Full wwPDB EM Validation Report (i)

May 12, 2024 – 04:08 pm BST

PDB ID	:	6RDK
EMDB ID	:	EMD-4821
Title	:	Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 1B, composite map
Authors	:	Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on	:	2019-04-12
Resolution	:	3.70 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:

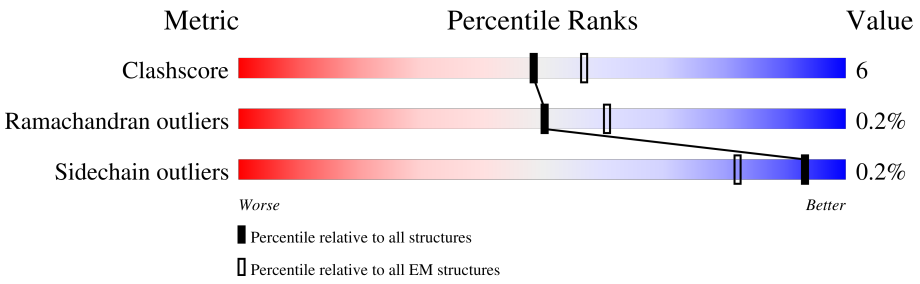
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.70 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	93% 6% •
2	1	618	84% 13% •
3	2	441	87% 13%
4	3	325	63% 12% 25%
5	4	294	87% 11% •
6	5	123	83% 17%
7	6	151	78% • 18%
8	7	190	76% 17% 7%

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Mol	Chain	Length	Quality of chain
9	8	89	82% 17% •
10	9	97	91% 9%
11	A	127	44% 14% 42%
11	B	127	46% 12% 42%
11	C	127	45% 13% 42%
11	D	127	45% 13% 42%
11	E	127	51% 7% 42%
11	F	127	46% 12% 42%
11	G	127	39% 18% • 42%
11	H	127	47% 11% 42%
11	I	127	43% 15% • 42%
11	J	127	46% 11% • 42%
12	M	327	60% 6% 34%
13	P	229	69% 15% 16%
14	Q	74	80% 18% •
15	R	199	74% 15% 11%
16	S	317	73% 14% 13%
17	T	562	79% 14% • 7%
17	U	562	77% 15% 7%
17	V	562	75% 17% 7%
18	X	574	77% 17% 6%
18	Y	574	74% 17% 9%
18	Z	574	80% 13% 6%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 53748 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 Mitochondrial ATP synthase subunit ASA2.

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 Mitochondrial ATP synthase subunit ASA9.

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	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	542	4115	2586	696	820	13	0	0
18	Y	521	3957	2485	670	789	13	0	0
18	Z	538	4087	2568	692	814	13	0	0

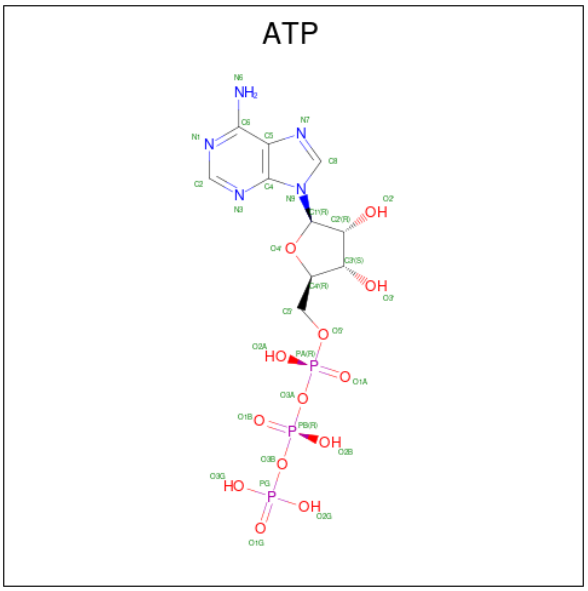
There are 6 discrepancies between the modelled and reference sequences:

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

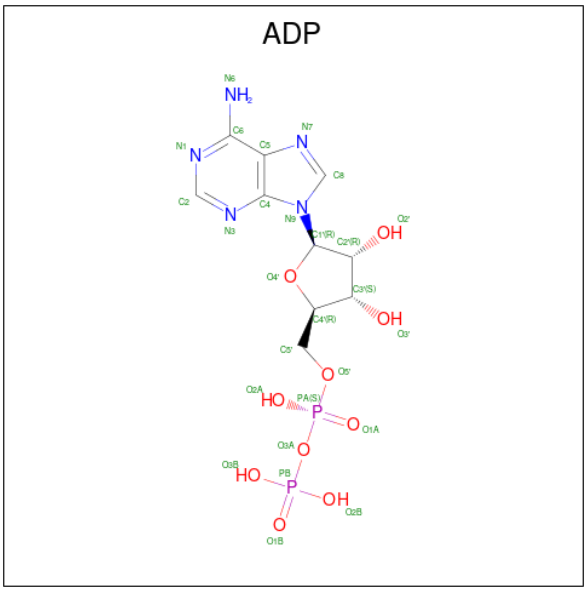


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	Y	1	Total	Mg	0
			1	1	

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



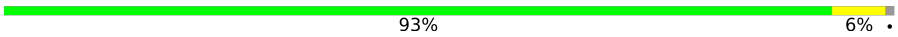
Mol	Chain	Residues	Atoms					AltConf
22	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

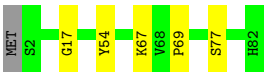
3 Residue-property plots (i)

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

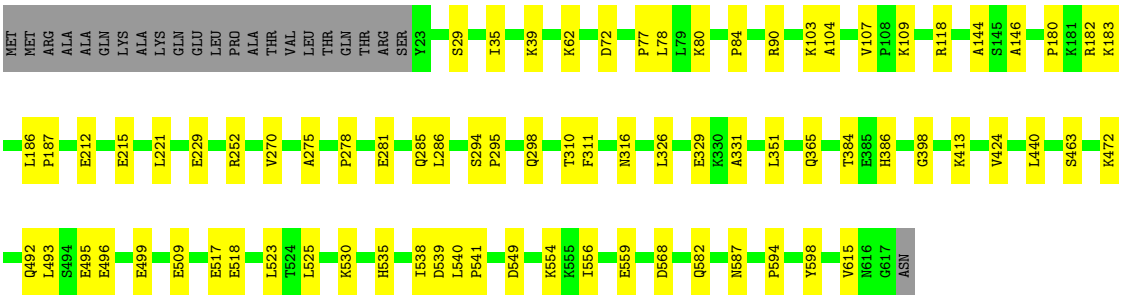
Chain 0:





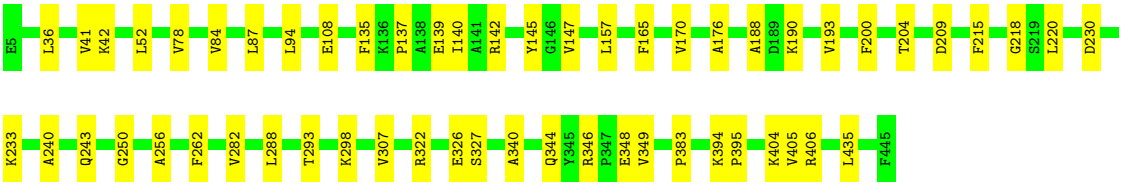
• Molecule 2: ATP synthase associated protein ASA1

Chain 1:



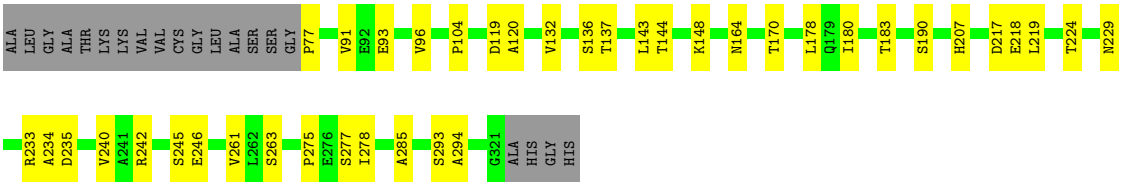
• Molecule 3: Mitochondrial ATP synthase subunit ASA2

Chain 2:



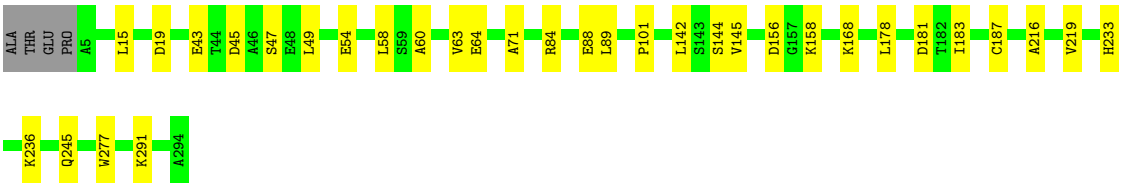
• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3:



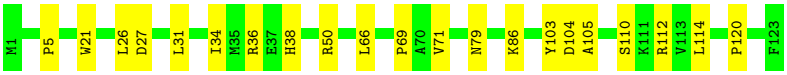
• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4:



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

Chain 5:



• Molecule 7: Mitochondrial ATP synthase subunit ASA6

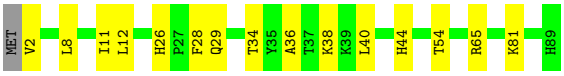
Chain 6:

• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7:

• Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8:



• Molecule 10: Mitochondrial ATP synthase subunit ASA9

Chain 9: 91% 9%

M1 L52 N60 T65 I66 G67 W73 T76 W77 V78 K83 N97

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain A: 44% 14% 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 A70

L71 A72 G73 V74 G75 S84 L85 I86 N92 I95 Q98 Y102 F107 E111 S112 I113 A114 L115 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain B: 46% 12% 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 G63 A64 G65 C66 A67

T68 I69 A70 L71 A72 G73 V74 L78 L85 I86 N92 F107 I113 A114 L115 L118 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain C: 45% 13% 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 A67 T68 I69 A70 L71

A72 L78 G79 V80 R91 N92 L99 F107 A108 L109 T110 E111 S112 I113 L118 L119 V120 V121 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

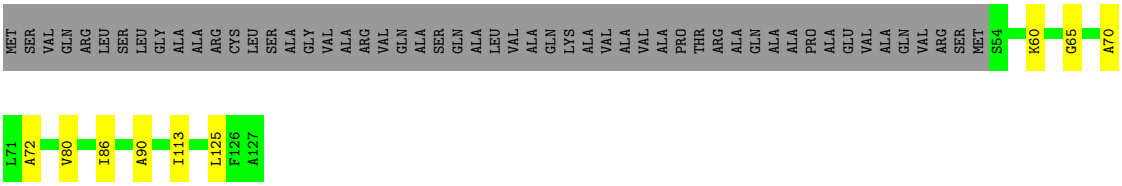
Chain D: 45% 13% 42%

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 V55 L56 A57 A58 S59 K60

A70 L71 A72 G73 V74 V80 L85 N92 I113 A114 L115 L118 L119 V120 V121 I124 A127

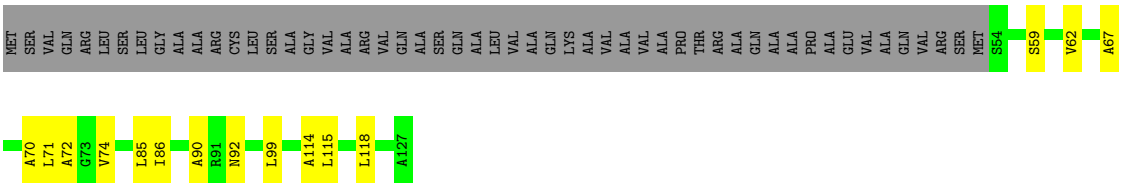
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain E: 51% 7% 42%



