Full wwPDB EM Validation Report (i)

May 14, 2024 – 03:27 am BST

PDB ID	:	6REP
EMDB ID	:	EMD-4853
Title	:	Cryo-EM structure of Polytomella F-ATP synthase, Primary rotary state 3, composite map
Authors	:	Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on	:	2019-04-12
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 (i) 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 (1)) were used in the production of this report:

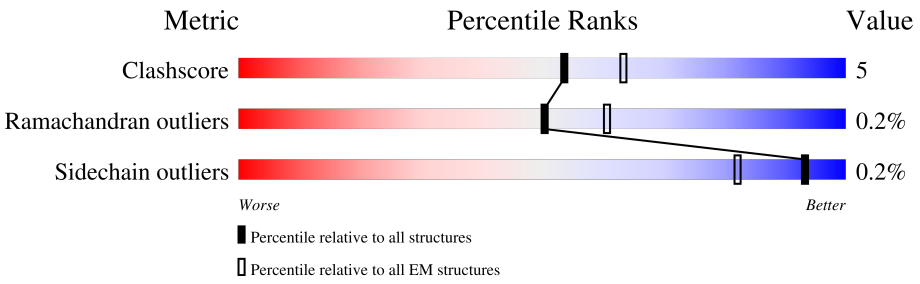
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	82	95% • •
2	1	618	88% 8% •
3	2	441	87% 13%
4	3	325	68% 7% 25%
5	4	294	88% 11% •
6	5	123	83% 17%
7	6	151	75% 7% 18%
8	7	190	81% 12% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	8	89	88% 11%
10	9	97	93% 7%
11	A	127	54% 42%
11	B	127	49% 9% 42%
11	C	127	54% 5% 42%
11	D	127	52% 6% 42%
11	E	127	48% 10% 42%
11	F	127	50% 9% 42%
11	G	127	45% 13% 42%
11	H	127	48% 10% 42%
11	I	127	53% 6% 42%
11	J	127	47% 11% 42%
12	M	327	58% 8% 34%
13	P	229	65% 19% 16%
14	Q	74	81% 15%
15	R	199	76% 13% 11%
16	S	317	71% 16% 13%
17	T	562	81% 11% 7%
17	U	562	83% 10% 7%
17	V	562	79% 14% 7%
18	X	574	79% 15% 6%
18	Y	574	79% 11% 9%
18	Z	574	79% 15% 6%

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 53782 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	81	607	388	107	110	2	0	0

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	595	4661	2958	798	900	5	0	0

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	2	441	3163	2020	532	611	0	0

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	245	1874	1204	299	370	1	0	0

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	290	2177	1385	356	434	2	0	0

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	123	986	640	172	170	4	0	0

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	124	926	599	154	172	1	0	0

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	176	1347	860	227	259	1	0	0

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	8	88	692	456	115	121	0	0

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	97	776	514	124	132	6	0	0

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	74	514	340	83	88	3	0	0
11	B	74	514	340	83	88	3	0	0
11	C	74	514	340	83	88	3	0	0
11	D	74	514	340	83	88	3	0	0
11	E	74	514	340	83	88	3	0	0
11	F	74	514	340	83	88	3	0	0
11	G	74	514	340	83	88	3	0	0
11	H	74	514	340	83	88	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	74	514	340	83	88	3	0	0
11	J	74	514	340	83	88	3	0	0

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	217	1640	1077	267	288	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	P	193	1532	988	250	290	4	0	0

- Molecule 14 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	72	561	358	102	99	2	0	0

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	177	1303	833	213	256	1	0	0

- Molecule 16 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	277	2130	1327	377	416	10	0	0

- Molecule 17 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	523	3979	2537	703	728	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	U	523	3980	2537	703	729	11	0	0
17	V	520	3962	2527	700	724	11	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	539	4095	2572	693	817	13	0	0
18	Y	521	3957	2485	670	789	13	0	0
18	Z	542	4115	2586	696	820	13	0	0

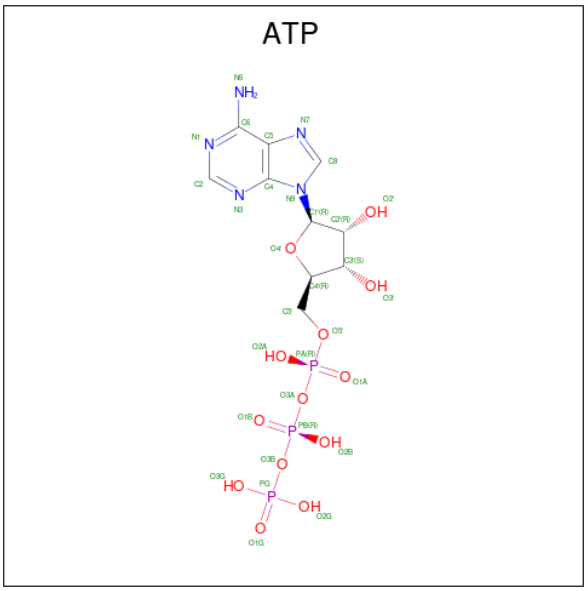
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
19	M	1	1	1	0

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

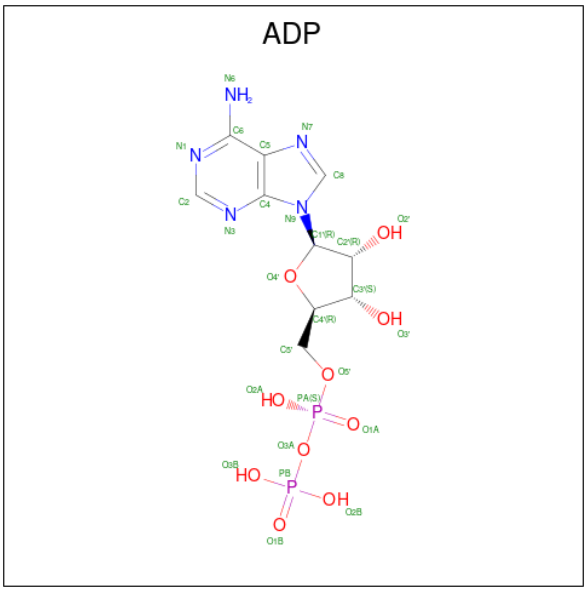


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	T	1	Total	Mg	0
			1	1	
21	U	1	Total	Mg	0
			1	1	
21	V	1	Total	Mg	0
			1	1	
21	X	1	Total	Mg	0
			1	1	
21	Z	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 23 is water.

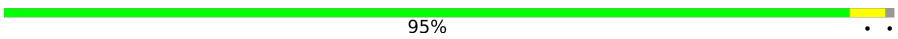
Mol	Chain	Residues	Atoms		AltConf
23	1	1	Total	O	0
			1	1	
23	5	3	Total	O	0
			3	3	
23	6	1	Total	O	0
			1	1	
23	C	2	Total	O	0
			2	2	
23	D	1	Total	O	0
			1	1	
23	M	18	Total	O	0
			18	18	

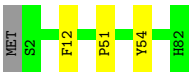
3 Residue-property plots (i)

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

• Molecule 1: ASA-10: Polytomella F-ATP synthase associated subunit 10

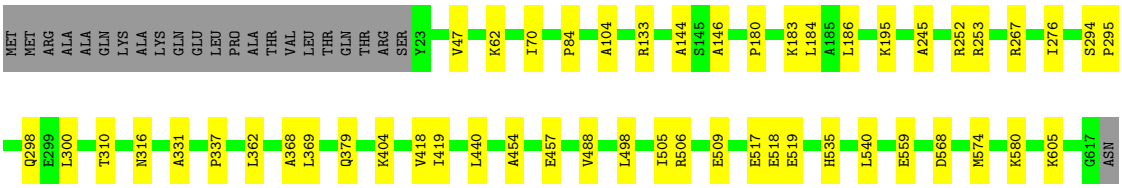
Chain 0:





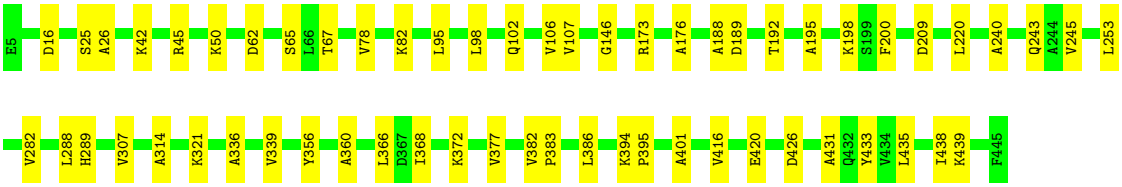
• Molecule 2: ATP synthase associated protein ASA1

Chain 1:



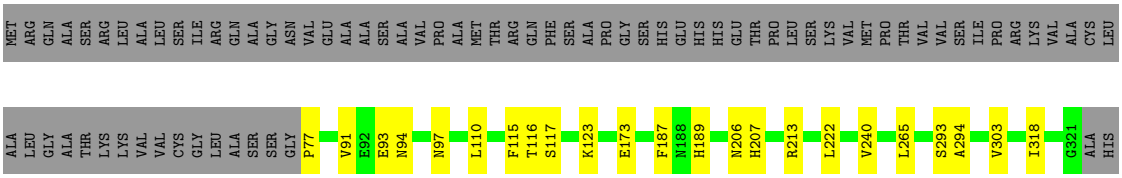
• Molecule 3: ASA-2: Polytomella F-ATP synthase associated subunit 2

Chain 2:



• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3:

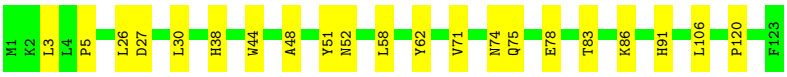


• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4:

• Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5:



• Molecule 7: Mitochondrial ATP synthase subunit ASA6

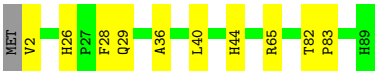
Chain 6:

• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7:

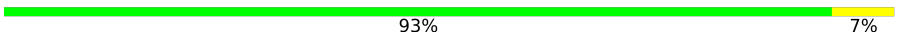
• Molecule 9: Mitochondrial ATP synthase subunit ASA8

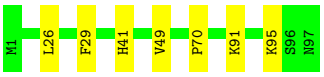
Chain 8:



• Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9:





• Molecule 11: Mitochondrial ATP synthase subunit c

Chain A: 54% • 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 A70 V74 L99

T110 A114 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain B: 49% 9% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 S59 V62 V74

V80 N92 L104 F107 E111 A114 L119 V120 L123 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain C: 54% 5% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 A72 G73 V74 V80

P93 A114 L119 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain D: 52% 6% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 A70 L71 A72 G73 V74

G75 A90 I95 A114 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

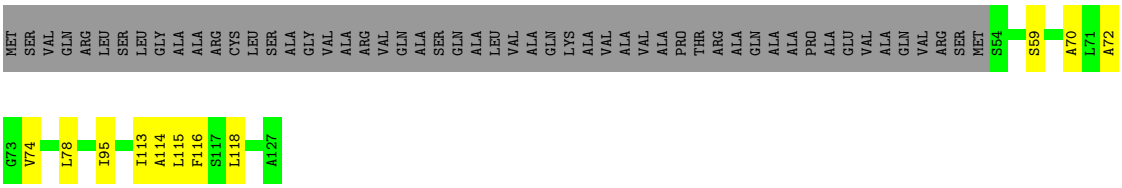
Chain E: 48% 10% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 V62 A70 L71 A72

G73 V74 A90 R91 I95 A103 F107 A114 L115 F116 S117 L123 A127

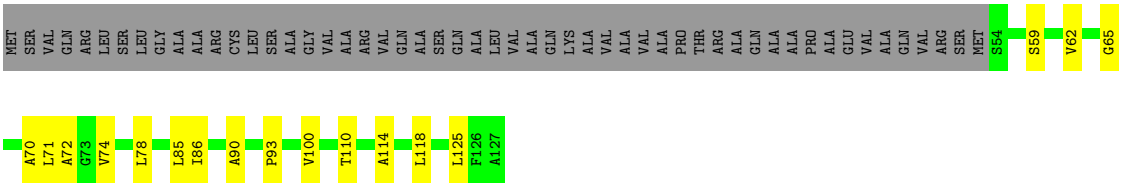
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain F: 50% 9% 42%



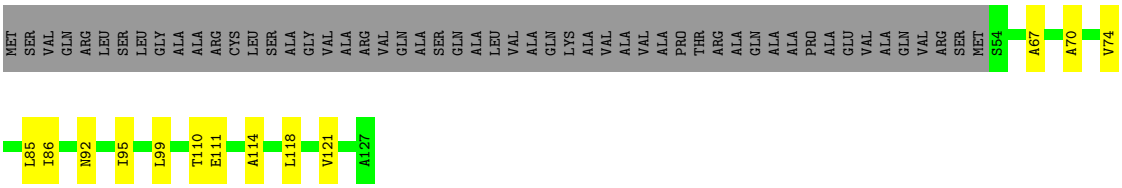
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain G: 45% 13% 42%



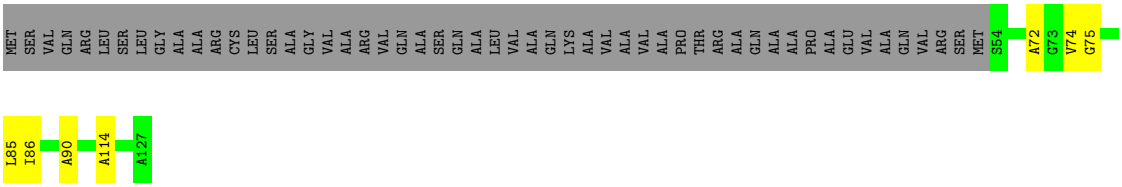
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain H: 48% 10% 42%



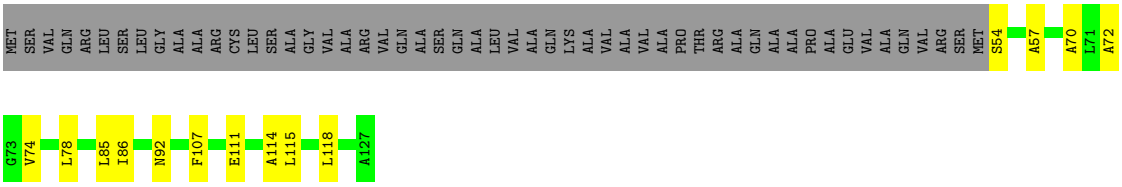
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain I: 53% 6% 42%



• Molecule 11: Mitochondrial ATP synthase subunit c

Chain J: 47% 11% 42%



• Molecule 12: Mitochondrial ATP synthase subunit 6

Chain M: 58% 8% 34%

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

SER PRO LEU ASN VAL LYS LEU PRO GLY MET SER CYS SER SER ILE LEU LEU PRO LYS THR SER ARG ILE ALA VAL PRO PHE GLY ASN GLN THR MET ALA MET S95 S96 K101 G112 P126 D143 T153 T154 F155 T158 N163 T175 K199 T200 G201 P205

GLY HIS PHE ILE PRO GLY GLY THR PRO TRP PRO MET ALA F219 P223 I227 H248 T249 L250 L251 L259 S264 L281 V285 E288 A292 D313 K321 K324 LYS ILE HIS

- Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P: 65% 19% 16%

MET LEU ALA ARG VAL ALA SER VAL ALA LEU ARG ARG ALA GLU GLY LYS ILE MET PRO GLN MET VAL ARG ALA LEU SER VAL SER ALA ALA SER ALA ALA GLN ALA GLU L37 K38 L39 P40 T41 A42 P43 L44 T49 Q52 T55 L56 L57 W58 Q59 A62 K63 E64 N65 Q66

K69 V70 Q71 D72 E73 L80 K103 K110 I117 L121 Y141 L144 M145 K149 K150 E151 V152 T155 V156 I157 L170 F182 V185 M186 Q187 L194 L195 V199 D208 T211 A212 K213 I229

- Molecule 14: epsilon: Polytomella F-ATP synthase epsilon subunit

Chain Q: 81% 15%

MET CYS A3 R18 R28 K32 K36 A39 R48 Q49 A50 P51 D54 A59 S60 K61 V62 M74

- Molecule 15: Mitochondrial ATP synthase subunit delta

Chain R: 76% 13% 11%

MET PHE GLY LEU LYS ARG ALA VAL THR VAL GLY ARG ARG PHE ILE SER THR SER ALA ALA ARG MET E23 T34 E35 V36 W37 N38 K39 K40 L45 I46 V47 P48 E49 K58 K86 D87 T88 V89 V90 G96 H104 E117 L118 H119 K126 V136 N139

