Full wwPDB EM Validation Report (i)

May 12, 2024 – 04:48 pm BST

PDB ID	:	6RE8
EMDB ID	:	EMD-4845
Title	:	Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 2D, composite map
Authors	:	Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on	:	2019-04-12
Resolution	:	3.80 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:

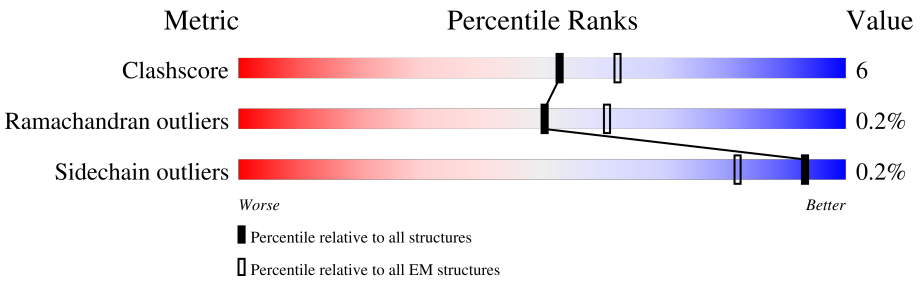
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.80 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	87% 12% •
2	1	618	86% 11% •
3	2	441	85% 15%
4	3	325	65% 11% 25%
5	4	294	90% 8% •
6	5	123	92% 8%
7	6	151	75% 7% 18%
8	7	190	78% 14% 7%

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Mol	Chain	Length	Quality of chain
9	8	89	81% 18%
10	9	97	88% 12%
11	A	127	46% 12% 42%
11	B	127	44% 14% 42%
11	C	127	46% 12% 42%
11	D	127	48% 10% 42%
11	E	127	43% 14% 42%
11	F	127	50% 9% 42%
11	G	127	48% 10% 42%
11	H	127	46% 13% 42%
11	I	127	50% 9% 42%
11	J	127	46% 13% 42%
12	M	327	60% 7% 34%
13	P	229	71% 13% 16%
14	Q	74	80% 18%
15	R	199	80% 9% 11%
16	S	317	73% 14% 13%
17	T	562	77% 16% 7%
17	U	562	79% 14% 7%
17	V	562	78% 14% 7%
18	X	574	79% 15% 6%
18	Y	574	78% 12% 9%
18	Z	574	80% 14% 6%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 53720 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

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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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	U	523	3978	2537	702	728	11	0	0
17	V	520	3961	2527	700	723	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	538	4087	2568	692	814	13	0	0
18	Y	520	3952	2484	669	786	13	0	0
18	Z	539	4095	2572	693	817	13	0	0

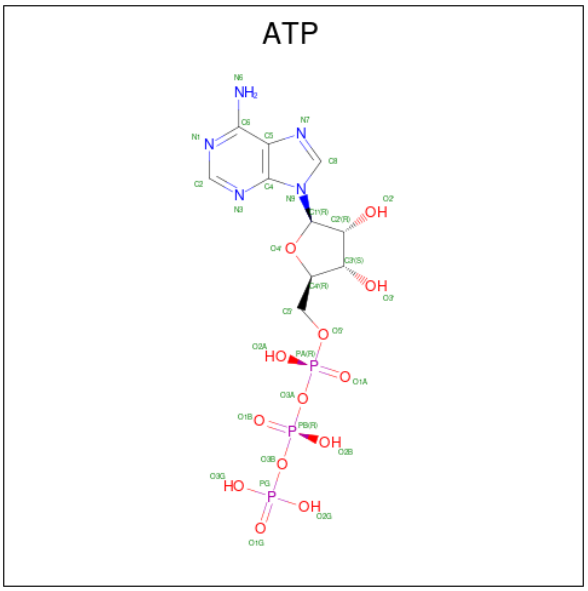
There are 6 discrepancies between the modelled and reference sequences:

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: $C_{10}H_{16}N_5O_{13}P_3$).

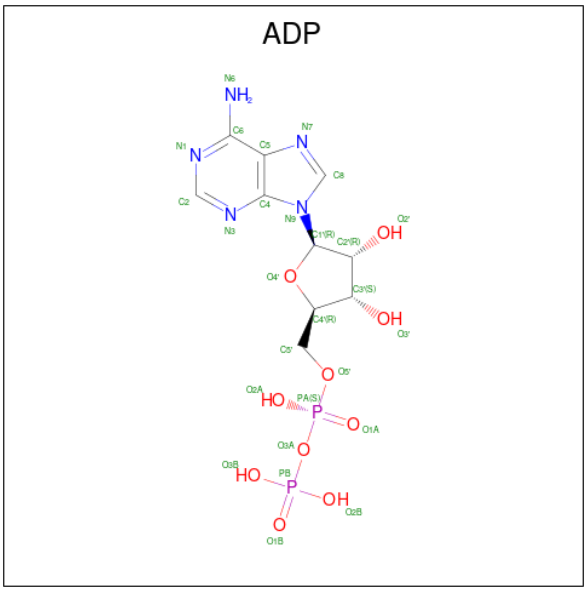


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	Y	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: $C_{10}H_{15}N_5O_{10}P_2$).



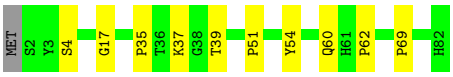
Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

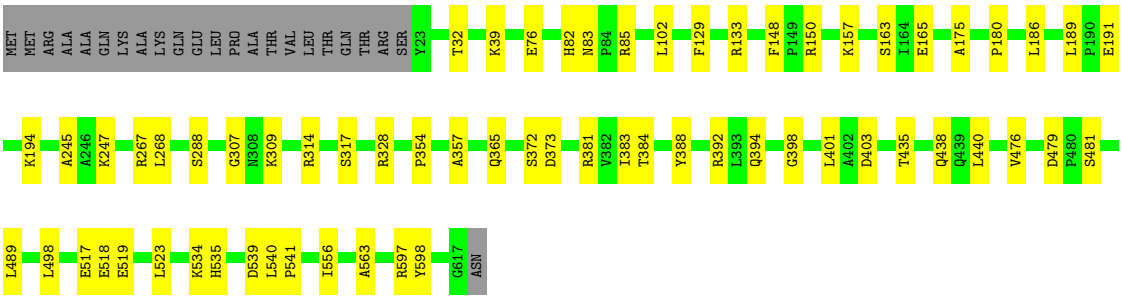
• Molecule 1: ASA-10: Polytomella F-ATP synthase associated subunit 10

Chain 0:



• Molecule 2: ATP synthase associated protein ASA1

Chain 1:

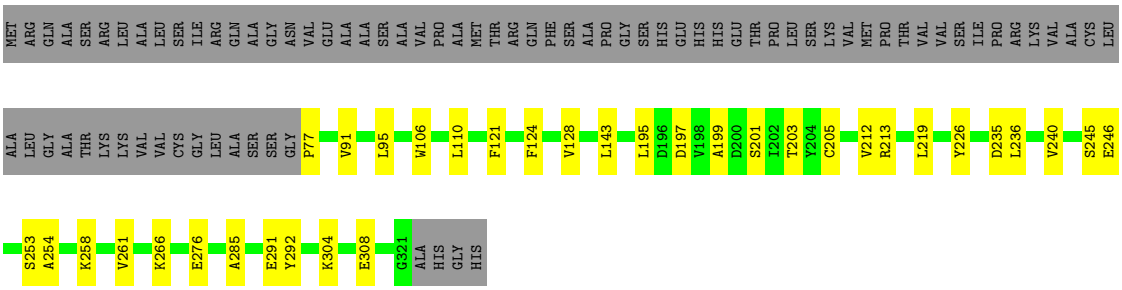


• Molecule 3: ASA-2: Polytomella F-ATP synthase associated subunit 2

Chain 2:

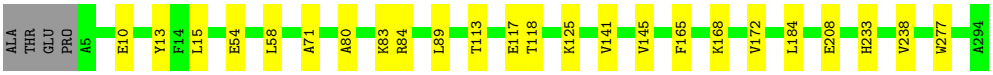
• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3:



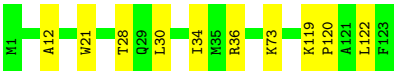
• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4:



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

Chain 5:



• Molecule 7: Mitochondrial ATP synthase subunit ASA6

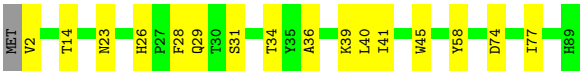
Chain 6:

• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7:

• Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8:

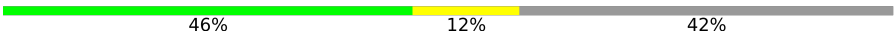


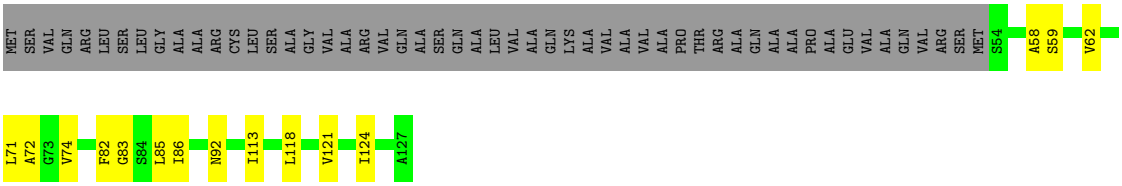
• Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9:

• Molecule 11: Mitochondrial ATP synthase subunit c

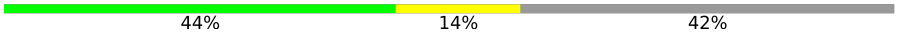
Chain A:

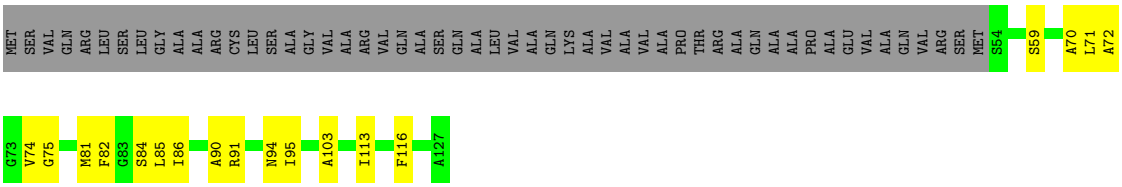




• Molecule 11: Mitochondrial ATP synthase subunit c

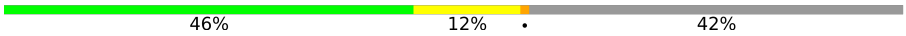
Chain B:

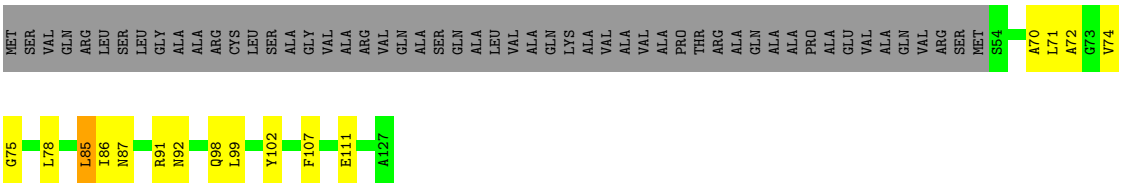




• Molecule 11: Mitochondrial ATP synthase subunit c

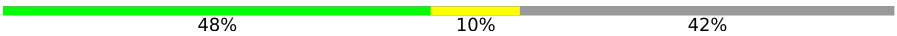
Chain C:

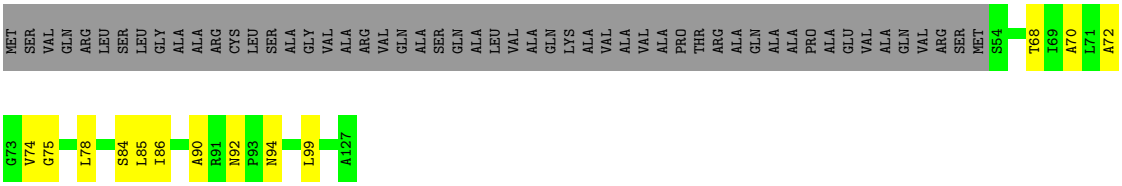




• Molecule 11: Mitochondrial ATP synthase subunit c

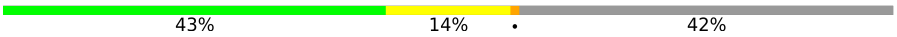
Chain D:

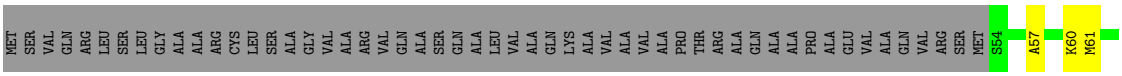


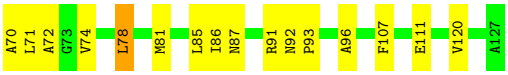


• Molecule 11: Mitochondrial ATP synthase subunit c

Chain E:

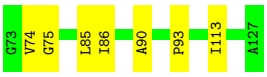






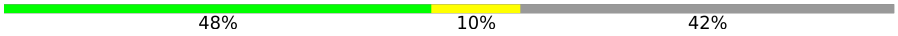
• Molecule 11: Mitochondrial ATP synthase subunit c

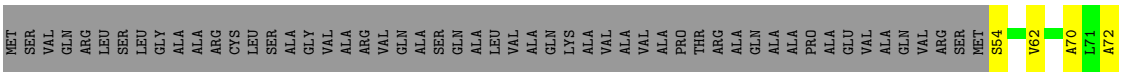
Chain F:



• Molecule 11: Mitochondrial ATP synthase subunit c

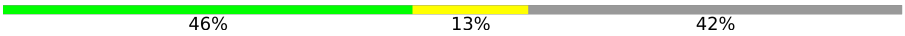
Chain G:

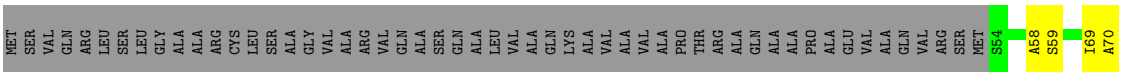


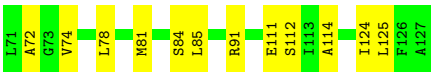


• Molecule 11: Mitochondrial ATP synthase subunit c

Chain H:

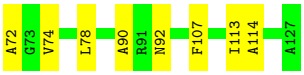






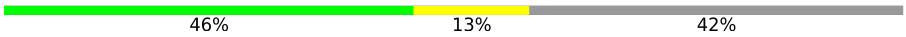
• Molecule 11: Mitochondrial ATP synthase subunit c

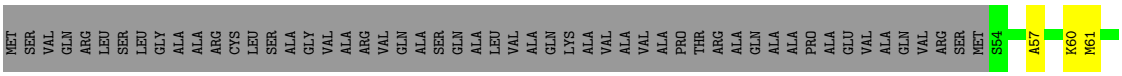
Chain I:



• Molecule 11: Mitochondrial ATP synthase subunit c

Chain J:





A70 L71 V74 L78 I86 A90 I95 Q98 L99 F107 T110 I113 A114 A127

• Molecule 12: Mitochondrial ATP synthase subunit 6

Chain M: 60% 7% 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 GLY ASN GLN THR MET ALA MET S95 S96 V97 T107 L110 N131 P136 D143 S147 N163 W189 K199 T200 G201 F202 K203 F204

P205 GLY HIS PHE ILE PRO GLY GLY THR PRO TRP PRO MET ALA F219 P223 T226 A233 N243 L254 M257 S264 V271 F275 A292 K324 LYS ILE HIS

• Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P: 71% 13% • 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 L44 L74 L99 K103 L134 V137 M145 H148 K149 K150 E151 V152 Y153 C154 T155

V156 I157 T158 P161 V168 E169 L170 T171 K172 E175 D179 L184 V185 M186 Q187 E201 F202 S203 D204 R205 M209 I229

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

Chain Q: 80% 18% •

MET CYS A3 P4 R10 D25 R28 N29 V30 L31 K32 E33 P34 F35 K36 I45 H46 F47 R48 D54 N74

• Molecule 15: Mitochondrial ATP synthase subunit delta

Chain R: 80% 9% 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 V47 P51 S52 N53 Y54 K58 Q64 Y75 Q83 V90 D95 E117 N139 D153 Q154 A159 V160 K161 A199