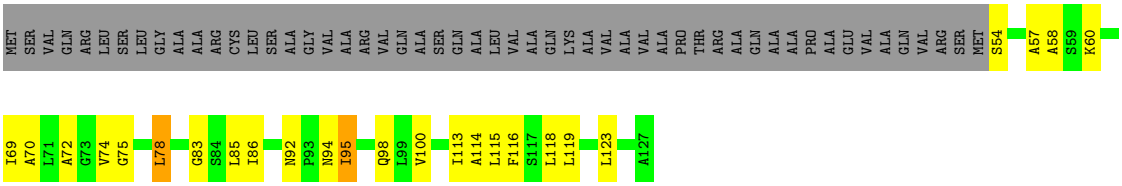
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain F: 46% 12% 42%



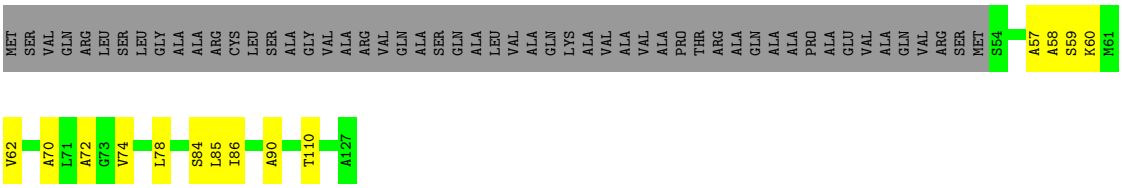
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain G: 39% 18% • 42%



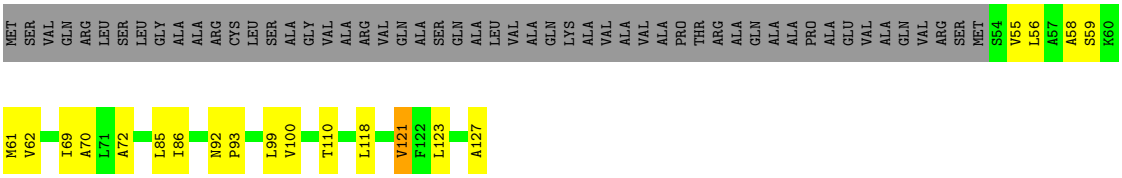
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain H: 47% 11% 42%



• Molecule 11: Mitochondrial ATP synthase subunit c

Chain I: 43% 15% • 42%



• Molecule 11: Mitochondrial ATP synthase subunit c

Chain J: 46% 11% • 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 V55 L56 A57 A58 A70

L71 A72 L85 I86 N87 N92 P93 N94 I95 F107 E111 I124 A127

- Molecule 12: Mitochondrial ATP synthase subunit 6

Chain M: 60% 6% 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 K101 D132 T150 N163 V186 A190 T193 T200 G201 P205 GLY HIS PHE ILE PRO GLY

GLY THR PRO TRP PRO MET ALA F219 I227 T230 F231 R232 S235 R239 M244 L251 L284 V285 E288 V291 K324 LYS ILE HIS

- Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P: 69% 15% 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 L46 A51 Q52 T55 L56 V70 E73 L74 Y75 I78 E79 K82 A91

L109 K119 K120 L121 A124 S132 A133 L134 V137 Y153 C154 I157 E166 L184 V185 M186 Q187 E188 K189 V207 D208 M209 S210 T211 V215 V222 I229

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

Chain Q: 80% 18%

MET CYS A3 L17 N21 I22 K32 E33 P34 F35 K36 R42 Q43 Q49 Y52 K61 N67 K71 N74

- Molecule 15: Mitochondrial ATP synthase subunit delta

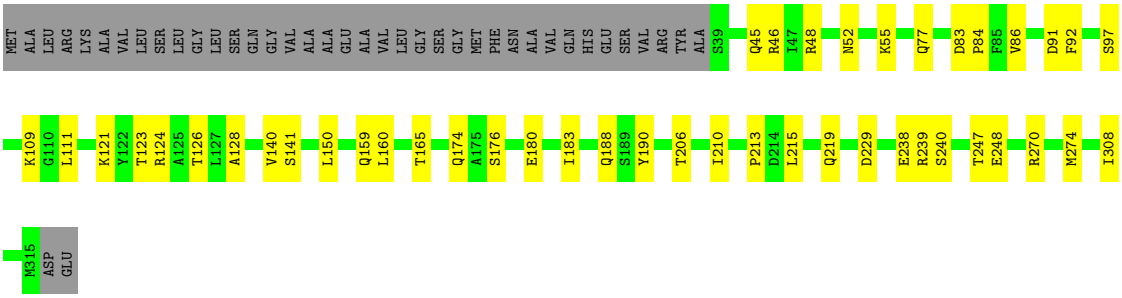
Chain R: 74% 15% 11%

MET PHE GLY LEU LYS ARG ALA VAL THR VAL GLY ARG ARG PHE ILE SER THR SER ALA ALA ARG MET E23 A28 G29 P30 T34 N38 K39 K40 A41 P42 L45 I46 V47 P48 E49 A59 F74 S79 S82 K86 D87 T88 V89 V90 G99 S103

H119 S120 H137 P138 D143 E148 K161 L164 E175 Q178 R182 A199

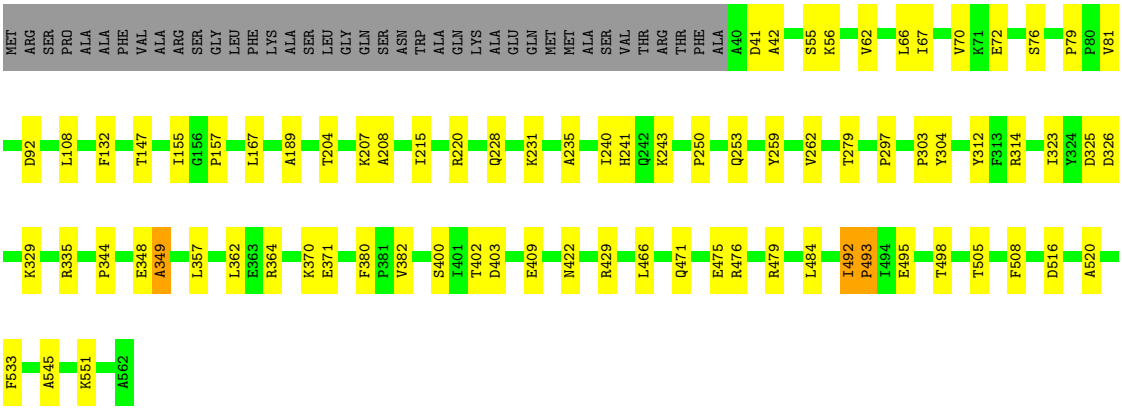
- Molecule 16: ATP synthase gamma chain, mitochondrial

Chain S: 73% 14% 13%



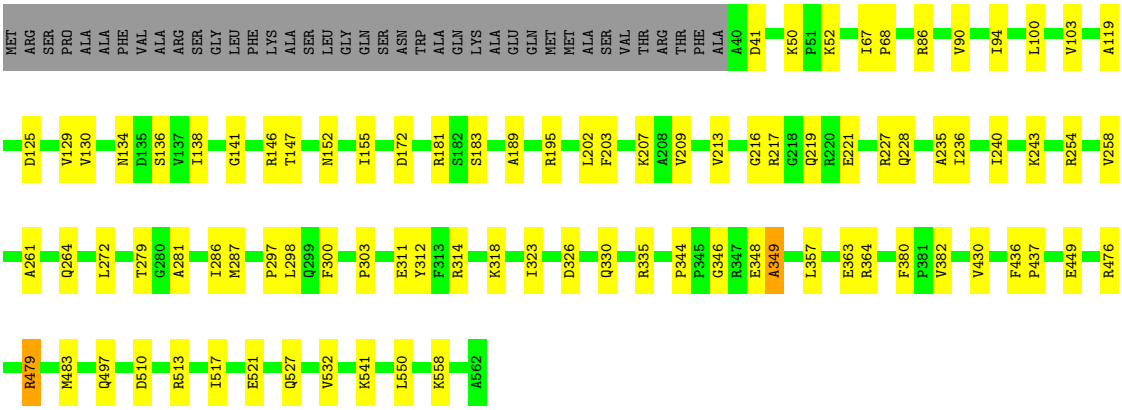
• Molecule 17: ATP synthase subunit alpha

Chain T:



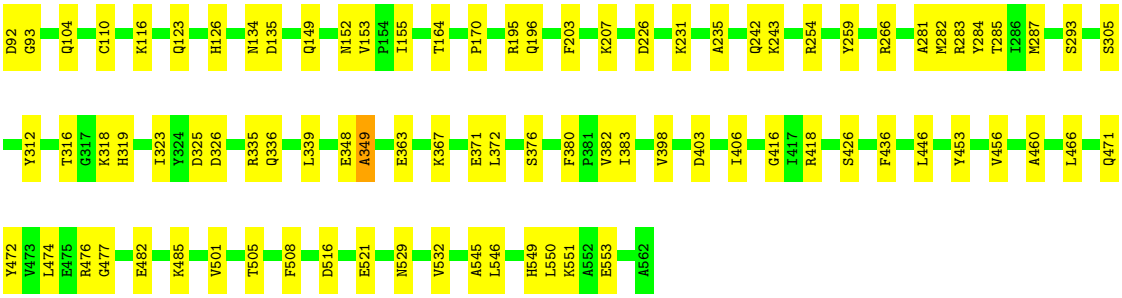
• Molecule 17: ATP synthase subunit alpha

Chain U:



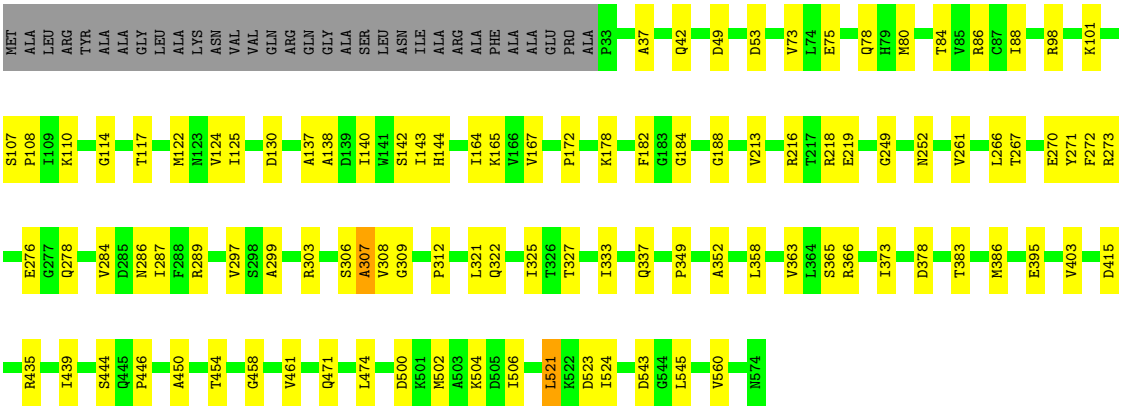
• Molecule 17: ATP synthase subunit alpha