E175 F176 E177 Q178 N181 A199

- Molecule 16: ATP synthase gamma chain, mitochondrial

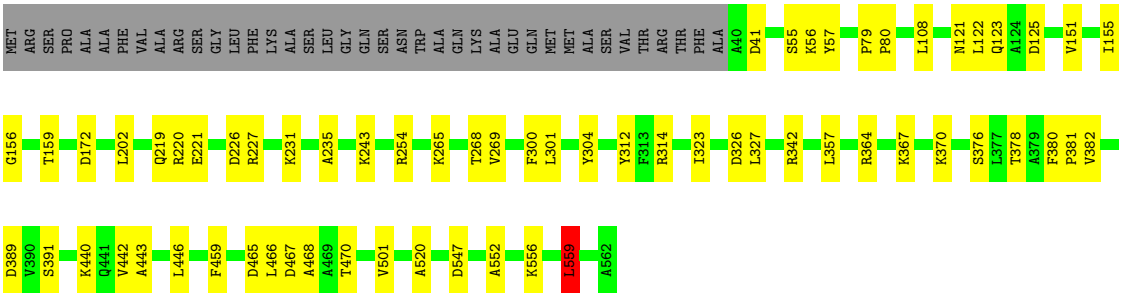
Chain S: 71% 16% 13%

MET ALA LEU ARG LYS ALA VAL LEU SER LEU GLY LEU SER GLN GLY VAL ALA ALA GLU ALA VAL LEU GLY SER GLY MET PHE ASN ALA VAL GLN HIS GLU SER VAL ARG TYR ALA S39 M60 K61 M62 R79 F92 V95 K99 S100 V101 V102 S107 L111 N116

I119 T120 K121 Y122 T123 R124 L127 A128 T129 T130 E131 K135 D136 V137 V138 I153 R157 Y158 Q159 I162 I178 V179 E180 E181 L182 P187 F197 K204 I210 L211 S212 P213 D214 L215 L216 E217 K218 Q219 D222 R239 V242 L243 R244 D245 L246

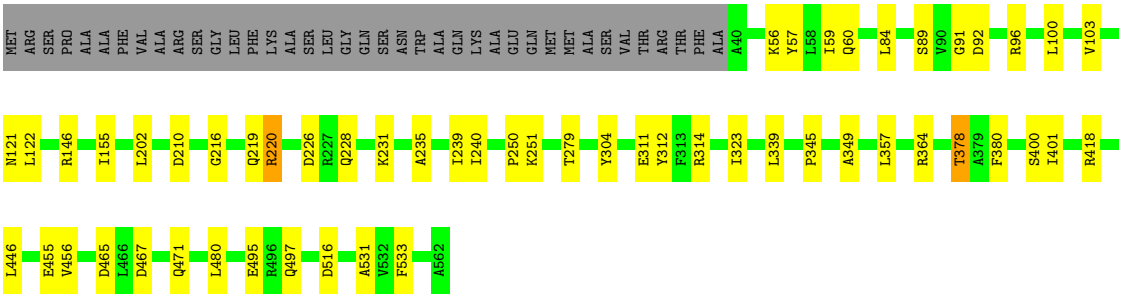
• Molecule 17: ATP synthase subunit alpha

Chain T:



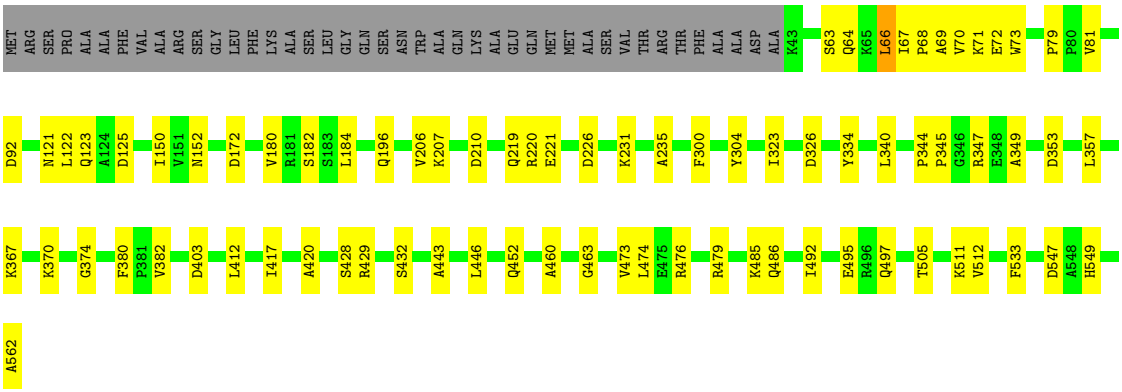
• Molecule 17: ATP synthase subunit alpha

Chain U:



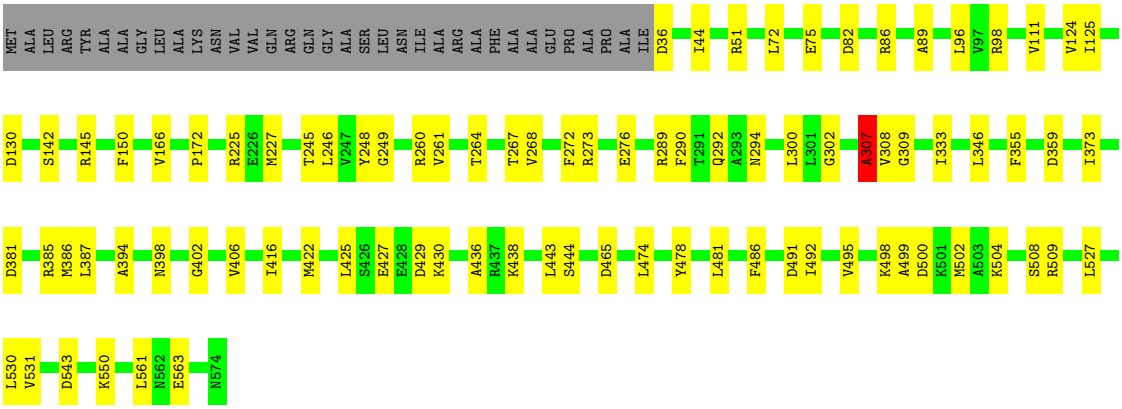
• Molecule 17: ATP synthase subunit alpha

Chain V:



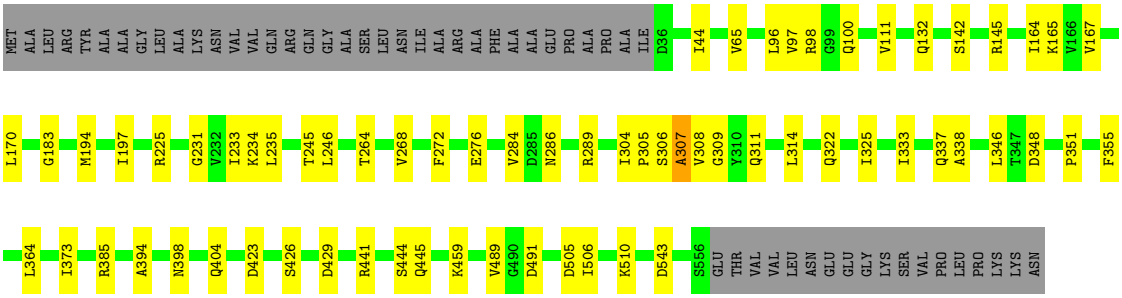
• Molecule 18: ATP synthase subunit beta

Chain X:



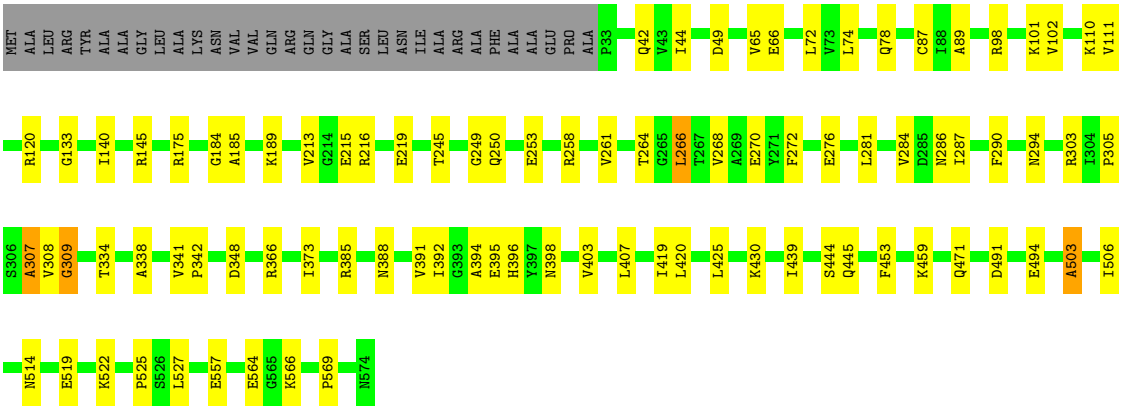
• Molecule 18: ATP synthase subunit beta

Chain Y:



• Molecule 18: ATP synthase subunit beta

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163259	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 ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	43.890	Depositor
Minimum map value	-26.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.061	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0	0.48	0/628	0.54	0/856
2	1	0.47	0/4750	0.52	0/6434
3	2	0.38	0/3212	0.55	0/4371
4	3	0.43	0/1911	0.53	1/2601 (0.0%)
5	4	0.44	0/2216	0.51	0/3000
6	5	0.57	0/1011	0.66	3/1376 (0.2%)
7	6	0.50	0/946	0.55	0/1287
8	7	0.54	0/1374	0.54	0/1865
9	8	0.53	0/715	0.58	0/974
10	9	0.40	0/802	0.51	0/1084
11	A	0.32	0/520	0.52	0/704
11	B	0.33	0/520	0.56	0/704
11	C	0.36	0/519	0.56	1/701 (0.1%)
11	D	0.40	0/520	0.52	0/704
11	E	0.41	0/520	0.52	0/704
11	F	0.38	0/520	0.53	0/704
11	G	0.35	0/520	0.52	0/704
11	H	0.33	0/520	0.53	0/704
11	I	0.33	0/520	0.48	0/704
11	J	0.33	0/520	0.57	0/704
12	M	0.54	0/1683	0.60	0/2295
13	P	0.43	0/1553	0.59	0/2093
14	Q	0.43	0/574	0.54	0/774
15	R	0.42	0/1336	0.53	0/1827
16	S	0.43	0/2153	0.57	0/2901
17	T	0.55	0/4048	0.60	2/5481 (0.0%)
17	U	0.54	0/4049	0.61	1/5481 (0.0%)
17	V	0.55	0/4031	0.58	0/5456
18	X	0.51	0/4155	0.58	0/5630
18	Y	0.52	0/4015	0.56	0/5440
18	Z	0.53	0/4176	0.60	1/5659 (0.0%)
All	All	0.49	0/54537	0.57	9/73922 (0.0%)

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
13	P	0	2
17	U	0	1
18	X	0	1
18	Y	0	1
18	Z	0	2
All	All	0	7

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	U	467	ASP	CB-CG-OD1	6.77	124.40	118.30
6	5	106	LEU	CA-CB-CG	6.47	130.18	115.30
4	3	77	PRO	N-CA-CB	5.87	110.34	103.30
17	T	122	LEU	CA-CB-CG	5.77	128.58	115.30
6	5	106	LEU	CB-CG-CD2	-5.40	101.82	111.00
18	Z	266	LEU	CA-CB-CG	5.38	127.68	115.30
17	T	559	LEU	CA-CB-CG	5.06	126.93	115.30
6	5	58	LEU	C-N-CA	-5.04	109.09	121.70
11	C	119	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	P	110	LYS	Peptide
13	P	185	VAL	Peptide
17	U	250	PRO	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Z	307	ALA	Peptide
18	Z	503	ALA	Mainchain