• Molecule 16: ATP synthase gamma chain, mitochondrial

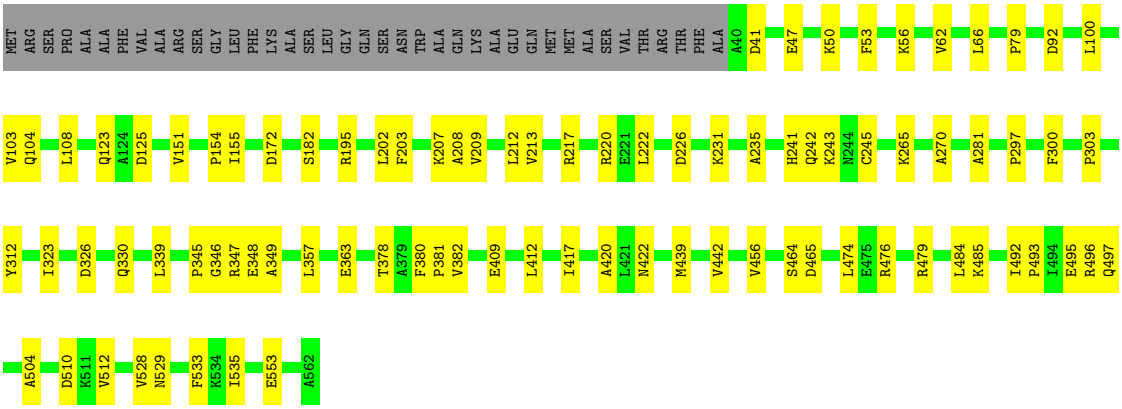
Chain S: 73% 14% • 13%

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 R79 V86 D91 V95 K99 A104 V105 C112 N116 L127 V140

S141 I142 R147 L150 I153 R157 L160 D164 Q174 A175 S176 L177 E180 Q188 S189 Y190 Q191 I192 L193 F194 N195 K196 F197 P205 A208 T209 I210 L211 S212 P213 D214 L215 L216 E217 D229 D232 R239 R244 D245 L246 T247 H250 L304

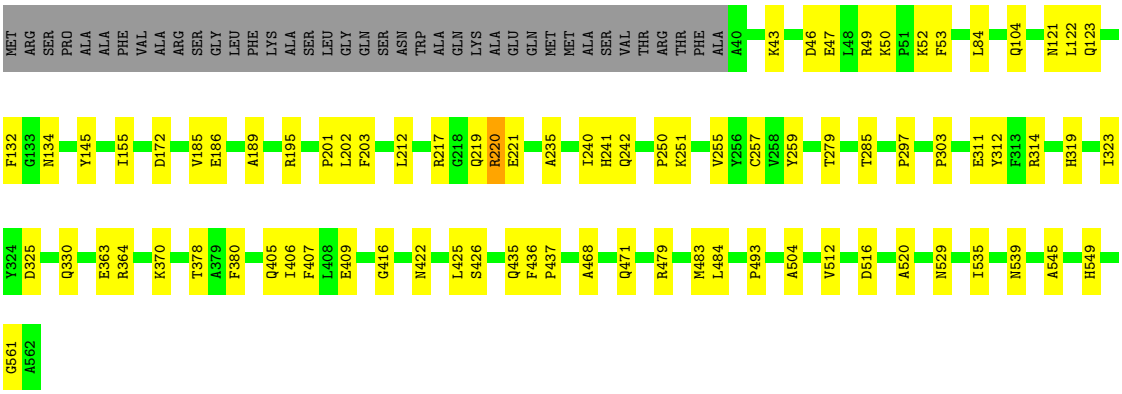
• Molecule 17: ATP synthase subunit alpha

Chain T:



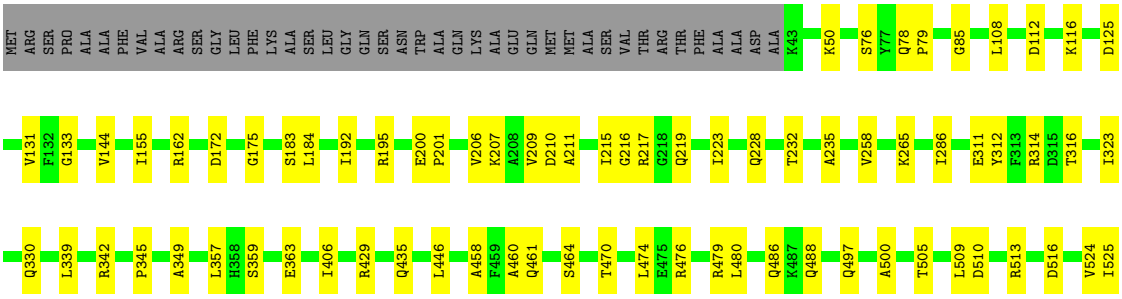
• Molecule 17: ATP synthase subunit alpha

Chain U:



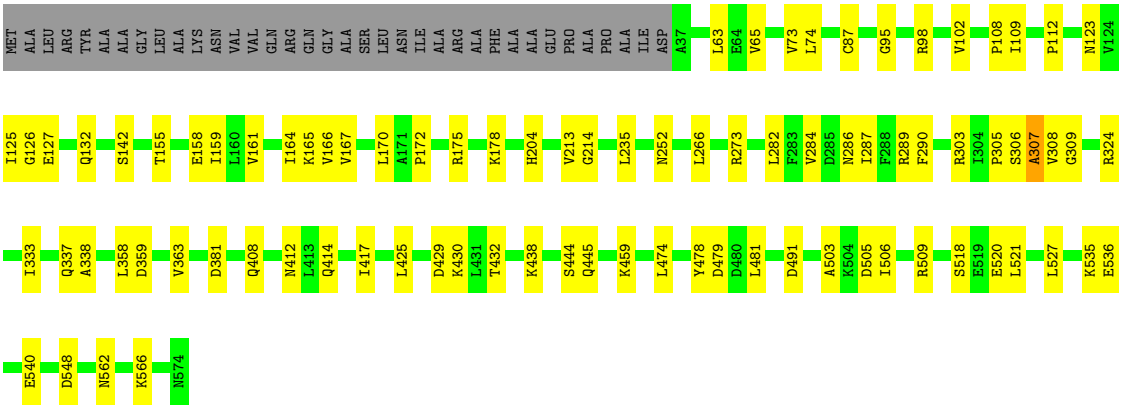
• Molecule 17: ATP synthase subunit alpha

Chain V:



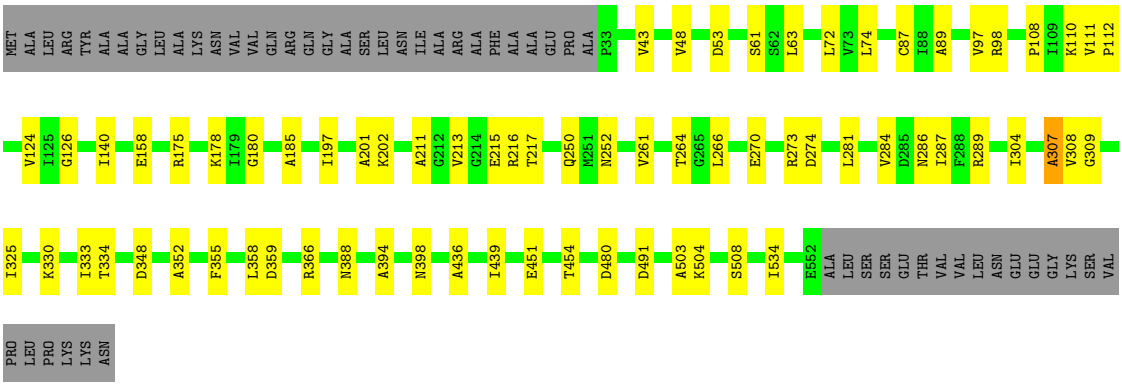
• Molecule 18: ATP synthase subunit beta

Chain X:



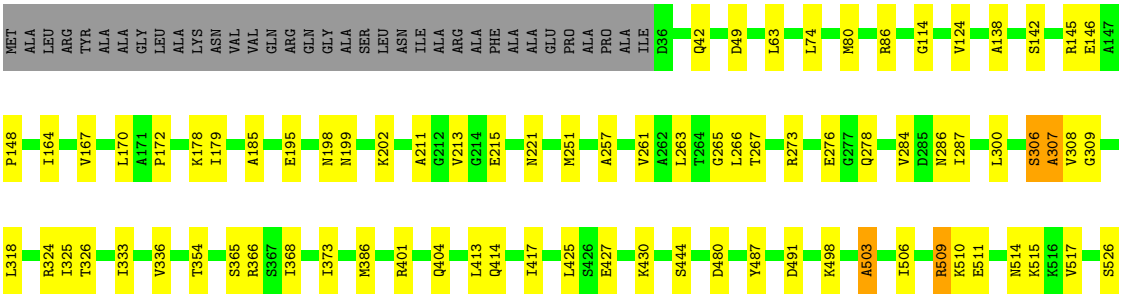
• Molecule 18: ATP synthase subunit beta

Chain Y:



• Molecule 18: ATP synthase subunit beta

Chain Z:



K529
D543
N574

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16363	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	25.996	Depositor
Minimum map value	-14.870	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.023	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: ATP, ADP, MG, 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	0.30	0/628	0.45	0/856
2	1	0.30	0/4750	0.47	1/6434 (0.0%)
3	2	0.29	0/3212	0.51	0/4371
4	3	0.31	0/1911	0.50	1/2601 (0.0%)
5	4	0.30	0/2216	0.46	0/3000
6	5	0.32	0/1011	0.56	0/1376
7	6	0.30	0/946	0.49	0/1287
8	7	0.32	0/1374	0.49	0/1865
9	8	0.31	0/715	0.51	0/974
10	9	0.30	0/802	0.50	0/1084
11	A	0.28	0/520	0.53	0/704
11	B	0.28	0/520	0.59	0/704
11	C	0.28	0/519	0.57	1/701 (0.1%)
11	D	0.28	0/520	0.49	0/704
11	E	0.28	0/520	0.53	0/704
11	F	0.30	0/520	0.52	0/704
11	G	0.29	0/520	0.49	0/704
11	H	0.31	0/520	0.48	0/704
11	I	0.28	0/520	0.54	0/704
11	J	0.29	0/520	0.56	0/704
12	M	0.33	0/1683	0.56	0/2295
13	P	0.32	0/1553	0.55	1/2093 (0.0%)
14	Q	0.30	0/574	0.49	0/774
15	R	0.31	0/1336	0.51	0/1827
16	S	0.30	0/2153	0.50	0/2901
17	T	0.34	0/4048	0.53	0/5481
17	U	0.33	0/4047	0.53	0/5479
17	V	0.34	0/4030	0.52	0/5456
18	X	0.34	0/4147	0.53	0/5619
18	Y	0.34	0/4011	0.52	0/5435
18	Z	0.33	0/4155	0.55	2/5630 (0.0%)
All	All	0.32	0/54501	0.52	6/73875 (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
6	5	0	1
18	X	0	1
18	Y	0	2
18	Z	0	1
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Z	543	ASP	CB-CG-OD1	6.62	124.26	118.30
4	3	77	PRO	N-CA-CB	5.92	110.40	103.30
13	P	44	LEU	CA-CB-CG	5.73	128.49	115.30
18	Z	413	LEU	CA-CB-CG	5.63	128.26	115.30
2	1	388	TYR	C-N-CA	5.29	134.92	121.70
11	C	85	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	119	LYS	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Y	503	ALA	Mainchain
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	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	4661	0	4695	42	0
3	2	3163	0	3262	41	0
4	3	1874	0	1826	22	0
5	4	2177	0	2169	19	0
6	5	986	0	1021	9	0
7	6	926	0	941	10	0
8	7	1347	0	1345	22	0
9	8	692	0	694	13	0
10	9	776	0	757	10	0
11	A	514	0	554	12	0
11	B	514	0	554	17	0
11	C	514	0	553	16	0
11	D	514	0	554	13	0
11	E	514	0	554	16	0
11	F	514	0	554	11	0
11	G	514	0	554	13	0
11	H	514	0	554	14	0
11	I	514	0	554	11	0
11	J	514	0	554	13	0
12	M	1640	0	1665	18	0
13	P	1532	0	1603	28	0
14	Q	561	0	565	11	0
15	R	1303	0	1266	13	0
16	S	2130	0	2180	30	0
17	T	3979	0	4119	56	0
17	U	3978	0	4116	53	0
17	V	3961	0	4105	51	0
18	X	4087	0	4110	54	0
18	Y	3952	0	3964	45	0
18	Z	4095	0	4114	50	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	0	0
20	V	31	0	12	2	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	Y	1	0	0	0	0
21	Z	1	0	0	0	0
22	Y	27	0	12	0	0
22	Z	27	0	12	1	0
All	All	53720	0	54700	609	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 6.

