67 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	R	70/141 (50%)	67 (96%)	3 (4%)	0	100	100
8	S	185/213 (87%)	174 (94%)	10 (5%)	1 (0%)	25	61
9	T	79/103 (77%)	77 (98%)	2 (2%)	0	100	100
10	U	41/71 (58%)	41 (100%)	0	0	100	100
11	V	210/238 (88%)	207 (99%)	3 (1%)	0	100	100
12	W	79/88 (90%)	76 (96%)	3 (4%)	0	100	100
13	a	219/226 (97%)	207 (94%)	12 (6%)	0	100	100
14	c	67/76 (88%)	66 (98%)	1 (2%)	0	100	100
15	d	151/166 (91%)	140 (93%)	11 (7%)	0	100	100
16	i	40/58 (69%)	38 (95%)	2 (5%)	0	100	100
18	A	503/550 (92%)	495 (98%)	8 (2%)	0	100	100
18	B	476/550 (86%)	467 (98%)	9 (2%)	0	100	100
18	C	489/550 (89%)	475 (97%)	14 (3%)	0	100	100
All	All	5016/6479 (77%)	4875 (97%)	140 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	S	77	LYS

### 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	8	28/66 (42%)	26 (93%)	2 (7%)	12	40
2	D	374/452 (83%)	362 (97%)	12 (3%)	34	67
2	E	375/452 (83%)	360 (96%)	15 (4%)	27	61
2	F	375/452 (83%)	371 (99%)	4 (1%)	70	87
3	G	225/231 (97%)	221 (98%)	4 (2%)	54	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	104/127 (82%)	98 (94%)	6 (6%)	17	48
5	I	37/109 (34%)	36 (97%)	1 (3%)	40	71
6	J	31/85 (36%)	31 (100%)	0	100	100
7	K	49/103 (48%)	44 (90%)	5 (10%)	6	24
7	L	48/103 (47%)	47 (98%)	1 (2%)	48	77
7	M	49/103 (48%)	47 (96%)	2 (4%)	26	60
7	N	48/103 (47%)	44 (92%)	4 (8%)	9	34
7	O	48/103 (47%)	41 (85%)	7 (15%)	2	12
7	P	49/103 (48%)	45 (92%)	4 (8%)	9	34
7	Q	49/103 (48%)	46 (94%)	3 (6%)	15	46
7	R	48/103 (47%)	44 (92%)	4 (8%)	9	34
8	S	161/186 (87%)	148 (92%)	13 (8%)	9	34
9	T	60/85 (71%)	60 (100%)	0	100	100
10	U	25/60 (42%)	25 (100%)	0	100	100
11	V	185/207 (89%)	183 (99%)	2 (1%)	70	87
12	W	63/76 (83%)	61 (97%)	2 (3%)	34	67
13	a	185/199 (93%)	170 (92%)	15 (8%)	9	34
14	c	18/69 (26%)	18 (100%)	0	100	100
15	d	115/144 (80%)	107 (93%)	8 (7%)	12	41
16	i	28/47 (60%)	28 (100%)	0	100	100
18	A	402/443 (91%)	390 (97%)	12 (3%)	36	69
18	B	382/443 (86%)	378 (99%)	4 (1%)	73	88
18	C	396/443 (89%)	383 (97%)	13 (3%)	33	67
All	All	3957/5200 (76%)	3814 (96%)	143 (4%)	32	64

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	8	5	ASP
1	8	28	ILE
2	D	102	THR
2	D	139	LEU
2	D	159	GLU
2	D	168	LEU

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Mol	Chain	Res	Type
2	D	231	VAL
2	D	343	VAL
2	D	349	ASN
2	D	369	SER
2	D	390	THR
2	D	407	ASP
2	D	520	LEU
2	D	559	VAL
2	E	135	THR
2	E	167	VAL
2	E	178	VAL
2	E	181	GLU
2	E	189	VAL
2	E	204	GLN
2	E	224	ILE
2	E	226	VAL
2	E	231	VAL
2	E	304	THR
2	E	307	VAL
2	E	343	VAL
2	E	344	LEU
2	E	349	ASN
2	E	524	VAL
2	F	168	LEU
2	F	258	ILE
2	F	371	VAL
2	F	469	ILE
3	G	64	LYS
3	G	131	VAL
3	G	133	VAL
3	G	194	ILE
4	H	62	THR
4	H	87	VAL
4	H	101	SER
4	H	106	VAL
4	H	107	ASN
4	H	112	VAL
5	I	44	ILE
7	K	2	ILE
7	K	25	ILE
7	K	33	ILE
7	K	47	PHE

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Mol	Chain	Res	Type
7	K	56	LEU
7	L	70	LEU
7	M	9	ILE
7	M	33	ILE
7	N	2	ILE
7	N	46	LEU
7	N	62	LEU
7	N	71	ILE
7	O	9	ILE
7	O	32	LEU
7	O	36	TYR
7	O	43	LYS
7	O	46	LEU
7	O	56	LEU
7	O	69	PHE
7	P	18	VAL
7	P	25	ILE
7	P	54	PHE
7	P	65	LEU
7	Q	16	VAL
7	Q	42	LEU
7	Q	65	LEU
7	R	4	THR
7	R	56	LEU
7	R	66	MET
7	R	72	LEU
8	S	4	LEU
8	S	11	ILE
8	S	15	GLU
8	S	33	GLU
8	S	62	ARG
8	S	67	LYS
8	S	76	GLU
8	S	81	LEU
8	S	138	LEU
8	S	142	LEU
8	S	144	LYS
8	S	169	LYS
8	S	171	VAL
11	V	78	THR
11	V	168	LEU
12	W	151	LYS

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Mol	Chain	Res	Type
12	W	178	HIS
13	a	17	LEU
13	a	33	THR
13	a	66	GLN
13	a	68	TRP
13	a	102	LEU
13	a	122	LYS
13	a	141	LEU
13	a	145	GLU
13	a	149	LEU
13	a	160	LEU
13	a	169	LEU
13	a	173	LEU
13	a	193	PHE
13	a	198	LEU
13	a	216	LEU
15	d	52	ILE
15	d	53	ASP
15	d	69	ASP
15	d	124	ASN
15	d	125	ILE
15	d	143	THR
15	d	146	ASP
15	d	152	TYR
18	A	114	VAL
18	A	142	VAL
18	A	200	VAL
18	A	224	ASP
18	A	312	ASP
18	A	370	ILE
18	A	397	THR
18	A	423	THR
18	A	437	LEU
18	A	449	PHE
18	A	453	LEU
18	A	505	THR
18	C	87	LEU
18	C	138	VAL
18	C	142	VAL
18	C	168	THR
18	C	190	GLN
18	C	229	GLN