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	0	607	0	584	2	0
2	1	4661	0	4695	32	0
3	2	3163	0	3262	37	0
4	3	1874	0	1826	13	0
5	4	2177	0	2169	22	0
6	5	986	0	1021	17	0
7	6	926	0	941	10	0
8	7	1347	0	1345	23	0
9	8	692	0	694	7	0
10	9	776	0	757	5	0
11	A	514	0	554	4	0
11	B	514	0	554	9	0
11	C	514	0	553	4	0
11	D	514	0	554	7	0
11	E	514	0	554	12	0
11	F	514	0	554	9	0
11	G	514	0	554	14	0
11	H	514	0	554	12	0
11	I	514	0	554	6	0
11	J	514	0	554	11	0
12	M	1640	0	1665	24	0
13	P	1532	0	1603	63	0
14	Q	561	0	565	10	0
15	R	1303	0	1266	16	0
16	S	2130	0	2180	38	0
17	T	3979	0	4118	50	0
17	U	3980	0	4119	40	0
17	V	3962	0	4105	72	0
18	X	4095	0	4113	61	0
18	Y	3957	0	3967	40	0
18	Z	4115	0	4137	57	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	1	0
20	V	31	0	12	1	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	X	1	0	0	0	0
21	Z	1	0	0	0	0
22	X	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Z	27	0	12	0	0
23	1	1	0	0	0	0
23	5	3	0	0	0	0
23	6	1	0	0	0	0
23	C	2	0	0	0	0
23	D	1	0	0	0	0
23	M	18	0	0	6	0
All	All	53782	0	54731	592	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 (592) 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)
13:P:39:LEU:CD2	17:V:73:TRP:CH2	2.20	1.24
13:P:39:LEU:CD2	17:V:73:TRP:HH2	1.53	1.18
13:P:37:LEU:HD13	17:V:73:TRP:CE2	1.69	1.17
13:P:37:LEU:HB2	17:V:73:TRP:CZ2	1.82	1.14
14:Q:51:PRO:HD2	14:Q:59:ALA:HB3	1.13	1.10
12:M:288:GLU:OE1	23:M:701:HOH:O	1.66	1.10
17:T:466:LEU:HG	17:T:467:ASP:H	1.07	1.07
13:P:39:LEU:HD21	17:V:73:TRP:CH2	1.88	1.03
14:Q:51:PRO:HD2	14:Q:59:ALA:CB	1.93	0.97
13:P:37:LEU:CD1	17:V:73:TRP:CE2	2.45	0.93
17:T:466:LEU:HD23	17:T:470:THR:OG1	1.71	0.90
13:P:37:LEU:HB2	17:V:73:TRP:HZ2	1.28	0.89
17:T:466:LEU:HG	17:T:467:ASP:N	1.87	0.88
12:M:199:LYS:HE3	12:M:313:ASP:OD1	1.74	0.88
14:Q:49:GLN:O	14:Q:60:SER:O	1.94	0.86
13:P:39:LEU:HD23	17:V:73:TRP:HH2	1.39	0.85
13:P:117:ILE:HD13	17:V:69:ALA:HB1	1.57	0.85
13:P:37:LEU:HD13	17:V:73:TRP:CD2	2.13	0.83
13:P:39:LEU:HD21	17:V:73:TRP:CZ3	2.15	0.81
13:P:64:GLU:OE2	17:V:70:VAL:HA	1.81	0.80
18:X:465:ASP:HB3	18:X:491:ASP:OD2	1.81	0.79
13:P:39:LEU:HD23	17:V:73:TRP:CH2	2.15	0.77
18:X:498:LYS:O	18:X:502:MET:HG2	1.84	0.77
13:P:141:TYR:O	13:P:145:MET:HG2	1.86	0.76
17:T:466:LEU:CD2	17:T:470:THR:HG21	2.17	0.75
14:Q:48:ARG:HB3	14:Q:62:VAL:HG13	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:37:LEU:CB	17:V:73:TRP:CZ2	2.69	0.73
13:P:37:LEU:HD13	17:V:73:TRP:CZ2	2.24	0.73
14:Q:51:PRO:CD	14:Q:59:ALA:HB3	2.07	0.73
13:P:39:LEU:HD22	17:V:73:TRP:HH2	1.51	0.72
17:T:466:LEU:CG	17:T:467:ASP:H	1.93	0.71
17:T:466:LEU:HD23	17:T:470:THR:CB	2.20	0.71
12:M:199:LYS:NZ	23:M:702:HOH:O	2.24	0.70
13:P:39:LEU:HD22	17:V:73:TRP:CH2	2.25	0.70
17:V:196:GLN:HE22	17:V:370:LYS:HE2	1.55	0.70
17:V:63:SER:O	17:V:67:ILE:HG12	1.93	0.69
12:M:223:PRO:O	12:M:227:ILE:HG12	1.92	0.68
13:P:40:PRO:O	13:P:59:GLN:HG2	1.92	0.68
2:1:316:ASN:HD21	2:1:331:ALA:H	1.41	0.67
12:M:248:HIS:HB3	23:M:718:HOH:O	1.94	0.67
8:7:123:HIS:HD2	8:7:125:GLU:H	1.41	0.66
13:P:64:GLU:OE2	17:V:71:LYS:N	2.28	0.65
18:Z:388:ASN:HD22	18:Z:391:VAL:HG23	1.60	0.65
18:X:498:LYS:O	18:X:502:MET:CG	2.44	0.65
11:B:74:VAL:HG11	11:B:114:ALA:HB2	1.76	0.65
4:3:93:GLU:OE1	4:3:123:LYS:NZ	2.30	0.64
13:P:44:LEU:HD23	13:P:144:LEU:HD23	1.78	0.64
11:G:74:VAL:HG11	11:G:114:ALA:HB2	1.79	0.63
3:2:394:LYS:HD3	3:2:395:PRO:HD2	1.80	0.63
17:V:121:ASN:HB3	17:V:123:GLN:HE21	1.62	0.63
17:T:466:LEU:HD21	17:T:470:THR:HG21	1.80	0.63
18:Y:506:ILE:HG22	18:Y:510:LYS:HD3	1.81	0.63
2:1:517:GLU:HG2	2:1:518:GLU:HG3	1.79	0.63
13:P:117:ILE:HD13	17:V:69:ALA:CB	2.29	0.62
17:T:466:LEU:HD23	17:T:470:THR:HG21	1.80	0.62
17:T:235:ALA:HB1	17:T:323:ILE:HD13	1.82	0.62
18:Z:395:GLU:OE2	18:Z:471:GLN:NE2	2.33	0.62
17:T:466:LEU:HD23	17:T:470:THR:CG2	2.30	0.62
13:P:44:LEU:HD23	13:P:44:LEU:H	1.63	0.62
5:4:6:VAL:HG11	5:4:11:VAL:HG13	1.80	0.62
13:P:44:LEU:CD2	13:P:144:LEU:HD23	2.28	0.61
15:R:37:TRP:HD1	16:S:129:THR:HG21	1.65	0.61
18:Z:184:GLY:O	18:Z:366:ARG:NH2	2.33	0.61
8:7:170:HIS:HD2	8:7:172:ALA:H	1.50	0.60
3:2:321:LYS:HZ2	5:4:16:SER:HB2	1.66	0.60
16:S:213:PRO:HA	16:S:217:GLU:HB3	1.83	0.59
15:R:40:LYS:HD2	16:S:129:THR:HA	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:276:ASN:ND2	17:V:463:GLY:O	2.35	0.59
3:2:245:VAL:HG22	3:2:288:LEU:HD13	1.84	0.59
2:1:295:PRO:HA	2:1:298:GLN:HG2	1.85	0.59
17:T:219:GLN:NE2	17:T:221:GLU:OE1	2.35	0.59
17:U:210:ASP:HB2	17:U:497:GLN:HE22	1.68	0.59
13:P:152:VAL:HG12	13:P:152:VAL:O	2.01	0.59
13:P:39:LEU:CD2	17:V:73:TRP:CZ3	2.77	0.59
11:I:90:ALA:O	11:J:92:ASN:ND2	2.35	0.59
18:Z:216:ARG:HB2	18:Z:219:GLU:HG3	1.84	0.59
2:1:418:VAL:HG23	2:1:419:ILE:HG13	1.85	0.58
11:J:107:PHE:O	11:J:111:GLU:HB2	2.02	0.58
18:X:394:ALA:O	18:X:398:ASN:ND2	2.36	0.58
18:Z:110:LYS:HB3	18:Z:140:ILE:HG22	1.85	0.58
18:Z:216:ARG:O	18:Z:250:GLN:NE2	2.37	0.58
3:2:339:VAL:HG13	3:2:431:ALA:HB2	1.86	0.58
17:T:121:ASN:HB2	18:Y:44:ILE:HG12	1.85	0.58
2:1:253:ARG:HD2	2:1:369:LEU:HB3	1.84	0.58
15:R:23:GLU:N	16:S:222:ASP:OD2	2.37	0.57
18:X:111:VAL:HG11	18:X:264:THR:HG23	1.85	0.57
2:1:267:ARG:NH1	2:1:519:GLU:OE1	2.37	0.57
17:U:455:GLU:HG3	17:U:456:VAL:HG13	1.87	0.57
3:2:377:VAL:HG11	3:2:438:ILE:HG23	1.87	0.57
7:6:108:LEU:HD11	12:M:281:LEU:HD13	1.86	0.57
17:T:226:ASP:O	17:T:231:LYS:NZ	2.35	0.57
20:V:1001:ATP:O2G	18:Y:385:ARG:NH1	2.37	0.57
12:M:248:HIS:CD2	23:M:718:HOH:O	2.57	0.56
17:V:479:ARG:NH1	17:V:512:VAL:O	2.38	0.56
18:Y:306:SER:OG	18:Y:307:ALA:N	2.37	0.56
17:T:151:VAL:HG11	17:T:301:LEU:HD21	1.87	0.56
3:2:195:ALA:HA	3:2:198:LYS:HE3	1.85	0.56
17:V:210:ASP:HB2	17:V:497:GLN:HE22	1.71	0.56
17:V:219:GLN:NE2	17:V:221:GLU:OE1	2.39	0.56
13:P:40:PRO:HG3	13:P:62:ALA:HB3	1.88	0.55
13:P:150:LYS:HA	13:P:182:PHE:CE2	2.41	0.55
18:X:86:ARG:NH2	18:X:300:LEU:O	2.39	0.55
18:Z:42:GLN:HE21	18:Z:44:ILE:HD11	1.72	0.55
3:2:188:ALA:HB2	3:2:220:LEU:HD22	1.88	0.55
15:R:35:GLU:O	15:R:39:LYS:NZ	2.39	0.55
11:A:70:ALA:HA	11:J:72:ALA:HB2	1.88	0.55
4:3:293:SER:OG	4:3:294:ALA:N	2.40	0.55
2:1:180:PRO:HG2	2:1:183:LYS:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:72:ALA:HB2	11:E:70:ALA:HA	1.89	0.55
16:S:79:ARG:NH2	16:S:197:PHE:O	2.40	0.55
18:Z:403:VAL:HG13	18:Z:439:ILE:HD12	1.89	0.55
13:P:43:PRO:HD3	13:P:58:TRP:CH2	2.41	0.55
16:S:131:GLU:OE1	16:S:157:ARG:NH2	2.40	0.55
2:1:368:ALA:O	2:1:379:GLN:NE2	2.35	0.55
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.89	0.54
18:X:500:ASP:O	18:X:504:LYS:HG2	2.07	0.54
18:Y:373:ILE:HG23	18:Y:444:SER:HB3	1.89	0.54
3:2:253:LEU:HD11	3:2:401:ALA:HB2	1.88	0.54
11:A:110:THR:HG22	11:J:78:LEU:HB3	1.88	0.54
17:U:122:LEU:HD23	18:X:98:ARG:HG3	1.89	0.54
18:Z:253:GLU:O	18:Z:258:ARG:NH1	2.40	0.54
17:T:254:ARG:NH1	18:Y:543:ASP:OD1	2.41	0.54
3:2:209:ASP:OD1	3:2:209:ASP:N	2.41	0.54
17:V:220:ARG:HH12	18:Z:216:ARG:HD3	1.71	0.54
16:S:119:ILE:O	16:S:123:THR:N	2.40	0.54
13:P:44:LEU:HD23	13:P:44:LEU:N	2.23	0.54
17:U:465:ASP:HB2	17:U:471:GLN:HB2	1.90	0.53
7:6:141:ASN:O	7:6:144:LYS:NZ	2.39	0.53
8:7:47:GLU:HG3	8:7:60:GLN:HG3	1.90	0.53
16:S:239:ARG:HA	16:S:242:VAL:HG12	1.89	0.53
13:P:37:LEU:HD12	13:P:37:LEU:N	2.24	0.53
17:T:108:LEU:HG	17:T:151:VAL:HG22	1.89	0.53
11:I:74:VAL:HG11	11:I:114:ALA:HB2	1.90	0.53
17:U:100:LEU:O	18:X:98:ARG:NH2	2.42	0.53
5:4:74:LEU:HD23	5:4:219:VAL:HG13	1.90	0.53
11:C:93:PRO:HB3	11:D:95:ILE:HD13	1.91	0.53
13:P:157:ILE:HB	13:P:199:VAL:HG22	1.90	0.53
18:Y:272:PHE:HD1	18:Y:276:GLU:HG3	1.73	0.53
17:U:235:ALA:HB1	17:U:323:ILE:HG12	1.91	0.53
18:Y:231:GLY:O	18:Y:234:LYS:NZ	2.41	0.53
17:U:314:ARG:NH2	17:U:364:ARG:O	2.42	0.52
18:X:51:ARG:NH1	18:X:82:ASP:O	2.42	0.52
11:B:92:ASN:OD1	11:B:92:ASN:N	2.42	0.52
13:P:156:VAL:HG11	13:P:170:LEU:HD21	1.91	0.52
16:S:210:ILE:HD11	16:S:254:THR:HG21	1.90	0.52
3:2:282:VAL:HG12	3:2:314:ALA:HB2	1.90	0.52
10:9:26:LEU:HA	10:9:29:PHE:HD2	1.75	0.52
13:P:49:THR:H	13:P:52:GLN:HE21	1.56	0.52
17:U:323:ILE:HG13	17:U:380:PHE:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:304:TYR:OH	17:V:357:LEU:O	2.25	0.52
12:M:163:ASN:ND2	12:M:175:THR:OG1	2.43	0.52
13:P:150:LYS:HA	13:P:182:PHE:CD2	2.44	0.52
17:V:326:ASP:H	17:V:382:VAL:HB	1.74	0.52
17:T:466:LEU:CG	17:T:467:ASP:N	2.62	0.52
13:P:71:GLN:OE1	13:P:145:MET:CE	2.57	0.52
2:1:84:PRO:HG2	6:5:71:VAL:HG11	1.91	0.52
18:Z:42:GLN:HG2	18:Z:49:ASP:HB2	1.92	0.52
4:3:265:LEU:HD22	4:3:303:VAL:HG11	1.91	0.52
5:4:63:VAL:HA	5:4:92:LEU:HD11	1.92	0.52
11:F:74:VAL:HG11	11:F:114:ALA:HB2	1.91	0.52
18:Y:286:ASN:H	18:Y:338:ALA:HB3	1.73	0.52
3:2:95:LEU:HA	3:2:98:LEU:HD12	1.91	0.52
5:4:6:VAL:HG12	5:4:8:LYS:H	1.75	0.52
17:T:155:ILE:HD12	17:T:312:TYR:HB2	1.92	0.51
17:U:240:ILE:HG23	17:U:279:THR:HG21	1.93	0.51
17:V:323:ILE:HG12	17:V:380:PHE:HB2	1.91	0.51
17:V:122:LEU:HD23	18:Z:98:ARG:HG3	1.93	0.51
7:6:115:SER:HG	10:9:41:HIS:HD1	1.53	0.51
11:E:74:VAL:HG11	11:E:114:ALA:HB2	1.93	0.51
17:V:220:ARG:NH1	17:V:403:ASP:OD2	2.38	0.51
18:X:425:LEU:HB3	18:X:429:ASP:HB2	1.93	0.51
12:M:101:LYS:NZ	23:M:707:HOH:O	2.42	0.51
13:P:80:LEU:HD21	17:U:59:ILE:HA	1.91	0.51
17:V:207:LYS:H	17:V:486:GLN:HE22	1.58	0.51
18:Y:142:SER:O	18:Y:145:ARG:NH2	2.44	0.51
18:Y:164:ILE:HB	18:Y:167:VAL:HB	1.93	0.51
17:U:531:ALA:HB1	18:X:531:VAL:HG21	1.93	0.51
5:4:145:VAL:HG21	5:4:165:PHE:HA	1.93	0.51
11:A:74:VAL:HG11	11:A:114:ALA:HB2	1.91	0.51
17:U:84:LEU:HG	18:X:563:GLU:HG3	1.92	0.51
17:V:67:ILE:HB	17:V:68:PRO:HD3	1.92	0.51
18:Y:394:ALA:O	18:Y:398:ASN:ND2	2.44	0.51
2:1:404:LYS:NZ	6:5:74:ASN:OD1	2.40	0.51
17:V:226:ASP:O	17:V:231:LYS:NZ	2.43	0.51
16:S:213:PRO:HG3	16:S:244:ARG:HA	1.93	0.50
17:U:304:TYR:OH	17:U:357:LEU:O	2.28	0.50
13:P:40:PRO:HD3	13:P:63:LYS:HE2	1.92	0.50
13:P:195:LEU:O	13:P:211:THR:OG1	2.29	0.50
3:2:173:ARG:HG3	8:7:67:ARG:HH12	1.76	0.50
3:2:240:ALA:H	3:2:243:GLN:HE21	1.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:347:ARG:NH2	18:Z:348:ASP:OD2	2.40	0.50
18:X:75:GLU:OE2	18:X:260:ARG:NE	2.41	0.50
13:P:194:LEU:HD21	13:P:199:VAL:HG13	1.93	0.50
18:X:142:SER:O	18:X:145:ARG:NH2	2.43	0.50
18:X:427:GLU:HA	18:X:430:LYS:HB2	1.94	0.50
18:Y:165:LYS:NZ	18:Y:489:VAL:O	2.36	0.50
2:1:104:ALA:HB1	2:1:294:SER:HB2	1.93	0.50
16:S:308:ILE:HD13	18:Y:304:ILE:HG23	1.94	0.50
2:1:47:VAL:HG23	8:7:103:LEU:HD11	1.94	0.50
17:V:344:PRO:HB3	18:Z:305:PRO:HG3	1.94	0.50
18:Y:111:VAL:HG11	18:Y:264:THR:HG23	1.92	0.50
18:X:422:MET:HG2	18:X:425:LEU:HD12	1.93	0.50
17:U:91:GLY:HA3	18:Z:78:GLN:HG2	1.93	0.49
18:X:145:ARG:HH12	18:X:267:THR:HG23	1.76	0.49
3:2:382:VAL:HG13	3:2:386:LEU:HB2	1.94	0.49
6:5:86:LYS:NZ	8:7:135:ASP:OD1	2.44	0.49
16:S:107:SER:HB2	16:S:116:ASN:HD21	1.76	0.49
2:1:559:GLU:OE2	4:3:207:HIS:NE2	2.40	0.49
16:S:101:VAL:HG11	16:S:182:LEU:HD22	1.94	0.49
18:Y:426:SER:HB2	18:Y:429:ASP:HB2	1.94	0.49
3:2:82:LYS:HA	5:4:84:ARG:HD3	1.93	0.49
18:X:527:LEU:HA	18:X:530:LEU:HD12	1.94	0.49
8:7:170:HIS:CD2	8:7:172:ALA:H	2.30	0.49
17:T:304:TYR:OH	17:T:357:LEU:O	2.29	0.49
3:2:78:VAL:HA	8:7:74:ILE:HB	1.95	0.49
10:9:70:PRO:HA	12:M:264:SER:HA	1.93	0.49
11:C:72:ALA:HB2	11:D:70:ALA:HA	1.93	0.49
3:2:435:LEU:HG	3:2:439:LYS:HE2	1.94	0.49
11:G:72:ALA:HB2	11:H:70:ALA:HA	1.94	0.49
18:X:172:PRO:HG2	18:X:386:MET:HB2	1.94	0.49
1:0:12:PHE:HB3	7:6:75:ALA:HB2	1.95	0.49
13:P:37:LEU:CD1	17:V:73:TRP:CD1	2.95	0.49
17:T:125:ASP:OD1	17:T:125:ASP:N	2.44	0.49
17:U:228:GLN:HE22	18:Z:385:ARG:HH21	1.61	0.49
18:Z:425:LEU:HB2	18:Z:430:LYS:HG3	1.93	0.49
2:1:70:ILE:HG13	2:1:133:ARG:HH11	1.78	0.49
13:P:69:LYS:NZ	17:U:57:TYR:OH	2.39	0.49
16:S:131:GLU:HA	16:S:135:LYS:HE2	1.95	0.49
17:T:342:ARG:NH2	18:X:302:GLY:O	2.46	0.49
2:1:184:LEU:HG	2:1:488:VAL:HG21	1.95	0.49
3:2:16:ASP:OD1	3:2:50:LYS:NZ	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:192:ASN:OD1	5:4:192:ASN:N	2.46	0.49
15:R:49:GLU:HG3	16:S:204:LYS:HB3	1.95	0.49
17:U:155:ILE:HD12	17:U:312:TYR:HB2	1.95	0.48
18:X:166:VAL:HG23	18:X:443:LEU:HD22	1.95	0.48
18:X:290:PHE:O	18:X:294:ASN:ND2	2.42	0.48
18:Z:185:ALA:O	18:Z:366:ARG:NH2	2.46	0.48
3:2:107:VAL:HG12	3:2:146:GLY:HA3	1.94	0.48
11:E:90:ALA:HA	11:F:95:ILE:HD11	1.94	0.48
11:I:75:GLY:HA3	11:J:74:VAL:HG22	1.95	0.48
5:4:187:CYS:HB2	8:7:184:ASN:HD21	1.78	0.48
11:D:74:VAL:HG11	11:D:114:ALA:HB2	1.95	0.48
15:R:117:GLU:HG3	15:R:126:LYS:HG2	1.95	0.48
18:X:249:GLY:HA3	18:X:261:VAL:HG11	1.95	0.48
18:X:406:VAL:HG22	18:X:436:ALA:HB2	1.95	0.48
18:Y:423:ASP:N	18:Y:423:ASP:OD1	2.47	0.48
11:H:118:LEU:HA	11:H:121:VAL:HG22	1.95	0.48
17:V:125:ASP:OD1	17:V:125:ASP:N	2.46	0.48
18:X:465:ASP:HB3	18:X:491:ASP:CG	2.34	0.48
18:Y:286:ASN:HB3	18:Y:289:ARG:HG3	1.95	0.48
18:Z:272:PHE:HD1	18:Z:276:GLU:HG3	1.78	0.48
15:R:104:HIS:HB3	15:R:136:VAL:HG11	1.95	0.48
11:J:54:SER:HB2	11:J:57:ALA:HB3	1.94	0.48
17:V:428:SER:O	17:V:432:SER:OG	2.27	0.48
18:Z:445:GLN:NE2	18:Z:459:LYS:O	2.42	0.48
3:2:420:GLU:OE1	3:2:433:TYR:OH	2.28	0.48
4:3:91:VAL:HG23	4:3:93:GLU:H	1.79	0.48
11:D:90:ALA:HA	11:E:95:ILE:HD11	1.96	0.48
13:P:66:GLN:HE21	13:P:69:LYS:HD3	1.79	0.48
16:S:138:VAL:HG13	16:S:159:GLN:HB2	1.95	0.48
17:U:56:LYS:HD2	17:U:60:GLN:HE21	1.78	0.48
18:Z:564:GLU:HG3	18:Z:566:LYS:HG2	1.95	0.48
16:S:162:ILE:HD13	16:S:178:ILE:HG23	1.96	0.48
18:Y:441:ARG:O	18:Y:444:SER:OG	2.32	0.48
2:1:506:ARG:NH1	2:1:509:GLU:OE1	2.47	0.48
18:Z:66:GLU:HG3	18:Z:101:LYS:HD3	1.96	0.48
2:1:535:HIS:HB3	2:1:540:LEU:HB2	1.96	0.47
10:9:49:VAL:HG23	12:M:259:LEU:HD23	1.95	0.47
18:X:438:LYS:NZ	18:X:481:LEU:O	2.47	0.47
2:1:276:ILE:HD12	2:1:300:LEU:HG	1.97	0.47
10:9:91:LYS:O	10:9:95:LYS:NZ	2.39	0.47
17:T:172:ASP:OD2	17:T:172:ASP:N	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:443:ALA:HA	17:V:446:LEU:HB3	1.95	0.47
18:Y:445:GLN:NE2	18:Y:459:LYS:O	2.43	0.47
18:Z:145:ARG:HA	18:Z:145:ARG:HD3	1.68	0.47
18:X:492:ILE:HD12	18:X:495:VAL:CG1	2.43	0.47
18:X:492:ILE:HD12	18:X:495:VAL:HG11	1.95	0.47
18:Z:419:ILE:HG13	18:Z:420:LEU:HG	1.95	0.47
1:0:51:PRO:HD2	1:0:54:TYR:HB2	1.96	0.47
9:8:26:HIS:HB3	9:8:29:GLN:HG3	1.97	0.47
11:E:91:ARG:HB3	15:R:96:GLY:HA3	1.97	0.47
17:T:265:LYS:NZ	18:X:359:ASP:OD1	2.45	0.47
17:T:314:ARG:NH1	17:T:364:ARG:O	2.47	0.47
17:U:516:ASP:N	17:U:516:ASP:OD2	2.47	0.47
16:S:197:PHE:N	16:S:261:GLU:OE1	2.40	0.47
17:T:326:ASP:H	17:T:382:VAL:HB	1.79	0.47
18:Y:183:GLY:HA2	18:Y:364:LEU:HB2	1.96	0.47
18:Y:322:GLN:OE1	18:Y:337:GLN:NE2	2.38	0.47
4:3:187:PHE:O	4:3:189:HIS:N	2.48	0.47
11:J:74:VAL:HG11	11:J:114:ALA:HB2	1.95	0.47
6:5:83:THR:O	8:7:119:TYR:OH	2.23	0.47
12:M:95:SER:OG	12:M:96:SER:N	2.48	0.47
17:U:92:ASP:OD1	18:Z:78:GLN:NE2	2.47	0.47
11:G:93:PRO:HG3	11:H:95:ILE:HD13	1.97	0.47
13:P:73:GLU:OE2	17:U:57:TYR:OH	2.27	0.47
17:V:152:ASN:HD22	17:V:182:SER:HB2	1.79	0.47
2:1:186:LEU:HD13	2:1:440:LEU:HB2	1.96	0.47
3:2:356:TYR:HB3	3:2:368:ILE:HA	1.97	0.47
11:E:115:LEU:HD22	12:M:250:LEU:HD13	1.96	0.47
13:P:150:LYS:HB3	13:P:182:PHE:HD2	1.79	0.47
15:R:175:GLU:HA	15:R:178:GLN:HG2	1.97	0.47
17:U:251:LYS:HG2	18:X:543:ASP:HA	1.97	0.47
18:X:486:PHE:CD2	18:X:495:VAL:HG21	2.49	0.47
18:Y:311:GLN:HG3	18:Y:314:LEU:HB2	1.97	0.47
18:Z:514:ASN:OD1	18:Z:514:ASN:N	2.48	0.47
6:5:75:GLN:HA	6:5:78:GLU:HG2	1.97	0.47
16:S:308:ILE:HD11	18:Y:305:PRO:HD2	1.97	0.47
3:2:360:ALA:HB2	3:2:366:LEU:HD21	1.96	0.46
6:5:3:LEU:HD11	11:E:123:LEU:HD11	1.97	0.46
12:M:163:ASN:HB3	12:M:292:ALA:HB1	1.97	0.46
17:U:226:ASP:O	17:U:231:LYS:NZ	2.46	0.46
11:F:78:LEU:HB3	11:G:110:THR:HG22	1.96	0.46
11:H:86:ILE:HG21	11:I:85:LEU:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:239:ILE:HD11	17:U:323:ILE:HD13	1.96	0.46
18:Y:132:GLN:HE22	18:Y:235:LEU:HD13	1.79	0.46
5:4:64:GLU:HG2	17:T:55:SER:HB2	1.97	0.46
11:D:71:LEU:HD12	11:E:117:SER:HB3	1.97	0.46
11:G:78:LEU:HB3	11:H:110:THR:HG22	1.97	0.46
18:X:225:ARG:HA	18:X:225:ARG:HD3	1.77	0.46
18:Y:505:ASP:N	18:Y:505:ASP:OD1	2.48	0.46
2:1:245:ALA:HB1	2:1:498:LEU:HD13	1.98	0.46
11:I:86:ILE:HG21	11:J:85:LEU:HA	1.97	0.46
17:U:339:LEU:HD21	17:U:345:PRO:HB3	1.97	0.46
2:1:252:ARG:HG3	2:1:505:ILE:HG21	1.98	0.46
5:4:178:LEU:HD11	8:7:183:THR:HG21	1.97	0.46
18:X:246:LEU:HD13	18:X:248:TYR:HE2	1.80	0.46
4:3:213:ARG:NH1	12:M:143:ASP:OD1	2.49	0.46
4:3:318:ILE:HD11	12:M:321:LYS:HE2	1.97	0.46
11:B:119:LEU:O	11:B:123:LEU:N	2.48	0.46
14:Q:32:LYS:O	14:Q:36:LYS:N	2.41	0.46
17:U:89:SER:OG	17:U:96:ARG:NH2	2.42	0.46
18:X:307:ALA:O	18:X:309:GLY:N	2.39	0.46
18:Z:290:PHE:O	18:Z:294:ASN:ND2	2.45	0.46
8:7:86:HIS:HE1	8:7:155:SER:HB3	1.81	0.46
18:Y:284:VAL:HB	18:Y:337:GLN:HG2	1.98	0.46
18:Z:284:VAL:HG11	18:Z:287:ILE:HD13	1.96	0.46
11:I:72:ALA:HB2	11:J:70:ALA:HA	1.98	0.46
11:F:72:ALA:HB2	11:G:70:ALA:HA	1.98	0.46
17:V:235:ALA:HB1	17:V:323:ILE:HD13	1.97	0.46
7:6:143:LEU:HD12	7:6:143:LEU:HA	1.73	0.46
11:G:85:LEU:HD21	11:G:100:VAL:HG12	1.97	0.46
13:P:39:LEU:HD23	13:P:39:LEU:N	2.31	0.46
13:P:57:LEU:HD13	13:P:121:LEU:HD22	1.98	0.45
17:U:92:ASP:OD2	18:Z:303:ARG:NH2	2.49	0.45
18:X:416:ILE:HD11	18:X:425:LEU:HD21	1.98	0.45
18:X:508:SER:OG	18:X:509:ARG:N	2.47	0.45
18:Z:213:VAL:HG22	18:Z:261:VAL:HG13	1.97	0.45
18:Z:407:LEU:HG	18:Z:439:ILE:HD11	1.97	0.45
11:B:59:SER:HA	11:B:62:VAL:HG12	1.98	0.45
14:Q:54:ASP:OD1	14:Q:54:ASP:N	2.48	0.45
17:V:123:GLN:O	18:Z:98:ARG:NH1	2.42	0.45
18:X:387:LEU:HD12	18:X:387:LEU:HA	1.84	0.45
18:Z:373:ILE:HG23	18:Z:444:SER:HB2	1.98	0.45
6:5:27:ASP:OD2	9:8:44:HIS:NE2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:202:LEU:HD13	17:U:378:THR:HG21	1.99	0.45
17:V:334:TYR:OH	17:V:353:ASP:OD2	2.29	0.45