All (609) 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)
18:Z:514:ASN:O	18:Z:517:VAL:HG22	1.18	1.28
13:P:184:LEU:HD12	13:P:184:LEU:O	1.48	1.10
18:Z:514:ASN:O	18:Z:517:VAL:CG2	1.99	1.10
13:P:154:CYS:SG	13:P:185:VAL:O	2.33	0.86
3:2:82:LYS:O	3:2:86:GLU:HB2	1.78	0.83
18:X:503:ALA:O	18:X:506:ILE:HG12	1.77	0.83
13:P:154:CYS:SG	13:P:186:MET:SD	2.81	0.79
13:P:187:GLN:HA	13:P:187:GLN:NE2	2.00	0.75
13:P:154:CYS:SG	13:P:186:MET:HA	2.26	0.74
18:Z:195:GLU:O	18:Z:199:ASN:HB2	1.87	0.74
13:P:148:HIS:C	13:P:150:LYS:H	1.93	0.70
13:P:184:LEU:O	13:P:184:LEU:CD1	2.36	0.70
12:M:271:VAL:O	12:M:275:PHE:HB2	1.92	0.69
16:S:213:PRO:O	16:S:217:GLU:HB3	1.91	0.69
18:Z:425:LEU:HB2	18:Z:430:LYS:HG3	1.75	0.69
15:R:64:GLN:HE21	15:R:139:ASN:HD22	1.42	0.68
13:P:148:HIS:O	13:P:150:LYS:N	2.29	0.66
17:U:189:ALA:HB3	18:X:252:ASN:HD22	1.62	0.65
18:Y:197:ILE:O	18:Y:201:ALA:HB3	1.97	0.64
2:1:598:TYR:HH	9:8:2:VAL:N	1.96	0.64
8:7:170:HIS:HD2	8:7:172:ALA:H	1.43	0.64
16:S:190:TYR:HB2	16:S:210:ILE:HB	1.78	0.63
11:D:86:ILE:HG21	11:E:85:LEU:HA	1.80	0.63
17:T:326:ASP:H	17:T:382:VAL:HB	1.64	0.63
11:B:72:ALA:HB2	11:C:70:ALA:HA	1.82	0.62
18:X:518:SER:HB2	18:X:521:LEU:HB2	1.80	0.62
11:J:74:VAL:HG21	11:J:114:ALA:HB2	1.81	0.62
17:U:185:VAL:HG23	17:U:186:GLU:HG2	1.82	0.62
11:E:72:ALA:HB2	11:F:70:ALA:HA	1.81	0.62
17:T:528:VAL:HG13	17:T:553:GLU:HG2	1.81	0.61
17:V:470:THR:O	17:V:474:LEU:HB2	2.00	0.61
18:X:286:ASN:H	18:X:338:ALA:HB3	1.66	0.60
11:F:72:ALA:HB2	11:G:70:ALA:HA	1.83	0.60
11:H:69:ILE:HD13	11:I:69:ILE:HB	1.83	0.60
17:T:203:PHE:O	17:T:242:GLN:NE2	2.33	0.60
5:4:277:TRP:HE1	17:T:41:ASP:HA	1.67	0.60
11:J:74:VAL:HG23	11:J:110:THR:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:515:LYS:O	18:Z:517:VAL:HG13	2.01	0.60
8:7:50:VAL:HB	8:7:57:ALA:HB3	1.84	0.60
15:R:58:LYS:O	15:R:139:ASN:ND2	2.35	0.60
11:G:72:ALA:HB2	11:H:70:ALA:HA	1.83	0.59
11:I:74:VAL:HG11	11:I:114:ALA:HB2	1.83	0.59
17:T:330:GLN:HE22	17:T:357:LEU:HD11	1.67	0.59
11:F:75:GLY:HA3	11:G:74:VAL:HG12	1.85	0.59
2:1:102:LEU:H	2:1:288:SER:HB2	1.68	0.59
11:B:75:GLY:HA3	11:C:74:VAL:HG12	1.85	0.59
11:D:72:ALA:HB2	11:E:70:ALA:HA	1.85	0.59
18:Z:266:LEU:HD21	18:Z:324:ARG:HB2	1.85	0.59
4:3:258:LYS:HD2	4:3:291:GLU:HG3	1.85	0.59
17:V:500:ALA:HB2	17:V:525:ILE:HD11	1.86	0.58
17:V:235:ALA:HB1	17:V:323:ILE:HD13	1.85	0.58
17:V:192:ILE:O	18:Z:221:ASN:ND2	2.36	0.58
9:8:31:SER:HG	9:8:34:THR:HG1	1.51	0.58
13:P:148:HIS:C	13:P:150:LYS:N	2.55	0.58
18:X:408:GLN:O	18:X:412:ASN:HB2	2.04	0.58
18:Y:72:LEU:HD11	18:Y:89:ALA:HB1	1.85	0.58
18:Y:266:LEU:HD11	18:Y:325:ILE:HG12	1.84	0.58
16:S:95:VAL:HG21	16:S:211:LEU:HD21	1.85	0.58
17:U:314:ARG:NH2	17:U:364:ARG:O	2.37	0.58
18:Y:216:ARG:O	18:Y:250:GLN:NE2	2.37	0.57
1:0:37:LYS:O	1:0:60:GLN:NE2	2.37	0.57
18:Z:373:ILE:HG23	18:Z:444:SER:HB2	1.87	0.57
17:T:439:MET:HA	17:T:442:VAL:HG12	1.85	0.57
17:U:195:ARG:NH2	17:U:363:GLU:O	2.37	0.57
17:V:479:ARG:HE	17:V:510:ASP:HA	1.69	0.57
11:E:71:LEU:HD22	11:F:113:ILE:HG23	1.87	0.57
17:T:209:VAL:HG23	17:T:213:VAL:HG23	1.86	0.57
18:Z:427:GLU:HA	18:Z:430:LYS:HB2	1.87	0.57
3:2:382:VAL:HG21	3:2:399:VAL:HG11	1.84	0.57
17:T:125:ASP:OD1	17:T:125:ASP:N	2.37	0.57
3:2:383:PRO:HA	3:2:418:ALA:HB3	1.85	0.57
11:I:69:ILE:HA	11:J:70:ALA:HB2	1.87	0.57
15:R:34:THR:HG22	15:R:47:VAL:HG11	1.86	0.57
3:2:79:GLU:OE1	8:7:15:LEU:N	2.38	0.57
4:3:253:SER:OG	4:3:254:ALA:N	2.38	0.56
17:V:509:LEU:HD11	17:V:524:VAL:HG21	1.86	0.56
18:Z:86:ARG:NH2	18:Z:300:LEU:O	2.38	0.56
2:1:186:LEU:HD13	2:1:440:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:147:ARG:NH2	17:V:464:SER:OG	2.37	0.56
16:S:213:PRO:HD3	16:S:247:THR:HG21	1.87	0.56
17:T:409:GLU:OE1	17:T:422:ASN:ND2	2.39	0.56
18:Y:217:THR:OG1	18:Y:252:ASN:ND2	2.38	0.56
17:V:476:ARG:NH1	17:V:505:THR:O	2.38	0.56
18:Z:510:LYS:O	18:Z:511:GLU:HG2	2.06	0.56
18:Y:286:ASN:HB3	18:Y:289:ARG:HG2	1.87	0.56
18:Y:307:ALA:O	18:Y:309:GLY:N	2.36	0.56
17:T:202:LEU:HD22	17:T:378:THR:HG21	1.88	0.56
8:7:39:VAL:HG12	8:7:48:VAL:HG23	1.88	0.56
9:8:41:ILE:O	9:8:45:TRP:HB3	2.04	0.56
11:A:71:LEU:HA	11:A:74:VAL:HG12	1.88	0.56
11:D:90:ALA:O	11:E:92:ASN:ND2	2.39	0.56
17:V:201:PRO:O	17:V:217:ARG:NH2	2.39	0.56
17:T:347:ARG:NH2	18:Y:348:ASP:OD1	2.37	0.56
18:Z:414:GLN:HA	18:Z:417:ILE:HG12	1.87	0.56
11:H:74:VAL:HG11	11:H:114:ALA:HB2	1.88	0.56
17:V:265:LYS:NZ	18:Y:359:ASP:OD1	2.39	0.56
17:U:259:TYR:OH	17:U:325:ASP:OD2	2.23	0.55
8:7:19:THR:O	8:7:67:ARG:NH2	2.39	0.55
17:U:405:GLN:NE2	17:U:425:LEU:O	2.40	0.55
18:Z:178:LYS:HD3	18:Z:325:ILE:HB	1.87	0.55
18:Z:273:ARG:NH1	18:Z:326:THR:O	2.39	0.55
4:3:304:LYS:NZ	4:3:308:GLU:OE2	2.37	0.55
11:H:72:ALA:HB2	11:I:70:ALA:HA	1.88	0.55
11:D:68:THR:HG21	11:E:120:VAL:HG21	1.89	0.55
16:S:79:ARG:NH2	16:S:197:PHE:O	2.39	0.55
11:E:86:ILE:HG21	11:F:85:LEU:HA	1.89	0.55
18:X:164:ILE:HB	18:X:167:VAL:HG22	1.88	0.55
17:U:535:ILE:O	17:U:539:ASN:ND2	2.40	0.55
11:A:72:ALA:HB2	11:B:70:ALA:HA	1.89	0.54
16:S:112:CYS:SG	16:S:116:ASN:ND2	2.80	0.54
16:S:229:ASP:OD1	16:S:239:ARG:NH1	2.41	0.54
17:T:456:VAL:HG11	17:T:474:LEU:HB2	1.88	0.54
17:V:311:GLU:HG2	17:V:314:ARG:HE	1.73	0.54
18:X:363:VAL:HG21	18:X:381:ASP:HB2	1.89	0.54
18:Z:307:ALA:O	18:Z:309:GLY:N	2.40	0.54
2:1:384:THR:HG21	2:1:398:GLY:HA3	1.90	0.54
17:T:226:ASP:O	17:T:231:LYS:NZ	2.39	0.54
17:U:220:ARG:NH1	17:U:363:GLU:OE2	2.40	0.54
18:X:73:VAL:HG11	18:X:125:ILE:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:185:ALA:O	18:Z:366:ARG:NH2	2.40	0.54
11:A:92:ASN:ND2	11:J:90:ALA:O	2.41	0.54
4:3:258:LYS:HE3	4:3:292:TYR:HA	1.90	0.54
17:T:92:ASP:OD1	18:X:303:ARG:NE	2.41	0.54
3:2:195:ALA:HA	3:2:198:LYS:HE3	1.89	0.54
11:C:86:ILE:HG21	11:D:85:LEU:HA	1.90	0.54
18:X:214:GLY:O	18:X:289:ARG:NH1	2.42	0.54
11:F:71:LEU:HD12	11:G:113:ILE:HG23	1.90	0.53
11:H:111:GLU:HG3	11:I:113:ILE:HD11	1.90	0.53
14:Q:10:ARG:NH2	16:S:245:ASP:OD2	2.41	0.53
14:Q:47:PHE:HB3	16:S:174:GLN:HE21	1.73	0.53
5:4:89:LEU:HB3	8:7:172:ALA:HB2	1.90	0.53
11:D:92:ASN:OD1	11:D:94:ASN:ND2	2.42	0.53
14:Q:31:LEU:HD22	15:R:154:GLN:HG3	1.90	0.53
11:E:57:ALA:HA	11:E:60:LYS:HE3	1.91	0.53
11:G:98:GLN:NE2	11:G:102:TYR:OH	2.41	0.53
17:T:476:ARG:NH1	17:T:510:ASP:OD1	2.42	0.53
11:B:113:ILE:HA	11:B:116:PHE:HB2	1.91	0.53
11:J:57:ALA:HA	11:J:60:LYS:HE2	1.91	0.53
11:A:113:ILE:HD11	11:J:71:LEU:HD22	1.89	0.53
17:T:535:ILE:HG22	18:Y:534:ILE:HD11	1.91	0.53
17:U:203:PHE:O	17:U:242:GLN:NE2	2.36	0.53
17:V:342:ARG:HD3	18:Y:304:ILE:HD11	1.90	0.53
4:3:213:ARG:NH2	12:M:143:ASP:OD2	2.41	0.53
12:M:223:PRO:HA	12:M:226:THR:HG22	1.91	0.53
17:T:479:ARG:NH2	17:T:512:VAL:O	2.42	0.53
3:2:73:ILE:HD13	3:2:84:VAL:HG22	1.90	0.53
17:V:339:LEU:HD21	17:V:345:PRO:HB3	1.90	0.53
11:C:107:PHE:O	11:C:111:GLU:HG2	2.09	0.52
11:I:72:ALA:HB2	11:J:70:ALA:HA	1.91	0.52
17:V:200:GLU:HG3	17:V:217:ARG:HB2	1.92	0.52
18:X:158:GLU:OE2	18:X:175:ARG:NH1	2.41	0.52
18:Y:491:ASP:OD1	18:Y:491:ASP:N	2.40	0.52
2:1:157:LYS:O	8:7:98:ASN:ND2	2.43	0.52
11:C:72:ALA:HB2	11:D:70:ALA:HA	1.92	0.52
11:F:74:VAL:HG13	11:G:113:ILE:HD13	1.90	0.52
17:T:417:ILE:HG23	17:T:485:LYS:HZ2	1.75	0.52
11:C:75:GLY:HA3	11:D:74:VAL:HG12	1.92	0.52
3:2:188:ALA:HB2	3:2:220:LEU:HD22	1.90	0.52
5:4:145:VAL:HG11	5:4:165:PHE:HB2	1.90	0.52
17:U:409:GLU:HG3	17:U:422:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:108:LEU:HD11	17:V:116:LYS:HB3	1.90	0.52
3:2:197:LEU:HD21	3:2:217:LEU:HD11	1.91	0.52
18:Z:215:GLU:OE2	18:Z:286:ASN:ND2	2.43	0.52
1:0:51:PRO:HD2	1:0:54:TYR:HB2	1.91	0.52
11:I:78:LEU:HD11	11:I:107:PHE:HD1	1.75	0.52
14:Q:32:LYS:HG2	14:Q:34:PRO:HD2	1.92	0.52
17:U:416:GLY:O	18:Z:401:ARG:NH2	2.42	0.52
17:V:78:GLN:NE2	17:V:79:PRO:O	2.43	0.52
14:Q:25:ASP:OD2	14:Q:28:ARG:NH1	2.42	0.52
14:Q:45:ILE:HG21	16:S:177:LEU:HD12	1.91	0.52
17:U:251:LYS:HD3	18:X:540:GLU:OE2	2.09	0.52
13:P:175:GLU:HG2	13:P:184:LEU:HD21	1.91	0.52
17:T:207:LYS:NZ	17:T:485:LYS:O	2.42	0.52
17:V:155:ILE:HD12	17:V:312:TYR:HB2	1.93	0.52
17:V:162:ARG:NH2	17:V:175:GLY:O	2.39	0.52
17:V:195:ARG:NH2	17:V:363:GLU:O	2.43	0.52
18:Y:284:VAL:HG11	18:Y:287:ILE:HD13	1.92	0.52
18:Z:211:ALA:HB2	18:Z:265:GLY:HA3	1.92	0.52
17:U:219:GLN:NE2	17:U:221:GLU:OE1	2.42	0.51
18:X:165:LYS:NZ	18:X:444:SER:O	2.35	0.51
11:F:90:ALA:O	11:G:92:ASN:ND2	2.42	0.51
15:R:90:VAL:HB	15:R:117:GLU:HB2	1.90	0.51
17:V:311:GLU:OE2	17:V:314:ARG:NH1	2.43	0.51
17:U:122:LEU:HB3	18:X:98:ARG:HD3	1.92	0.51
17:V:207:LYS:HG3	17:V:486:GLN:HE21	1.74	0.51
18:X:159:ILE:HD12	18:X:172:PRO:HB3	1.92	0.51
2:1:328:ARG:NH1	10:9:12:GLU:OE1	2.42	0.51
3:2:282:VAL:HG21	5:4:15:LEU:HD13	1.92	0.51
13:P:187:GLN:NE2	13:P:187:GLN:CA	2.73	0.51
17:T:323:ILE:HG13	17:T:380:PHE:HB2	1.92	0.51
11:B:94:ASN:ND2	14:Q:4:PRO:O	2.42	0.51
17:U:47:GLU:OE2	17:U:52:LYS:NZ	2.39	0.51
4:3:203:THR:HG21	4:3:235:ASP:HB2	1.92	0.51
11:A:85:LEU:HA	11:J:86:ILE:HG21	1.92	0.51
18:X:213:VAL:HG11	18:X:290:PHE:HB2	1.92	0.51
3:2:119:GLU:N	5:4:208:GLU:OE1	2.44	0.51
16:S:210:ILE:HG23	16:S:250:HIS:HD2	1.76	0.51
11:B:85:LEU:HD13	11:B:103:ALA:HB2	1.92	0.51
18:X:520:GLU:HG2	18:X:521:LEU:HG	1.93	0.51
2:1:392:ARG:NH2	2:1:394:GLN:OE1	2.43	0.51
18:Y:213:VAL:HG22	18:Y:261:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:418:ALA:HA	3:2:421:PHE:HB3	1.93	0.51
17:V:330:GLN:HE22	17:V:357:LEU:HD11	1.76	0.51
8:7:99:GLU:OE2	8:7:100:ARG:NH1	2.44	0.50
18:Z:164:ILE:HB	18:Z:167:VAL:HB	1.92	0.50
17:V:460:ALA:HB2	17:V:474:LEU:HD11	1.94	0.50
18:X:425:LEU:O	18:X:430:LYS:NZ	2.44	0.50
1:0:17:GLY:O	6:5:21:TRP:NE1	2.44	0.50
2:1:556:ILE:HG21	6:5:36:ARG:HA	1.93	0.50
2:1:597:ARG:NH1	4:3:197:ASP:OD2	2.43	0.50
3:2:346:ARG:NH1	13:P:161:PRO:O	2.44	0.50
13:P:149:LYS:HD3	13:P:151:GLU:OE2	2.11	0.50
17:T:241:HIS:HE1	17:T:493:PRO:HA	1.76	0.50
18:X:273:ARG:HD3	18:X:333:ILE:HG13	1.93	0.50
11:C:78:LEU:HD11	11:C:107:PHE:HD1	1.76	0.50
18:X:548:ASP:OD1	18:X:548:ASP:N	2.42	0.50
2:1:372:SER:OG	2:1:373:ASP:N	2.45	0.50
3:2:42:LYS:NZ	8:7:69:LEU:O	2.43	0.50
16:S:105:VAL:HG22	16:S:142:ILE:HD12	1.94	0.50
17:T:347:ARG:HG2	17:T:348:GLU:HG3	1.94	0.50
5:4:71:ALA:HB2	8:7:84:VAL:HG12	1.93	0.50
17:U:172:ASP:OD1	17:U:172:ASP:N	2.43	0.50
17:V:429:ARG:NH2	22:Z:601:ADP:O2B	2.44	0.50
18:Z:306:SER:OG	18:Z:307:ALA:N	2.43	0.50
3:2:197:LEU:HD22	3:2:225:GLU:HG3	1.94	0.50
9:8:26:HIS:HD2	9:8:28:PHE:H	1.60	0.50
11:B:86:ILE:HG23	11:C:99:LEU:HD22	1.94	0.50
11:C:98:GLN:NE2	11:C:102:TYR:OH	2.45	0.50
17:T:346:GLY:HA2	18:Y:309:GLY:HA3	1.93	0.50
18:Y:185:ALA:O	18:Y:366:ARG:NH1	2.42	0.50
18:Y:394:ALA:O	18:Y:398:ASN:ND2	2.44	0.50
18:Z:170:LEU:HD22	18:Z:404:GLN:HE21	1.77	0.50
15:R:153:ASP:OD1	15:R:153:ASP:N	2.41	0.50
17:U:202:LEU:HD22	17:U:378:THR:HG21	1.93	0.50
18:X:491:ASP:OD1	18:X:491:ASP:N	2.44	0.50
17:T:339:LEU:HD21	17:T:345:PRO:HB3	1.92	0.49
17:U:516:ASP:O	17:U:520:ALA:N	2.44	0.49
17:V:488:GLN:NE2	18:Y:388:ASN:OD1	2.46	0.49
18:X:266:LEU:HD13	18:X:282:LEU:HD22	1.93	0.49
18:Y:180:GLY:HA3	18:Y:358:LEU:HD13	1.94	0.49
16:S:141:SER:HB2	16:S:150:LEU:HD12	1.94	0.49
17:V:513:ARG:HH11	17:V:516:ASP:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:526:SER:HB3	18:Z:529:LYS:HG2	1.93	0.49
2:1:180:PRO:HB2	2:1:489:LEU:HD21	1.93	0.49
11:C:87:ASN:ND2	11:D:84:SER:OG	2.45	0.49
17:U:201:PRO:HB3	17:U:435:GLN:HA	1.93	0.49
4:3:245:SER:OG	4:3:246:GLU:N	2.46	0.49
11:A:118:LEU:HA	11:A:121:VAL:HG12	1.94	0.49
13:P:153:TYR:HA	13:P:185:VAL:HG22	1.93	0.49
17:V:211:ALA:O	17:V:435:GLN:NE2	2.45	0.49
17:V:535:ILE:HD11	17:V:546:LEU:HD13	1.93	0.49
17:T:265:LYS:NZ	18:X:359:ASP:OD1	2.45	0.49
17:U:203:PHE:HE2	17:U:436:PHE:HB2	1.77	0.49
18:Z:510:LYS:O	18:Z:511:GLU:CG	2.61	0.49
2:1:267:ARG:NE	7:6:150:SER:O	2.42	0.49
18:X:112:PRO:HD2	18:X:126:GLY:HA3	1.92	0.49
12:M:163:ASN:HB3	12:M:292:ALA:HB1	1.95	0.49
17:T:297:PRO:HA	17:T:300:PHE:HB3	1.94	0.49
17:V:458:ALA:HA	17:V:461:GLN:HE22	1.77	0.49
3:2:366:LEU:HD22	3:2:378:LEU:HD11	1.94	0.49
13:P:145:MET:HG3	13:P:149:LYS:HD2	1.95	0.49
18:Z:491:ASP:N	18:Z:491:ASP:OD1	2.42	0.49
6:5:30:LEU:HD13	12:M:110:LEU:HG	1.95	0.49
11:C:74:VAL:O	11:C:78:LEU:HB2	2.13	0.49
17:U:46:ASP:HB2	17:U:49:ARG:HH11	1.78	0.49
3:2:67:THR:HG21	3:2:102:GLN:HG2	1.95	0.48
16:S:195:ASN:HA	16:S:205:PRO:HA	1.94	0.48
2:1:563:ALA:HA	9:8:39:LYS:HE2	1.94	0.48
11:A:82:PHE:HB3	11:B:81:MET:HE3	1.93	0.48
13:P:74:LEU:HD22	13:P:134:LEU:HD11	1.94	0.48
17:U:545:ALA:O	17:U:549:HIS:ND1	2.38	0.48
3:2:36:LEU:HD22	3:2:41:VAL:HG11	1.95	0.48
4:3:276:GLU:OE2	12:M:131:ASN:ND2	2.46	0.48
17:V:201:PRO:HA	17:V:216:GLY:HA2	1.96	0.48
17:V:206:VAL:HB	17:V:209:VAL:HG12	1.96	0.48
11:E:87:ASN:O	11:E:91:ARG:HB2	2.14	0.48
16:S:140:VAL:HG22	16:S:160:LEU:HB3	1.96	0.48
17:T:529:ASN:ND2	17:T:553:GLU:OE2	2.47	0.48
16:S:213:PRO:HG3	16:S:244:ARG:HA	1.95	0.48
7:6:107:VAL:HG11	10:9:48:GLY:HA3	1.95	0.48
17:U:217:ARG:HE	17:U:319:HIS:CD2	2.32	0.48
18:Z:172:PRO:HG2	18:Z:386:MET:HB2	1.96	0.48
1:0:69:PRO:HD2	10:9:83:LYS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:125:ASP:OD1	17:V:125:ASP:N	2.46	0.48
2:1:539:ASP:N	2:1:539:ASP:OD1	2.47	0.48
11:E:61:MET:SD	11:F:60:LYS:NZ	2.80	0.48
13:P:134:LEU:HA	13:P:137:VAL:HG12	1.96	0.48
17:U:257:CYS:HB2	17:U:285:THR:HG22	1.96	0.48
18:X:478:TYR:HB3	18:X:481:LEU:HD12	1.94	0.48
2:1:175:ALA:HB1	2:1:476:VAL:HG21	1.96	0.48
17:V:112:ASP:OD1	17:V:112:ASP:N	2.47	0.48
5:4:113:THR:HG22	5:4:125:LYS:HE3	1.95	0.47
17:U:217:ARG:HE	17:U:319:HIS:HD2	1.60	0.47
18:Y:281:LEU:HD23	18:Y:334:THR:HB	1.94	0.47
4:3:212:VAL:HG22	12:M:136:PRO:HG3	1.96	0.47
6:5:12:ALA:HB2	9:8:58:TYR:HD2	1.79	0.47
10:9:80:GLN:HB3	10:9:86:ALA:HB2	1.96	0.47
17:T:476:ARG:NH2	17:T:504:ALA:O	2.40	0.47
17:V:210:ASP:HB2	17:V:497:GLN:HE22	1.80	0.47
18:Y:273:ARG:HD3	18:Y:333:ILE:HG13	1.96	0.47
3:2:268:VAL:HG13	3:2:269:VAL:HG13	1.96	0.47
10:9:65:THR:HG23	10:9:67:GLY:H	1.78	0.47
11:H:81:MET:O	11:H:84:SER:OG	2.30	0.47
3:2:147:VAL:HG11	3:2:157:LEU:HD23	1.97	0.47
8:7:73:LYS:HA	8:7:73:LYS:HD3	1.72	0.47
13:P:203:SER:O	17:U:43:LYS:NZ	2.42	0.47
18:Z:124:VAL:HG21	18:Z:257:ALA:HB1	1.97	0.47
18:Z:179:ILE:HD12	18:Z:336:VAL:HG22	1.96	0.47
11:A:86:ILE:HG21	11:B:85:LEU:HA	1.97	0.47
16:S:127:LEU:HD23	16:S:157:ARG:HH11	1.79	0.47
18:X:562:ASN:ND2	18:X:566:LYS:O	2.47	0.47
18:Y:270:GLU:O	18:Y:274:ASP:HB2	2.15	0.47
2:1:479:ASP:OD2	2:1:481:SER:OG	2.33	0.47
4:3:219:LEU:HD22	4:3:240:VAL:HG13	1.96	0.47
17:T:155:ILE:HD12	17:T:312:TYR:HB2	1.96	0.47
11:A:124:ILE:HB	11:J:61:MET:HG3	1.97	0.47
13:P:156:VAL:HG12	13:P:187:GLN:O	2.15	0.47
17:U:134:ASN:ND2	18:Z:146:GLU:OE2	2.48	0.47
17:U:323:ILE:HG12	17:U:380:PHE:HB2	1.95	0.47
17:V:228:GLN:N	20:V:1001:ATP:O3G	2.46	0.47
18:Z:213:VAL:HG22	18:Z:261:VAL:HG13	1.96	0.47