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Mol	Chain	Res	Type
18	C	341	VAL
18	C	377	VAL
18	C	417	VAL
18	C	453	LEU
18	C	461	LEU
18	C	469	GLU
18	C	542	GLU
18	B	200	VAL
18	B	370	ILE
18	B	397	THR
18	B	482	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	116	GLN
2	D	126	ASN
2	D	131	GLN
2	D	269	HIS
2	D	338	GLN
2	D	349	ASN
2	E	131	GLN
2	E	204	GLN
2	E	313	GLN
2	E	349	ASN
2	E	453	ASN
2	F	263	ASN
2	F	269	HIS
2	F	286	ASN
2	F	341	GLN
2	F	385	GLN
2	F	459	HIS
3	G	107	HIS
3	G	145	HIS
3	G	236	ASN
3	G	250	GLN
3	G	259	ASN
4	H	73	HIS
5	I	6	GLN
5	I	16	GLN
5	I	41	ASN
6	J	66	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	K	39	ASN
7	L	44	GLN
7	L	45	GLN
7	N	45	GLN
7	P	39	ASN
7	P	44	GLN
7	Q	45	GLN
7	R	39	ASN
8	S	10	GLN
8	S	29	GLN
8	S	84	ASN
8	S	180	GLN
10	U	6	GLN
11	V	146	HIS
11	V	155	ASN
11	V	187	ASN
11	V	204	HIS
12	W	168	ASN
13	a	4	ASN
13	a	61	HIS
13	a	152	GLN
13	a	168	HIS
18	A	306	HIS
18	A	484	GLN
18	A	520	GLN
18	C	190	GLN
18	C	229	GLN
18	C	233	ASN
18	C	251	GLN
18	C	306	HIS
18	C	373	GLN
18	C	384	ASN
18	C	484	GLN
18	C	520	GLN
18	B	303	ASN
18	B	323	GLN
18	B	514	HIS

### 5.3.3 RNA ⓘ

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 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$
19	ADP	F	601	20	24,29,29	0.88	0	29,45,45	1.22	3 (10%)
21	ATP	A	601	20	28,33,33	0.71	0	34,52,52	0.61	1 (2%)
21	ATP	B	601	20	28,33,33	0.98	1 (3%)	34,52,52	0.63	1 (2%)
21	ATP	C	601	20	28,33,33	0.69	0	34,52,52	0.61	1 (2%)
19	ADP	D	601	20	24,29,29	0.86	0	29,45,45	1.17	3 (10%)

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
19	ADP	F	601	20	-	1/12/32/32	0/3/3/3
21	ATP	A	601	20	-	6/18/38/38	0/3/3/3
21	ATP	B	601	20	-	3/18/38/38	0/3/3/3
21	ATP	C	601	20	-	2/18/38/38	0/3/3/3
19	ADP	D	601	20	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	601	ATP	PA-O3A	-3.40	1.55	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	601	ADP	N3-C2-N1	-3.53	123.88	128.67
19	D	601	ADP	N3-C2-N1	-3.48	123.95	128.67
19	F	601	ADP	C4-C5-N7	-2.53	106.66	109.34
19	D	601	ADP	C4-C5-N7	-2.40	106.80	109.34
21	B	601	ATP	C5-C6-N6	2.40	123.97	120.31
21	C	601	ATP	C5-C6-N6	2.31	123.83	120.31
21	A	601	ATP	C5-C6-N6	2.30	123.82	120.31
19	D	601	ADP	O4'-C1'-N9	2.12	111.56	108.75
19	F	601	ADP	C4'-O4'-C1'	2.03	111.79	109.92

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	601	ATP	PB-O3B-PG-O2G
21	C	601	ATP	C5'-O5'-PA-O1A
19	D	601	ADP	O4'-C4'-C5'-O5'
21	A	601	ATP	PA-O3A-PB-O1B
21	A	601	ATP	PB-O3B-PG-O1G
19	F	601	ADP	C5'-O5'-PA-O1A
21	A	601	ATP	C5'-O5'-PA-O1A
21	B	601	ATP	C5'-O5'-PA-O1A
21	B	601	ATP	C5'-O5'-PA-O2A
21	B	601	ATP	C5'-O5'-PA-O3A
21	C	601	ATP	PA-O3A-PB-O2B
21	A	601	ATP	PA-O3A-PB-O2B
21	A	601	ATP	PG-O3B-PB-O1B

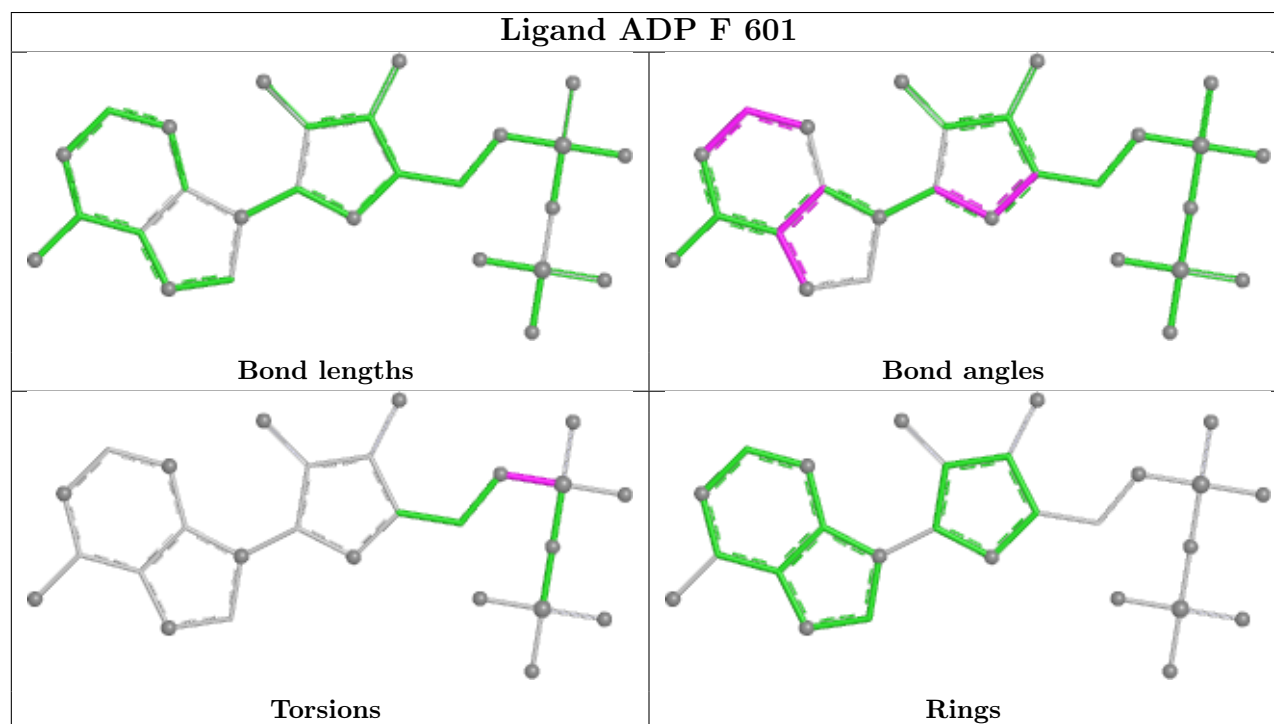
There are no ring outliers.