Chain V:



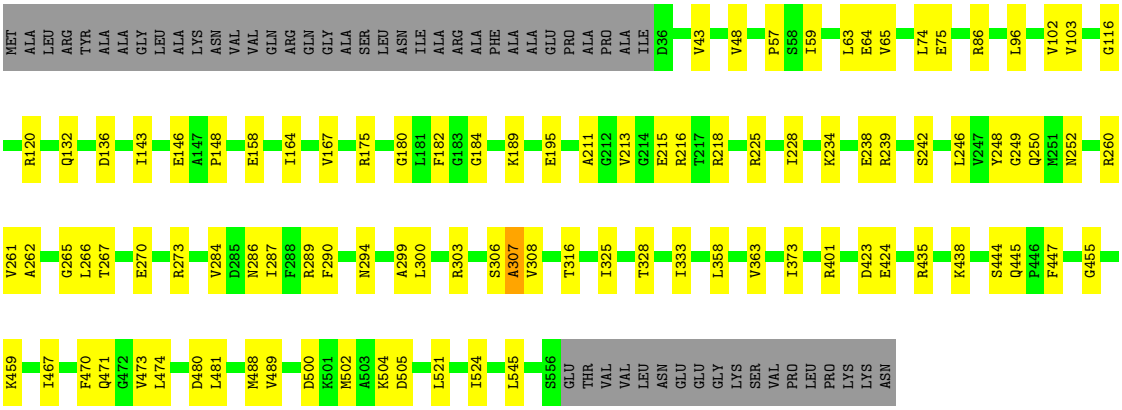
- Molecule 18: ATP synthase subunit beta

Chain X:



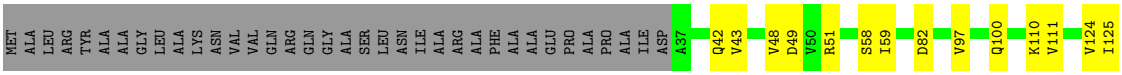
- Molecule 18: ATP synthase subunit beta

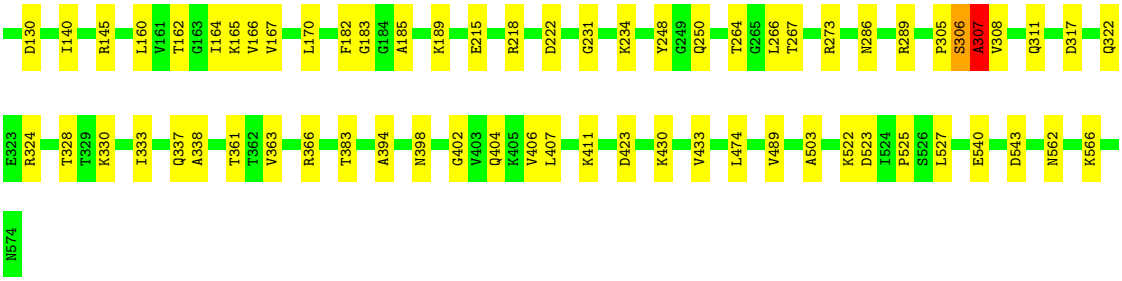
Chain Y:



- Molecule 18: ATP synthase subunit beta

Chain Z:




D130
I140
R145
L160
V161
T162
G163
I164
K165
V166
V167
L170
F182
G183
G184
A185
K189
E215
R218
D222
G231
K234
Y248
G249
Q250
T264
G265
L266
T267
R273
N286
R289
P305
S306
A307
V308
Q311
D317
Q322
E323
R324
T328
T329
K330
I333
Q337
A338
T361
T362
V363
R366
T383
A394
N398
G402
V403
Q404
K405
V406
L407
K411
D423
K430
V433
L474
V489
A503
K522
D523
I524
P525
S526
L527
E540
D543
N562
K566
N574

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72402	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	29.917	Depositor
Minimum map value	-16.990	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.026	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, ATP, ADP, 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	0.31	0/628	0.47	0/856
2	1	0.31	0/4750	0.49	0/6434
3	2	0.30	0/3212	0.53	1/4371 (0.0%)
4	3	0.33	0/1911	0.52	1/2601 (0.0%)
5	4	0.31	0/2216	0.48	0/3000
6	5	0.35	0/1011	0.56	0/1376
7	6	0.32	0/946	0.53	0/1287
8	7	0.35	0/1374	0.50	0/1865
9	8	0.36	0/715	0.53	0/974
10	9	0.31	0/802	0.50	0/1084
11	A	0.32	0/520	0.50	0/704
11	B	0.29	0/520	0.56	0/704
11	C	0.30	0/519	0.56	0/701
11	D	0.30	0/520	0.52	0/704
11	E	0.28	0/520	0.52	0/704
11	F	0.29	0/520	0.56	0/704
11	G	0.30	0/520	0.63	1/704 (0.1%)
11	H	0.29	0/520	0.57	0/704
11	I	0.30	0/520	0.53	0/704
11	J	0.30	0/520	0.53	0/704
12	M	0.35	0/1683	0.58	0/2295
13	P	0.32	0/1553	0.53	0/2093
14	Q	0.29	0/574	0.46	0/774
15	R	0.32	0/1336	0.52	0/1827
16	S	0.30	0/2153	0.52	0/2901
17	T	0.37	0/4048	0.54	1/5481 (0.0%)
17	U	0.37	0/4049	0.56	0/5481
17	V	0.36	0/4031	0.53	0/5456
18	X	0.37	0/4176	0.53	1/5659 (0.0%)
18	Y	0.34	0/4015	0.55	1/5440 (0.0%)
18	Z	0.35	0/4147	0.56	2/5619 (0.0%)
All	All	0.34	0/54529	0.53	8/73911 (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
5	4	0	1
17	T	0	2
17	U	0	1
17	V	0	1
18	X	0	1
18	Y	0	1
18	Z	0	2
All	All	0	9