5:4:54:GLU:O	5:4:58:LEU:HB2	2.14	0.47
5:4:80:ALA:HA	5:4:83:LYS:HB2	1.97	0.47
17:T:47:GLU:HA	17:T:50:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:303:PRO:HG2	17:U:330:GLN:HG3	1.97	0.47
2:1:435:THR:HG23	2:1:438:GLN:H	1.79	0.47
11:A:59:SER:HA	11:A:62:VAL:HG12	1.97	0.47
17:U:104:GLN:HB3	18:X:95:GLY:HA2	1.97	0.47
3:2:15:ILE:HG22	3:2:47:LEU:HD11	1.97	0.46
18:Z:273:ARG:HD3	18:Z:333:ILE:HG13	1.96	0.46
18:Z:515:LYS:O	18:Z:515:LYS:HG2	2.15	0.46
14:Q:54:ASP:OD2	14:Q:54:ASP:N	2.49	0.46
17:T:303:PRO:HG2	17:T:330:GLN:HG3	1.97	0.46
18:X:166:VAL:HG23	18:X:170:LEU:HD12	1.98	0.46
18:X:307:ALA:O	18:X:309:GLY:N	2.41	0.46
18:X:445:GLN:NE2	18:X:459:LYS:O	2.49	0.46
18:Y:215:GLU:OE2	18:Y:286:ASN:ND2	2.48	0.46
2:1:381:ARG:NH2	2:1:403:ASP:OD1	2.49	0.46
4:3:199:ALA:HA	4:3:236:LEU:HD13	1.98	0.46
16:S:150:LEU:HD23	16:S:153:ILE:HD11	1.96	0.46
2:1:191:GLU:HA	2:1:194:LYS:HG2	1.98	0.46
17:T:202:LEU:HB2	17:T:217:ARG:HG2	1.98	0.46
3:2:70:LEU:HD12	3:2:106:VAL:HG22	1.98	0.46
17:U:240:ILE:HD12	17:U:279:THR:HG21	1.96	0.46
17:U:529:ASN:HD22	18:X:527:LEU:HD11	1.81	0.46
18:X:63:LEU:HB2	18:X:74:LEU:HB2	1.98	0.46
3:2:215:PHE:HA	3:2:250:GLY:HA3	1.97	0.46
4:3:261:VAL:HG11	4:3:285:ALA:HB2	1.97	0.46
15:R:160:VAL:HG23	15:R:161:LYS:HD2	1.98	0.46
17:V:50:LYS:HA	17:V:50:LYS:HD3	1.79	0.46
2:1:540:LEU:HD12	2:1:541:PRO:HD2	1.97	0.46
17:T:492:ILE:O	17:T:497:GLN:NE2	2.42	0.46
18:X:429:ASP:HA	18:X:432:THR:HG22	1.97	0.46
18:X:503:ALA:O	18:X:506:ILE:CG1	2.56	0.46
18:Y:158:GLU:HG2	18:Y:175:ARG:HB3	1.97	0.46
16:S:99:LYS:O	16:S:188:GLN:N	2.39	0.46
16:S:304:LEU:HD21	18:X:305:PRO:HB2	1.98	0.46
17:T:270:ALA:HB1	18:X:155:THR:HG22	1.97	0.46
3:2:188:ALA:HB1	3:2:222:PHE:HE2	1.80	0.46
10:9:56:ASN:OD1	10:9:56:ASN:N	2.49	0.46
17:V:76:SER:O	17:V:76:SER:OG	2.33	0.46
18:X:266:LEU:HD21	18:X:324:ARG:HB2	1.98	0.46
2:1:245:ALA:HB1	2:1:498:LEU:HD13	1.98	0.45
3:2:288:LEU:HD23	3:2:307:VAL:HG11	1.97	0.45
5:4:141:VAL:HG21	5:4:172:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:183:SER:OG	17:V:184:LEU:N	2.49	0.45
15:R:75:TYR:OH	15:R:83:GLN:NE2	2.50	0.45
2:1:76:GLU:OE2	2:1:133:ARG:NH2	2.50	0.45
3:2:390:THR:HG22	3:2:392:PRO:HD2	1.98	0.45
12:M:201:GLY:HA3	12:M:203:LYS:HE3	1.97	0.45
17:T:123:GLN:O	18:Y:98:ARG:NH1	2.39	0.45
17:T:243:LYS:HG3	17:T:281:ALA:HA	1.99	0.45
18:X:123:ASN:HD21	18:X:127:GLU:HB2	1.82	0.45
18:Y:211:ALA:HB3	18:Y:284:VAL:HG22	1.97	0.45
18:Z:284:VAL:HG11	18:Z:287:ILE:HD13	1.98	0.45
2:1:354:PRO:HG2	7:6:51:LEU:HB3	1.99	0.45
11:E:107:PHE:O	11:E:111:GLU:HG2	2.16	0.45
15:R:51:PRO:HB2	16:S:86:VAL:HG11	1.98	0.45
17:T:495:GLU:HG3	17:T:533:PHE:HB3	1.98	0.45
18:X:178:LYS:HB3	18:X:358:LEU:HD23	1.99	0.45
18:Y:110:LYS:HB3	18:Y:140:ILE:HG22	1.97	0.45
11:E:92:ASN:OD1	11:E:92:ASN:N	2.50	0.45
2:1:129:PHE:HZ	2:1:133:ARG:HH21	1.64	0.45
3:2:46:ARG:HH12	6:5:122:LEU:H	1.63	0.45
16:S:188:GLN:HB3	16:S:216:LEU:HD12	1.98	0.45
3:2:78:VAL:HA	8:7:74:ILE:HB	1.99	0.45
4:3:128:VAL:HG21	4:3:143:LEU:HD11	1.98	0.45
5:4:71:ALA:O	5:4:84:ARG:NH2	2.44	0.45
11:A:58:ALA:O	11:B:59:SER:OG	2.29	0.45
16:S:192:ILE:HB	16:S:208:ALA:HB3	1.99	0.45
17:V:258:VAL:HG22	17:V:286:ILE:HB	1.99	0.45
18:Z:276:GLU:OE1	18:Z:278:GLN:NE2	2.50	0.45
18:X:108:PRO:HB2	18:X:142:SER:HB2	1.99	0.45
18:X:161:VAL:O	18:X:204:HIS:NE2	2.38	0.45
18:Z:63:LEU:HB2	18:Z:74:LEU:HB2	1.98	0.45
5:4:117:GLU:HG2	5:4:118:THR:HG23	1.99	0.45
17:U:242:GLN:HB3	17:U:255:VAL:HG13	1.99	0.45
7:6:32:VAL:H	9:8:14:THR:HG21	1.82	0.45
18:Y:185:ALA:HB3	18:Y:366:ARG:HH22	1.82	0.45
3:2:377:VAL:HG21	3:2:438:ILE:HG23	1.99	0.44
7:6:130:ARG:O	7:6:136:THR:OG1	2.35	0.44
8:7:82:ILE:HG23	17:T:53:PHE:HD2	1.83	0.44
17:T:195:ARG:NH1	17:T:363:GLU:OE1	2.49	0.44
13:P:156:VAL:HG21	13:P:170:LEU:HD21	1.99	0.44
2:1:267:ARG:NH1	2:1:519:GLU:OE1	2.47	0.44
14:Q:48:ARG:NE	16:S:164:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:208:ALA:HA	17:T:484:LEU:HD22	2.00	0.44
18:X:284:VAL:HG11	18:X:287:ILE:HD13	1.99	0.44
18:X:284:VAL:HB	18:X:337:GLN:HG2	1.98	0.44
3:2:82:LYS:HA	5:4:84:ARG:HD3	1.99	0.44
7:6:143:LEU:HD11	7:6:148:SER:HB3	2.00	0.44
17:T:241:HIS:CD2	17:T:245:CYS:HG	2.36	0.44
17:V:359:SER:OG	18:Z:251:MET:O	2.32	0.44
18:Y:436:ALA:HA	18:Y:439:ILE:HG12	1.98	0.44
3:2:416:VAL:HG13	3:2:433:TYR:HE1	1.81	0.44
5:4:141:VAL:HG13	5:4:168:LYS:HE2	2.00	0.44
9:8:26:HIS:HB3	9:8:29:GLN:HG3	1.99	0.44
18:Z:198:ASN:HA	18:Z:202:LYS:HB2	1.99	0.44
3:2:321:LYS:HE3	5:4:13:TYR:HA	1.99	0.44
9:8:36:ALA:HA	9:8:40:LEU:HB3	2.00	0.44
11:C:86:ILE:HG23	11:D:99:LEU:HD22	1.98	0.44
17:U:155:ILE:HD12	17:U:312:TYR:HB2	2.00	0.44
2:1:307:GLY:HA3	2:1:534:LYS:HE3	2.00	0.44
4:3:91:VAL:O	4:3:95:LEU:N	2.49	0.44
11:I:92:ASN:OD1	11:I:92:ASN:N	2.49	0.44
14:Q:30:VAL:HG13	15:R:159:ALA:HB3	1.99	0.44
18:Y:74:LEU:HB3	18:Y:87:CYS:HB3	2.00	0.44
1:0:35:PRO:HB3	1:0:39:THR:HG23	2.00	0.44
11:B:90:ALA:O	11:C:92:ASN:ND2	2.48	0.44
11:G:62:VAL:HG23	11:H:59:SER:HB2	1.99	0.44
17:U:468:ALA:HA	17:U:471:GLN:HG2	2.00	0.44
1:0:62:PRO:HG2	7:6:95:LYS:HB2	2.00	0.44
11:B:86:ILE:HG21	11:C:85:LEU:HA	1.99	0.44
17:T:412:LEU:HB2	17:T:420:ALA:HB1	2.00	0.44
17:V:446:LEU:HD12	17:V:480:LEU:HD13	1.99	0.44
18:Z:263:LEU:O	18:Z:267:THR:OG1	2.33	0.44
18:Z:510:LYS:O	18:Z:511:GLU:OE2	2.35	0.44
11:I:78:LEU:HD13	11:J:113:ILE:HD11	2.00	0.43
13:P:168:VAL:O	13:P:172:LYS:NZ	2.46	0.43
18:Y:63:LEU:HB2	18:Y:74:LEU:HB2	2.00	0.43
10:9:64:PRO:HG2	12:M:257:MET:HE2	2.00	0.43
11:B:71:LEU:HA	11:B:74:VAL:HG22	2.00	0.43
17:T:241:HIS:NE2	17:T:245:CYS:SG	2.91	0.43
11:E:78:LEU:HB2	11:E:81:MET:HE2	2.00	0.43
17:T:235:ALA:HB1	17:T:323:ILE:HG12	1.99	0.43
17:U:370:LYS:HA	17:U:370:LYS:HD3	1.84	0.43
18:Y:112:PRO:HD2	18:Y:126:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:75:GLY:HA3	11:E:74:VAL:HG22	1.99	0.43
11:F:93:PRO:HB3	11:G:95:ILE:HD13	2.01	0.43
18:X:414:GLN:HA	18:X:417:ILE:HD12	2.01	0.43
11:J:78:LEU:HD11	11:J:107:PHE:HD1	1.84	0.43
17:U:250:PRO:C	17:U:251:LYS:HG2	2.39	0.43
2:1:401:LEU:HD22	6:5:73:LYS:HB3	2.01	0.43
11:H:112:SER:HB2	12:M:243:ASN:HD21	1.84	0.43
18:Y:61:SER:HA	18:Y:108:PRO:HA	2.00	0.43
11:E:91:ARG:NH1	15:R:95:ASP:O	2.51	0.43
17:T:464:SER:OG	17:T:465:ASP:N	2.51	0.43
1:0:4:SER:OG	2:1:317:SER:O	2.27	0.43
13:P:155:THR:HB	13:P:201:GLU:HB2	2.01	0.43
14:Q:32:LYS:O	14:Q:36:LYS:N	2.50	0.43
17:T:100:LEU:HB3	17:T:103:VAL:HB	2.00	0.43
17:V:223:ILE:HG12	17:V:406:ILE:HD12	2.00	0.43
18:X:65:VAL:HG22	18:X:102:VAL:HG22	2.01	0.43
18:X:165:LYS:HB2	18:X:165:LYS:HE3	1.84	0.43
18:Y:352:ALA:HA	18:Y:355:PHE:HD2	1.84	0.43
18:Y:480:ASP:OD1	18:Y:480:ASP:N	2.37	0.43
18:Z:42:GLN:HB3	18:Z:49:ASP:HB2	2.00	0.43
3:2:108:GLU:HB2	3:2:142:ARG:HB3	2.01	0.43
11:H:91:ARG:NH2	16:S:232:ASP:OD2	2.52	0.43
17:U:235:ALA:HB1	17:U:323:ILE:HG21	2.00	0.43
18:X:74:LEU:HB3	18:X:87:CYS:HB3	2.01	0.43
18:Z:318:LEU:HD21	18:Z:354:THR:HB	2.01	0.43
18:Z:503:ALA:HA	18:Z:506:ILE:HG12	2.01	0.43
2:1:83:ASN:HD21	2:1:85:ARG:HB2	1.84	0.43
3:2:206:SER:OG	3:2:209:ASP:OD2	2.37	0.43
4:3:266:LYS:HD2	4:3:266:LYS:HA	1.78	0.43
13:P:153:TYR:CD1	13:P:185:VAL:HG21	2.54	0.43
17:T:222:LEU:HA	17:T:381:PRO:HG2	2.00	0.43
17:V:172:ASP:N	17:V:172:ASP:OD1	2.44	0.43
7:6:143:LEU:HD12	7:6:143:LEU:HA	1.85	0.42
12:M:254:LEU:HD12	12:M:254:LEU:HA	1.92	0.42
15:R:52:SER:HB3	16:S:91:ASP:HB2	2.02	0.42
17:U:241:HIS:HE1	17:U:493:PRO:HA	1.84	0.42
4:3:201:SER:HA	4:3:205:CYS:HB2	2.01	0.42
11:B:82:PHE:HE1	11:B:103:ALA:HB1	1.83	0.42
16:S:212:SER:HB3	16:S:215:LEU:HB2	2.00	0.42
2:1:247:LYS:HD2	2:1:247:LYS:HA	1.83	0.42
2:1:309:LYS:O	2:1:314:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:53:LEU:HD23	10:9:53:LEU:HA	1.90	0.42
17:U:406:ILE:HA	17:U:426:SER:HB2	2.01	0.42
17:V:85:GLY:O	17:V:144:VAL:N	2.45	0.42
18:Y:274:ASP:HA	18:Y:330:LYS:HD2	2.00	0.42
3:2:111:GLY:HA3	3:2:146:GLY:HA2	2.01	0.42
16:S:176:SER:O	16:S:180:GLU:HG2	2.19	0.42
17:T:62:VAL:O	17:T:66:LEU:N	2.49	0.42
17:T:108:LEU:HB2	17:T:151:VAL:HA	2.01	0.42
18:Y:178:LYS:N	18:Y:359:ASP:OD2	2.45	0.42
18:Y:202:LYS:HE3	18:Y:202:LYS:HB3	1.96	0.42
2:1:82:HIS:NE2	8:7:120:TYR:O	2.52	0.42
8:7:36:LYS:HB2	8:7:51:ALA:HB3	2.00	0.42
17:U:84:LEU:HD11	17:U:145:TYR:HD1	1.84	0.42
17:U:512:VAL:HG13	17:U:561:GLY:HA3	2.01	0.42
18:Y:43:VAL:HG22	18:Y:48:VAL:HG13	2.02	0.42
6:5:34:ILE:HD13	12:M:107:THR:HG23	2.01	0.42
7:6:104:ASN:HD21	10:9:49:VAL:HG12	1.83	0.42
2:1:268:LEU:HD22	2:1:357:ALA:HB1	2.01	0.42
5:4:233:HIS:CG	8:7:153:LEU:HD11	2.55	0.42
13:P:204:ASP:OD1	13:P:205:ARG:NH1	2.51	0.42
17:T:154:PRO:HA	17:T:182:SER:HA	2.02	0.42
17:U:212:LEU:HD11	17:U:484:LEU:HD13	2.00	0.42
3:2:80:HIS:CE1	3:2:82:LYS:HB3	2.55	0.42
11:B:91:ARG:HE	11:C:91:ARG:HH12	1.67	0.42
12:M:147:SER:O	12:M:147:SER:OG	2.33	0.42
15:R:51:PRO:HA	15:R:54:TYR:HD2	1.84	0.42
17:U:84:LEU:HD12	17:U:84:LEU:HA	1.91	0.42
17:V:108:LEU:HD21	17:V:116:LYS:HD2	2.01	0.42
17:V:550:LEU:HA	17:V:553:GLU:HB2	2.01	0.42
18:Z:142:SER:O	18:Z:145:ARG:NH1	2.53	0.42
2:1:365:GLN:HG2	2:1:383:ILE:HD12	2.02	0.42
3:2:66:LEU:HD22	3:2:90:PRO:HB2	2.01	0.42
4:3:121:PHE:HA	4:3:124:PHE:HB2	2.01	0.42
11:B:95:ILE:HD12	11:B:95:ILE:HA	1.93	0.42
11:D:78:LEU:HD12	11:D:78:LEU:HA	1.89	0.42
11:I:90:ALA:HB2	11:J:99:LEU:HD21	2.02	0.42
13:P:99:LEU:HG	13:P:103:LYS:HE2	2.02	0.42
17:V:345:PRO:HB2	17:V:349:ALA:HA	2.02	0.42
11:G:86:ILE:HG21	11:H:85:LEU:HA	2.02	0.42
12:M:189:TRP:CD2	12:M:233:ALA:HB2	2.55	0.42
13:P:209:MET:HG2	17:T:79:PRO:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:104:GLN:HG2	18:Y:97:VAL:HG22	2.01	0.42
11:C:71:LEU:HB2	11:D:70:ALA:HB1	2.02	0.41
11:J:95:ILE:HG22	11:J:98:GLN:HB3	2.01	0.41
17:V:215:ILE:HA	17:V:219:GLN:HE21	1.85	0.41
18:X:535:LYS:NZ	18:X:536:GLU:O	2.51	0.41
18:Y:451:GLU:HA	18:Y:454:THR:HG22	2.01	0.41
18:Z:480:ASP:OD1	18:Z:480:ASP:N	2.53	0.41
3:2:62:ASP:OD1	3:2:62:ASP:N	2.39	0.41
9:8:26:HIS:CD2	9:8:28:PHE:H	2.38	0.41
2:1:535:HIS:HB3	2:1:540:LEU:HB2	2.01	0.41
3:2:370:ILE:HB	3:2:377:VAL:HG12	2.02	0.41
5:4:10:GLU:HG2	5:4:58:LEU:HD11	2.02	0.41
10:9:70:PRO:HA	12:M:264:SER:HA	2.01	0.41
18:Z:487:TYR:O	18:Z:498:LYS:NZ	2.47	0.41
2:1:189:LEU:HD13	2:1:194:LYS:HB3	2.02	0.41
3:2:337:THR:HG22	3:2:434:VAL:HG11	2.02	0.41
12:M:199:LYS:HA	12:M:199:LYS:HD3	1.84	0.41
18:X:505:ASP:O	18:X:509:ARG:N	2.53	0.41
18:Y:504:LYS:O	18:Y:508:SER:N	2.54	0.41
18:Z:365:SER:HB3	18:Z:368:ILE:HD12	2.03	0.41
2:1:39:LYS:HD2	2:1:39:LYS:HA	1.85	0.41
17:U:132:PHE:CE1	17:U:297:PRO:HB2	2.55	0.41
18:X:438:LYS:HE3	18:X:479:ASP:HA	2.03	0.41
2:1:163:SER:OG	2:1:165:GLU:OE2	2.37	0.41
4:3:235:ASP:N	4:3:235:ASP:OD1	2.54	0.41
9:8:23:ASN:HB3	12:M:97:VAL:HG23	2.02	0.41
11:H:58:ALA:O	11:I:59:SER:OG	2.38	0.41
17:T:493:PRO:HD2	17:T:496:ARG:HD2	2.03	0.41
2:1:148:PHE:O	2:1:150:ARG:NH2	2.54	0.41
6:5:28:THR:HG23	9:8:28:PHE:HB3	2.01	0.41
8:7:123:HIS:HD2	8:7:125:GLU:H	1.69	0.41
17:U:250:PRO:O	17:U:251:LYS:HG2	2.21	0.41
17:U:407:PHE:CE2	17:U:409:GLU:HG2	2.56	0.41
18:X:109:ILE:HD13	18:X:125:ILE:HG22	2.03	0.41
18:X:287:ILE:HD12	18:X:290:PHE:HB3	2.03	0.41
2:1:32:THR:OG1	8:7:163:ALA:O	2.35	0.41
2:1:267:ARG:HG3	2:1:523:LEU:HD21	2.03	0.41
3:2:6:ASN:ND2	8:7:58:ALA:O	2.54	0.41
4:3:106:TRP:O	4:3:110:LEU:HB2	2.21	0.41
4:3:213:ARG:NH1	12:M:143:ASP:OD1	2.49	0.41
5:4:184:LEU:HD23	8:7:184:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:86:ILE:HG21	11:G:85:LEU:HA	2.02	0.41
11:G:54:SER:O	11:G:54:SER:OG	2.34	0.41
16:S:104:ALA:HA	16:S:193:LEU:HB2	2.03	0.41
17:T:172:ASP:OD1	17:T:172:ASP:N	2.53	0.41
17:U:407:PHE:HE2	17:U:409:GLU:HG2	1.86	0.41
17:V:559:LEU:HA	17:V:560:PRO:HD3	1.96	0.41
18:X:474:LEU:HD23	18:X:474:LEU:HA	1.94	0.41
18:Y:111:VAL:HG11	18:Y:264:THR:HG23	2.03	0.41
18:Z:80:MET:SD	18:Z:86:ARG:NE	2.90	0.41
18:Z:124:VAL:HG22	18:Z:261:VAL:HB	2.03	0.41
18:Z:506:ILE:HA	18:Z:509:ARG:HH21	1.86	0.41
8:7:153:LEU:HD23	8:7:153:LEU:HA	1.93	0.41
13:P:175:GLU:HA	13:P:184:LEU:CD2	2.51	0.41
17:U:121:ASN:HD22	17:U:123:GLN:HE21	1.68	0.41
17:V:232:THR:OG1	20:V:1001:ATP:O2B	2.39	0.41
4:3:195:LEU:O	4:3:226:TYR:OH	2.34	0.40
7:6:52:LYS:HB2	7:6:52:LYS:HE2	1.88	0.40
18:Y:53:ASP:OD1	18:Y:53:ASP:N	2.53	0.40
5:4:238:VAL:HG21	8:7:142:GLU:HB3	2.03	0.40
11:G:125:LEU:HD21	11:H:124:ILE:HG22	2.04	0.40
13:P:179:ASP:OD1	13:P:179:ASP:N	2.54	0.40
18:X:132:GLN:HE22	18:X:235:LEU:HD13	1.86	0.40
18:Z:114:GLY:HA3	18:Z:138:ALA:HB3	2.04	0.40
2:1:517:GLU:HG2	2:1:518:GLU:HG3	2.04	0.40
11:A:83:GLY:O	11:B:84:SER:OG	2.34	0.40
11:E:93:PRO:HA	11:E:96:ALA:HB2	2.04	0.40
17:T:212:LEU:HD11	17:T:484:LEU:HD13	2.03	0.40
17:T:345:PRO:HB2	17:T:349:ALA:HA	2.03	0.40
17:U:311:GLU:OE2	17:U:364:ARG:NE	2.44	0.40
3:2:128:VAL:HG21	3:2:143:VAL:HG11	2.03	0.40
9:8:74:ASP:HA	9:8:77:ILE:HG22	2.03	0.40
11:H:125:LEU:HD23	11:H:125:LEU:HA	1.95	0.40
17:U:50:LYS:HE3	17:U:52:LYS:HD2	2.03	0.40
17:V:131:VAL:HG12	17:V:133:GLY:H	1.85	0.40
6:5:122:LEU:HD23	6:5:122:LEU:HA	1.92	0.40
11:H:78:LEU:HD23	11:H:78:LEU:HA	1.89	0.40
17:U:436:PHE:HA	17:U:437:PRO:HD3	1.98	0.40
17:U:483:MET:HG2	17:U:504:ALA:HB2	2.03	0.40
18:Y:124:VAL:HG12	18:Y:261:VAL:HB	2.04	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%)	74 (94%)	5 (6%)	0	100	100
2	1	593/618 (96%)	576 (97%)	17 (3%)	0	100	100
3	2	439/441 (100%)	424 (97%)	14 (3%)	1 (0%)	47	79
4	3	243/325 (75%)	236 (97%)	7 (3%)	0	100	100
5	4	288/294 (98%)	276 (96%)	12 (4%)	0	100	100
6	5	121/123 (98%)	111 (92%)	9 (7%)	1 (1%)	19	57
7	6	122/151 (81%)	110 (90%)	12 (10%)	0	100	100
8	7	174/190 (92%)	169 (97%)	5 (3%)	0	100	100
9	8	86/89 (97%)	80 (93%)	6 (7%)	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%)	72 (100%)	0	0	100	100
11	C	71/127 (56%)	71 (100%)	0	0	100	100
11	D	72/127 (57%)	72 (100%)	0	0	100	100
11	E	72/127 (57%)	72 (100%)	0	0	100	100
11	F	72/127 (57%)	70 (97%)	2 (3%)	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%)	71 (99%)	1 (1%)	0	100	100
12	M	213/327 (65%)	208 (98%)	5 (2%)	0	100	100
13	P	191/229 (83%)	178 (93%)	12 (6%)	1 (0%)	29	66
14	Q	70/74 (95%)	67 (96%)	3 (4%)	0	100	100
15	R	175/199 (88%)	167 (95%)	8 (5%)	0	100	100
16	S	275/317 (87%)	262 (95%)	12 (4%)	1 (0%)	34	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	521/562 (93%)	501 (96%)	19 (4%)	1 (0%)	47	79
17	U	521/562 (93%)	493 (95%)	28 (5%)	0	100	100
17	V	518/562 (92%)	499 (96%)	19 (4%)	0	100	100
18	X	536/574 (93%)	510 (95%)	24 (4%)	2 (0%)	34	70
18	Y	518/574 (90%)	484 (93%)	33 (6%)	1 (0%)	47	79
18	Z	537/574 (94%)	499 (93%)	34 (6%)	4 (1%)	22	60
All	All	7034/8234 (85%)	6718 (96%)	304 (4%)	12 (0%)	50	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	X	308	VAL
18	Y	308	VAL
18	Z	308	VAL
13	P	149	LYS
18	Z	307	ALA
17	T	56	LYS
16	S	213	PRO
18	Z	306	SER
3	2	383	PRO
18	X	306	SER
18	Z	148	PRO
6	5	120	PRO