17:V:549:HIS:HB3	18:Z:527:LEU:HD12	1.99	0.45
18:Z:215:GLU:OE2	18:Z:286:ASN:ND2	2.37	0.45
2:1:568:ASP:HB2	2:1:580:LYS:HE3	1.99	0.45
6:5:5:PRO:O	9:8:65:ARG:NH1	2.49	0.45
17:V:547:ASP:N	17:V:547:ASP:OD1	2.49	0.45
5:4:260:LYS:HG2	5:4:261:GLY:H	1.82	0.45
13:P:64:GLU:OE2	17:V:70:VAL:CA	2.59	0.45
16:S:215:LEU:O	16:S:219:GLN:NE2	2.50	0.45
18:Z:111:VAL:HG11	18:Z:264:THR:HG23	1.98	0.45
6:5:91:HIS:ND1	8:7:138:TYR:OH	2.32	0.45
11:B:80:VAL:HG22	11:C:80:VAL:HG11	1.98	0.45
17:U:240:ILE:HD12	17:U:279:THR:HG21	1.98	0.45
17:V:345:PRO:HB2	17:V:349:ALA:HA	1.99	0.45
18:Y:170:LEU:HD22	18:Y:404:GLN:HG3	1.98	0.45
18:Y:325:ILE:HG23	18:Y:333:ILE:HG22	1.99	0.45
18:Z:557:GLU:HG3	18:Z:569:PRO:HB3	1.98	0.45
12:M:155:PHE:HA	12:M:158:THR:HG22	1.98	0.45
13:P:44:LEU:CD2	13:P:44:LEU:N	2.80	0.45
18:X:499:ALA:HA	18:X:502:MET:HB2	1.98	0.45
18:Y:233:ILE:HD11	18:Y:246:LEU:HD13	1.98	0.45
17:T:323:ILE:HG12	17:T:380:PHE:HB2	1.99	0.45
13:P:40:PRO:CG	13:P:62:ALA:HB3	2.46	0.44
16:S:119:ILE:HA	16:S:122:TYR:HB2	1.99	0.44
17:T:202:LEU:HD22	17:T:378:THR:HG21	1.99	0.44
17:T:442:VAL:HG12	17:T:501:VAL:HG12	1.99	0.44
6:5:62:TYR:OH	7:6:146:PHE:O	2.22	0.44
3:2:189:ASP:OD1	3:2:192:THR:OG1	2.34	0.44
9:8:26:HIS:CD2	9:8:28:PHE:H	2.35	0.44
11:E:72:ALA:HB2	11:F:70:ALA:HA	1.99	0.44
17:U:216:GLY:N	17:U:219:GLN:OE1	2.50	0.44
17:U:311:GLU:OE1	17:U:364:ARG:NE	2.44	0.44
18:Z:245:THR:HG21	18:Z:268:VAL:HG11	1.99	0.44
18:Z:249:GLY:HA3	18:Z:261:VAL:HG11	1.99	0.44
11:G:59:SER:HA	11:G:62:VAL:HG12	2.00	0.44
17:T:547:ASP:N	17:T:547:ASP:OD1	2.48	0.44
18:Z:281:LEU:HD23	18:Z:334:THR:HB	2.00	0.44
2:1:454:ALA:HA	2:1:457:GLU:HG2	1.98	0.44
3:2:67:THR:HG22	3:2:106:VAL:HG23	1.99	0.44
14:Q:18:ARG:NH2	16:S:180:GLU:OE1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:206:VAL:HA	17:V:486:GLN:HE22	1.83	0.44
18:Z:120:ARG:NH2	18:Z:133:GLY:O	2.42	0.44
5:4:6:VAL:HG13	5:4:10:GLU:HB2	1.99	0.44
7:6:132:MET:HB3	12:M:112:GLY:HA3	2.00	0.44
11:B:104:LEU:HA	11:B:107:PHE:HB3	1.99	0.44
15:R:45:LEU:HD21	16:S:121:LYS:HE2	2.00	0.44
17:V:511:LYS:HG3	17:V:562:ALA:HB1	1.99	0.44
18:X:72:LEU:HD11	18:X:89:ALA:HB1	2.00	0.44
18:X:130:ASP:OD1	18:X:130:ASP:N	2.51	0.44
18:X:289:ARG:NH1	18:X:292:GLN:OE1	2.50	0.44
3:2:25:SER:OG	3:2:26:ALA:N	2.51	0.44
3:2:416:VAL:HG23	3:2:433:TYR:HE1	1.83	0.44
5:4:101:PRO:HG3	8:7:170:HIS:CD2	2.52	0.44
5:4:141:VAL:HG21	5:4:172:VAL:HG21	1.99	0.44
11:H:111:GLU:O	11:H:114:ALA:N	2.51	0.44
17:T:367:LYS:HD2	17:T:376:SER:HB3	1.99	0.44
17:V:417:ILE:HA	17:V:485:LYS:HD2	1.98	0.44
18:X:478:TYR:HB3	18:X:481:LEU:HD12	1.99	0.44
18:Z:394:ALA:O	18:Z:398:ASN:ND2	2.50	0.44
11:E:103:ALA:O	11:E:107:PHE:N	2.45	0.44
16:S:92:PHE:HB2	16:S:211:LEU:HD11	2.00	0.44
16:S:127:LEU:HD11	16:S:137:VAL:HG11	2.00	0.44
17:T:443:ALA:HA	17:T:446:LEU:HB3	2.00	0.44
17:V:460:ALA:HB1	17:V:474:LEU:HD21	2.00	0.44
18:Y:97:VAL:HB	18:Y:100:GLN:HG3	1.99	0.44
6:5:51:TYR:HE2	7:6:143:LEU:HD13	1.82	0.43
14:Q:28:ARG:HB3	14:Q:39:ALA:HB1	2.00	0.43
17:U:220:ARG:NH2	17:U:401:ILE:O	2.50	0.43
18:Y:65:VAL:HG11	18:Y:96:LEU:HD11	2.00	0.43
3:2:67:THR:HG21	3:2:102:GLN:HB3	2.00	0.43
5:4:277:TRP:HE1	17:T:41:ASP:HA	1.83	0.43
11:B:111:GLU:O	11:B:114:ALA:N	2.51	0.43
8:7:69:LEU:HD12	8:7:69:LEU:HA	1.89	0.43
18:X:402:GLY:HA3	18:X:474:LEU:HD21	2.01	0.43
11:G:86:ILE:HG21	11:H:85:LEU:HA	2.00	0.43
11:G:90:ALA:HA	11:H:95:ILE:HD11	2.00	0.43
5:4:190:SER:OG	5:4:191:ALA:N	2.52	0.43
16:S:212:SER:HB3	16:S:215:LEU:HB2	1.99	0.43
17:T:79:PRO:HA	17:T:80:PRO:HD3	1.87	0.43
17:T:389:ASP:OD1	17:T:391:SER:OG	2.34	0.43
17:U:100:LEU:HD13	17:U:103:VAL:HG11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:373:ILE:HG23	18:X:444:SER:HB3	2.00	0.43
6:5:48:ALA:O	6:5:52:ASN:ND2	2.36	0.43
11:H:92:ASN:N	11:H:92:ASN:OD1	2.50	0.43
17:V:64:GLN:NE2	17:V:79:PRO:HG2	2.33	0.43
2:1:195:LYS:HA	2:1:195:LYS:HD3	1.85	0.43
11:G:71:LEU:HD11	11:G:118:LEU:HD21	2.00	0.43
12:M:248:HIS:HD2	23:M:718:HOH:O	2.00	0.43
17:U:121:ASN:HB2	18:X:44:ILE:HG12	2.01	0.43
17:V:92:ASP:HB2	17:V:340:LEU:HD13	2.00	0.43
17:V:367:LYS:NZ	17:V:374:GLY:O	2.44	0.43
18:X:273:ARG:HD3	18:X:333:ILE:HG13	2.01	0.43
11:H:74:VAL:HG11	11:H:114:ALA:HB2	1.99	0.43
13:P:71:GLN:OE1	13:P:145:MET:HE2	2.18	0.43
16:S:62:MET:HB2	17:T:459:PHE:HZ	1.84	0.43
17:T:156:GLY:O	17:T:159:THR:OG1	2.33	0.43
17:T:440:LYS:HB2	17:T:440:LYS:HE3	1.83	0.43
18:X:272:PHE:HD1	18:X:276:GLU:HG3	1.83	0.43
18:Z:74:LEU:HB3	18:Z:87:CYS:HB3	2.00	0.43
3:2:78:VAL:HG22	8:7:74:ILE:HG13	2.01	0.43
18:Z:266:LEU:O	18:Z:270:GLU:N	2.43	0.43
3:2:426:ASP:OD1	3:2:426:ASP:N	2.49	0.43
4:3:116:THR:OG1	4:3:117:SER:N	2.52	0.43
8:7:149:SER:H	8:7:149:SER:HG	1.62	0.43
11:B:120:VAL:HA	11:B:123:LEU:HB3	2.00	0.43
13:P:42:ALA:CB	13:P:55:THR:HG23	2.49	0.43
13:P:121:LEU:HB2	17:V:66:LEU:HD21	2.00	0.43
16:S:60:MET:HE3	16:S:60:MET:HB3	1.85	0.43
16:S:124:ARG:HD2	16:S:153:ILE:HD11	2.00	0.43
5:4:66:GLY:HA3	5:4:92:LEU:HD13	2.00	0.42
11:B:111:GLU:OE2	11:B:111:GLU:HA	2.19	0.42
12:M:200:THR:OG1	12:M:201:GLY:N	2.52	0.42
12:M:251:LEU:HD21	12:M:285:VAL:HG22	2.01	0.42
13:P:149:LYS:HB2	13:P:149:LYS:NZ	2.34	0.42
15:R:90:VAL:HB	15:R:117:GLU:HB3	2.00	0.42
16:S:211:LEU:HD22	16:S:216:LEU:HD23	2.00	0.42
17:T:123:GLN:O	18:Y:98:ARG:NH2	2.48	0.42
17:T:268:THR:OG1	18:X:385:ARG:NH1	2.46	0.42
17:T:370:LYS:HA	17:T:370:LYS:HD3	1.80	0.42
18:Z:519:GLU:HA	18:Z:522:LYS:HE2	2.00	0.42
17:T:227:ARG:HH22	18:X:346:LEU:HD13	1.84	0.42
17:V:70:VAL:HG12	17:V:72:GLU:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:65:GLY:HA2	11:H:67:ALA:HB2	2.00	0.42
15:R:58:LYS:O	15:R:139:ASN:ND2	2.52	0.42
17:T:55:SER:O	17:T:57:TYR:N	2.50	0.42
17:V:370:LYS:HA	17:V:370:LYS:HD3	1.74	0.42
18:X:96:LEU:HD23	18:X:96:LEU:HA	1.91	0.42
18:Z:307:ALA:O	18:Z:309:GLY:N	2.46	0.42
2:1:62:LYS:HD2	2:1:144:ALA:HB3	2.01	0.42
2:1:310:THR:HG21	2:1:337:PRO:HB3	2.01	0.42
13:P:150:LYS:CA	13:P:182:PHE:HD2	2.32	0.42
15:R:88:THR:HB	15:R:119:HIS:HB2	2.00	0.42
16:S:95:VAL:HB	16:S:216:LEU:HD21	2.01	0.42
17:T:227:ARG:NH2	18:X:381:ASP:OD1	2.52	0.42
17:V:67:ILE:N	17:V:68:PRO:CD	2.82	0.42
18:Z:392:ILE:HB	18:Z:396:HIS:HD1	1.84	0.42
2:1:568:ASP:OD2	6:5:38:HIS:NE2	2.43	0.42
3:2:45:ARG:NH2	8:7:74:ILE:O	2.47	0.42
5:4:71:ALA:HB2	8:7:84:VAL:HG12	2.01	0.42
11:A:99:LEU:HD22	11:J:86:ILE:HG23	2.00	0.42
17:T:327:LEU:HD22	17:T:381:PRO:HB3	2.01	0.42
4:3:173:GLU:HA	4:3:206:ASN:HD21	1.84	0.42
6:5:26:LEU:HD21	12:M:153:THR:HG23	2.01	0.42
8:7:23:LEU:HD23	8:7:23:LEU:HA	1.79	0.42
17:T:552:ALA:O	17:T:556:LYS:NZ	2.49	0.42
18:Z:175:ARG:O	18:Z:334:THR:OG1	2.28	0.42
18:X:124:VAL:HG13	18:X:125:ILE:HG23	2.01	0.42
18:Z:503:ALA:HA	18:Z:506:ILE:HG12	2.01	0.42
2:1:574:MET:HB2	12:M:126:PRO:HD3	2.02	0.42
2:1:605:LYS:O	2:1:605:LYS:HG2	2.20	0.42
3:2:336:ALA:HA	3:2:339:VAL:HG12	2.02	0.42
6:5:91:HIS:CG	8:7:111:THR:HG21	2.55	0.42
7:6:76:LYS:HB2	7:6:76:LYS:HE3	1.89	0.42
13:P:150:LYS:CA	13:P:182:PHE:CD2	3.03	0.42
15:R:177:GLU:O	15:R:181:ASN:N	2.52	0.42
18:X:227:MET:HE1	18:X:246:LEU:HD21	2.02	0.42
11:G:86:ILE:HG23	11:H:99:LEU:HB3	2.01	0.42
13:P:63:LYS:HE3	17:V:73:TRP:CH2	2.55	0.42
13:P:208:ASP:HB3	13:P:213:LYS:HD2	2.02	0.42
18:Y:346:LEU:HD22	18:Y:355:PHE:HE1	1.85	0.42
5:4:141:VAL:HG13	5:4:168:LYS:HE2	2.01	0.42
8:7:173:ILE:HD12	8:7:173:ILE:HA	1.90	0.42
13:P:150:LYS:CB	13:P:182:PHE:HD2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:466:LEU:CD2	17:T:470:THR:CG2	2.91	0.42
17:U:146:ARG:HG2	18:X:561:LEU:HD12	2.01	0.42
17:V:429:ARG:HD2	18:Z:453:PHE:HB2	2.01	0.42
18:X:36:ASP:OD1	18:X:36:ASP:N	2.51	0.42
3:2:62:ASP:OD1	3:2:62:ASP:N	2.43	0.41
4:3:110:LEU:HB3	4:3:115:PHE:HB3	2.01	0.41
13:P:103:LYS:HD3	13:P:103:LYS:HA	1.83	0.41
17:U:446:LEU:HD13	17:U:480:LEU:HD22	2.02	0.41
17:V:495:GLU:HG3	17:V:533:PHE:HB3	2.02	0.41
11:C:74:VAL:HG11	11:C:114:ALA:HB2	2.02	0.41
15:R:86:LYS:HG3	15:R:118:LEU:HD12	2.01	0.41
16:S:99:LYS:HB3	16:S:187:PRO:HA	2.02	0.41
17:T:520:ALA:HB2	17:T:559:LEU:HD13	2.02	0.41
18:Z:491:ASP:H	18:Z:494:GLU:HG3	1.86	0.41
9:8:82:THR:HA	9:8:83:PRO:HD3	1.92	0.41
14:Q:48:ARG:HB2	14:Q:62:VAL:HG22	2.01	0.41
3:2:289:HIS:HB2	3:2:307:VAL:HG12	2.02	0.41
6:5:26:LEU:HA	6:5:30:LEU:HB2	2.02	0.41
11:E:62:VAL:HG23	11:F:59:SER:HB2	2.01	0.41
17:U:400:SER:HB2	18:X:289:ARG:HH22	1.85	0.41
17:V:150:ILE:HB	17:V:184:LEU:HD22	2.03	0.41
17:V:235:ALA:HB1	17:V:323:ILE:HG21	2.01	0.41
18:X:245:THR:HG21	18:X:268:VAL:HG11	2.02	0.41
18:Y:491:ASP:OD1	18:Y:491:ASP:N	2.53	0.41
5:4:159:THR:HG22	5:4:161:GLY:H	1.85	0.41
13:P:150:LYS:HB3	13:P:182:PHE:HA	2.02	0.41
13:P:155:THR:HA	13:P:187:GLN:HB3	2.02	0.41
18:Z:341:VAL:HA	18:Z:342:PRO:HD3	1.77	0.41
16:S:310:GLY:HA2	17:U:345:PRO:HD2	2.02	0.41
17:T:243:LYS:HB3	17:T:243:LYS:HE3	1.74	0.41
17:V:476:ARG:NH1	17:V:505:THR:O	2.40	0.41
2:1:362:LEU:HD23	2:1:362:LEU:HA	1.86	0.41
11:F:115:LEU:HA	11:F:118:LEU:HB2	2.02	0.41
11:J:115:LEU:HA	11:J:118:LEU:HB2	2.03	0.41
12:M:199:LYS:HD2	12:M:199:LYS:HA	1.84	0.41
16:S:102:VAL:HG21	16:S:127:LEU:HD13	2.03	0.41
2:1:517:GLU:HA	9:8:2:VAL:HG12	2.02	0.41
18:Y:96:LEU:HD12	18:Y:96:LEU:HA	1.94	0.41
18:Z:72:LEU:HD11	18:Z:89:ALA:HB1	2.02	0.41
3:2:42:LYS:NZ	8:7:69:LEU:O	2.45	0.41
6:5:44:TRP:CE3	7:6:142:GLY:HA3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:125:LEU:HD23	11:G:125:LEU:HA	1.94	0.41
16:S:123:THR:O	16:S:127:LEU:N	2.47	0.41
18:X:550:LYS:HB3	18:X:550:LYS:HE2	1.76	0.41
3:2:176:ALA:HB2	3:2:200:PHE:HZ	1.86	0.41
16:S:60:MET:HE1	16:S:111:LEU:HD13	2.03	0.41
17:U:345:PRO:HB2	17:U:349:ALA:HA	2.03	0.41
3:2:372:LYS:HB3	3:2:372:LYS:HE2	1.87	0.40
5:4:72:LEU:HD13	5:4:222:ILE:HG21	2.02	0.40
11:F:118:LEU:HD23	11:F:118:LEU:HA	1.94	0.40
18:Y:194:MET:HA	18:Y:197:ILE:HD12	2.02	0.40
18:Z:65:VAL:HG22	18:Z:102:VAL:HG22	2.02	0.40
3:2:62:ASP:OD1	3:2:65:SER:OG	2.34	0.40
13:P:71:GLN:OE1	13:P:145:MET:HE1	2.20	0.40
4:3:94:ASN:HA	4:3:97:ASN:HB2	2.03	0.40
11:D:75:GLY:HA3	11:E:74:VAL:HG22	2.04	0.40
11:F:113:ILE:HA	11:F:116:PHE:HB2	2.02	0.40
15:R:34:THR:HG22	15:R:47:VAL:HG21	2.03	0.40
16:S:246:LEU:O	16:S:250:HIS:N	2.52	0.40
17:T:269:VAL:HG23	18:X:150:PHE:HE2	1.87	0.40
20:U:1001:ATP:O2A	18:Z:385:ARG:NH2	2.40	0.40
17:V:172:ASP:OD1	17:V:172:ASP:N	2.49	0.40
17:V:452:GLN:HG3	17:V:473:VAL:HG21	2.03	0.40
18:Y:225:ARG:HA	18:Y:225:ARG:HD3	1.90	0.40
4:3:222:LEU:HD23	4:3:240:VAL:HG21	2.04	0.40
17:V:412:LEU:HB2	17:V:420:ALA:HB1	2.04	0.40
18:X:346:LEU:HD22	18:X:355:PHE:HZ	1.86	0.40
18:Y:245:THR:HG21	18:Y:268:VAL:HG11	2.02	0.40
18:Z:189:LYS:HD2	18:Z:338:ALA:HB1	2.04	0.40
9:8:36:ALA:HA	9:8:40:LEU:HB3	2.01	0.40
17:U:495:GLU:HG3	17:U:533:PHE:HB3	2.04	0.40
17:V:123:GLN:HA	18:Z:42:GLN:HB2	2.02	0.40
17:V:207:LYS:HG3	17:V:492:ILE:HD12	2.04	0.40
18:Y:348:ASP:HB3	18:Y:351:PRO:HD2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
2	1	593/618 (96%)	573 (97%)	20 (3%)	0	100	100
3	2	439/441 (100%)	410 (93%)	28 (6%)	1 (0%)	47	79
4	3	243/325 (75%)	236 (97%)	7 (3%)	0	100	100
5	4	288/294 (98%)	275 (96%)	13 (4%)	0	100	100
6	5	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	19	54
7	6	122/151 (81%)	111 (91%)	11 (9%)	0	100	100
8	7	174/190 (92%)	171 (98%)	3 (2%)	0	100	100
9	8	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
10	9	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
11	A	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	B	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	C	71/127 (56%)	70 (99%)	1 (1%)	0	100	100
11	D	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	E	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	F	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	G	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	H	72/127 (57%)	72 (100%)	0	0	100	100
11	I	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
12	M	213/327 (65%)	205 (96%)	8 (4%)	0	100	100
13	P	191/229 (83%)	176 (92%)	14 (7%)	1 (0%)	29	64
14	Q	70/74 (95%)	67 (96%)	2 (3%)	1 (1%)	11	40
15	R	175/199 (88%)	166 (95%)	9 (5%)	0	100	100
16	S	275/317 (87%)	265 (96%)	9 (3%)	1 (0%)	34	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	521/562 (93%)	494 (95%)	24 (5%)	3 (1%)	25	59
17	U	521/562 (93%)	492 (94%)	29 (6%)	0	100	100
17	V	518/562 (92%)	491 (95%)	27 (5%)	0	100	100
18	X	537/574 (94%)	508 (95%)	27 (5%)	2 (0%)	34	69
18	Y	519/574 (90%)	496 (96%)	21 (4%)	2 (0%)	34	69
18	Z	540/574 (94%)	505 (94%)	32 (6%)	3 (1%)	25	59
All	All	7039/8234 (86%)	6695 (95%)	329 (5%)	15 (0%)	50	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	T	468	ALA
18	X	308	VAL
18	Y	308	VAL
18	Z	308	VAL
3	2	383	PRO
13	P	186	MET
14	Q	60	SER
17	T	56	LYS
17	T	465	ASP
18	X	307	ALA
18	Z	525	PRO
6	5	120	PRO
16	S	213	PRO
18	Y	309	GLY
18	Z	309	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	493 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	312/312 (100%)	312 (100%)	0	100	100
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
6	5	107/107 (100%)	107 (100%)	0	100	100
7	6	96/115 (84%)	96 (100%)	0	100	100
8	7	140/150 (93%)	140 (100%)	0	100	100
9	8	71/72 (99%)	71 (100%)	0	100	100
10	9	79/79 (100%)	79 (100%)	0	100	100
11	A	50/86 (58%)	50 (100%)	0	100	100
11	B	50/86 (58%)	50 (100%)	0	100	100
11	C	50/86 (58%)	50 (100%)	0	100	100
11	D	50/86 (58%)	50 (100%)	0	100	100
11	E	50/86 (58%)	50 (100%)	0	100	100
11	F	50/86 (58%)	50 (100%)	0	100	100
11	G	50/86 (58%)	50 (100%)	0	100	100
11	H	50/86 (58%)	50 (100%)	0	100	100
11	I	50/86 (58%)	50 (100%)	0	100	100
11	J	50/86 (58%)	50 (100%)	0	100	100
12	M	178/272 (65%)	178 (100%)	0	100	100
13	P	171/196 (87%)	171 (100%)	0	100	100
14	Q	56/58 (97%)	55 (98%)	1 (2%)	59	82
15	R	134/151 (89%)	134 (100%)	0	100	100
16	S	235/265 (89%)	235 (100%)	0	100	100
17	T	419/448 (94%)	416 (99%)	3 (1%)	84	93
17	U	419/448 (94%)	416 (99%)	3 (1%)	84	93
17	V	418/448 (93%)	414 (99%)	4 (1%)	76	90
18	X	447/469 (95%)	447 (100%)	0	100	100
18	Y	430/469 (92%)	430 (100%)	0	100	100
18	Z	449/469 (96%)	449 (100%)	0	100	100
All	All	5632/6445 (87%)	5621 (100%)	11 (0%)	93	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	Q	60	SER
17	T	220	ARG
17	T	300	PHE
17	T	559	LEU
17	U	220	ARG
17	U	378	THR
17	U	418	ARG
17	V	66	LEU
17	V	81	VAL
17	V	180	VAL
17	V	300	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	48	ASN
1	0	60	GLN
1	0	61	HIS
2	1	48	ASN
2	1	285	GLN
2	1	298	GLN
2	1	316	ASN
2	1	482	ASN
2	1	587	ASN
2	1	590	HIS
3	2	68	ASN
3	2	122	ASN
3	2	243	GLN
3	2	289	HIS
3	2	380	GLN
4	3	189	HIS
4	3	206	ASN
5	4	240	GLN
6	5	107	ASN
7	6	40	ASN
7	6	74	GLN
7	6	104	ASN
8	7	86	HIS
8	7	123	HIS
8	7	170	HIS
8	7	184	ASN
9	8	26	HIS
11	G	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I	94	ASN
11	J	92	ASN
11	J	94	ASN
12	M	108	ASN
12	M	163	ASN
13	P	52	GLN
13	P	66	GLN
13	P	223	ASN
14	Q	46	HIS
15	R	73	ASN
15	R	83	GLN
15	R	85	GLN
15	R	137	HIS
15	R	154	GLN
16	S	262	ASN
17	T	64	GLN
17	T	386	GLN
17	U	60	GLN
17	U	242	GLN
17	U	497	GLN
17	U	539	ASN
17	V	64	GLN
17	V	123	GLN
17	V	139	HIS
17	V	152	ASN
17	V	196	GLN
17	V	242	GLN
17	V	386	GLN
17	V	435	GLN
17	V	461	GLN
17	V	486	GLN
17	V	497	GLN
18	Y	132	GLN
18	Y	199	ASN
18	Y	252	ASN
18	Y	278	GLN
18	Y	294	ASN
18	Y	404	GLN
18	Z	42	GLN
18	Z	144	HIS
18	Z	199	ASN
18	Z	337	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	Z	388	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
20	ATP	T	1001	21	26,33,33	0.97	1 (3%)	31,52,52	1.36	5 (16%)
22	ADP	X	601	21	24,29,29	0.98	1 (4%)	29,45,45	1.37	5 (17%)
20	ATP	V	1001	21	26,33,33	0.94	0	31,52,52	1.36	5 (16%)
20	ATP	U	1001	21	26,33,33	0.94	1 (3%)	31,52,52	1.44	5 (16%)
22	ADP	Z	601	21	24,29,29	0.99	2 (8%)	29,45,45	1.32	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
20	ATP	T	1001	21	-	0/18/38/38	0/3/3/3
22	ADP	X	601	21	-	3/12/32/32	0/3/3/3
20	ATP	V	1001	21	-	2/18/38/38	0/3/3/3
20	ATP	U	1001	21	-	0/18/38/38	0/3/3/3
22	ADP	Z	601	21	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	601	ADP	C2'-C1'	-2.09	1.50	1.53
22	Z	601	ADP	C5-C4	2.04	1.46	1.40
20	T	1001	ATP	C5-C4	2.01	1.46	1.40
22	X	601	ADP	C2'-C1'	-2.01	1.50	1.53
20	U	1001	ATP	C5-C4	2.01	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	V	1001	ATP	N3-C2-N1	-3.59	123.06	128.68
20	U	1001	ATP	N3-C2-N1	-3.39	123.39	128.68
22	Z	601	ADP	C3'-C2'-C1'	3.33	105.99	100.98
22	X	601	ADP	N3-C2-N1	-3.23	123.63	128.68
20	T	1001	ATP	N3-C2-N1	-3.19	123.69	128.68
22	Z	601	ADP	N3-C2-N1	-3.09	123.84	128.68
22	X	601	ADP	PA-O3A-PB	-2.98	122.61	132.83
22	X	601	ADP	C3'-C2'-C1'	2.90	105.34	100.98
20	V	1001	ATP	PA-O3A-PB	-2.88	122.95	132.83
20	U	1001	ATP	PB-O3B-PG	-2.63	123.81	132.83
20	U	1001	ATP	C4-C5-N7	-2.57	106.72	109.40
20	U	1001	ATP	C3'-C2'-C1'	2.51	104.76	100.98
20	T	1001	ATP	PA-O3A-PB	-2.34	124.78	132.83
20	T	1001	ATP	PB-O3B-PG	-2.33	124.81	132.83
22	X	601	ADP	C4-C5-N7	-2.32	106.98	109.40
20	V	1001	ATP	C3'-C2'-C1'	2.31	104.45	100.98
20	T	1001	ATP	C4-C5-N7	-2.29	107.01	109.40
20	U	1001	ATP	PA-O3A-PB	-2.26	125.06	132.83
20	V	1001	ATP	C4-C5-N7	-2.24	107.06	109.40
22	Z	601	ADP	PA-O3A-PB	-2.14	125.49	132.83
22	X	601	ADP	O3B-PB-O2B	2.11	115.69	107.64
20	T	1001	ATP	C2'-C3'-C4'	2.10	106.71	102.64
20	V	1001	ATP	C2-N1-C6	2.04	122.25	118.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	X	601	ADP	C5'-O5'-PA-O1A
22	Z	601	ADP	C5'-O5'-PA-O2A
22	Z	601	ADP	C5'-O5'-PA-O3A
20	V	1001	ATP	O4'-C4'-C5'-O5'
22	Z	601	ADP	C3'-C4'-C5'-O5'
22	Z	601	ADP	O4'-C4'-C5'-O5'
22	X	601	ADP	C5'-O5'-PA-O3A
20	V	1001	ATP	C3'-C4'-C5'-O5'
22	X	601	ADP	C5'-O5'-PA-O2A
22	Z	601	ADP	C5'-O5'-PA-O1A