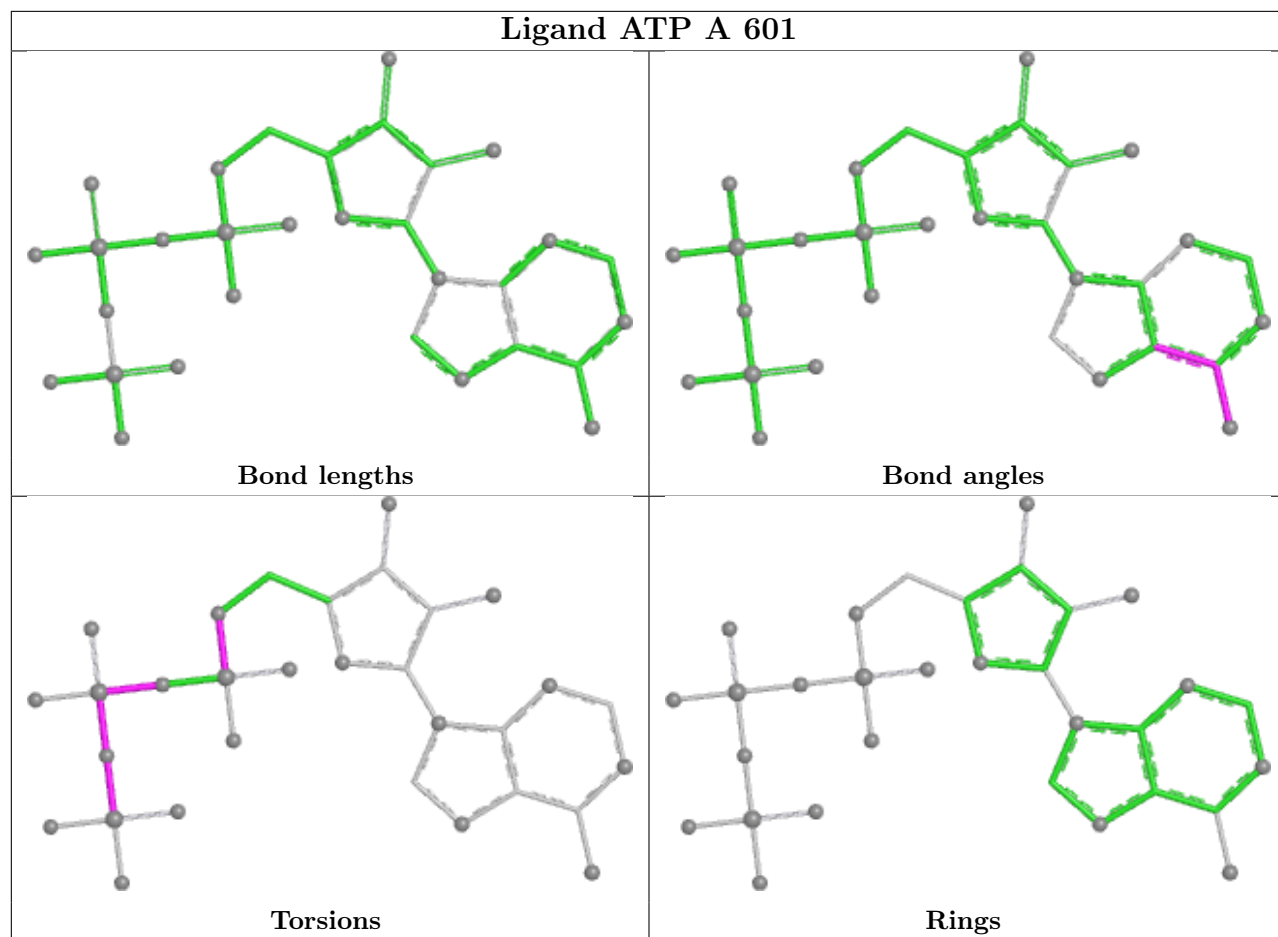
1 monomer is involved in 1 short contact:

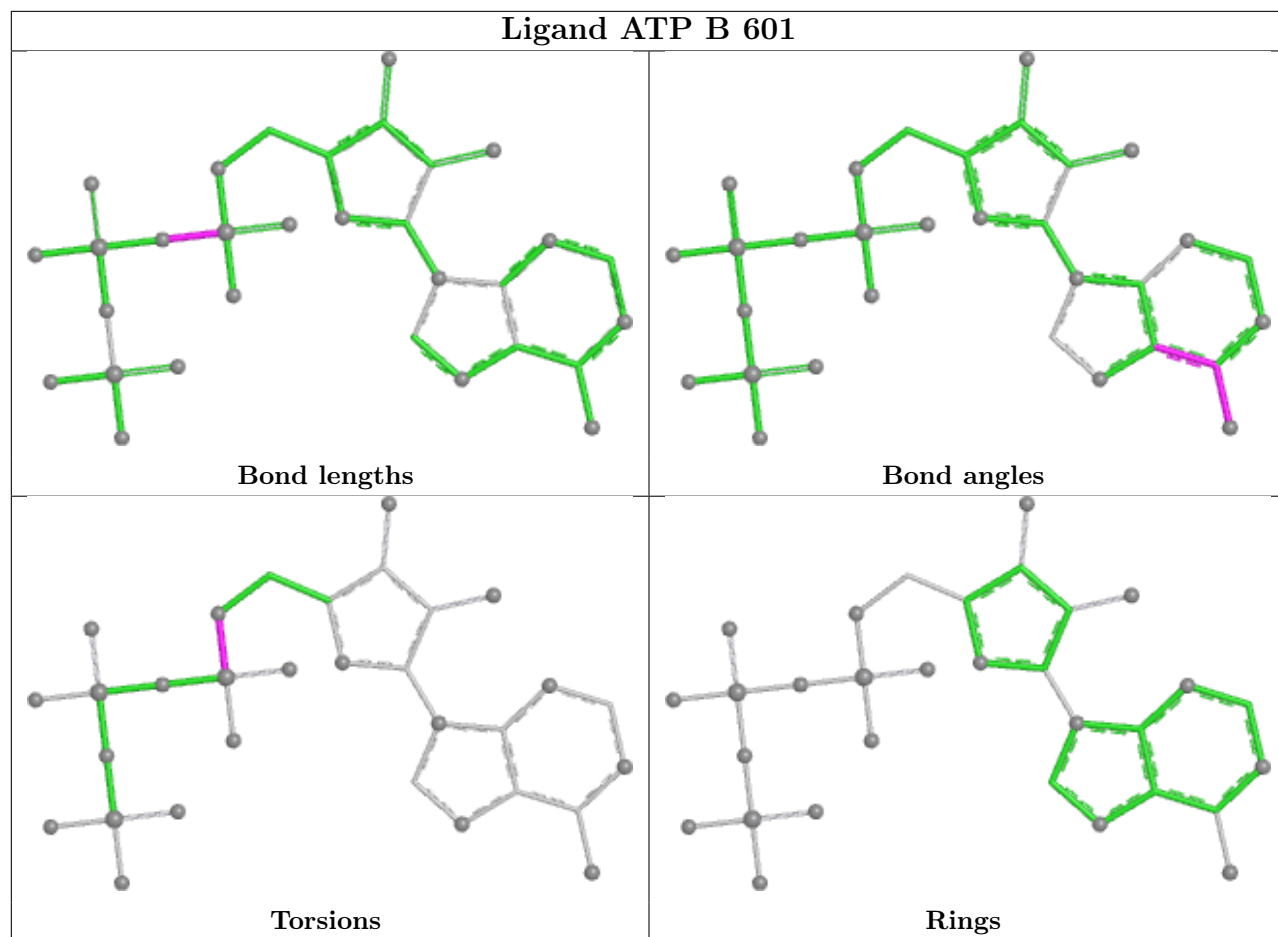
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F	601	ADP	1	0

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.