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
3	2	312/312 (100%)	310 (99%)	2 (1%)	86	92
4	3	195/258 (76%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	49 (98%)	1 (2%)	55	75
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%)	169 (99%)	2 (1%)	71	84
14	Q	56/58 (97%)	56 (100%)	0	100	100
15	R	134/151 (89%)	134 (100%)	0	100	100
16	S	235/265 (89%)	234 (100%)	1 (0%)	91	95
17	T	419/448 (94%)	418 (100%)	1 (0%)	93	97
17	U	419/448 (94%)	416 (99%)	3 (1%)	84	91
17	V	418/448 (93%)	417 (100%)	1 (0%)	93	97
18	X	446/469 (95%)	446 (100%)	0	100	100
18	Y	429/469 (92%)	429 (100%)	0	100	100
18	Z	447/469 (95%)	446 (100%)	1 (0%)	93	97
All	All	5628/6445 (87%)	5616 (100%)	12 (0%)	93	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	168	THR

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Mol	Chain	Res	Type
3	2	382	VAL
11	E	78	LEU
13	P	158	THR
13	P	187	GLN
16	S	147	ARG
17	T	220	ARG
17	U	53	PHE
17	U	220	ARG
17	U	479	ARG
17	V	316	THR
18	Z	509	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	316	ASN
2	1	394	GLN
2	1	531	HIS
3	2	59	GLN
3	2	68	ASN
3	2	74	ASN
3	2	153	ASN
3	2	243	GLN
4	3	87	ASN
4	3	309	ASN
5	4	38	GLN
5	4	240	GLN
7	6	40	ASN
8	7	102	GLN
8	7	123	HIS
8	7	170	HIS
8	7	184	ASN
9	8	26	HIS
10	9	97	ASN
11	A	92	ASN
11	C	87	ASN
11	C	98	GLN
11	D	94	ASN
11	G	98	GLN
11	H	98	GLN
12	M	108	ASN
12	M	121	ASN