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2	94	LEU	CA-CB-CG	6.77	130.88	115.30
11	G	78	LEU	CA-CB-CG	5.91	128.89	115.30
4	3	77	PRO	N-CA-CB	5.89	110.37	103.30
17	T	167	LEU	CA-CB-CG	5.82	128.69	115.30
18	Z	317	ASP	CB-CG-OD1	5.50	123.25	118.30
18	Z	222	ASP	CB-CG-OD2	5.16	122.95	118.30
18	X	521	LEU	CA-CB-CG	5.11	127.06	115.30
18	Y	521	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	4	47	SER	Peptide
17	T	348	GLU	Peptide
17	T	492	ILE	Peptide
17	U	348	GLU	Peptide
17	V	348	GLU	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	4	0
2	1	4661	0	4695	55	0
3	2	3163	0	3262	36	0
4	3	1874	0	1826	26	0
5	4	2177	0	2169	23	0
6	5	986	0	1021	17	0
7	6	926	0	941	4	0
8	7	1347	0	1345	31	0
9	8	692	0	694	11	0
10	9	776	0	757	7	0
11	A	514	0	554	15	0
11	B	514	0	554	14	0
11	C	514	0	553	20	0
11	D	514	0	554	15	0
11	E	514	0	554	9	0
11	F	514	0	554	13	0
11	G	514	0	554	21	0
11	H	514	0	554	15	0
11	I	514	0	554	19	0
11	J	514	0	554	17	0
12	M	1640	0	1665	14	0
13	P	1532	0	1603	32	0
14	Q	561	0	565	9	0
15	R	1303	0	1266	20	0
16	S	2130	0	2180	33	0
17	T	3979	0	4119	59	0
17	U	3980	0	4119	59	0
17	V	3962	0	4105	63	0
18	X	4115	0	4137	63	0
18	Y	3957	0	3967	62	0
18	Z	4087	0	4110	49	0
19	M	1	0	0	0	0
20	T	31	0	12	1	0
20	U	31	0	12	0	0
20	V	31	0	12	0	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	1	0	0	0	0
21	X	1	0	0	0	0
21	Y	1	0	0	0	0
22	X	27	0	12	1	0
22	Y	27	0	12	0	0
All	All	53748	0	54729	676	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 (676) 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)
11:C:107:PHE:O	11:C:111:GLU:HG2	1.30	1.25
11:J:107:PHE:CZ	11:J:111:GLU:OE1	2.19	0.95
16:S:83:ASP:OD1	16:S:84:PRO:CD	2.14	0.95
13:P:154:CYS:HB3	13:P:184:LEU:HD11	1.50	0.92
16:S:83:ASP:OD1	16:S:84:PRO:HD2	1.72	0.89
13:P:154:CYS:SG	13:P:185:VAL:O	2.31	0.86
13:P:153:TYR:HA	13:P:185:VAL:HG12	1.61	0.82
13:P:207:VAL:HG22	17:T:81:VAL:HG23	1.68	0.75
17:T:335:ARG:HD2	17:T:349:ALA:HB3	1.69	0.74
18:X:500:ASP:O	18:X:504:LYS:HG3	1.88	0.74
17:U:335:ARG:HD2	17:U:349:ALA:HB3	1.69	0.73
17:V:383:ILE:HG13	17:V:398:VAL:HG11	1.71	0.73
13:P:188:GLU:N	13:P:188:GLU:OE1	2.21	0.72
11:C:78:LEU:HD21	11:C:111:GLU:OE2	1.92	0.70
16:S:83:ASP:OD1	16:S:84:PRO:HD3	1.92	0.69
17:V:196:GLN:HE21	17:V:367:LYS:HE3	1.58	0.69
2:1:316:ASN:HD21	2:1:331:ALA:H	1.41	0.68
2:1:598:TYR:HH	9:8:2:VAL:N	1.91	0.68
16:S:213:PRO:HD3	16:S:247:THR:HG21	1.77	0.67
11:C:107:PHE:O	11:C:111:GLU:CG	2.26	0.66
18:Y:158:GLU:HG3	18:Y:175:ARG:HB3	1.76	0.66
17:V:335:ARG:HD2	17:V:349:ALA:HB3	1.77	0.66
18:Y:143:ILE:HA	18:Y:267:THR:HG21	1.78	0.66
18:X:143:ILE:HA	18:X:267:THR:HG21	1.77	0.65
17:V:155:ILE:HD12	17:V:312:TYR:HB2	1.78	0.65
18:Y:266:LEU:HD11	18:Y:325:ILE:HG12	1.79	0.65
18:Z:286:ASN:H	18:Z:338:ALA:HB3	1.61	0.64
18:X:523:ASP:H	18:X:524:ILE:HD12	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:330:GLN:HE22	17:U:357:LEU:HD11	1.63	0.64
11:H:86:ILE:HG21	11:I:85:LEU:HA	1.80	0.63
11:G:86:ILE:HG21	11:H:85:LEU:HA	1.80	0.63
15:R:42:PRO:HG2	15:R:45:LEU:HD13	1.81	0.63
13:P:209:MET:CE	17:T:79:PRO:HG2	2.29	0.62
13:P:153:TYR:HA	13:P:185:VAL:CG1	2.30	0.62
2:1:84:PRO:HG3	6:5:79:ASN:HD22	1.62	0.62
2:1:278:PRO:HG2	2:1:281:GLU:HB2	1.82	0.61
17:U:314:ARG:NH2	17:U:364:ARG:O	2.34	0.61
2:1:186:LEU:HD13	2:1:440:LEU:HB2	1.83	0.61
11:G:74:VAL:HG11	11:G:114:ALA:HB2	1.83	0.61
18:X:266:LEU:HD11	18:X:325:ILE:HG12	1.82	0.61
18:X:276:GLU:HB3	18:X:278:GLN:HE21	1.64	0.61
13:P:207:VAL:CG2	17:T:81:VAL:HG23	2.31	0.60
18:Z:266:LEU:HD21	18:Z:324:ARG:HB2	1.82	0.60
18:Y:180:GLY:HA3	18:Y:358:LEU:HD13	1.84	0.60
11:A:74:VAL:HG21	11:A:114:ALA:HB2	1.83	0.60
15:R:90:VAL:HA	15:R:99:GLY:HA2	1.83	0.60
11:B:78:LEU:HD12	11:C:113:ILE:HD11	1.84	0.60
5:4:183:ILE:HG22	8:7:184:ASN:HD22	1.67	0.60
14:Q:32:LYS:HG3	14:Q:34:PRO:HD2	1.84	0.60
17:V:153:VAL:HG11	17:V:305:SER:HB2	1.83	0.60
2:1:187:PRO:HG2	2:1:221:LEU:HB3	1.84	0.60
18:Z:328:THR:HG23	18:Z:330:LYS:H	1.67	0.59
17:V:203:PHE:O	17:V:242:GLN:NE2	2.34	0.59
18:Y:249:GLY:HA3	18:Y:261:VAL:HG21	1.84	0.59
11:G:75:GLY:HA3	11:H:74:VAL:HG22	1.85	0.59
13:P:209:MET:HE1	17:T:79:PRO:HD2	1.84	0.59
13:P:209:MET:HE2	17:T:79:PRO:HB2	1.84	0.59
5:4:71:ALA:HB2	8:7:84:VAL:HG12	1.85	0.59
17:T:235:ALA:HB1	17:T:323:ILE:HD13	1.84	0.59
17:T:545:ALA:HA	18:Y:524:ILE:HG22	1.85	0.59
18:Z:273:ARG:HD3	18:Z:333:ILE:HG13	1.84	0.59
18:Y:234:LYS:HB3	18:Y:238:GLU:HG3	1.85	0.59
11:J:107:PHE:CE2	11:J:111:GLU:OE1	2.55	0.59
18:X:435:ARG:NH1	18:X:474:LEU:O	2.36	0.59
18:Z:97:VAL:HG23	18:Z:100:GLN:HE21	1.68	0.59
18:X:284:VAL:HG11	18:X:287:ILE:HD13	1.83	0.58
2:1:77:PRO:HB2	2:1:80:LYS:HB2	1.85	0.58
4:3:91:VAL:HG13	4:3:93:GLU:H	1.68	0.58
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:79:SER:HA	16:S:77:GLN:HB3	1.86	0.58
17:U:437:PRO:HB2	17:U:541:LYS:HB3	1.85	0.58
18:Z:215:GLU:OE1	18:Z:289:ARG:NH1	2.37	0.58
15:R:59:ALA:HB1	15:R:138:PRO:HD2	1.86	0.58
18:X:178:LYS:HB3	18:X:358:LEU:HD23	1.86	0.58
11:A:107:PHE:O	11:A:111:GLU:HB2	2.03	0.58
11:G:85:LEU:HD21	11:G:100:VAL:HG22	1.86	0.58
17:V:104:GLN:HG2	18:Z:97:VAL:HG22	1.86	0.58
3:2:78:VAL:HB	8:7:74:ILE:HD12	1.85	0.57
14:Q:22:ILE:HG12	14:Q:71:LYS:HG2	1.86	0.57
11:C:91:ARG:O	15:R:182:ARG:NH2	2.38	0.57
11:I:72:ALA:HB2	11:J:70:ALA:HA	1.85	0.57
18:Z:402:GLY:HA3	18:Z:474:LEU:HD21	1.86	0.57
4:3:242:ARG:NH2	12:M:132:ASP:OD1	2.36	0.57
4:3:261:VAL:HG11	4:3:285:ALA:HB2	1.87	0.57
18:X:272:PHE:HD1	18:X:276:GLU:HG3	1.68	0.57
18:Z:423:ASP:OD1	18:Z:430:LYS:NZ	2.36	0.57
17:T:403:ASP:O	17:T:429:ARG:NH2	2.37	0.57
11:D:57:ALA:HA	11:D:60:LYS:HE2	1.87	0.57
11:A:72:ALA:HB2	11:B:70:ALA:HA	1.86	0.57
15:R:49:GLU:HB2	16:S:206:THR:HG22	1.87	0.57
18:Y:290:PHE:O	18:Y:294:ASN:ND2	2.38	0.57
17:U:227:ARG:HG2	17:U:228:GLN:HG2	1.87	0.56
17:V:195:ARG:NH2	17:V:363:GLU:O	2.39	0.56
18:Y:438:LYS:NZ	18:Y:481:LEU:O	2.37	0.56
11:F:115:LEU:HA	11:F:118:LEU:HB2	1.86	0.56
18:X:446:PRO:HB2	18:X:458:GLY:HA2	1.87	0.56
1:0:69:PRO:HD2	10:9:83:LYS:HD2	1.87	0.56
11:G:78:LEU:HB2	11:H:110:THR:HG23	1.87	0.56
2:1:180:PRO:HG2	2:1:183:LYS:HB3	1.87	0.56
11:G:57:ALA:HA	11:G:60:LYS:HE2	1.88	0.56
2:1:556:ILE:HG21	6:5:36:ARG:HA	1.88	0.56
17:T:323:ILE:HG12	17:T:380:PHE:HB2	1.87	0.56
11:C:78:LEU:CD2	11:C:111:GLU:OE2	2.55	0.55
12:M:232:ARG:HA	12:M:235:SER:HB3	1.88	0.55
17:T:409:GLU:OE1	17:T:422:ASN:ND2	2.39	0.55
17:U:207:LYS:NZ	17:U:521:GLU:OE1	2.38	0.55
18:Y:216:ARG:O	18:Y:250:GLN:NE2	2.39	0.55