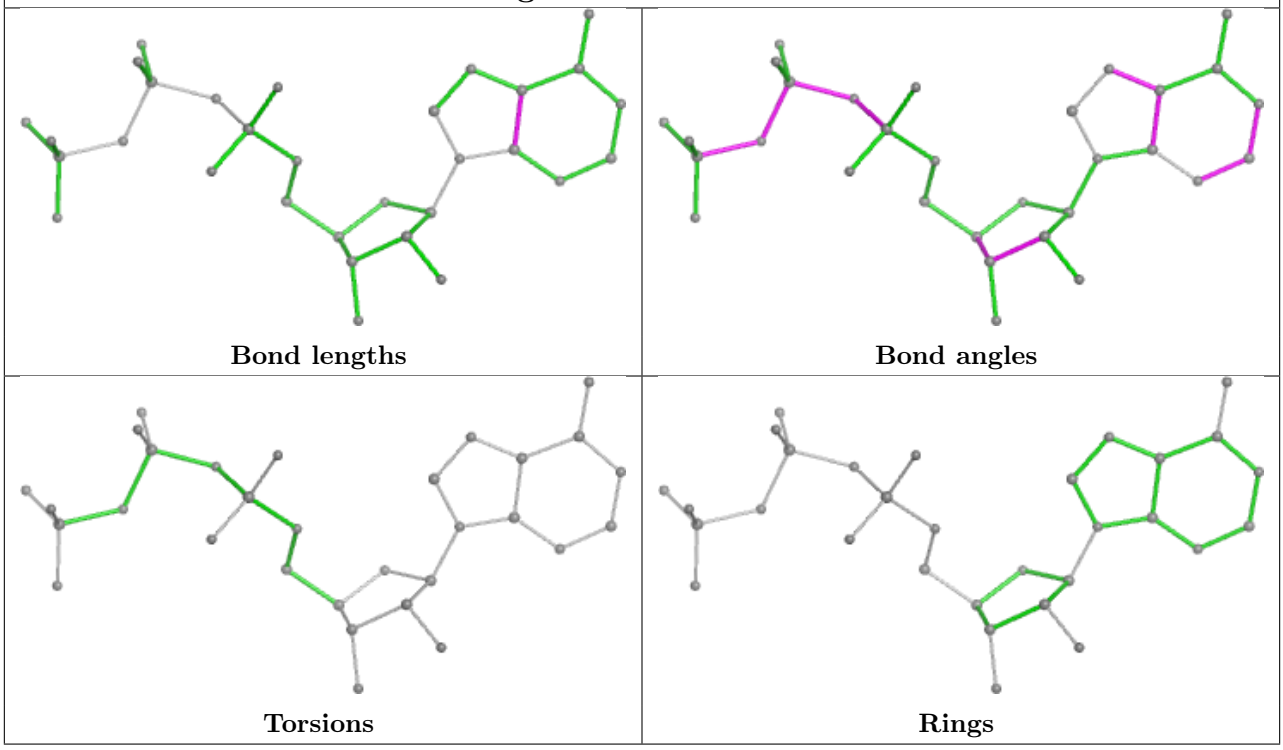
There are no ring outliers.