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Mol	Chain	Res	Type
12	M	243	ASN
12	M	295	GLN
13	P	83	GLN
13	P	140	ASN
13	P	148	HIS
13	P	187	GLN
13	P	220	ASN
15	R	64	GLN
15	R	73	ASN
15	R	83	GLN
15	R	85	GLN
16	S	70	ASN
16	S	116	ASN
16	S	174	GLN
16	S	250	HIS
16	S	262	ASN
17	T	64	GLN
17	T	152	ASN
17	U	104	GLN
17	U	123	GLN
17	U	139	HIS
17	U	241	HIS
17	U	248	GLN
17	U	264	GLN
17	U	319	HIS
17	U	527	GLN
17	U	539	ASN
17	V	60	GLN
17	V	78	GLN
17	V	149	GLN
17	V	242	GLN
17	V	244	ASN
17	V	264	GLN
17	V	271	GLN
17	V	278	GLN
17	V	386	GLN
17	V	497	GLN
18	X	132	GLN
18	X	199	ASN
18	X	278	GLN
18	X	404	GLN
18	Y	174	GLN

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Mol	Chain	Res	Type
18	Y	199	ASN
18	Y	252	ASN
18	Y	408	GLN
18	Y	412	ASN
18	Z	174	GLN
18	Z	440	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
22	ADP	Y	601	21	24,29,29	0.96	1 (4%)	29,45,45	1.52	4 (13%)
20	ATP	U	1001	21	26,33,33	0.89	1 (3%)	31,52,52	1.59	5 (16%)
20	ATP	V	1001	21	26,33,33	0.91	1 (3%)	31,52,52	1.58	5 (16%)
22	ADP	Z	601	21	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
20	ATP	T	1001	21	26,33,33	0.91	1 (3%)	31,52,52	1.51	5 (16%)

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
22	ADP	Y	601	21	-	5/12/32/32	0/3/3/3
20	ATP	U	1001	21	-	2/18/38/38	0/3/3/3
20	ATP	V	1001	21	-	5/18/38/38	0/3/3/3
22	ADP	Z	601	21	-	3/12/32/32	0/3/3/3
20	ATP	T	1001	21	-	0/18/38/38	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	C5-C4	2.47	1.47	1.40
22	Y	601	ADP	C5-C4	2.31	1.47	1.40
20	T	1001	ATP	C5-C4	2.27	1.46	1.40
20	V	1001	ATP	C5-C4	2.26	1.46	1.40
20	U	1001	ATP	C5-C4	2.21	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	PA-O3A-PB	-4.38	117.80	132.83
20	U	1001	ATP	PB-O3B-PG	-4.07	118.86	132.83
20	U	1001	ATP	PA-O3A-PB	-3.98	119.16	132.83
20	T	1001	ATP	PB-O3B-PG	-3.78	119.84	132.83
22	Y	601	ADP	C3'-C2'-C1'	3.73	106.60	100.98
22	Y	601	ADP	PA-O3A-PB	-3.49	120.84	132.83
22	Y	601	ADP	N3-C2-N1	-3.28	123.56	128.68
20	U	1001	ATP	N3-C2-N1	-3.22	123.64	128.68
22	Z	601	ADP	PA-O3A-PB	-3.22	121.79	132.83
20	V	1001	ATP	C3'-C2'-C1'	3.21	105.81	100.98
20	T	1001	ATP	N3-C2-N1	-3.18	123.70	128.68
22	Z	601	ADP	N3-C2-N1	-3.14	123.78	128.68
20	V	1001	ATP	N3-C2-N1	-3.11	123.82	128.68
20	T	1001	ATP	PA-O3A-PB	-3.04	122.38	132.83
22	Z	601	ADP	C3'-C2'-C1'	2.78	105.16	100.98
20	T	1001	ATP	C4-C5-N7	-2.59	106.70	109.40
20	U	1001	ATP	C4-C5-N7	-2.50	106.80	109.40
20	V	1001	ATP	C4-C5-N7	-2.48	106.81	109.40
22	Z	601	ADP	C4-C5-N7	-2.45	106.85	109.40
20	V	1001	ATP	PB-O3B-PG	-2.45	124.43	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	601	ADP	C4-C5-N7	-2.40	106.89	109.40
20	T	1001	ATP	C3'-C2'-C1'	2.22	104.31	100.98
20	U	1001	ATP	C3'-C2'-C1'	2.22	104.31	100.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	V	1001	ATP	C5'-O5'-PA-O3A
22	Y	601	ADP	C5'-O5'-PA-O3A
22	Y	601	ADP	O4'-C4'-C5'-O5'
22	Y	601	ADP	C3'-C4'-C5'-O5'
22	Z	601	ADP	O4'-C4'-C5'-O5'
22	Z	601	ADP	PB-O3A-PA-O1A
20	V	1001	ATP	C5'-O5'-PA-O1A
22	Y	601	ADP	C5'-O5'-PA-O1A
20	U	1001	ATP	PA-O3A-PB-O1B
20	V	1001	ATP	PB-O3A-PA-O2A
20	V	1001	ATP	O4'-C4'-C5'-O5'
20	U	1001	ATP	PA-O3A-PB-O2B
20	V	1001	ATP	PB-O3A-PA-O1A
22	Y	601	ADP	PB-O3A-PA-O2A
22	Z	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

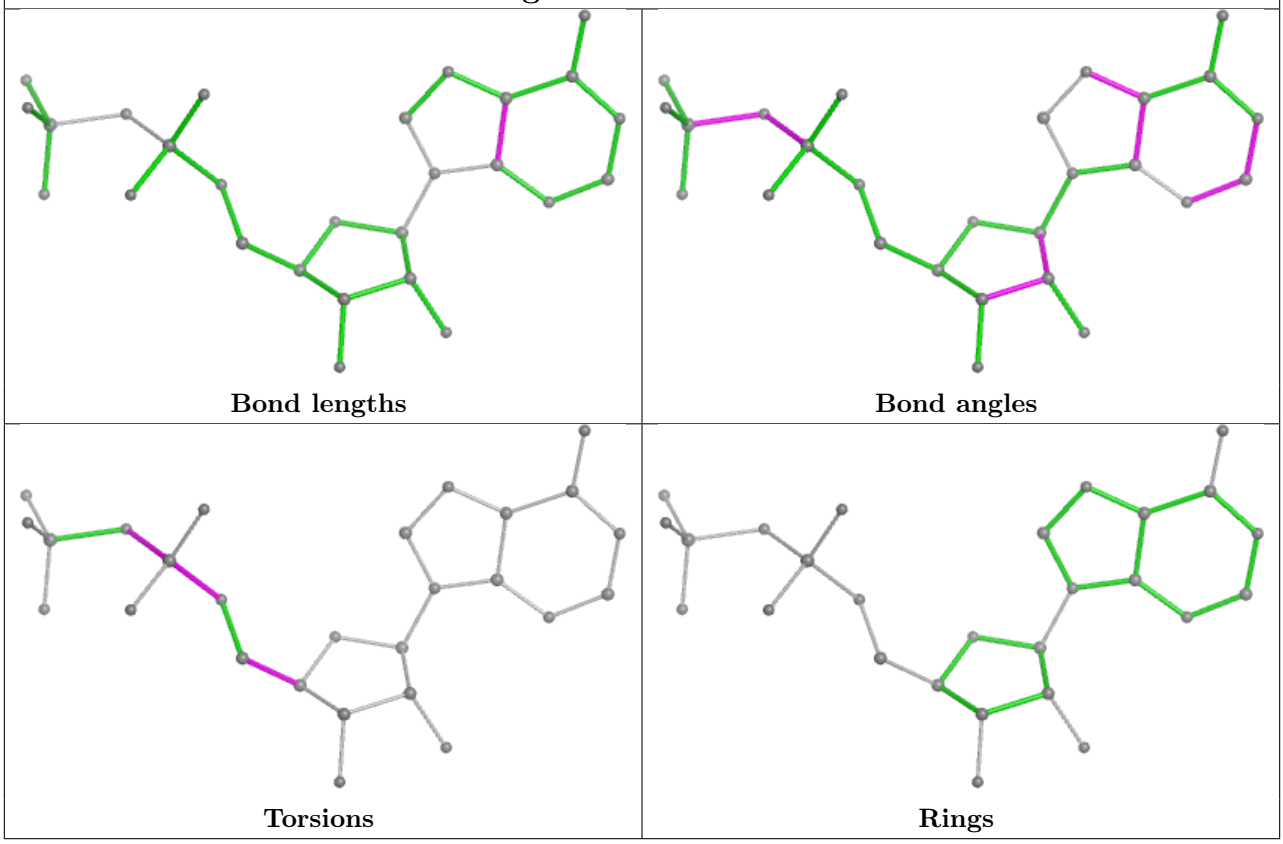
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	V	1001	ATP	2	0
22	Z	601	ADP	1	0

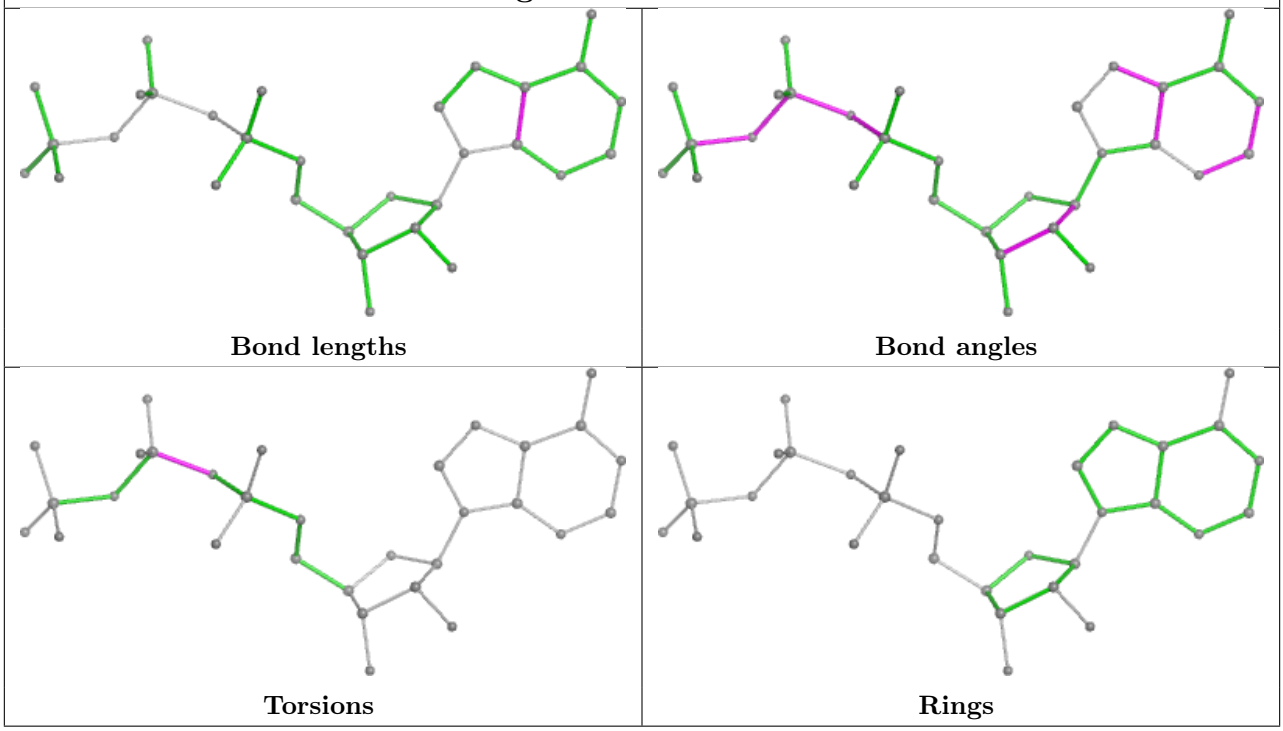
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