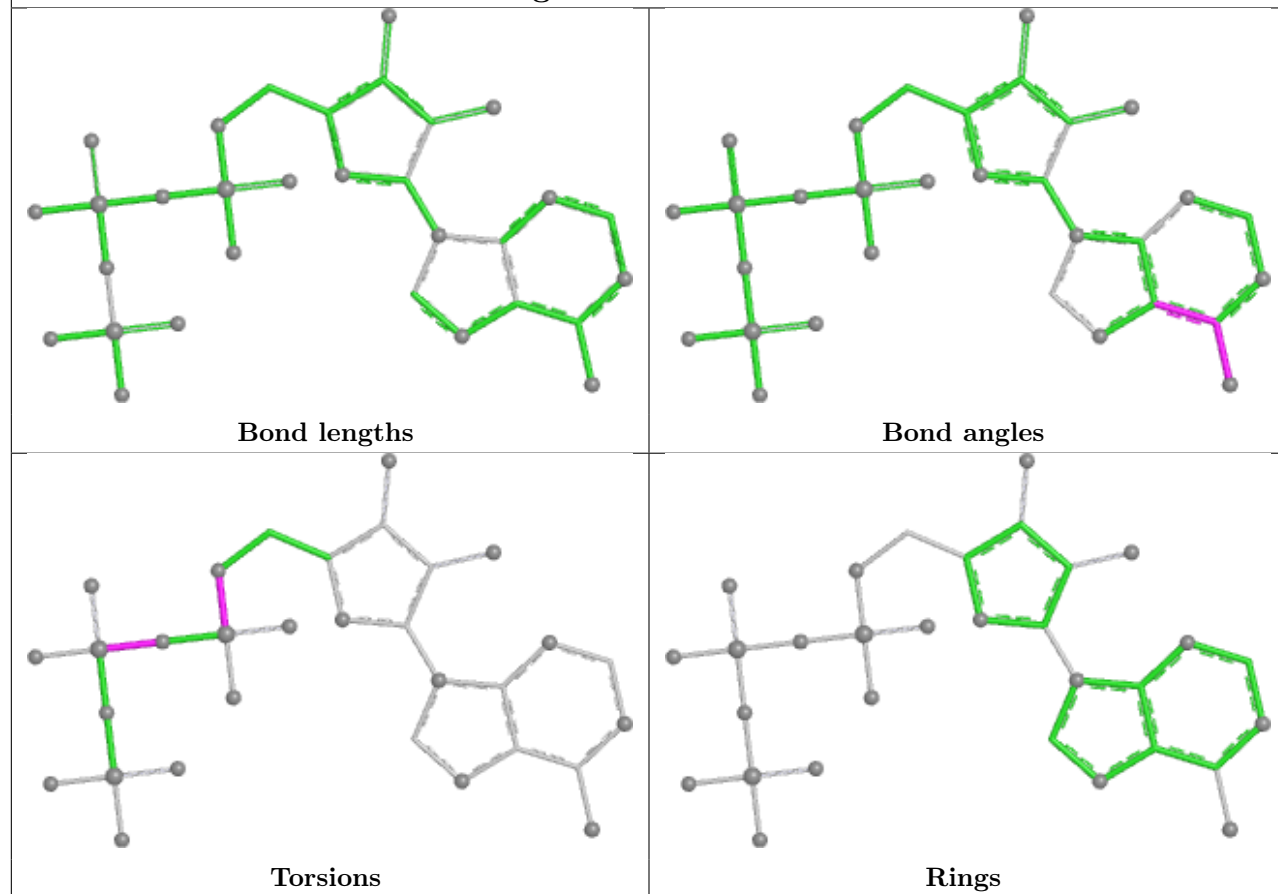




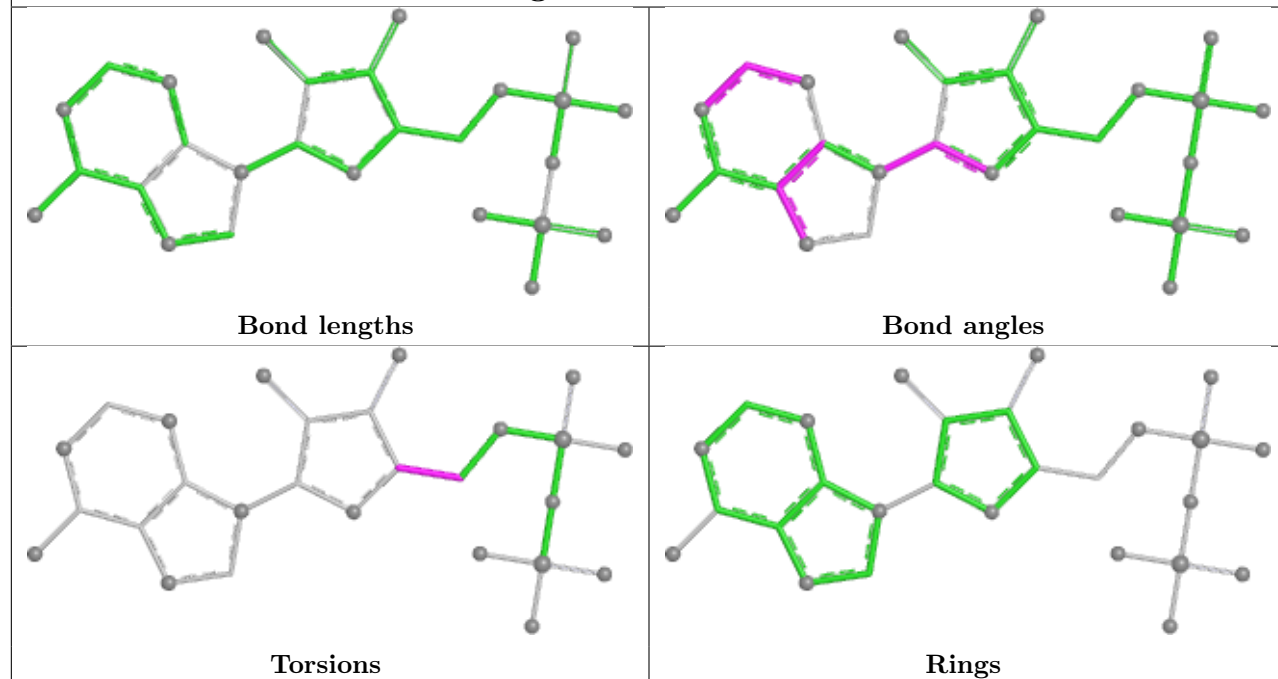




## Ligand ATP C 601



## Ligand ADP D 601



## 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.

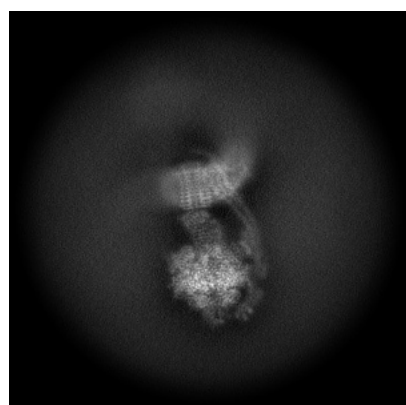
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45012. These allow visual inspection of the internal detail of the map and identification of artifacts.