2 monomers are involved in 2 short contacts:

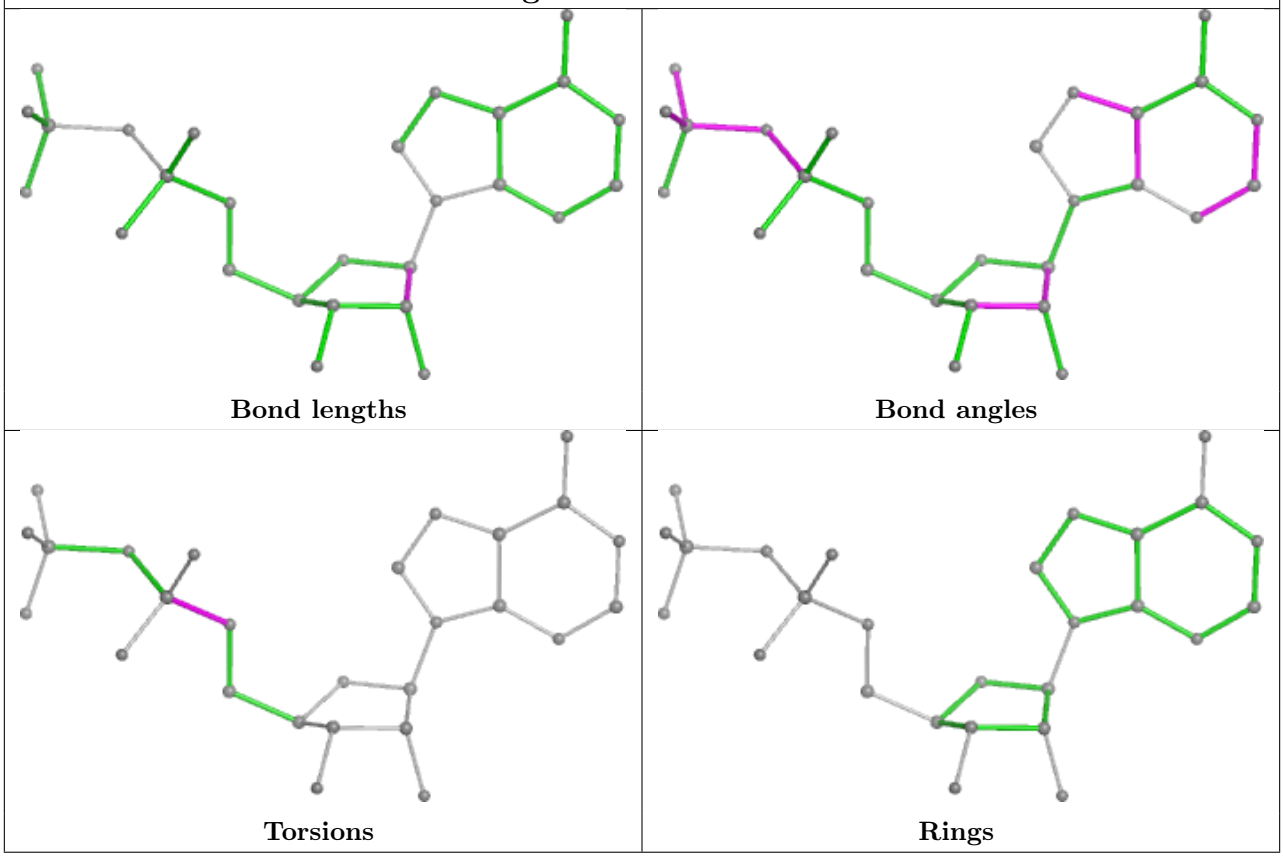
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	V	1001	ATP	1	0
20	U	1001	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