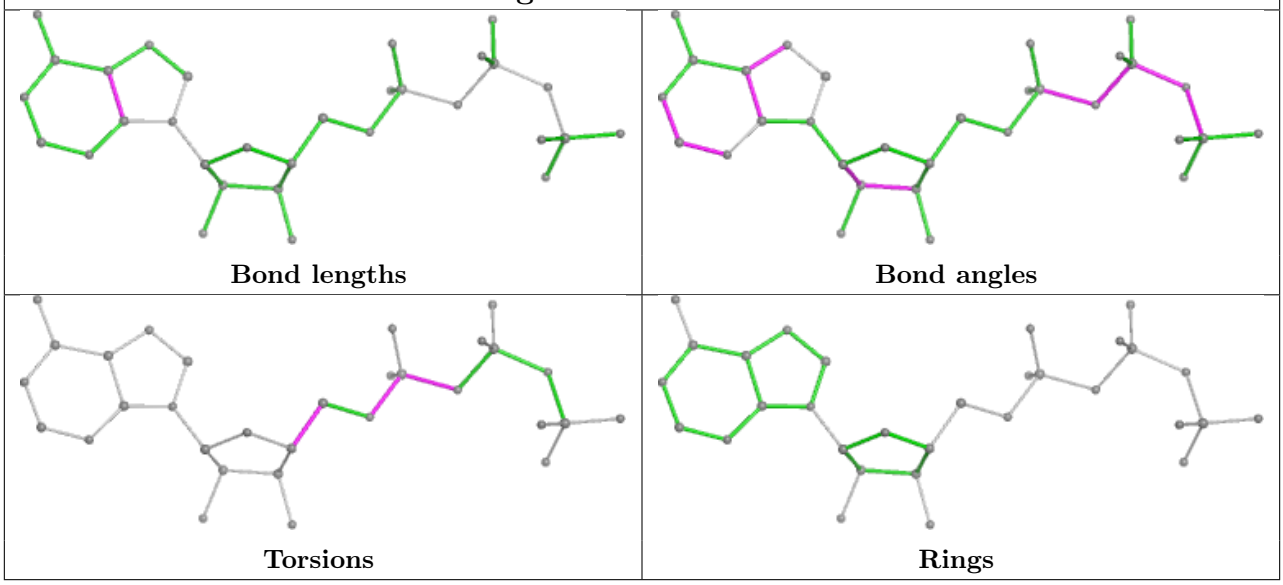
Ligand ADP Y 601



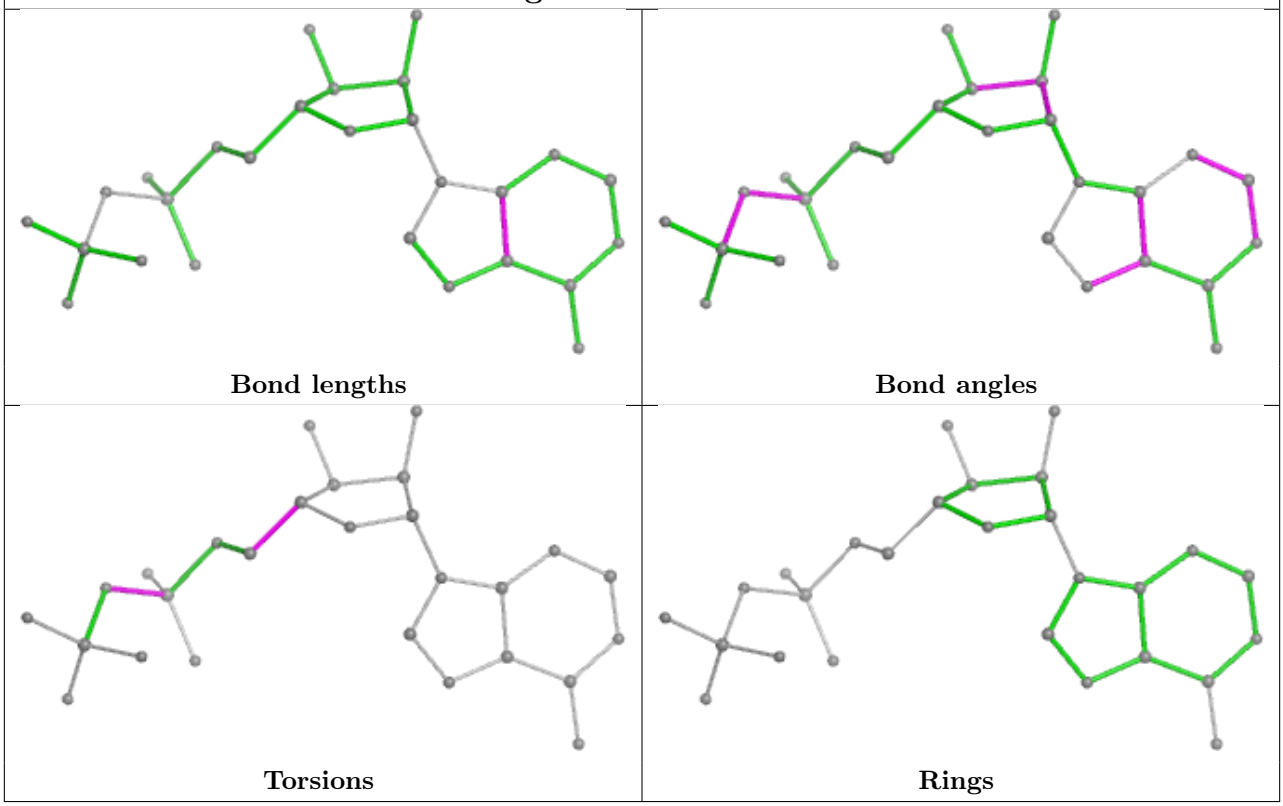
Ligand ATP U 1001

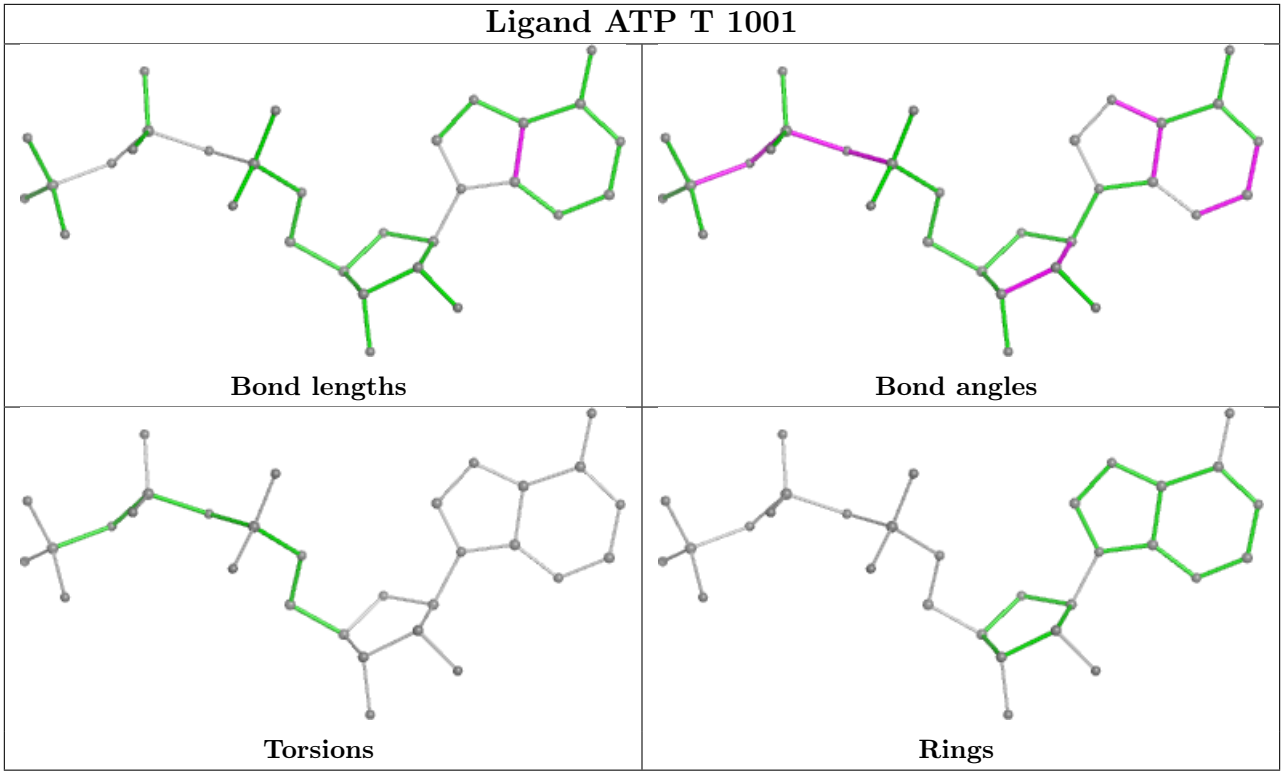


Ligand ATP V 1001



Ligand ADP Z 601





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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	3.68

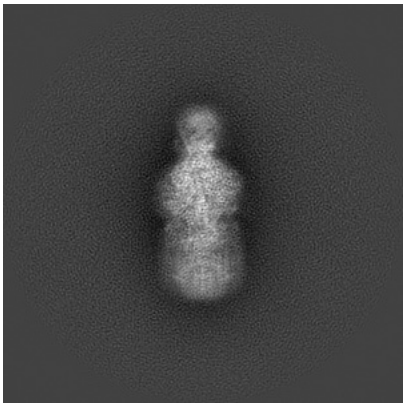
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4845. These allow visual inspection of the internal detail of the map and identification of artifacts.

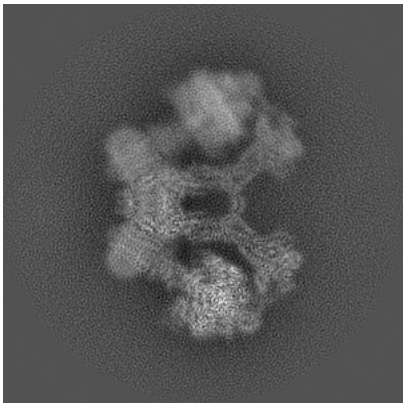
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

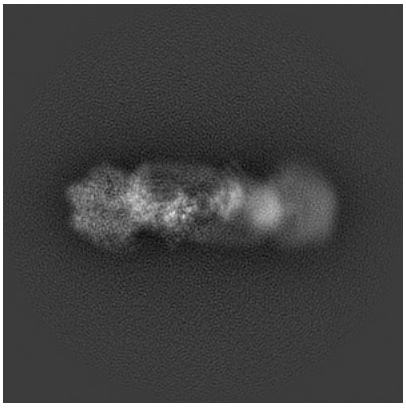
6.1.1 Primary map



X



Y

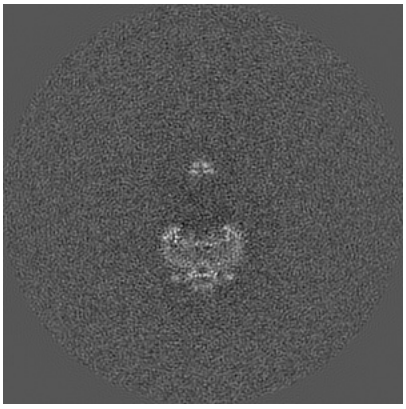


Z

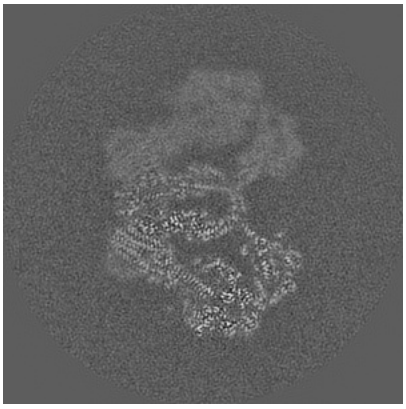
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

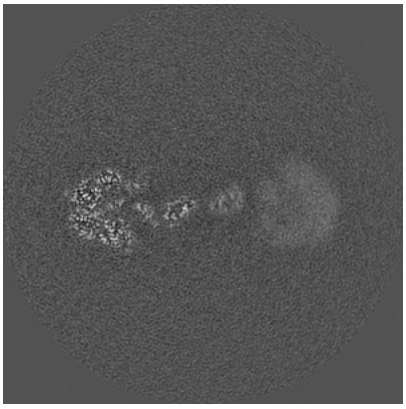
6.2.1 Primary map



X Index: 240



Y Index: 240

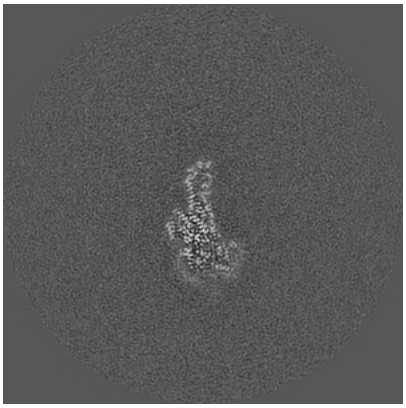


Z Index: 240

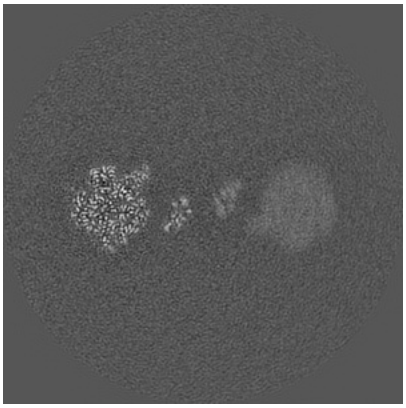
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 216

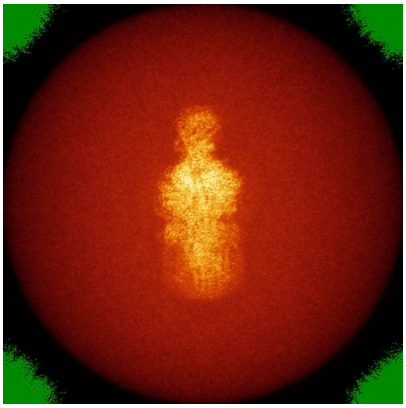
Y Index: 238

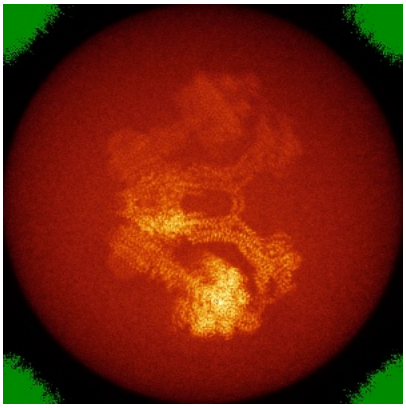

Z Index: 262

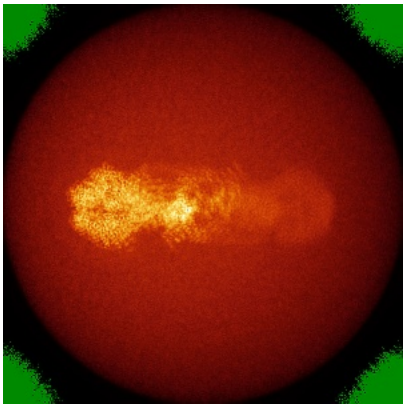
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

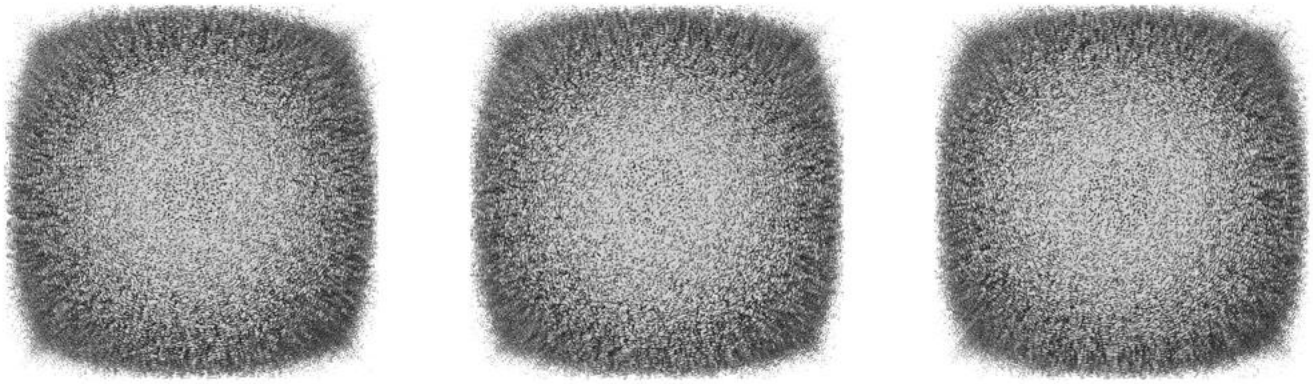

Y


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.

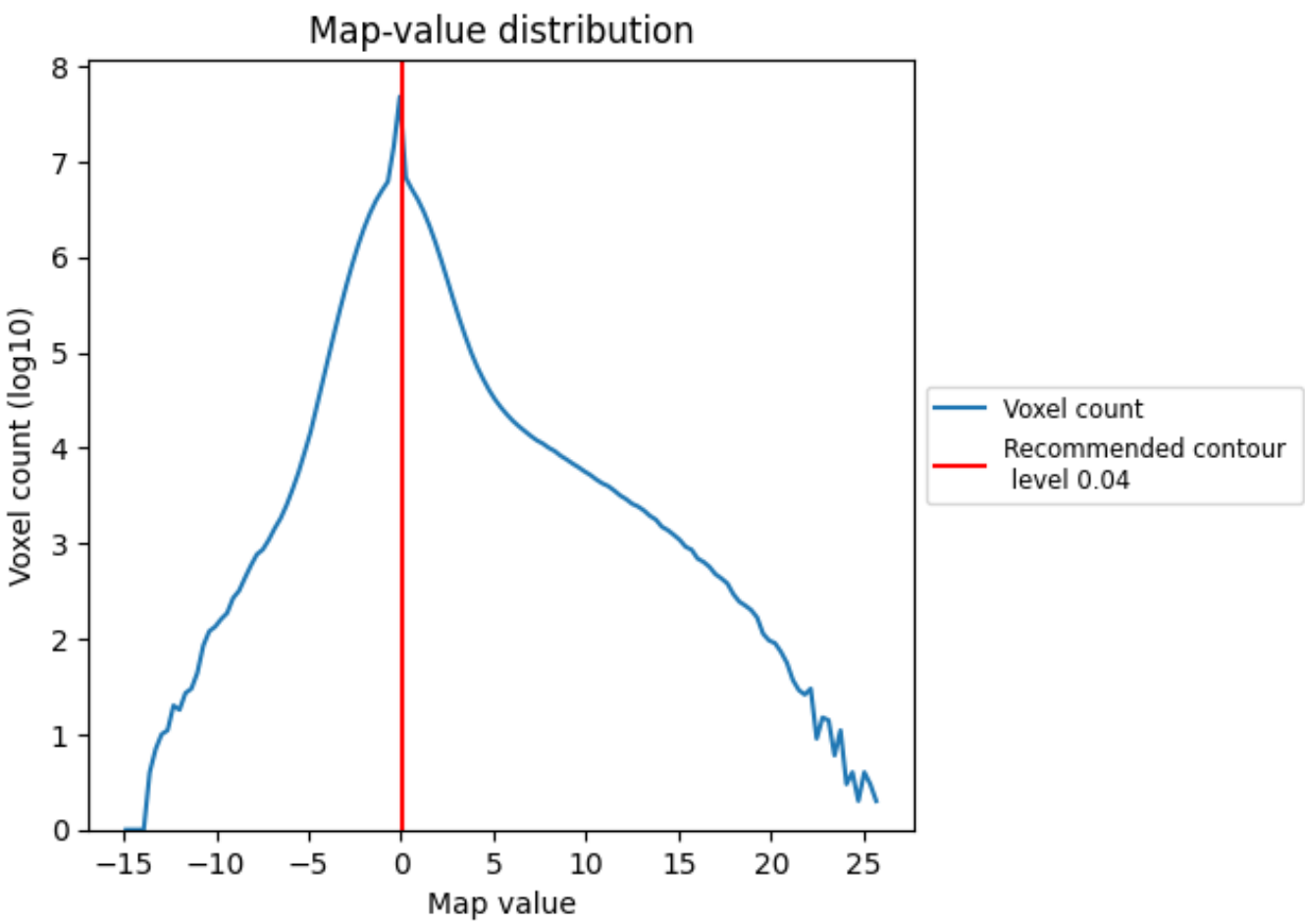
6.6 Mask visualisation (i)