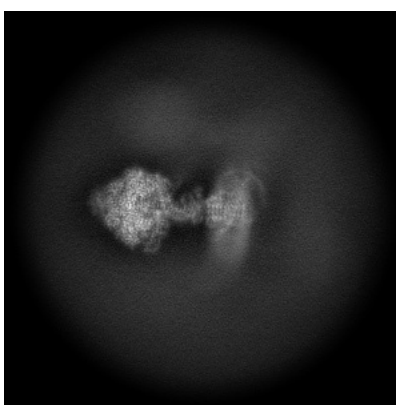
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

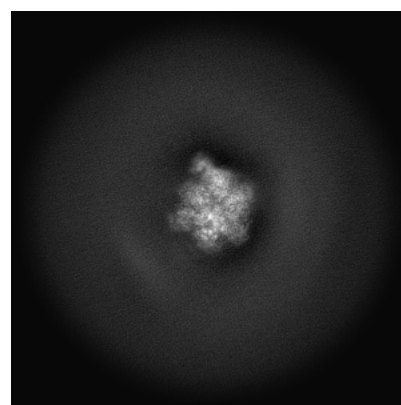
#### 6.1.1 Primary map



X



Y

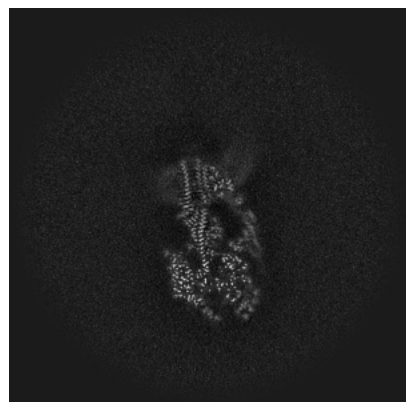


Z

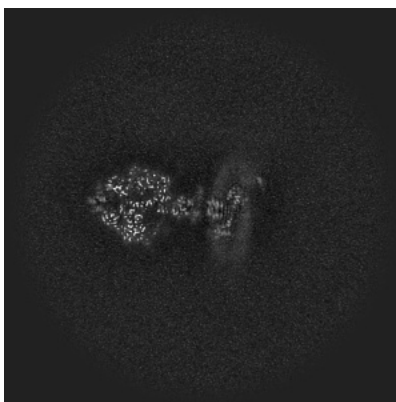
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

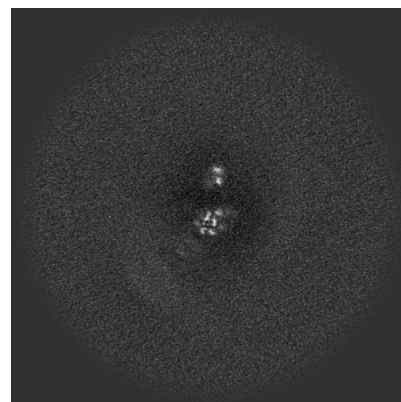
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

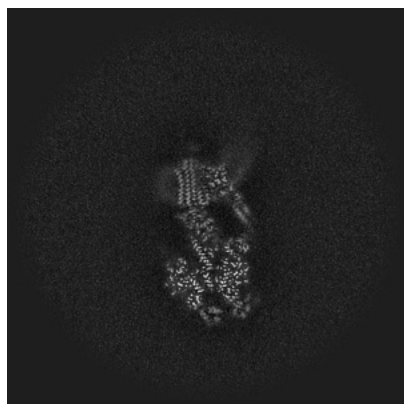


Z Index: 256

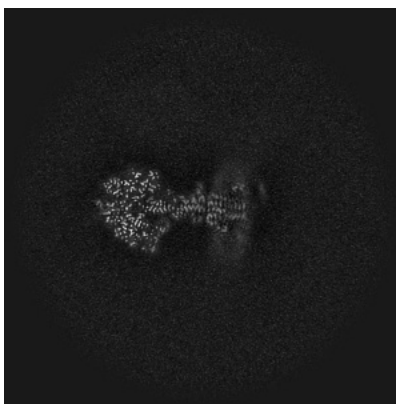
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

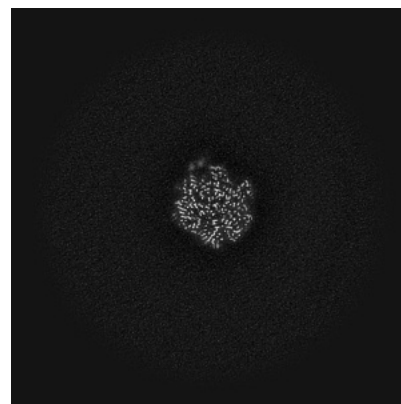
### 6.3.1 Primary map



X Index: 262



Y Index: 248

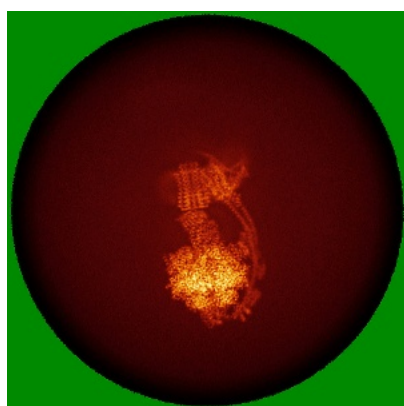


Z Index: 161

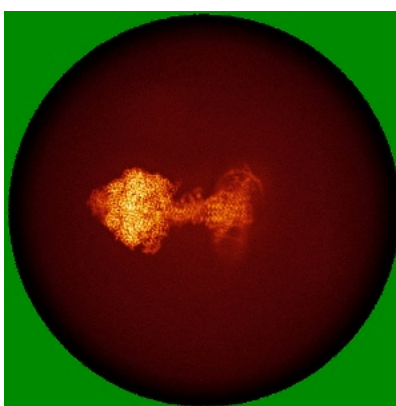
The images above show the largest variance slices of the map in three orthogonal directions.

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

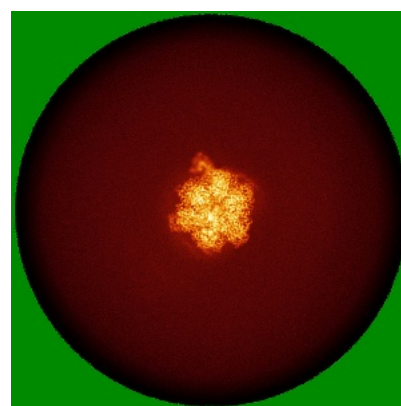
### 6.4.1 Primary map



X



Y

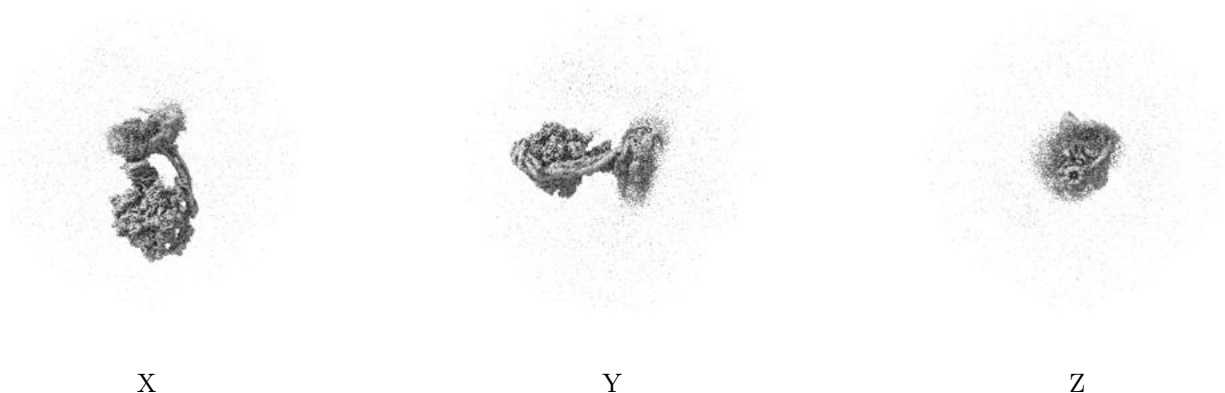


Z

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.