2:1:384:THR:HG21	2:1:398:GLY:HA3	1.88	0.55
17:U:207:LYS:NZ	17:U:483:MET:SD	2.79	0.55
17:V:70:VAL:HG23	17:V:73:TRP:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:508:PHE:HZ	17:V:551:LYS:HG3	1.71	0.55
3:2:142:ARG:NH1	8:7:25:ASP:OD2	2.40	0.55
11:I:58:ALA:HB2	11:J:56:LEU:HA	1.88	0.55
11:F:71:LEU:HB3	11:G:70:ALA:HB1	1.89	0.55
18:X:306:SER:OG	18:X:307:ALA:N	2.40	0.55
4:3:119:ASP:N	4:3:119:ASP:OD1	2.40	0.55
17:V:529:ASN:HD21	18:Z:527:LEU:HD13	1.72	0.55
18:Z:231:GLY:O	18:Z:234:LYS:NZ	2.38	0.55
9:8:36:ALA:HA	9:8:40:LEU:HB3	1.89	0.55
17:T:228:GLN:HE21	20:T:1001:ATP:H5'2	1.72	0.55
17:T:326:ASP:H	17:T:382:VAL:HB	1.72	0.55
17:U:219:GLN:NE2	17:U:221:GLU:OE2	2.39	0.55
17:U:272:LEU:HD23	17:U:287:MET:HE1	1.89	0.54
7:6:103:LEU:HB3	10:9:52:LEU:HD21	1.89	0.54
11:C:78:LEU:HD11	11:C:111:GLU:OE2	2.07	0.54
14:Q:42:ARG:NH2	15:R:148:GLU:OE2	2.40	0.54
3:2:215:PHE:HA	3:2:250:GLY:HA3	1.89	0.54
8:7:23:LEU:HD12	8:7:63:ALA:HA	1.89	0.54
17:U:90:VAL:HG13	18:Z:59:ILE:HD11	1.89	0.54
11:G:95:ILE:HG22	11:G:98:GLN:HB3	1.88	0.54
17:V:282:MET:HA	17:V:285:THR:HG22	1.89	0.54
2:1:326:LEU:HD23	2:1:329:GLU:HG3	1.90	0.54
11:G:94:ASN:HD21	15:R:103:SER:H	1.55	0.54
16:S:83:ASP:HA	16:S:86:VAL:HG22	1.89	0.54
17:T:314:ARG:NH1	17:T:364:ARG:O	2.41	0.54
17:V:316:THR:O	17:V:318:LYS:NZ	2.40	0.54
18:Z:164:ILE:HB	18:Z:167:VAL:HG22	1.89	0.54
2:1:107:VAL:HG11	2:1:286:LEU:HB2	1.90	0.54
13:P:56:LEU:HD11	17:V:67:ILE:HD11	1.90	0.54
16:S:180:GLU:HA	16:S:183:ILE:HB	1.89	0.54
6:5:86:LYS:NZ	8:7:135:ASP:OD1	2.40	0.54
17:T:81:VAL:O	17:T:81:VAL:HG13	2.08	0.54
17:U:125:ASP:OD1	17:U:125:ASP:N	2.40	0.54
4:3:144:THR:HG21	4:3:180:ILE:HG12	1.90	0.54
11:C:111:GLU:OE1	11:D:113:ILE:HD11	2.08	0.54
11:H:58:ALA:HB2	11:I:56:LEU:HG	1.89	0.54
18:X:188:GLY:HA2	22:X:601:ADP:H5'2	1.90	0.53
17:U:243:LYS:HG3	17:U:281:ALA:HA	1.91	0.53
11:A:95:ILE:HD13	11:J:93:PRO:HG3	1.90	0.53
2:1:212:GLU:HA	2:1:215:GLU:HB2	1.90	0.53
2:1:285:GLN:NE2	2:1:294:SER:OG	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:549:ASP:N	2:1:549:ASP:OD2	2.41	0.53
11:A:85:LEU:HA	11:J:86:ILE:HG21	1.91	0.53
17:T:92:ASP:OD1	18:X:303:ARG:NH2	2.42	0.53
11:D:71:LEU:HD12	11:E:113:ILE:HG23	1.91	0.53
17:V:135:ASP:HB3	18:Y:59:ILE:HD12	1.90	0.53
11:B:68:THR:HG21	11:C:120:VAL:HG11	1.90	0.53
18:X:42:GLN:HG2	18:X:49:ASP:HB2	1.91	0.53
4:3:235:ASP:OD1	4:3:235:ASP:N	2.42	0.53
17:T:495:GLU:HG3	17:T:533:PHE:HB3	1.91	0.53
17:U:209:VAL:HG23	17:U:213:VAL:HG23	1.90	0.53
17:U:240:ILE:HD12	17:U:279:THR:HG21	1.91	0.53
17:U:303:PRO:HG2	17:U:330:GLN:HG3	1.91	0.53
17:U:326:ASP:H	17:U:382:VAL:HB	1.74	0.53
17:V:266:ARG:HH11	17:V:293:SER:HB3	1.74	0.53
18:Y:184:GLY:O	18:Y:189:LYS:NZ	2.41	0.53
2:1:559:GLU:OE2	4:3:207:HIS:NE2	2.41	0.53
3:2:394:LYS:HE2	3:2:395:PRO:HD2	1.90	0.53
18:X:502:MET:O	18:X:506:ILE:HG23	2.09	0.53
3:2:84:VAL:HA	3:2:87:LEU:HD12	1.91	0.52
14:Q:32:LYS:O	14:Q:36:LYS:N	2.42	0.52
17:U:479:ARG:NH1	17:U:510:ASP:O	2.41	0.52
5:4:54:GLU:O	5:4:58:LEU:HB2	2.09	0.52
11:D:118:LEU:HA	11:D:121:VAL:HG12	1.91	0.52
18:X:75:GLU:OE2	18:X:144:HIS:NE2	2.41	0.52
11:G:119:LEU:O	11:G:123:LEU:HB2	2.09	0.52
18:X:322:GLN:OE1	18:X:337:GLN:NE2	2.40	0.52
11:C:68:THR:HG21	11:D:120:VAL:HG11	1.92	0.52
11:I:59:SER:HA	11:I:62:VAL:HG12	1.91	0.52
17:T:189:ALA:HB3	18:Y:252:ASN:HD22	1.73	0.52
17:V:472:TYR:OH	17:V:476:ARG:NH2	2.42	0.52
18:X:450:ALA:O	18:X:454:THR:OG1	2.27	0.52
2:1:84:PRO:HG2	6:5:71:VAL:HG11	1.90	0.52
10:9:65:THR:HG23	10:9:67:GLY:H	1.73	0.52
11:A:113:ILE:HG23	11:J:71:LEU:HD12	1.90	0.52
18:Y:273:ARG:HD3	18:Y:333:ILE:HG13	1.91	0.52
17:U:134:ASN:ND2	17:U:136:SER:OG	2.42	0.52
18:X:182:PHE:HB2	18:X:363:VAL:HA	1.92	0.52
18:X:395:GLU:OE2	18:X:471:GLN:NE2	2.43	0.52
11:E:72:ALA:HB2	11:F:70:ALA:HA	1.91	0.52
15:R:88:THR:HB	15:R:119:HIS:HB2	1.91	0.52
18:Y:270:GLU:OE1	18:Y:273:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:361:THR:HG23	18:Z:383:THR:H	1.74	0.52
16:S:48:ARG:O	16:S:52:ASN:ND2	2.43	0.52
17:T:259:TYR:OH	17:T:325:ASP:OD1	2.25	0.52
3:2:137:PRO:HA	3:2:140:ILE:HG12	1.92	0.51
18:Y:65:VAL:HG22	18:Y:102:VAL:HG22	1.92	0.51
2:1:275:ALA:HB3	2:1:351:LEU:HD13	1.91	0.51
2:1:295:PRO:HA	2:1:298:GLN:HG2	1.92	0.51
13:P:91:ALA:O	13:P:132:SER:OG	2.27	0.51
14:Q:43:GLN:NE2	14:Q:67:ASN:O	2.43	0.51
17:T:403:ASP:OD2	18:Y:218:ARG:NE	2.43	0.51
18:Z:183:GLY:HA3	18:Z:189:LYS:HD3	1.91	0.51
3:2:147:VAL:HG11	3:2:157:LEU:HD21	1.92	0.51
17:U:311:GLU:OE2	17:U:364:ARG:NE	2.41	0.51
18:X:108:PRO:HB2	18:X:142:SER:HB2	1.93	0.51
3:2:230:ASP:HA	3:2:233:LYS:HG2	1.92	0.51
18:Y:445:GLN:NE2	18:Y:459:LYS:O	2.41	0.51
18:Z:406:VAL:HG11	18:Z:474:LEU:CD1	2.40	0.51
17:U:297:PRO:HA	17:U:300:PHE:HB3	1.92	0.51
11:A:70:ALA:HA	11:J:72:ALA:HB2	1.91	0.51
11:F:86:ILE:HG21	11:G:85:LEU:HA	1.92	0.51
18:Y:164:ILE:HB	18:Y:167:VAL:HG22	1.92	0.51
11:F:59:SER:HA	11:F:62:VAL:HG12	1.91	0.51
13:P:222:VAL:HG23	17:T:66:LEU:HD11	1.93	0.51
3:2:209:ASP:OD1	8:7:67:ARG:NH2	2.42	0.51
3:2:340:ALA:HB1	3:2:435:LEU:HG	1.91	0.51
8:7:170:HIS:HD2	8:7:172:ALA:H	1.59	0.51
16:S:52:ASN:HA	16:S:55:LYS:HG2	1.93	0.51
17:T:155:ILE:HD12	17:T:312:TYR:HB2	1.93	0.51
18:X:373:ILE:HG23	18:X:444:SER:HB2	1.92	0.51
2:1:90:ARG:HH12	6:5:69:PRO:HD3	1.76	0.51
11:E:86:ILE:HG21	11:F:85:LEU:HA	1.93	0.51
12:M:251:LEU:HD13	12:M:284:LEU:HD22	1.93	0.51
18:X:184:GLY:O	18:X:366:ARG:NH2	2.42	0.51
2:1:104:ALA:HB1	2:1:294:SER:HB3	1.93	0.50
17:T:326:ASP:OD1	17:T:329:LYS:NZ	2.37	0.50
17:V:46:ASP:OD1	17:V:49:ARG:NH1	2.44	0.50
3:2:240:ALA:H	3:2:243:GLN:HE21	1.59	0.50
17:U:449:GLU:OE1	17:U:476:ARG:NH1	2.44	0.50
18:Z:43:VAL:HG12	18:Z:48:VAL:HG22	1.93	0.50
3:2:322:ARG:HH11	3:2:327:SER:HA	1.76	0.50
11:F:72:ALA:HB2	11:G:70:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:157:ILE:HG13	13:P:189:LYS:HB3	1.94	0.50
17:U:147:THR:HG22	18:X:560:VAL:HG12	1.94	0.50
17:V:516:ASP:OD1	17:V:516:ASP:N	2.44	0.50
4:3:219:LEU:HD22	4:3:240:VAL:HG13	1.94	0.50
2:1:310:THR:OG1	2:1:311:PHE:N	2.43	0.50
16:S:109:LYS:NZ	18:Y:424:GLU:OE2	2.40	0.50
18:X:270:GLU:OE2	18:X:273:ARG:NH2	2.44	0.50
3:2:346:ARG:HA	3:2:349:VAL:HG12	1.94	0.50
17:T:400:SER:HB2	18:Y:289:ARG:HH22	1.76	0.50
3:2:52:LEU:HD12	8:7:76:LEU:HD12	1.94	0.50
18:X:216:ARG:NH1	18:X:219:GLU:OE1	2.41	0.50
3:2:344:GLN:N	3:2:348:GLU:OE1	2.44	0.50
16:S:308:ILE:HD11	18:Z:305:PRO:HG2	1.94	0.50
17:T:304:TYR:OH	17:T:357:LEU:O	2.28	0.50
18:Y:215:GLU:OE1	18:Y:286:ASN:ND2	2.45	0.50
2:1:118:ARG:NH2	6:5:66:LEU:O	2.45	0.49