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

7 Map analysis (i)

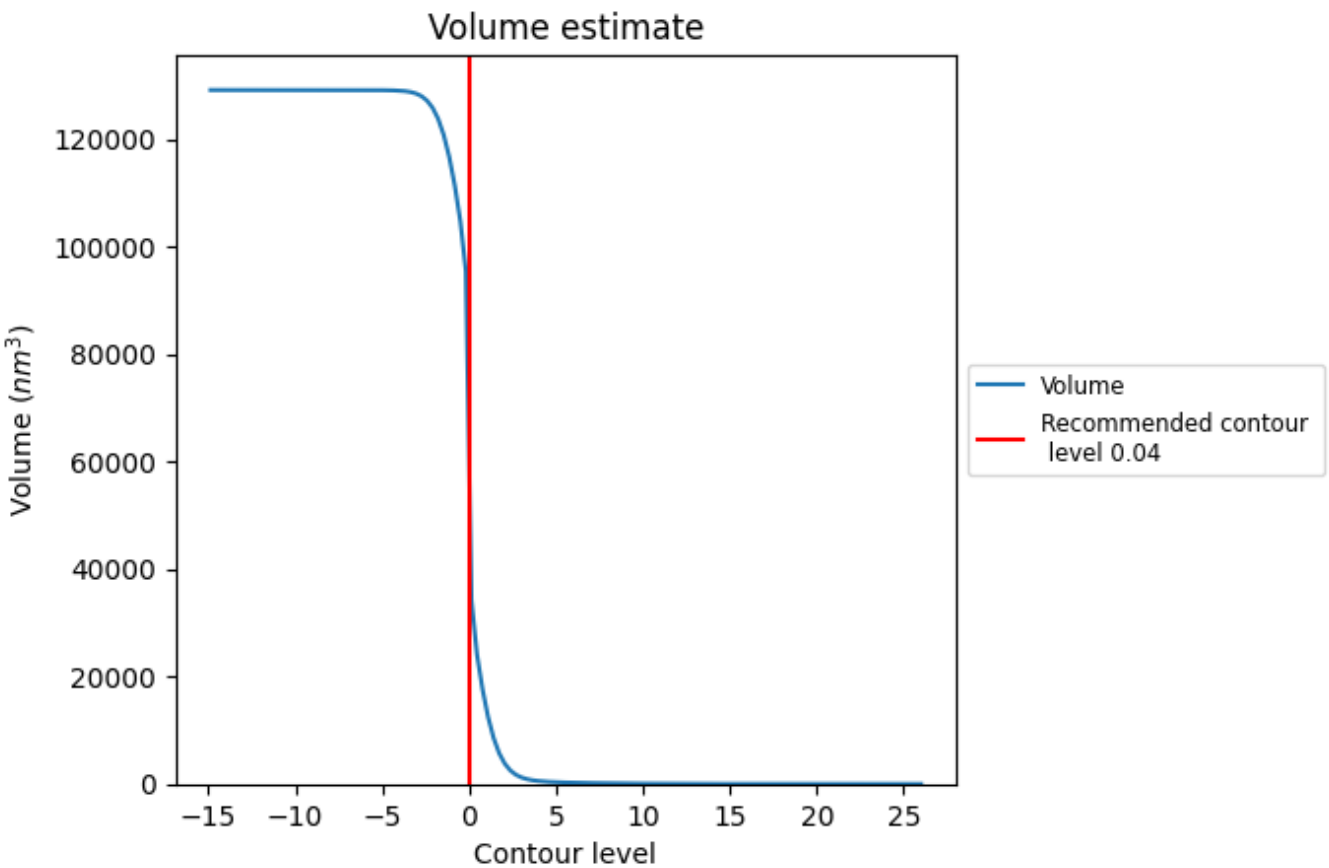
This section contains the results of statistical analysis of the map.

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.

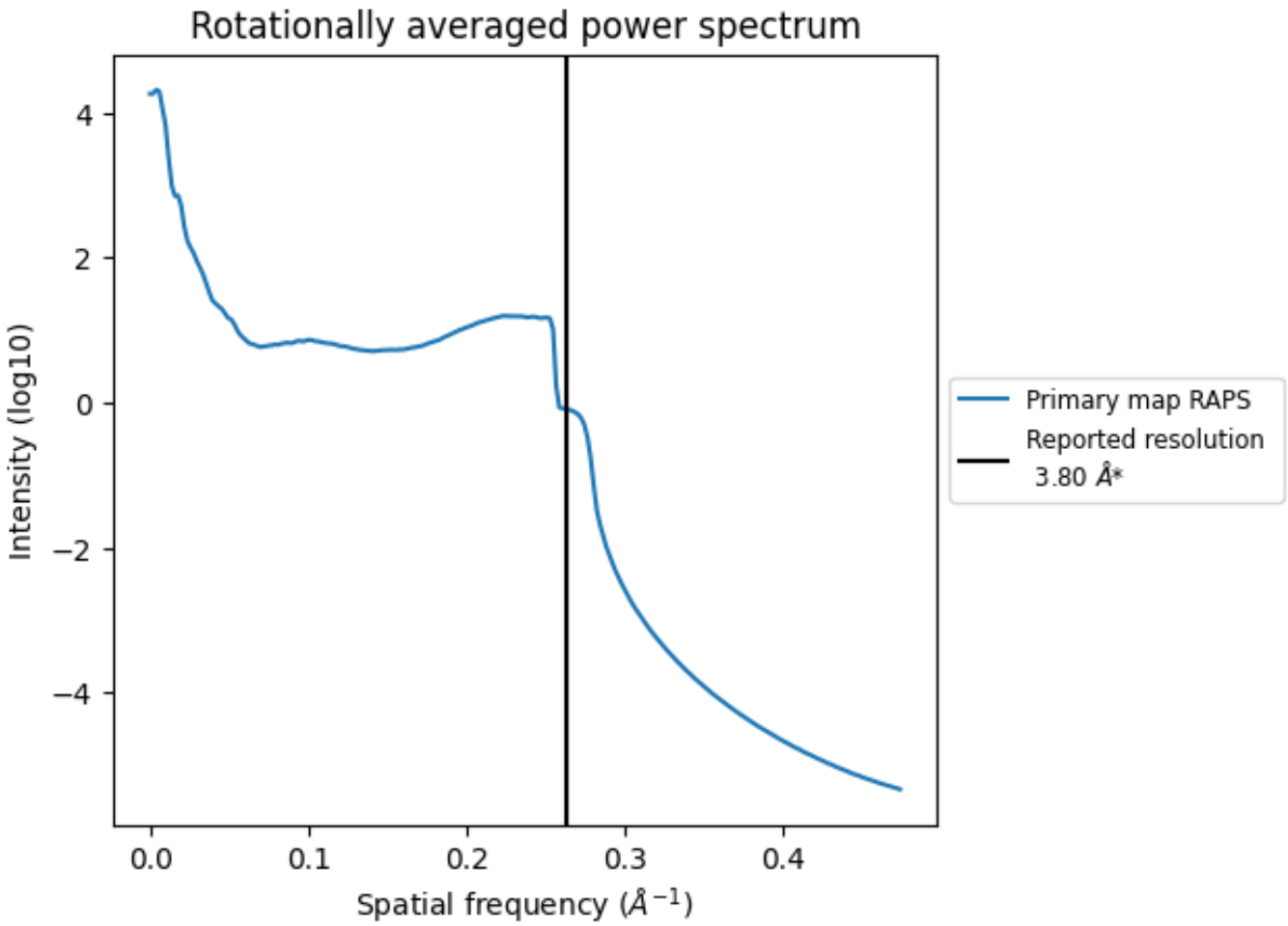
7.2 Volume estimate (i)



The volume at the recommended contour level is 52502 nm^3; this corresponds to an approximate mass of 47426 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 0.263 Å^{-1}

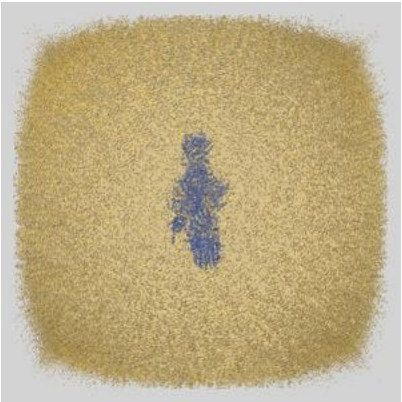
8 Fourier-Shell correlation (i)

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

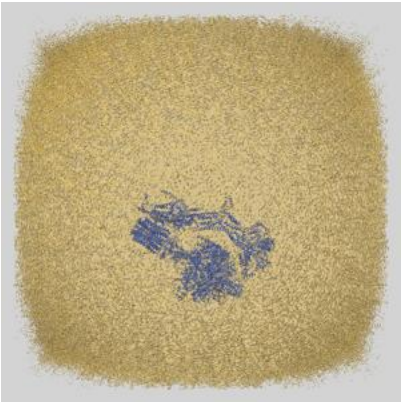
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4845 and PDB model 6RE8. Per-residue inclusion information can be found in section 3 on page 10.

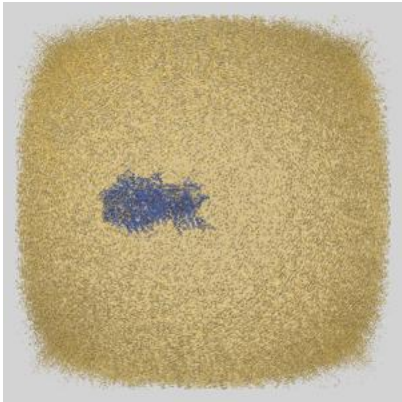
9.1 Map-model overlay (i)



X



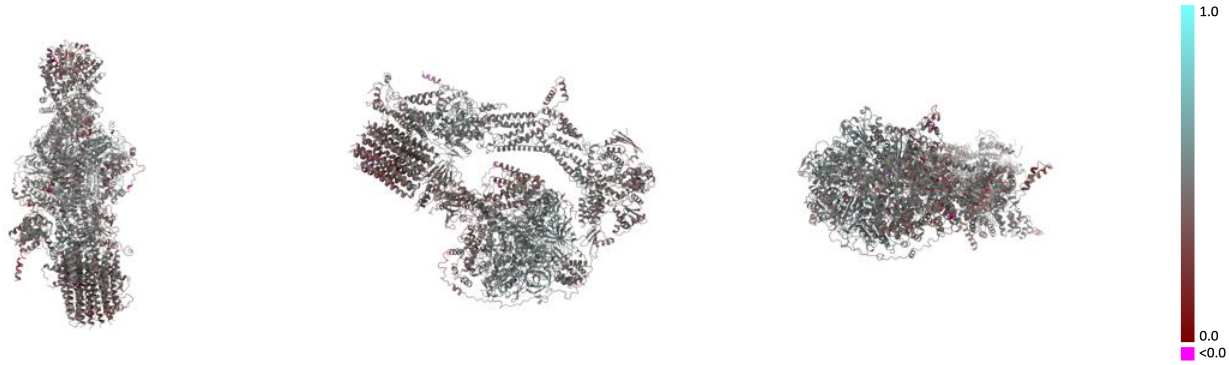
Y



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.

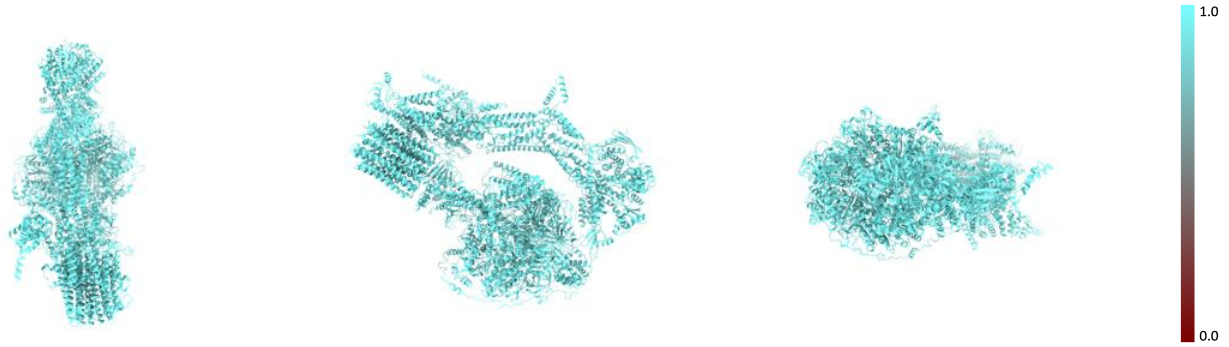
9.2 Q-score mapped to coordinate model (i)



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.

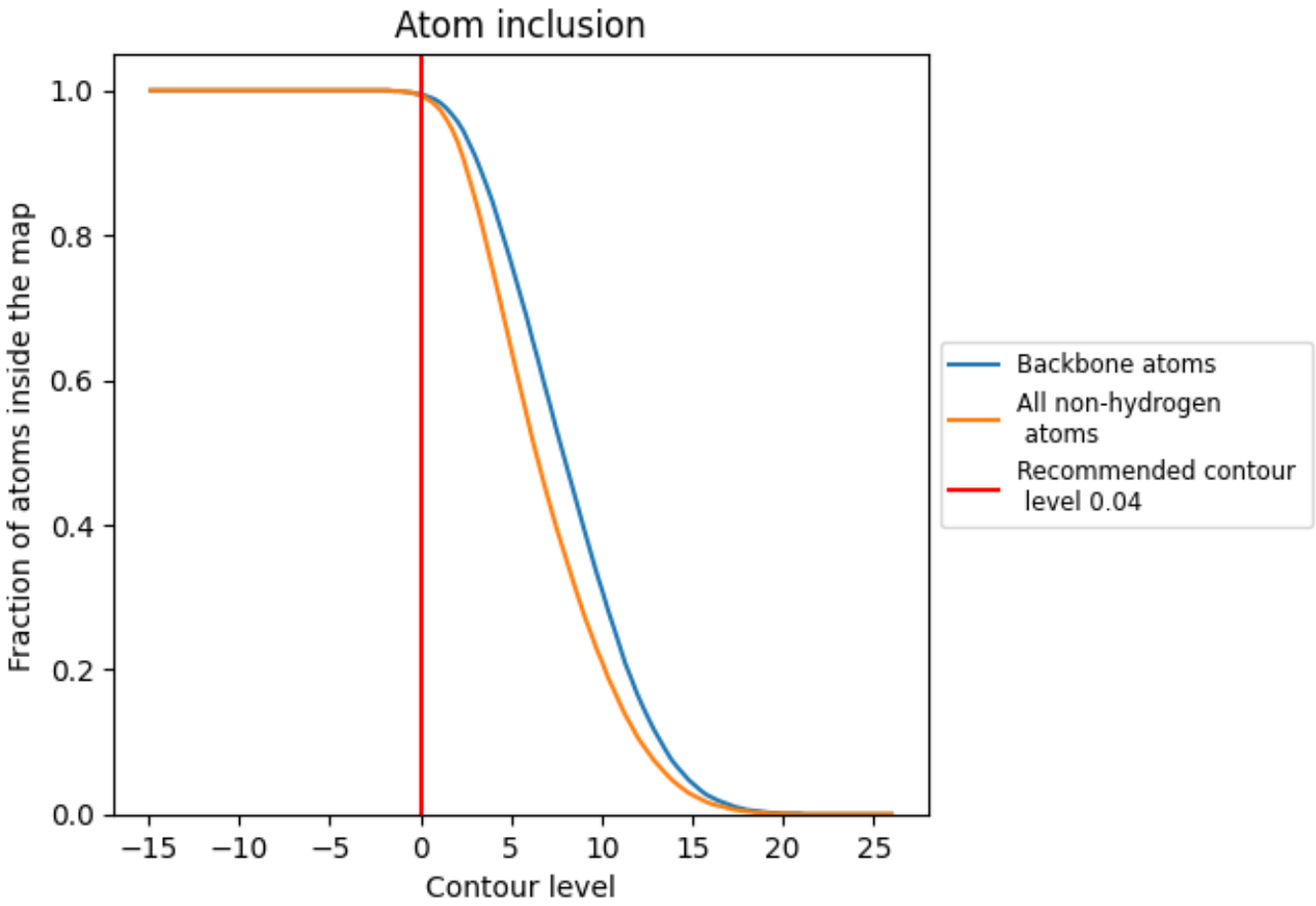
9.3 Atom inclusion mapped to coordinate model (i)



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, 99% of all backbone atoms, 99% 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	0.9930	0.4490
0	0.9930	0.4470
1	0.9960	0.4580
2	0.9960	0.4210
3	0.9950	0.4230
4	0.9960	0.4400
5	0.9940	0.4790
6	0.9950	0.4690
7	0.9970	0.4450
8	0.9940	0.4700
9	0.9950	0.4070
A	0.9920	0.3660
B	0.9880	0.3740
C	0.9900	0.3650
D	0.9940	0.3830
E	0.9880	0.3950
F	0.9840	0.4070
G	0.9800	0.4210
H	0.9800	0.4260
I	0.9900	0.4160
J	0.9880	0.3870
M	0.9920	0.4580
P	0.9910	0.4380
Q	0.9960	0.3990
R	0.9920	0.4020
S	0.9940	0.4180
T	0.9950	0.4820
U	0.9930	0.4630
V	0.9930	0.4750
X	0.9900	0.4650
Y	0.9950	0.4800
Z	0.9870	0.4550