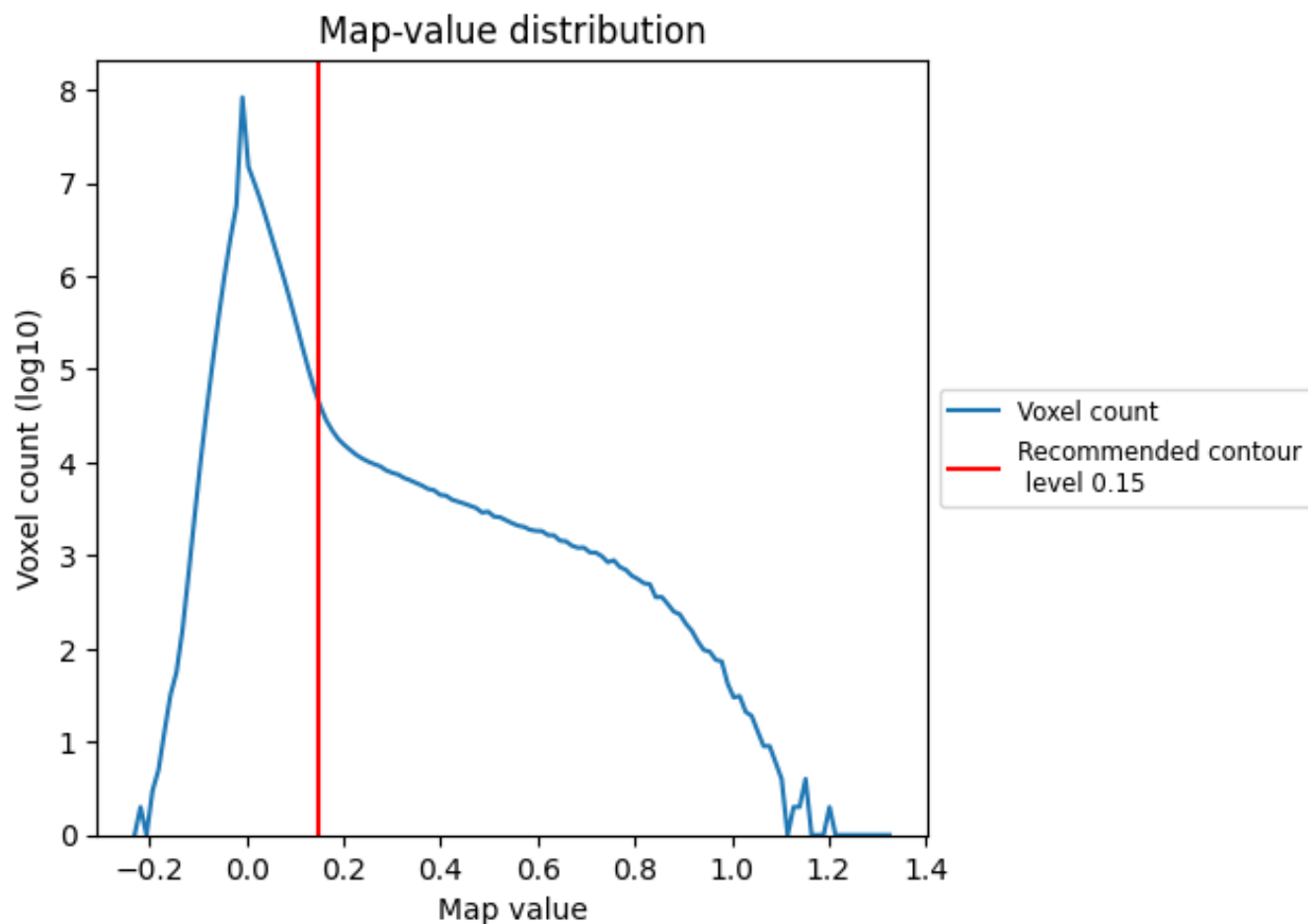
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

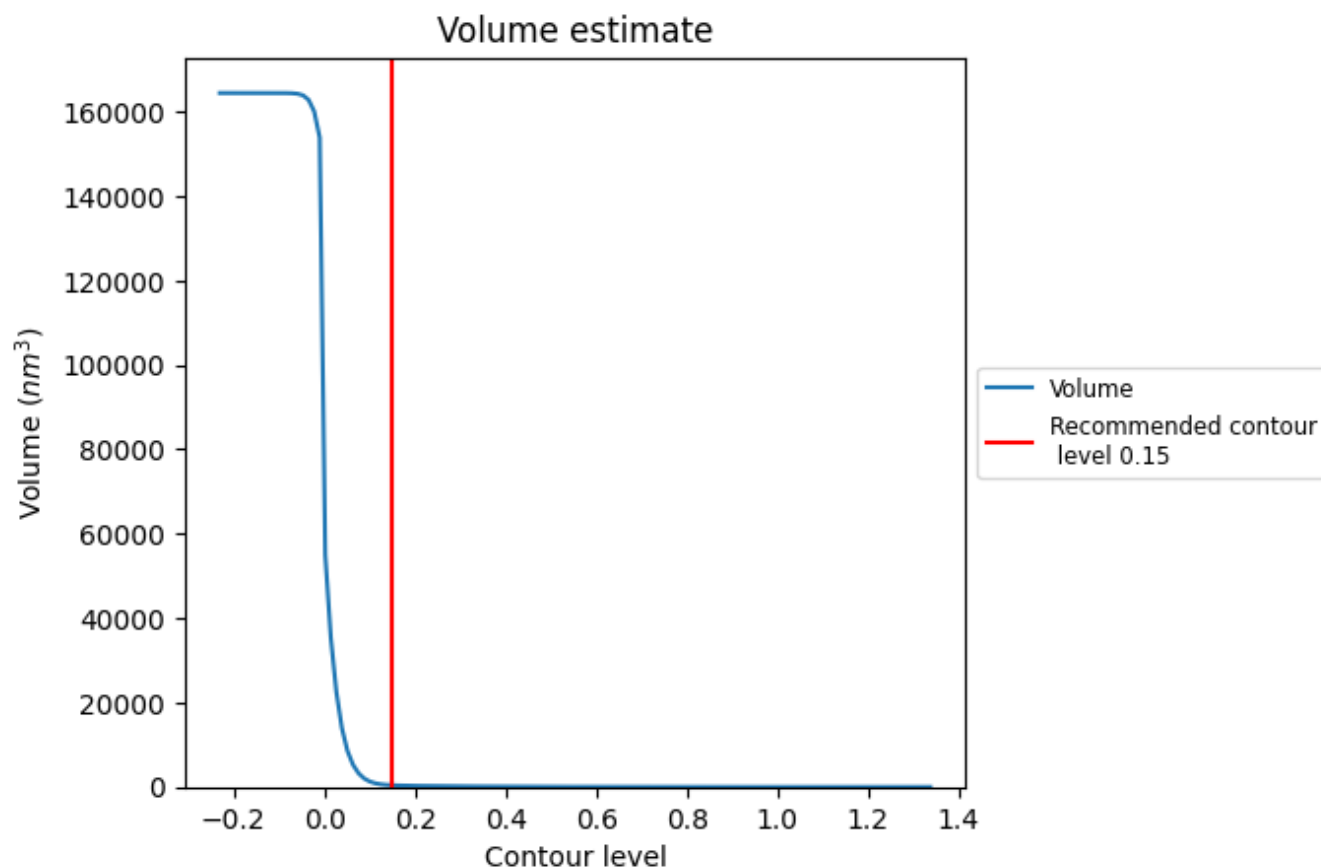
This section contains the results of statistical analysis of the map.