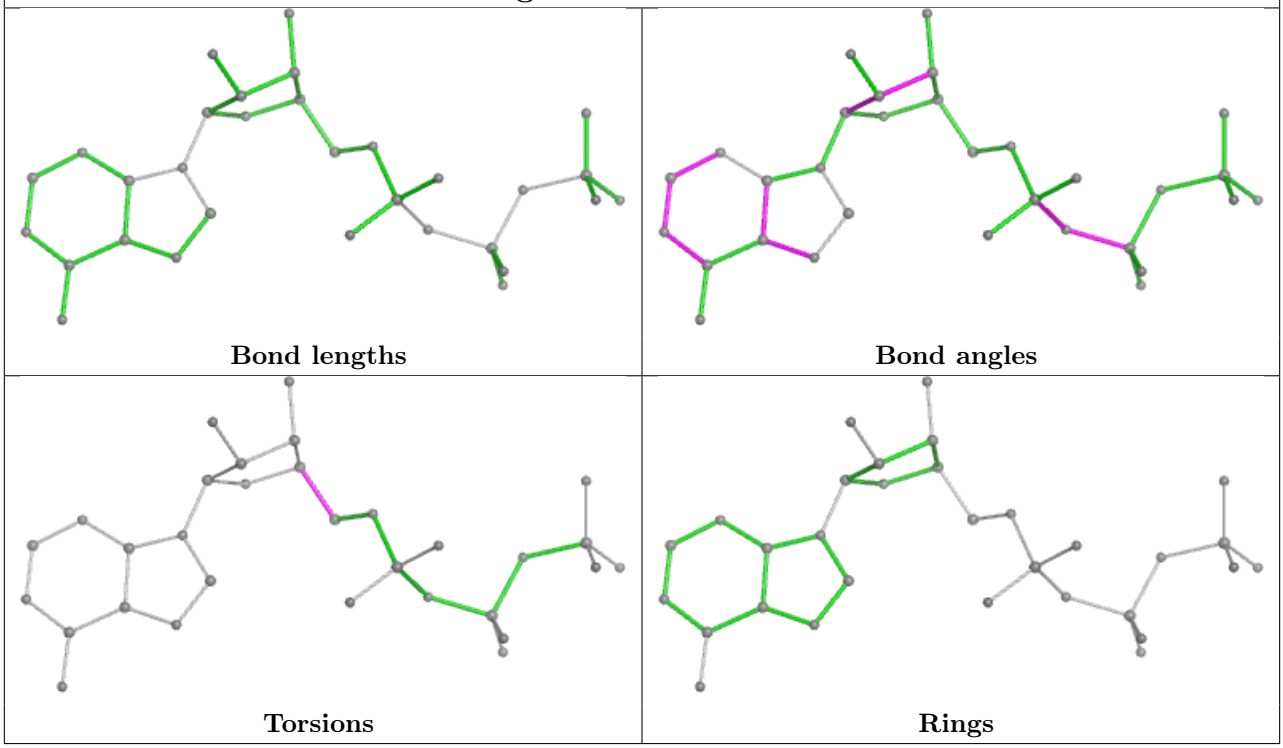
Ligand ATP T 1001



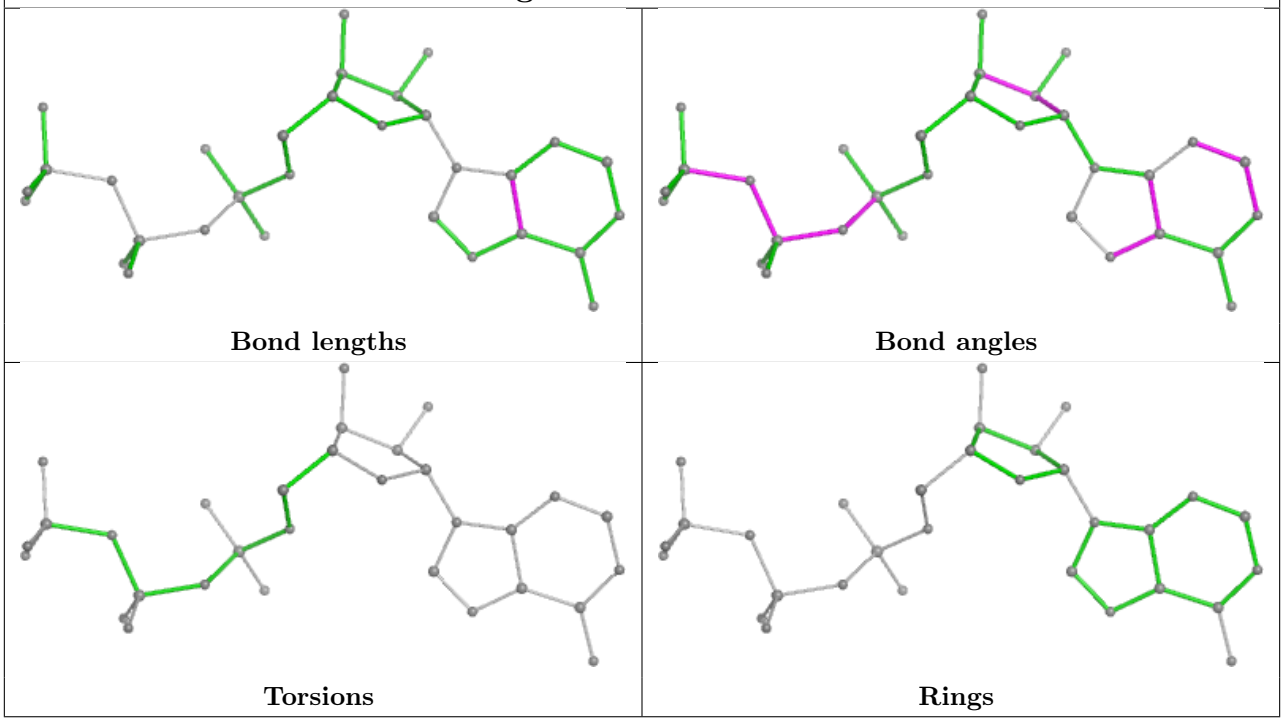
Ligand ADP X 601

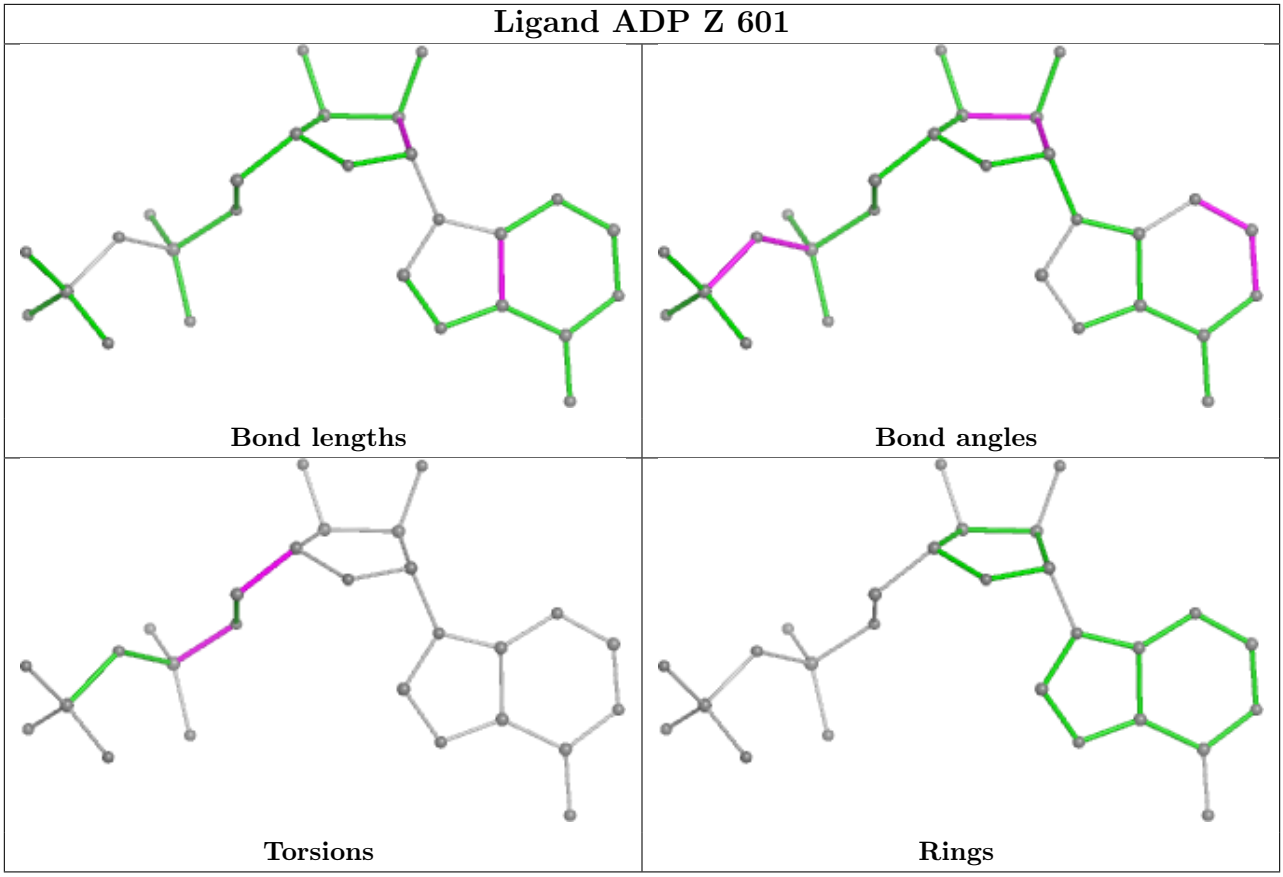


Ligand ATP V 1001



Ligand ATP U 1001





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
11	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	4.85

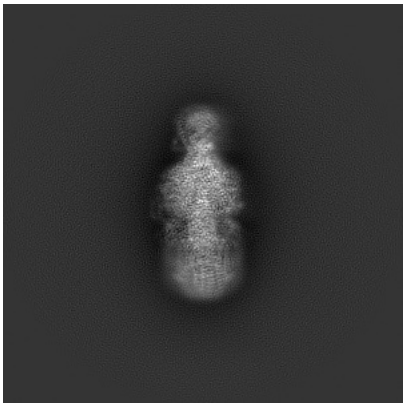
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4853. These allow visual inspection of the internal detail of the map and identification of artifacts.

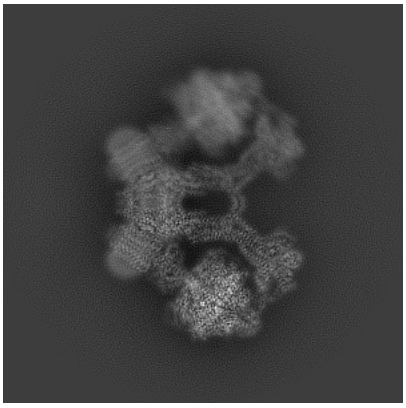
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

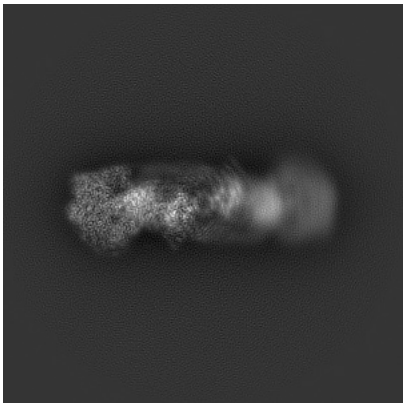
6.1.1 Primary map



X



Y

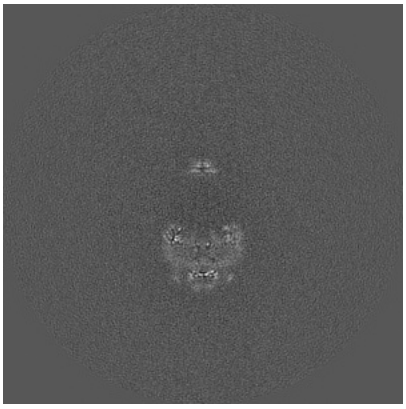


Z

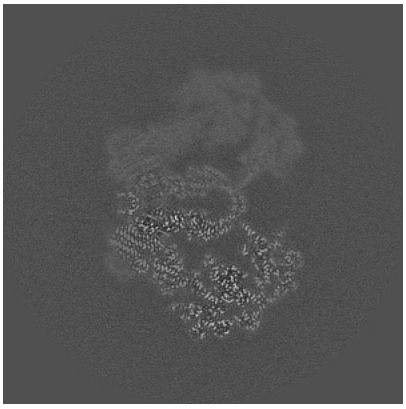
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

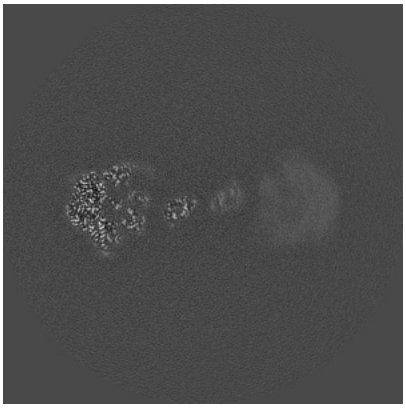
6.2.1 Primary map



X Index: 240



Y Index: 240

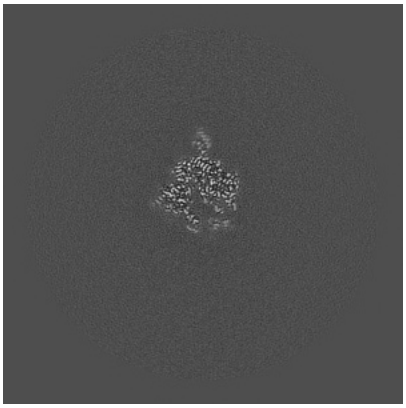


Z Index: 240

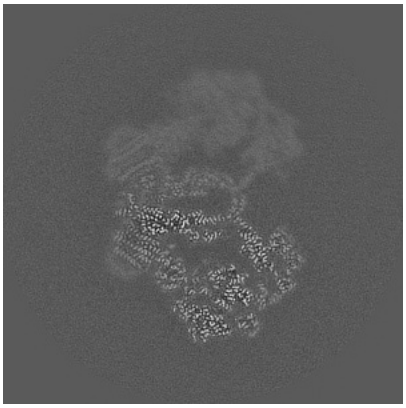
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 124



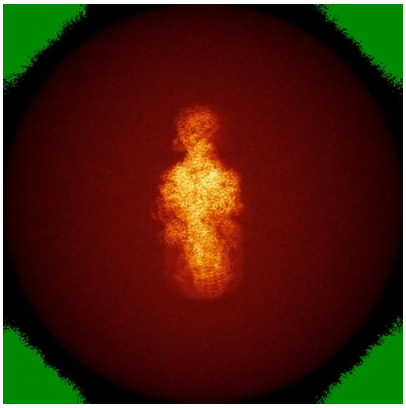
Y Index: 235

Z Index: 256

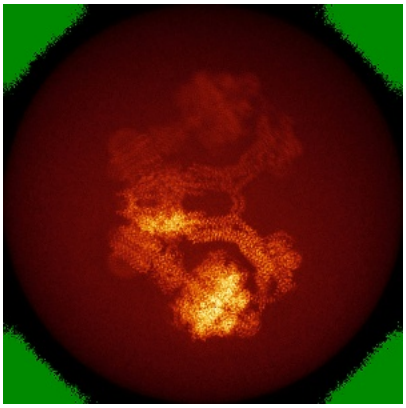
The images above show the largest variance slices of the map in three orthogonal directions.

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

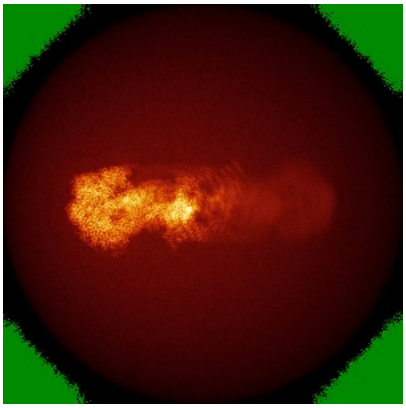
6.4.1 Primary map



X



Y

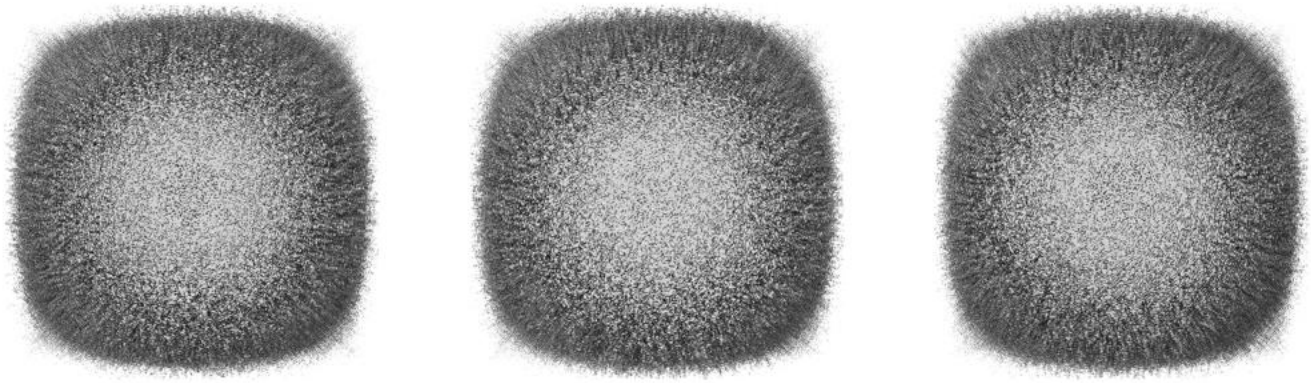


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

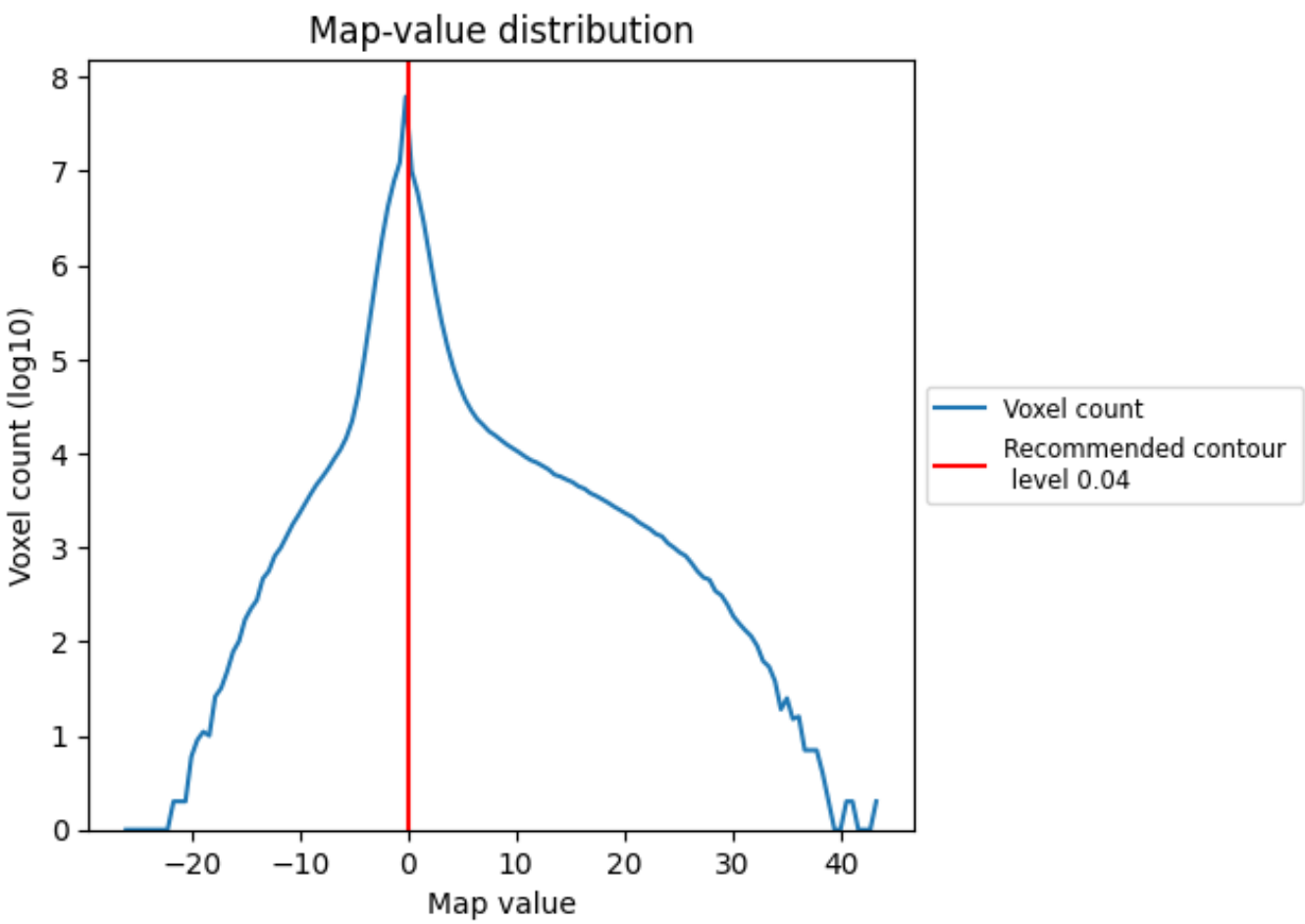
6.6 Mask visualisation (i)