5:4:245:GLN:HE22	8:7:149:SER:HB2	1.76	0.49
11:I:93:PRO:HB3	11:J:95:ILE:HG21	1.93	0.49
16:S:141:SER:HB3	16:S:150:LEU:HD12	1.94	0.49
17:U:318:LYS:HE2	18:X:545:LEU:HD23	1.94	0.49
17:U:254:ARG:NH2	18:X:543:ASP:OD1	2.44	0.49
18:Y:182:PHE:HB2	18:Y:363:VAL:HA	1.95	0.49
18:Z:394:ALA:O	18:Z:398:ASN:ND2	2.44	0.49
2:1:535:HIS:ND1	2:1:539:ASP:OD2	2.39	0.49
11:D:115:LEU:HD23	11:D:118:LEU:HD12	1.94	0.49
18:X:114:GLY:HA3	18:X:138:ALA:HB3	1.94	0.49
2:1:540:LEU:HD12	2:1:541:PRO:HD2	1.93	0.49
2:1:554:LYS:NZ	4:3:170:THR:O	2.37	0.49
11:F:71:LEU:HA	11:F:74:VAL:HG12	1.94	0.49
16:S:46:ARG:NH1	18:X:415:ASP:OD1	2.42	0.49
17:T:250:PRO:HD2	17:T:253:GLN:HE21	1.77	0.49
11:G:115:LEU:HA	11:G:118:LEU:HB2	1.95	0.49
11:I:86:ILE:HG21	11:J:85:LEU:HA	1.95	0.49
13:P:109:LEU:HD23	13:P:119:LYS:HA	1.93	0.49
17:U:203:PHE:HE1	17:U:436:PHE:HB2	1.77	0.49
11:I:86:ILE:HD13	11:J:85:LEU:HB2	1.95	0.49
18:Z:51:ARG:NH2	18:Z:82:ASP:O	2.45	0.49
1:0:17:GLY:O	6:5:21:TRP:NE1	2.46	0.49
16:S:140:VAL:HG22	16:S:160:LEU:HB3	1.95	0.49
17:V:549:HIS:NE2	18:Z:525:PRO:O	2.42	0.49
11:D:72:ALA:HB2	11:E:70:ALA:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:143:ASP:OD1	15:R:143:ASP:N	2.45	0.49
17:V:243:LYS:HG3	17:V:281:ALA:HA	1.94	0.49
17:V:259:TYR:HB3	17:V:287:MET:HG2	1.94	0.49
2:1:252:ARG:NH1	2:1:509:GLU:OE1	2.41	0.49
11:A:115:LEU:HD11	12:M:239:ARG:HB2	1.95	0.49
11:G:69:ILE:HA	11:H:70:ALA:HB2	1.94	0.49
17:V:283:ARG:NH1	18:Z:543:ASP:OD1	2.45	0.49
18:Y:502:MET:HA	18:Y:505:ASP:HB2	1.95	0.49
11:G:58:ALA:O	11:H:59:SER:OG	2.23	0.48
11:H:72:ALA:HB2	11:I:70:ALA:HA	1.94	0.48
13:P:79:GLU:HA	13:P:82:LYS:HD3	1.95	0.48
18:Y:120:ARG:NH1	18:Y:132:GLN:O	2.46	0.48
18:Y:306:SER:OG	18:Y:307:ALA:N	2.44	0.48
18:X:327:THR:HG22	18:X:333:ILE:H	1.78	0.48
18:Y:75:GLU:OE2	18:Y:260:ARG:NE	2.40	0.48
6:5:5:PRO:O	9:8:65:ARG:NH1	2.46	0.48
8:7:47:GLU:OE2	8:7:60:GLN:NE2	2.47	0.48
12:M:200:THR:OG1	12:M:201:GLY:N	2.46	0.48
15:R:30:PRO:HD3	16:S:91:ASP:HB3	1.94	0.48
18:X:80:MET:HB2	18:X:84:THR:HG23	1.95	0.48
14:Q:17:LEU:O	14:Q:21:ASN:ND2	2.40	0.48
11:B:86:ILE:HG23	11:C:99:LEU:HB2	1.95	0.48
16:S:109:LYS:O	16:S:270:ARG:NH2	2.46	0.48
16:S:229:ASP:OD1	16:S:239:ARG:NH1	2.46	0.48
17:U:172:ASP:OD1	17:U:172:ASP:N	2.46	0.48
3:2:256:ALA:HB3	3:2:262:PHE:HE1	1.78	0.48
4:3:293:SER:OG	4:3:294:ALA:N	2.46	0.48
4:3:277:SER:O	4:3:277:SER:OG	2.29	0.48
11:B:65:GLY:HA2	11:C:67:ALA:HB2	1.95	0.48
15:R:74:PHE:HB3	15:R:82:SER:HB3	1.95	0.48
17:U:136:SER:O	18:Z:58:SER:OG	2.30	0.48
17:U:323:ILE:HG13	17:U:380:PHE:HB2	1.95	0.48
17:V:476:ARG:NH1	17:V:505:THR:O	2.45	0.48
18:X:286:ASN:HB3	18:X:289:ARG:HG2	1.95	0.48
17:T:72:GLU:O	17:T:76:SER:OG	2.26	0.48
18:X:249:GLY:HA3	18:X:261:VAL:HG11	1.96	0.48
11:I:85:LEU:HD21	11:I:100:VAL:HG23	1.96	0.48
11:I:118:LEU:HA	11:I:121:VAL:HG12	1.94	0.48
12:M:227:ILE:HA	12:M:230:THR:HG22	1.96	0.48
17:T:220:ARG:H	17:T:220:ARG:HG2	1.52	0.48
17:T:516:ASP:O	17:T:520:ALA:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:181:ARG:NH2	17:U:183:SER:OG	2.47	0.48
17:V:446:LEU:HD22	17:V:501:VAL:HG21	1.95	0.48
18:Z:402:GLY:HA3	18:Z:474:LEU:CD2	2.44	0.48
14:Q:17:LEU:HB3	16:S:176:SER:HB2	1.95	0.48
18:Z:182:PHE:HB2	18:Z:363:VAL:HA	1.96	0.48
18:Z:185:ALA:O	18:Z:366:ARG:NH1	2.47	0.48
5:4:60:ALA:HA	5:4:63:VAL:HG12	1.96	0.47
11:A:98:GLN:NE2	11:A:102:TYR:OH	2.45	0.47
17:U:103:VAL:HA	17:U:146:ARG:HE	1.79	0.47
18:X:172:PRO:HG2	18:X:386:MET:HB2	1.96	0.47
16:S:215:LEU:O	16:S:219:GLN:NE2	2.47	0.47
17:V:207:LYS:NZ	17:V:521:GLU:OE2	2.47	0.47
17:V:418:ARG:HD2	18:Y:401:ARG:HH12	1.79	0.47
18:X:42:GLN:NE2	18:X:49:ASP:OD2	2.47	0.47
18:X:213:VAL:HG22	18:X:261:VAL:HG13	1.96	0.47
8:7:23:LEU:HG	8:7:66:LEU:HD12	1.94	0.47
8:7:40:ALA:HB3	8:7:47:GLU:H	1.78	0.47
11:A:75:GLY:HA3	11:B:74:VAL:HG22	1.96	0.47
11:G:113:ILE:HD12	11:G:116:PHE:HD2	1.79	0.47
10:9:76:THR:OG1	10:9:77:TRP:N	2.47	0.47
11:D:80:VAL:HG22	11:E:80:VAL:HG11	1.95	0.47
17:U:100:LEU:O	18:X:98:ARG:NH2	2.48	0.47
18:Y:234:LYS:H	18:Y:242:SER:HB3	1.79	0.47
2:1:270:VAL:O	2:1:530:LYS:NZ	2.48	0.47
4:3:132:VAL:O	4:3:164:ASN:ND2	2.48	0.47
5:4:144:SER:OG	5:4:168:LYS:NZ	2.47	0.47
7:6:43:SER:OG	7:6:46:ASN:OD1	2.27	0.47
11:J:92:ASN:OD1	11:J:92:ASN:N	2.46	0.47
16:S:45:GLN:HA	16:S:48:ARG:HG2	1.97	0.47
17:U:532:VAL:HG21	17:U:550:LEU:HD13	1.96	0.47
17:V:123:GLN:OE1	17:V:126:HIS:NE2	2.48	0.47
17:V:134:ASN:ND2	18:Y:146:GLU:OE2	2.48	0.47
4:3:190:SER:OG	4:3:229:ASN:ND2	2.48	0.47
17:V:254:ARG:NH2	18:Z:540:GLU:O	2.47	0.47
16:S:238:GLU:OE2	16:S:240:SER:OG	2.30	0.46
17:V:460:ALA:HB2	17:V:474:LEU:HD11	1.97	0.46
18:Z:110:LYS:HG2	18:Z:140:ILE:HG22	1.97	0.46
3:2:190:LYS:HA	3:2:193:VAL:HG12	1.97	0.46
9:8:26:HIS:HB3	9:8:29:GLN:HG3	1.96	0.46
16:S:183:ILE:HD13	16:S:248:GLU:HG2	1.97	0.46
17:T:344:PRO:HG2	18:Y:299:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:319:HIS:ND1	17:V:376:SER:OG	2.38	0.46
17:V:336:GLN:OE1	18:Y:316:THR:OG1	2.31	0.46
18:Y:444:SER:OG	18:Y:488:MET:SD	2.74	0.46
18:Z:42:GLN:HB2	18:Z:49:ASP:HB2	1.97	0.46
18:Z:311:GLN:H	18:Z:311:GLN:HG2	1.51	0.46
8:7:38:ASN:OD1	8:7:49:THR:OG1	2.29	0.46
17:U:207:LYS:HG2	17:U:497:GLN:HG3	1.98	0.46
18:Y:57:PRO:HG2	18:Y:63:LEU:HD21	1.98	0.46
5:4:49:LEU:HD11	13:P:215:VAL:HG12	1.98	0.46
11:H:86:ILE:HG23	11:I:99:LEU:HB3	1.96	0.46
17:V:283:ARG:NH2	17:V:284:TYR:OH	2.48	0.46
18:X:78:GLN:HB2	18:X:86:ARG:HB3	1.97	0.46
18:Z:430:LYS:HB3	18:Z:430:LYS:HE2	1.81	0.46
11:C:72:ALA:HB2	11:D:70:ALA:HA	1.98	0.46
11:H:90:ALA:O	11:I:92:ASN:ND2	2.48	0.46
17:T:370:LYS:NZ	17:T:371:GLU:OE2	2.41	0.46
3:2:282:VAL:HG21	5:4:15:LEU:HD22	1.97	0.46
9:8:81:LYS:HE2	9:8:81:LYS:HB3	1.75	0.46
11:A:59:SER:HA	11:A:62:VAL:HG12	1.96	0.46
11:G:54:SER:O	11:G:54:SER:OG	2.30	0.46
16:S:165:THR:OG1	16:S:174:GLN:NE2	2.49	0.46
17:T:67:ILE:HA	17:T:70:VAL:HG12	1.98	0.46
18:Y:116:GLY:HA3	18:Y:136:ASP:HB2	1.97	0.46
18:Y:423:ASP:N	18:Y:423:ASP:OD1	2.48	0.46
13:P:210:SER:OG	13:P:211:THR:N	2.48	0.46
8:7:38:ASN:OD1	8:7:38:ASN:N	2.47	0.46
8:7:39:VAL:HG12	8:7:48:VAL:HG12	1.98	0.46
12:M:163:ASN:ND2	12:M:244:MET:SD	2.89	0.46
17:V:110:CYS:HA	17:V:116:LYS:HA	1.97	0.46
6:5:26:LEU:HD23	12:M:150:THR:HG23	1.97	0.46
17:U:479:ARG:HA	17:U:517:ILE:HD13	1.97	0.46
18:Z:166:VAL:HG23	18:Z:170:LEU:HD12	1.98	0.46
18:Z:322:GLN:OE1	18:Z:337:GLN:NE2	2.40	0.46
4:3:96:VAL:HG11	4:3:120:ALA:HB1	1.98	0.46
11:C:78:LEU:CD1	11:C:111:GLU:OE2	2.65	0.45
15:R:86:LYS:HD3	15:R:120:SER:HB2	1.99	0.45