### 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.

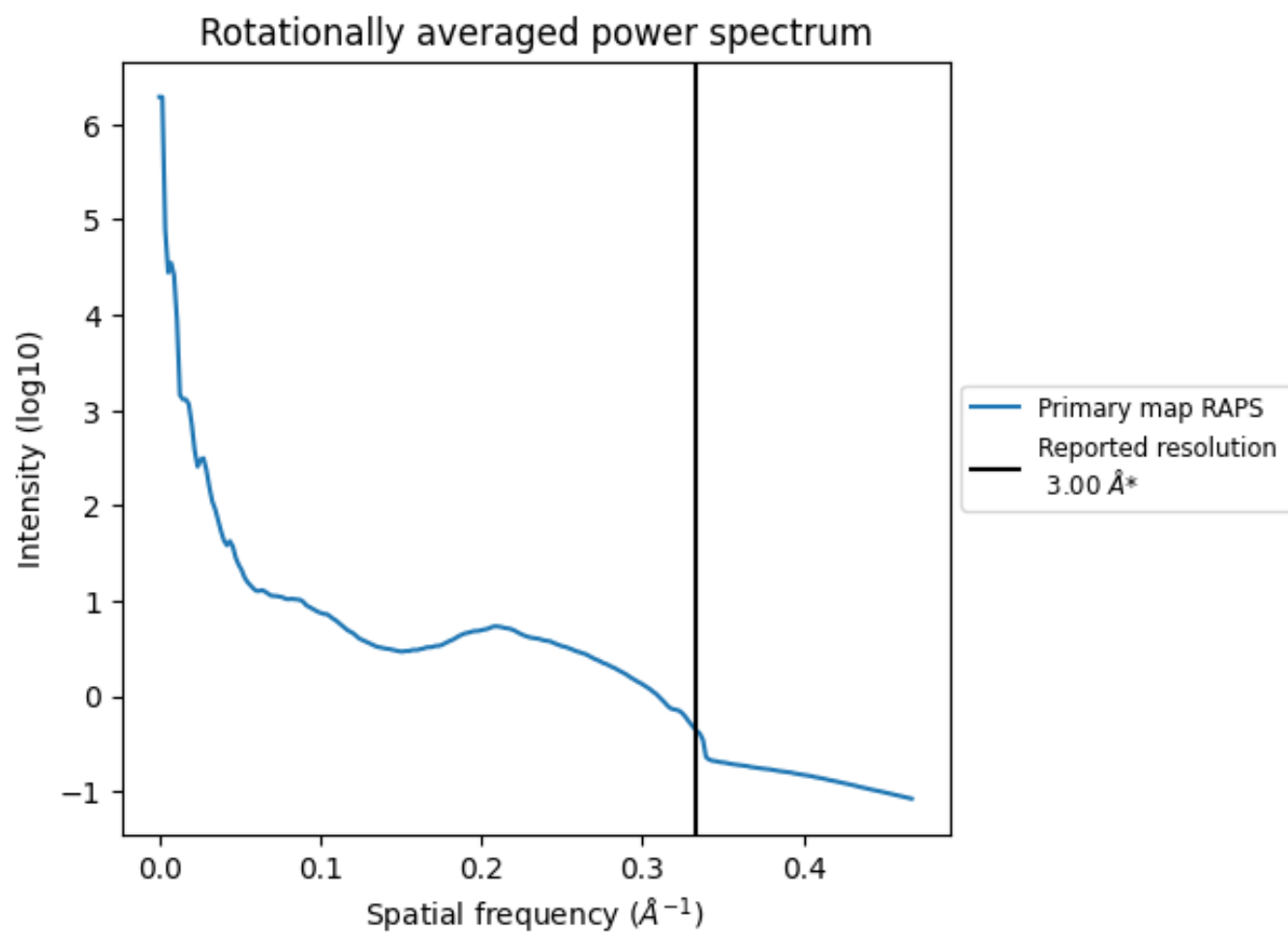
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404  $\text{nm}^3$ ; this corresponds to an approximate mass of 365 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 0.333 Å<sup>-1</sup>



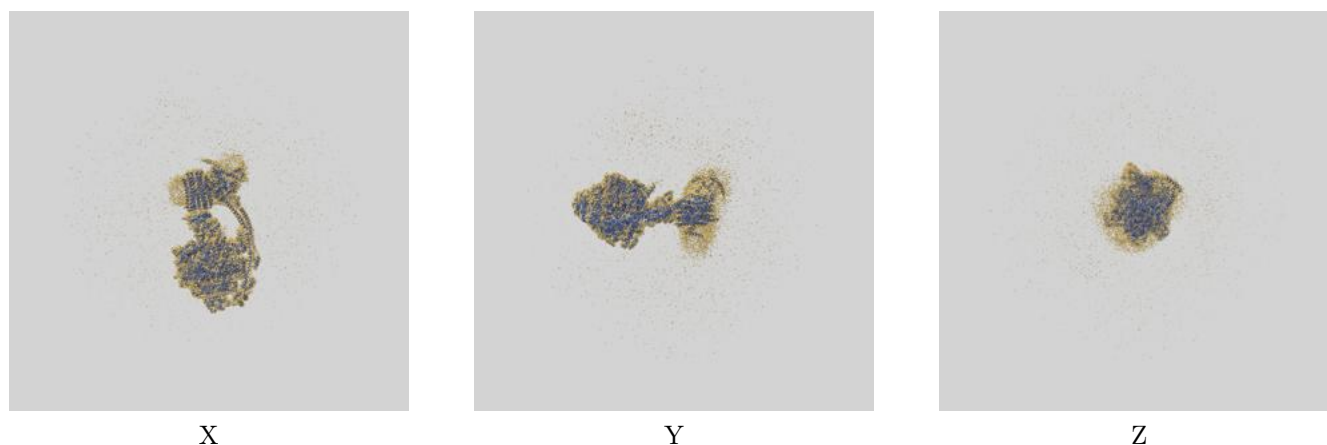
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

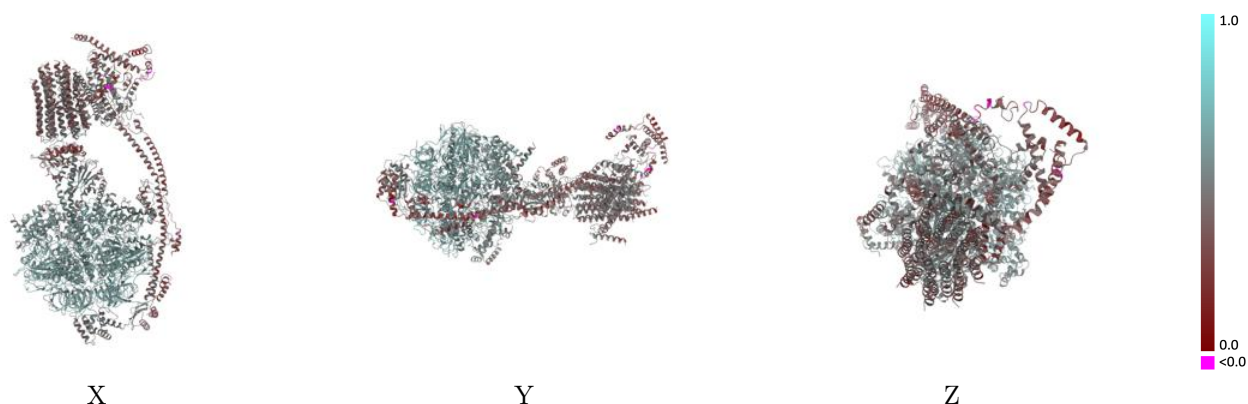
This section contains information regarding the fit between EMDB map EMD-45012 and PDB model 9BXU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