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

7 Map analysis (i)

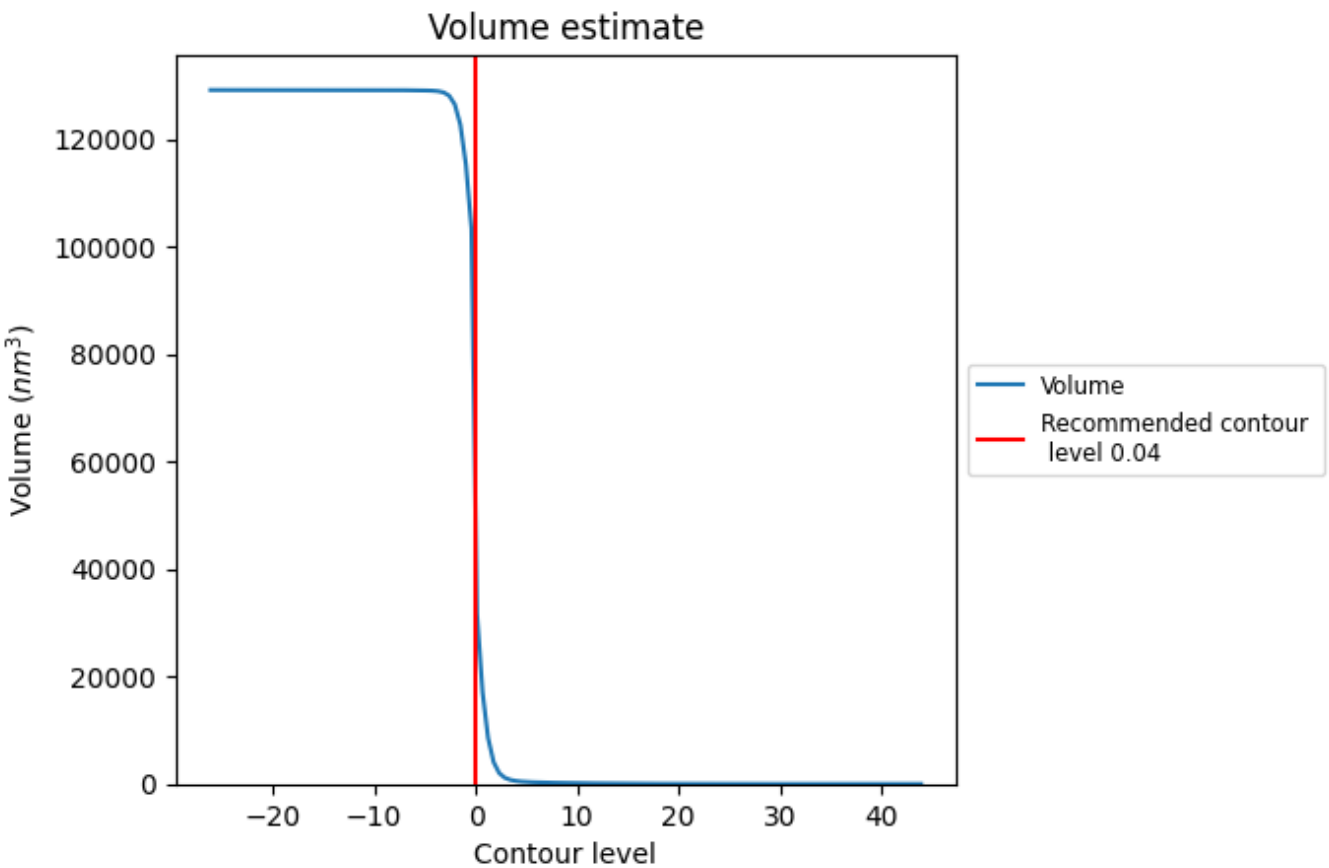
This section contains the results of statistical analysis of the map.

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.

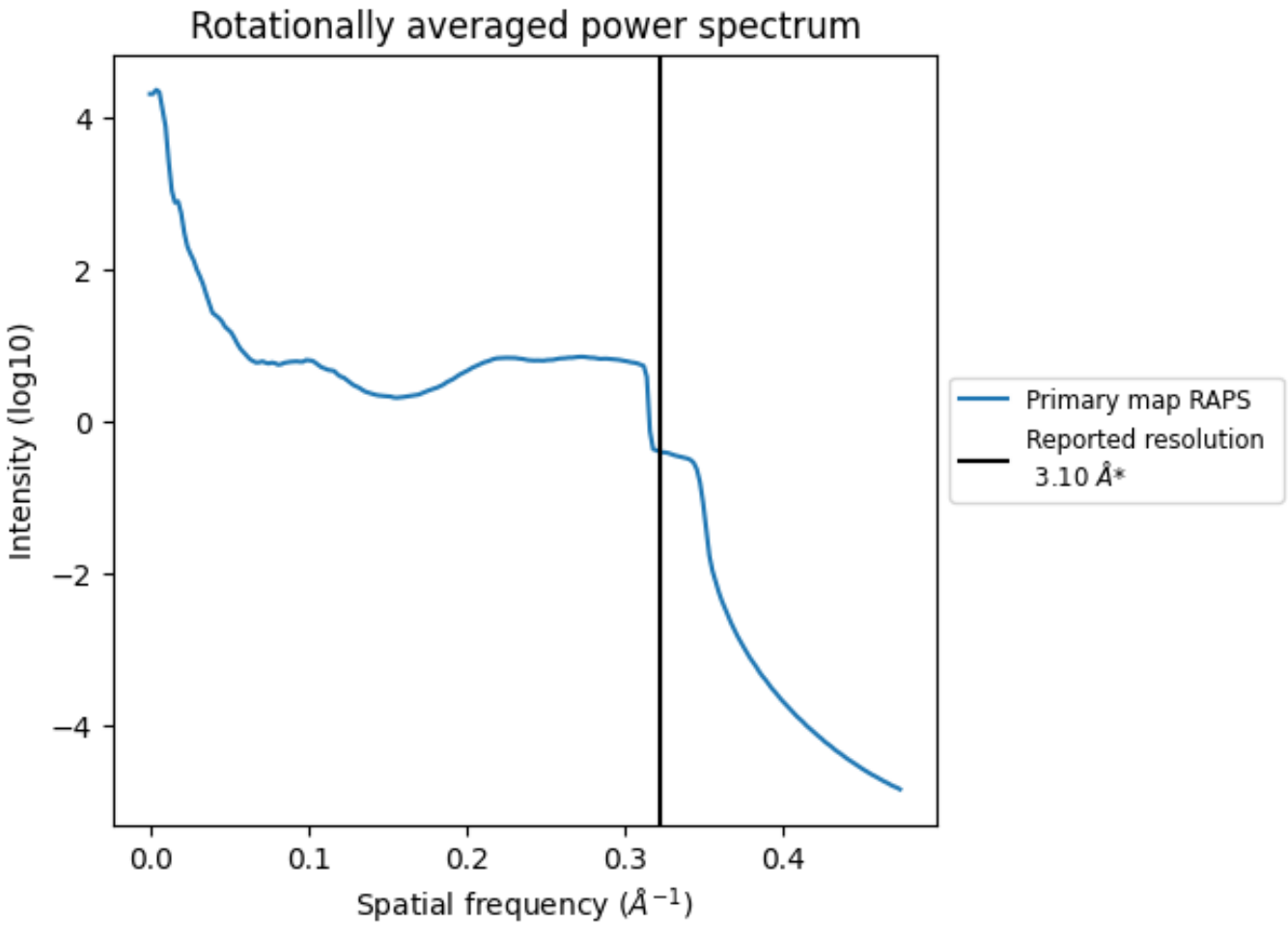
7.2 Volume estimate (i)



The volume at the recommended contour level is 45577 nm^3; this corresponds to an approximate mass of 41171 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

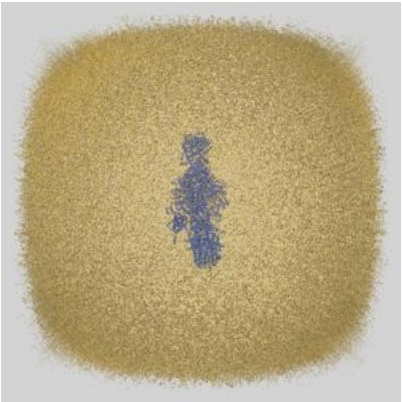
8 Fourier-Shell correlation (i)

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

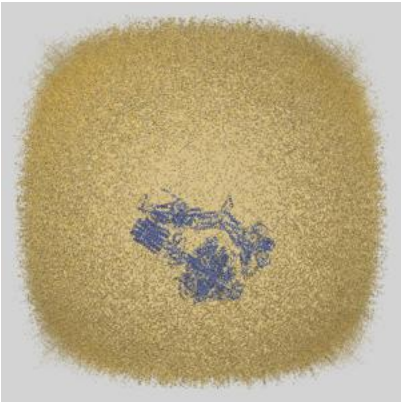
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4853 and PDB model 6REP. Per-residue inclusion information can be found in section 3 on page 10.

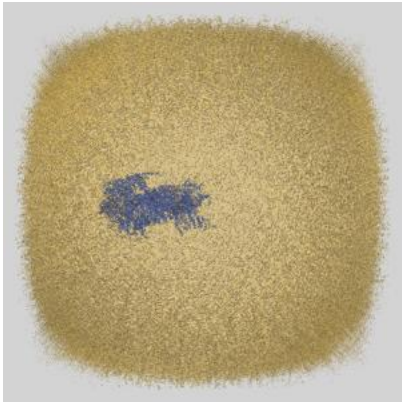
9.1 Map-model overlay (i)



X



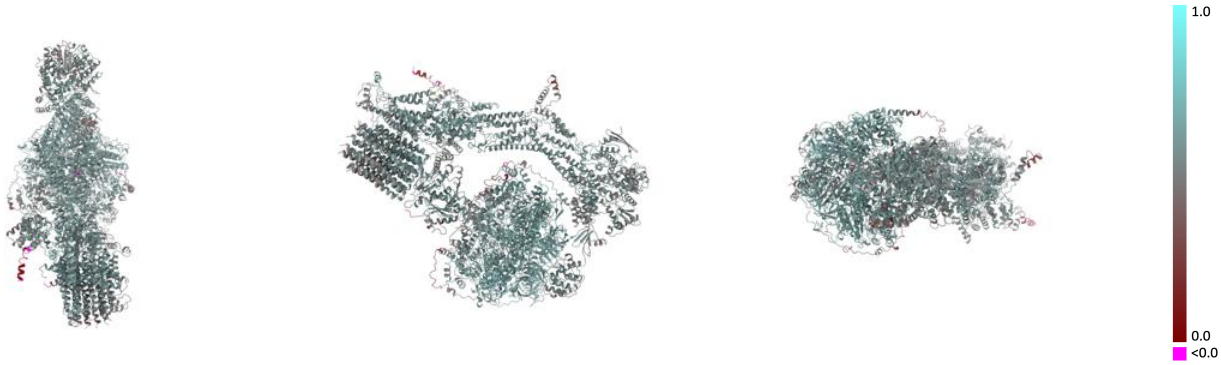
Y



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.

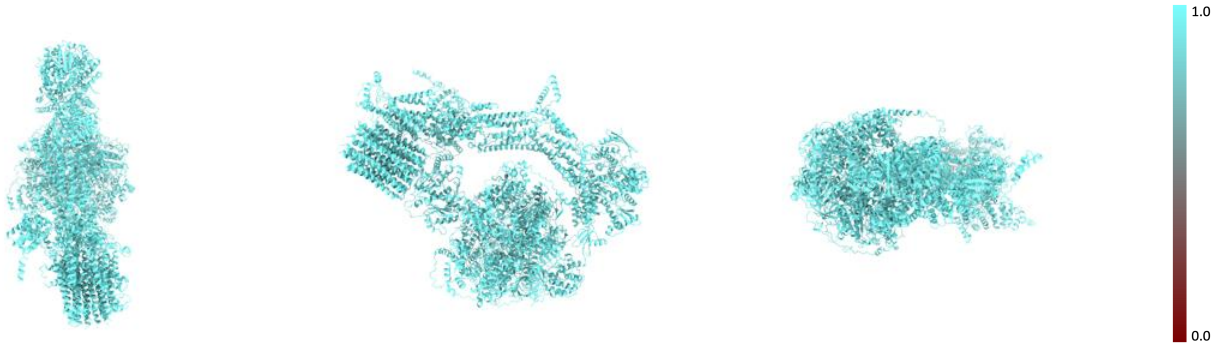
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

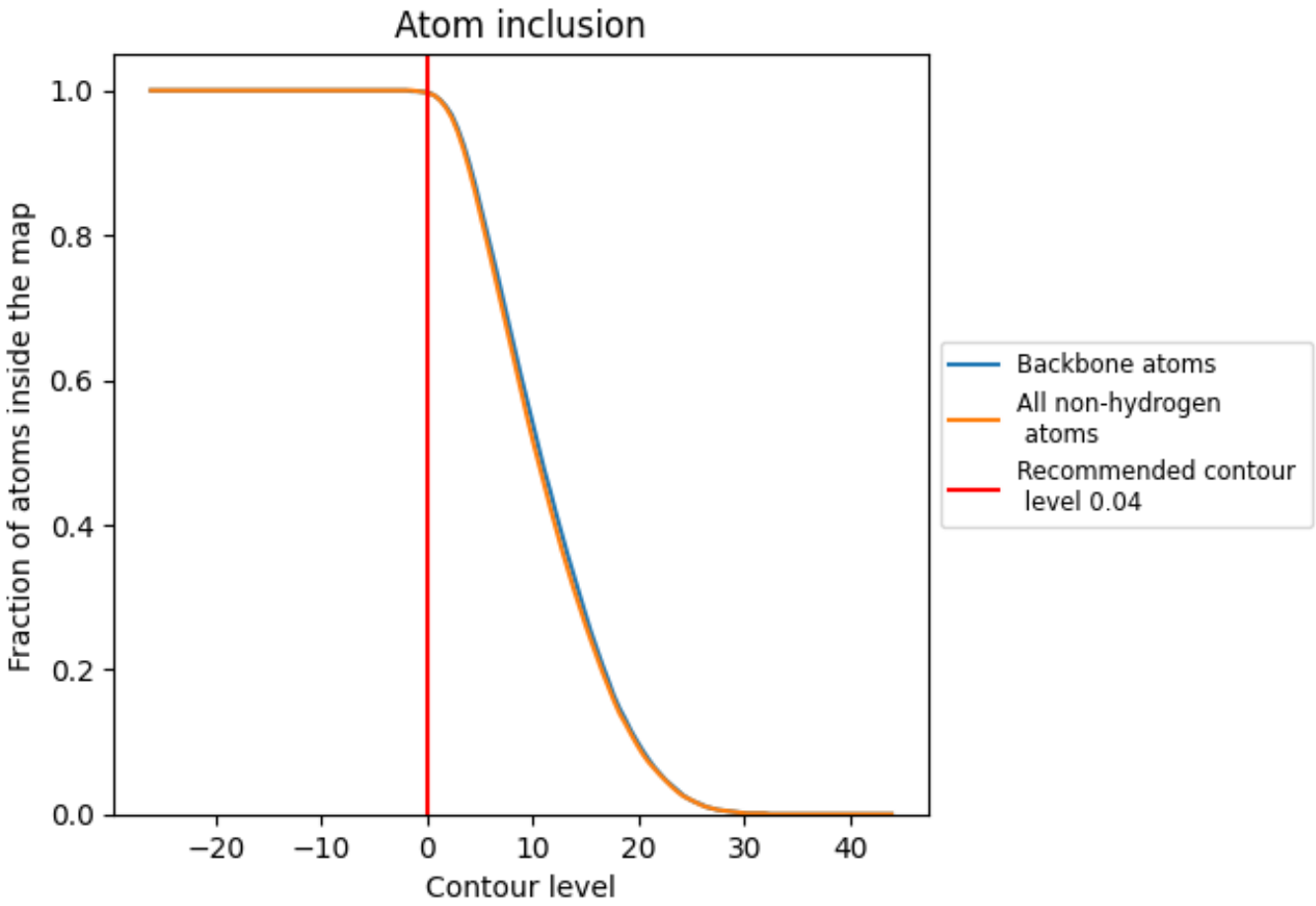
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9970	0.5600
0	0.9980	0.5510
1	0.9980	0.5560
2	0.9970	0.5230
3	0.9940	0.4920
4	0.9960	0.5260
5	0.9950	0.5810
6	0.9950	0.5620
7	0.9990	0.5600
8	0.9970	0.5720
9	0.9950	0.4950
A	0.9980	0.5000
B	0.9960	0.5190
C	0.9980	0.5470
D	0.9940	0.5620
E	0.9960	0.5700
F	0.9980	0.5510
G	1.0000	0.5270
H	1.0000	0.5230
I	0.9960	0.4990
J	0.9960	0.4900
M	0.9970	0.5630
P	0.9970	0.5290
Q	0.9910	0.5140
R	0.9970	0.5160
S	1.0000	0.5550
T	0.9920	0.5900
U	0.9970	0.5800
V	0.9990	0.5940
X	0.9970	0.5790
Y	0.9980	0.5870
Z	0.9970	0.5870