17:U:261:ALA:HB1	17:U:264:GLN:HG3	1.97	0.45
17:V:482:GLU:HA	17:V:485:LYS:HD3	1.97	0.45
18:X:216:ARG:HB2	18:X:219:GLU:HG3	1.97	0.45
18:Z:306:SER:OG	18:Z:307:ALA:N	2.46	0.45
5:4:156:ASP:OD2	5:4:158:LYS:NZ	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:86:ARG:NH1	17:U:141:GLY:O	2.49	0.45
18:X:403:VAL:HG13	18:X:439:ILE:HD12	1.97	0.45
18:Y:373:ILE:HG23	18:Y:444:SER:HB2	1.98	0.45
11:B:115:LEU:HA	11:B:118:LEU:HB2	1.99	0.45
11:C:80:VAL:HG12	11:D:80:VAL:HG11	1.98	0.45
17:U:235:ALA:HB1	17:U:323:ILE:HG12	1.96	0.45
17:V:323:ILE:HG12	17:V:380:PHE:HB2	1.98	0.45
3:2:135:PHE:HD2	3:2:139:GLU:HB3	1.82	0.45
9:8:54:THR:HG22	12:M:186:VAL:HG12	1.98	0.45
11:A:92:ASN:N	11:A:92:ASN:OD1	2.48	0.45
17:U:430:VAL:HG21	18:X:218:ARG:HD3	1.98	0.45
6:5:104:ASP:OD2	6:5:112:ARG:NE	2.48	0.45
8:7:117:ASP:OD1	8:7:117:ASP:N	2.45	0.45
11:G:72:ALA:HB2	11:H:70:ALA:HA	1.97	0.45
18:Z:130:ASP:OD2	18:Z:130:ASP:N	2.49	0.45
2:1:582:GLN:NE2	12:M:132:ASP:OD1	2.47	0.45
3:2:288:LEU:HD23	3:2:307:VAL:HG11	1.98	0.45
6:5:27:ASP:OD2	9:8:44:HIS:NE2	2.39	0.45
11:A:111:GLU:CD	11:B:113:ILE:HD11	2.37	0.45
17:U:189:ALA:HB3	18:X:252:ASN:HD22	1.81	0.45
17:V:235:ALA:HB1	17:V:323:ILE:HD13	1.99	0.45
17:V:453:TYR:CG	17:V:477:GLY:HA3	2.51	0.45
18:X:165:LYS:HG3	18:X:461:VAL:HG11	1.98	0.45
18:Y:286:ASN:HB3	18:Y:289:ARG:HG2	1.98	0.45
18:Y:470:PHE:HA	18:Y:473:VAL:HG12	1.98	0.45
2:1:496:GLU:HA	2:1:499:GLU:HG2	1.98	0.45
8:7:45:LYS:HE2	8:7:45:LYS:HB3	1.88	0.45
11:H:78:LEU:HB3	11:I:110:THR:HG22	1.99	0.45
17:V:371:GLU:HG2	17:V:372:LEU:HD12	1.98	0.45
18:X:117:THR:OG1	18:X:122:MET:SD	2.71	0.45
18:X:365:SER:HB2	18:X:378:ASP:HB2	1.99	0.45
18:Y:86:ARG:NH2	18:Y:300:LEU:O	2.50	0.45
2:1:109:LYS:HA	2:1:109:LYS:HD3	1.82	0.45
5:4:43:GLU:HG3	5:4:45:ASP:HB2	1.99	0.45
18:X:164:ILE:HB	18:X:167:VAL:HB	1.97	0.45
2:1:35:ILE:HD11	8:7:169:VAL:HG11	1.98	0.44
5:4:84:ARG:NH2	5:4:88:GLU:OE1	2.50	0.44
9:8:11:ILE:HG22	9:8:12:LEU:HG	1.98	0.44
13:P:124:ALA:HB2	17:V:65:LYS:HD2	1.99	0.44
17:U:136:SER:HA	18:Z:59:ILE:HB	2.00	0.44
2:1:62:LYS:HD2	2:1:144:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:568:ASP:OD2	6:5:38:HIS:NE2	2.50	0.44
5:4:89:LEU:HB3	8:7:172:ALA:HB2	1.98	0.44
13:P:209:MET:CE	17:T:79:PRO:CG	2.94	0.44
5:4:187:CYS:HB2	8:7:184:ASN:HD21	1.82	0.44
11:C:92:ASN:OD1	11:C:92:ASN:N	2.49	0.44
11:E:60:LYS:HB3	11:E:125:LEU:HD23	1.99	0.44
17:T:207:LYS:HD3	17:T:492:ILE:HD11	1.99	0.44
17:T:231:LYS:HE3	17:T:231:LYS:HB2	1.75	0.44
17:U:41:ASP:N	17:U:41:ASP:OD1	2.42	0.44
17:V:226:ASP:O	17:V:231:LYS:NZ	2.42	0.44
18:Y:284:VAL:HG11	18:Y:287:ILE:HD13	1.99	0.44
5:4:291:LYS:HE2	17:T:42:ALA:HB2	1.99	0.44
17:T:208:ALA:HA	17:T:484:LEU:HD22	1.99	0.44
18:X:130:ASP:OD1	18:X:130:ASP:N	2.41	0.44
18:Y:470:PHE:O	18:Y:474:LEU:HB2	2.17	0.44
3:2:176:ALA:HB2	3:2:200:PHE:HZ	1.82	0.44
4:3:136:SER:OG	4:3:137:THR:N	2.51	0.44
13:P:38:LYS:HD2	13:P:38:LYS:HA	1.84	0.44
17:U:155:ILE:HD12	17:U:312:TYR:HB2	1.98	0.44
2:1:78:LEU:HD12	2:1:493:LEU:HB2	2.00	0.44
8:7:70:SER:O	8:7:70:SER:OG	2.29	0.44
11:F:74:VAL:HG21	11:F:114:ALA:HB2	2.00	0.44
15:R:161:LYS:HA	15:R:164:LEU:HG	1.99	0.44
17:V:551:LYS:HE3	17:V:551:LYS:HB2	1.90	0.44
18:Y:480:ASP:OD1	18:Y:480:ASP:N	2.51	0.44
2:1:517:GLU:HG2	2:1:518:GLU:HG3	2.00	0.44
6:5:31:LEU:HA	6:5:34:ILE:HB	2.00	0.44
13:P:46:LEU:HD13	13:P:51:ALA:HB1	2.00	0.44
11:D:92:ASN:OD1	11:D:92:ASN:N	2.50	0.44
16:S:97:SER:HB2	16:S:188:GLN:HB2	1.99	0.44
17:T:475:GLU:OE2	17:T:479:ARG:NH2	2.40	0.44
17:T:204:THR:HG21	17:T:215:ILE:HD12	1.99	0.44
17:U:216:GLY:N	17:U:219:GLN:OE1	2.45	0.44
17:V:550:LEU:HA	17:V:553:GLU:HB2	2.00	0.44
9:8:34:THR:O	9:8:38:LYS:HB2	2.18	0.43
15:R:175:GLU:HA	15:R:178:GLN:HB2	2.00	0.43
17:T:243:LYS:HB3	17:T:243:LYS:HE3	1.80	0.43
18:X:73:VAL:HG21	18:X:125:ILE:HG21	2.00	0.43
18:Z:165:LYS:NZ	18:Z:489:VAL:O	2.36	0.43
5:4:19:ASP:OD1	5:4:19:ASP:N	2.51	0.43
5:4:216:ALA:HA	5:4:219:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:34:THR:HG22	15:R:47:VAL:HG21	2.00	0.43
15:R:59:ALA:HB2	15:R:137:HIS:HD2	1.82	0.43
16:S:121:LYS:HA	16:S:124:ARG:HG2	2.00	0.43
17:U:344:PRO:HD2	18:X:299:ALA:HB1	2.00	0.43
17:U:152:ASN:N	17:U:152:ASN:OD1	2.52	0.43
4:3:245:SER:OG	4:3:246:GLU:N	2.50	0.43
11:C:69:ILE:HA	11:D:70:ALA:HB2	2.01	0.43
17:U:67:ILE:HG23	17:U:68:PRO:HD3	1.99	0.43
17:U:258:VAL:HG22	17:U:286:ILE:HD12	2.01	0.43
17:V:403:ASP:OD2	18:Z:218:ARG:NE	2.50	0.43
18:Y:239:ARG:O	18:Y:242:SER:OG	2.31	0.43
18:Y:435:ARG:NH1	18:Y:474:LEU:O	2.51	0.43
11:I:123:LEU:HD12	11:I:127:ALA:HB3	2.01	0.43
18:Z:407:LEU:O	18:Z:411:LYS:HB2	2.19	0.43
5:4:178:LEU:HD11	8:7:183:THR:HG21	2.01	0.43
5:4:277:TRP:HE1	17:T:41:ASP:HA	1.84	0.43
14:Q:52:TYR:N	16:S:159:GLN:O	2.51	0.43
16:S:111:LEU:HB3	16:S:274:MET:HE3	2.00	0.43
17:V:149:GLN:HB3	17:V:152:ASN:HD21	1.84	0.43
18:Z:248:TYR:HB3	18:Z:250:GLN:HE21	1.83	0.43
2:1:463:SER:HB2	6:5:103:TYR:HE2	1.84	0.43
17:T:92:ASP:OD2	18:X:78:GLN:NE2	2.52	0.43
17:T:132:PHE:HE1	17:T:297:PRO:HB2	1.83	0.43
17:V:164:THR:HA	17:V:170:PRO:HA	2.00	0.43
5:4:181:ASP:OD1	5:4:181:ASP:N	2.49	0.43
18:Z:430:LYS:HA	18:Z:433:VAL:HB	2.01	0.43
2:1:182:ARG:HA	2:1:229:GLU:HA	2.01	0.43
2:1:413:LYS:HG3	2:1:424:VAL:HG21	1.99	0.43
11:G:83:GLY:O	11:H:84:SER:OG	2.37	0.43
11:G:92:ASN:OD1	11:G:92:ASN:N	2.49	0.43
18:X:137:ALA:HB1	18:X:140:ILE:HD11	2.00	0.43
18:Z:562:ASN:OD1	18:Z:566:LYS:N	2.48	0.43
2:1:39:LYS:HA	2:1:39:LYS:HD2	1.79	0.43
10:9:73:TRP:HE3	10:9:76:THR:HG21	1.83	0.43
11:J:55:VAL:HA	11:J:58:ALA:HB3	2.01	0.43
17:T:466:LEU:HD21	17:T:471:GLN:HG3	2.00	0.43
17:T:476:ARG:NH2	17:T:505:THR:O	2.51	0.43
13:P:132:SER:HA	17:V:48:LEU:HD22	2.00	0.42
15:R:40:LYS:NZ	16:S:128:ALA:O	2.50	0.42
17:T:62:VAL:O	17:T:66:LEU:HB3	2.19	0.42
17:U:202:LEU:HD12	17:U:217:ARG:HG3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:213:VAL:HG21	18:Y:262:ALA:HB2	2.01	0.42
18:Z:124:VAL:HG23	18:Z:125:ILE:HG23	2.01	0.42
3:2:108:GLU:HG2	3:2:145:TYR:HD1	1.84	0.42
4:3:148:LYS:HB2	4:3:183:THR:HG22	2.00	0.42
4:3:233:ARG:NH1	4:3:235:ASP:OD2	2.43	0.42
6:5:104:ASP:O	6:5:110:SER:OG	2.31	0.42
17:V:203:PHE:HE1	17:V:436:PHE:HB2	1.84	0.42
18:Z:160:LEU:O	18:Z:162:THR:OG1	2.36	0.42
3:2:42:LYS:NZ	8:7:69:LEU:O	2.43	0.42
3:2:406:ARG:HD3	3:2:406:ARG:HA	1.88	0.42
17:T:240:ILE:HG23	17:T:279:THR:HG21	2.00	0.42
18:Z:522:LYS:HG3	18:Z:523:ASP:H	1.84	0.42
2:1:587:ASN:HD21	4:3:207:HIS:CD2	2.38	0.42
11:A:86:ILE:HG21	11:B:85:LEU:HA	2.00	0.42
11:B:78:LEU:HD23	11:B:78:LEU:HA	1.87	0.42