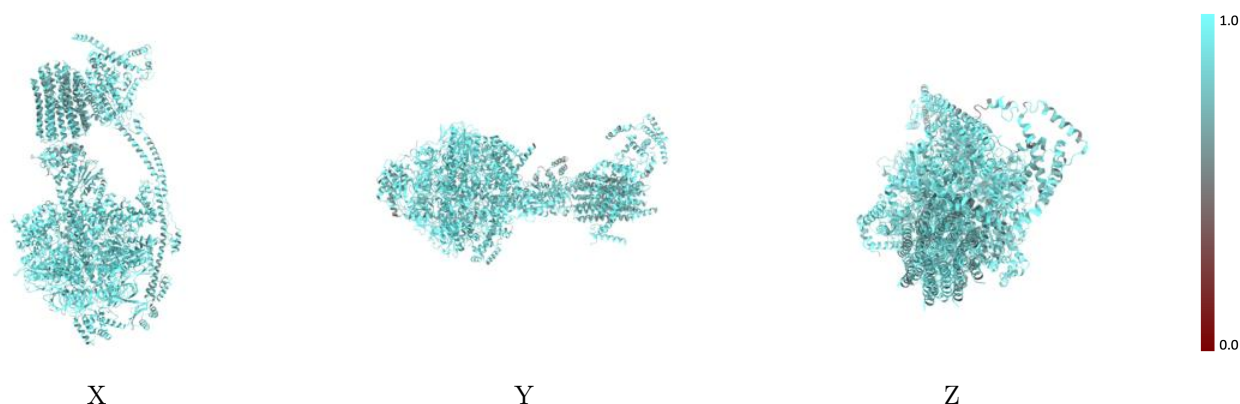
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



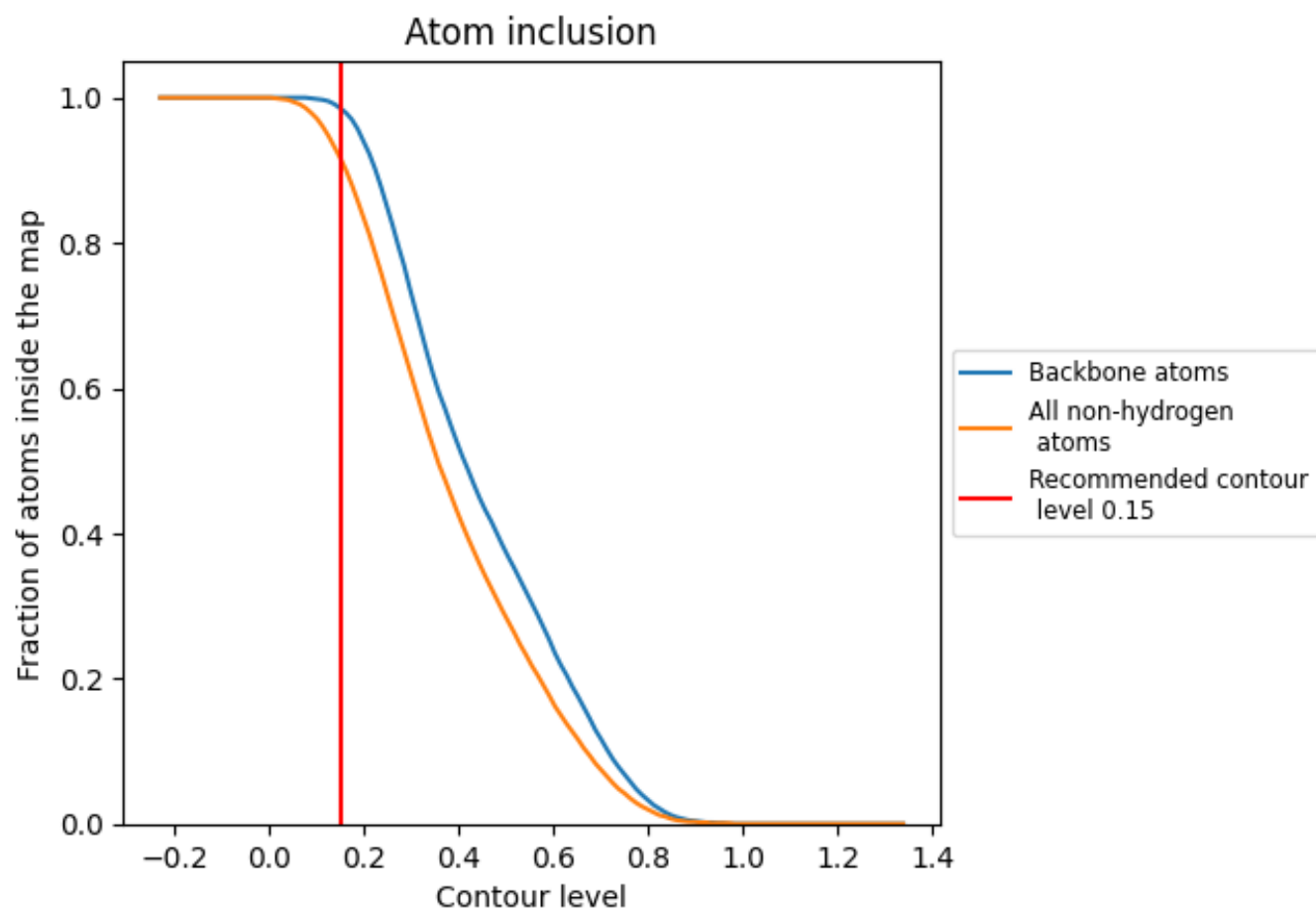
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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	 0.9160	 0.5070
8	 0.9100	 0.4780
A	 0.9730	 0.5860
B	 0.9560	 0.5570
C	 0.9520	 0.5670
D	 0.9680	 0.5940
E	 0.9570	 0.5760
F	 0.9680	 0.5890
G	 0.9160	 0.5140
H	 0.8360	 0.4060
I	 0.7960	 0.3930
J	 0.8950	 0.5420
K	 0.8290	 0.4000
L	 0.8160	 0.3940
M	 0.8270	 0.3970
N	 0.8140	 0.3980
O	 0.8120	 0.3880
P	 0.8090	 0.4030
Q	 0.8630	 0.4160
R	 0.8520	 0.4170
S	 0.8650	 0.4360
T	 0.7840	 0.3040
U	 0.8340	 0.3560
V	 0.8250	 0.3620
W	 0.8600	 0.3890
a	 0.8790	 0.4500
c	 0.9370	 0.3530
d	 0.8420	 0.3280
i	 0.8660	 0.3840
k	 0.9450	 0.4220