15:R:34:THR:O	15:R:38:ASN:ND2	2.52	0.42
18:X:287:ILE:HD11	18:X:321:LEU:HD21	2.01	0.42
18:Y:228:ILE:HD13	18:Y:228:ILE:HA	1.89	0.42
1:0:67:LYS:O	10:9:60:ASN:N	2.40	0.42
2:1:535:HIS:HB3	2:1:540:LEU:HB2	2.02	0.42
8:7:16:THR:O	8:7:73:LYS:NZ	2.43	0.42
8:7:170:HIS:CD2	8:7:172:ALA:H	2.37	0.42
11:D:74:VAL:HG23	11:E:113:ILE:HD13	2.02	0.42
17:T:157:PRO:HB3	18:Y:545:LEU:HD22	2.01	0.42
17:U:236:ILE:HD11	17:U:272:LEU:HD21	2.00	0.42
17:U:346:GLY:HA2	18:X:309:GLY:HA3	2.02	0.42
4:3:224:THR:HG21	4:3:263:SER:HB3	2.02	0.42
8:7:186:LEU:HD12	8:7:186:LEU:HA	1.89	0.42
10:9:76:THR:HG23	10:9:78:VAL:HG12	2.01	0.42
17:V:254:ARG:NH1	18:Z:543:ASP:OD2	2.53	0.42
2:1:29:SER:O	2:1:29:SER:OG	2.37	0.42
2:1:492:GLN:HA	2:1:495:GLU:HG2	2.01	0.42
3:2:293:THR:HG21	3:2:405:VAL:HG23	2.02	0.42
4:3:233:ARG:HE	4:3:233:ARG:HB3	1.68	0.42
5:4:142:LEU:HA	5:4:145:VAL:HG12	2.01	0.42
11:C:118:LEU:HA	11:C:121:VAL:HG12	2.02	0.42
12:M:288:GLU:HA	12:M:291:VAL:HG22	2.02	0.42
18:X:107:SER:HB2	18:X:110:LYS:HE3	2.02	0.42
18:Z:145:ARG:HH22	18:Z:267:THR:HG23	1.84	0.42
2:1:72:ASP:OD2	8:7:121:ARG:NH2	2.53	0.42
2:1:525:LEU:HD23	2:1:525:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:50:VAL:HG13	8:7:57:ALA:HB3	2.02	0.42
13:P:52:GLN:HA	13:P:55:THR:HG22	2.01	0.42
17:V:339:LEU:HD11	17:V:349:ALA:HB1	2.01	0.42
17:V:453:TYR:HA	17:V:456:VAL:HG22	2.01	0.42
18:Y:225:ARG:HA	18:Y:225:ARG:HD3	1.86	0.42
3:2:322:ARG:HG2	3:2:326:GLU:HB3	2.01	0.42
3:2:346:ARG:NH1	13:P:166:GLU:OE1	2.53	0.42
11:F:90:ALA:O	11:G:92:ASN:ND2	2.53	0.42
15:R:28:ALA:HB3	16:S:92:PHE:HD1	1.84	0.42
18:X:88:ILE:HD12	18:X:297:VAL:HG11	2.02	0.42
2:1:594:PRO:HG2	9:8:8:LEU:HD23	2.01	0.41
3:2:218:GLY:HA3	3:2:250:GLY:HA2	2.01	0.41
11:B:92:ASN:N	11:B:92:ASN:OD1	2.52	0.41
13:P:209:MET:HE2	17:T:79:PRO:HG2	2.02	0.41
17:V:545:ALA:O	17:V:549:HIS:ND1	2.52	0.41
18:Y:211:ALA:HB2	18:Y:265:GLY:HA3	2.03	0.41
2:1:365:GLN:HE21	2:1:386:HIS:HD2	1.67	0.41
3:2:36:LEU:HD22	3:2:41:VAL:HG21	2.01	0.41
5:4:233:HIS:HA	5:4:236:LYS:HE2	2.02	0.41
7:6:108:LEU:HG	12:M:285:VAL:HG21	2.00	0.41
11:D:124:ILE:HA	11:D:124:ILE:HD12	1.82	0.41
17:U:527:GLN:HE22	17:U:558:LYS:HB3	1.85	0.41
17:V:93:GLY:N	17:V:135:ASP:OD2	2.36	0.41
18:X:124:VAL:HG13	18:X:125:ILE:HG23	2.02	0.41
2:1:538:ILE:O	12:M:101:LYS:NZ	2.44	0.41
2:1:615:VAL:HA	4:3:234:ALA:HB2	2.02	0.41
4:3:217:ASP:OD1	4:3:217:ASP:N	2.53	0.41
11:J:107:PHE:HZ	11:J:111:GLU:OE1	1.92	0.41
12:M:190:ALA:HA	12:M:193:THR:HG22	2.02	0.41
13:P:134:LEU:HD23	13:P:134:LEU:HA	1.88	0.41
17:T:400:SER:O	18:Y:216:ARG:NH2	2.52	0.41
17:U:90:VAL:HG21	17:U:138:ILE:HB	2.02	0.41
17:V:416:GLY:O	18:Y:401:ARG:NH2	2.53	0.41
3:2:108:GLU:HG3	3:2:142:ARG:HG2	2.03	0.41
13:P:75:TYR:HA	13:P:78:ILE:HG12	2.02	0.41
18:Y:246:LEU:HD13	18:Y:248:TYR:HE2	1.85	0.41
18:Y:252:ASN:OD1	18:Y:252:ASN:N	2.50	0.41
18:Z:111:VAL:HG11	18:Z:264:THR:HG23	2.01	0.41
3:2:165:PHE:HD1	3:2:170:VAL:HG11	1.86	0.41
3:2:204:THR:HG21	3:2:209:ASP:HB2	2.02	0.41
3:2:404:LYS:HD3	3:2:404:LYS:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:84:SER:OG	11:J:87:ASN:ND2	2.53	0.41
11:E:65:GLY:HA2	11:F:67:ALA:HB2	2.03	0.41
11:I:69:ILE:HA	11:J:70:ALA:HB2	2.01	0.41
13:P:134:LEU:HA	13:P:137:VAL:HG12	2.02	0.41
17:T:108:LEU:O	17:T:147:THR:OG1	2.35	0.41
18:X:53:ASP:OD1	18:X:53:ASP:N	2.49	0.41
18:Y:195:GLU:HG3	18:Y:447:PHE:CG	2.55	0.41
2:1:530:LYS:HB3	2:1:530:LYS:HE2	1.94	0.41
6:5:105:ALA:HB1	6:5:114:LEU:HG	2.01	0.41
11:B:63:GLY:O	11:B:67:ALA:N	2.53	0.41
11:E:90:ALA:HB2	11:F:99:LEU:HD11	2.02	0.41
17:T:241:HIS:CE1	17:T:493:PRO:HA	2.56	0.41
17:V:326:ASP:H	17:V:382:VAL:HB	1.86	0.41
17:V:466:LEU:HD13	17:V:471:GLN:HG2	2.03	0.41
2:1:472:LYS:HD2	2:1:472:LYS:HA	1.89	0.41
11:I:55:VAL:O	11:I:59:SER:HB3	2.21	0.41
14:Q:49:GLN:HE21	14:Q:61:LYS:HG2	1.86	0.41
16:S:111:LEU:HD23	16:S:111:LEU:HA	1.97	0.41
17:T:495:GLU:HA	17:T:498:THR:HG22	2.02	0.41
17:U:119:ALA:HA	17:U:129:VAL:HG12	2.02	0.41
17:U:195:ARG:NH2	17:U:363:GLU:O	2.43	0.41
17:U:298:LEU:HD23	17:U:298:LEU:HA	1.92	0.41
3:2:188:ALA:HB2	3:2:220:LEU:HD22	2.03	0.41
5:4:64:GLU:OE1	17:T:55:SER:N	2.47	0.41
11:B:72:ALA:HB2	11:C:70:ALA:HA	2.03	0.41
17:T:262:VAL:HG11	17:T:303:PRO:HD3	2.03	0.41
17:T:508:PHE:HZ	17:T:551:LYS:HD3	1.86	0.41
17:U:236:ILE:O	17:U:240:ILE:HG12	2.21	0.41
17:V:406:ILE:HA	17:V:426:SER:HB2	2.02	0.41
18:X:110:LYS:HB3	18:X:140:ILE:HG22	2.02	0.41
18:Y:63:LEU:HB2	18:Y:74:LEU:HB2	2.03	0.41
18:Y:467:ILE:O	18:Y:471:GLN:HB2	2.21	0.41
18:Y:500:ASP:O	18:Y:504:LYS:HG3	2.21	0.41
2:1:103:LYS:HA	2:1:103:LYS:HD3	1.85	0.41
3:2:298:LYS:HA	3:2:298:LYS:HD2	1.91	0.41
11:D:55:VAL:HA	11:D:58:ALA:HB3	2.02	0.41
11:I:61:MET:HA	11:J:124:ILE:HD11	2.03	0.41
13:P:121:LEU:HD13	17:V:66:LEU:HD11	2.03	0.41
17:T:492:ILE:HA	17:T:493:PRO:HD3	1.95	0.41
18:X:306:SER:HB2	18:X:312:PRO:HA	2.02	0.41
18:Y:43:VAL:HG22	18:Y:48:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:87:LEU:HA	7:6:87:LEU:HD23	1.89	0.40
17:U:50:LYS:O	17:U:52:LYS:NZ	2.53	0.40
17:U:94:ILE:HG22	17:U:130:VAL:HG12	2.04	0.40
17:U:476:ARG:HA	17:U:476:ARG:HD3	1.94	0.40
17:V:259:TYR:OH	17:V:325:ASP:OD2	2.25	0.40
18:X:349:PRO:HA	18:X:352:ALA:HB3	2.03	0.40
4:3:104:PRO:HB3	4:3:143:LEU:HG	2.03	0.40
11:H:57:ALA:HA	11:H:60:LYS:HD3	2.03	0.40
11:H:62:VAL:HG23	11:I:59:SER:HB2	2.04	0.40
13:P:46:LEU:HD23	13:P:46:LEU:HA	1.90	0.40
17:V:92:ASP:OD2	18:Y:303:ARG:NE	2.54	0.40
18:X:114:GLY:HA2	18:X:271:TYR:CE2	2.56	0.40
18:Y:64:GLU:HB3	18:Y:103:VAL:HG23	2.03	0.40
18:Z:170:LEU:HD22	18:Z:404:GLN:HG3	2.03	0.40
2:1:270:VAL:HG21	2:1:523:LEU:HD13	2.02	0.40
4:3:178:LEU:HB3	4:3:218:GLU:HB3	2.03	0.40
11:B:107:PHE:CE1	11:C:109:LEU:HB3	2.57	0.40
17:T:220:ARG:HG3	17:T:402:THR:HA	2.02	0.40
1:0:54:TYR:HB3	1:0:77:SER:HB2	2.02	0.40
3:2:145:TYR:OH	8:7:16:THR:OG1	2.29	0.40
4:3:275:PRO:HD2	4:3:278:ILE:HB	2.03	0.40
6:5:50:ARG:HE	6:5:50:ARG:HB3	1.70	0.40
16:S:123:THR:HA	16:S:126:THR:HG22	2.03	0.40
16:S:190:TYR:HB2	16:S:210:ILE:HB	2.02	0.40
17:T:220:ARG:HD2	17:T:362:LEU:HB3	2.03	0.40
18:Y:96:LEU:HD23	18:Y:96:LEU:HA	1.93	0.40
5:4:101:PRO:HG3	8:7:170:HIS:CD2	2.57	0.40
9:8:26:HIS:CD2	9:8:28:PHE:H	2.38	0.40
11:F:92:ASN:OD1	11:F:92:ASN:N	2.54	0.40
13:P:70:VAL:HA	13:P:73:GLU:HB2	2.02	0.40
17:V:79:PRO:HA	17:V:80:PRO:HD3	1.95	0.40
17:V:532:VAL:HG23	17:V:546:LEU:HD11	2.02	0.40
18:X:37:ALA:HB1	18:X:101:LYS:HE3	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%)	73 (92%)	6 (8%)	0	100	100
2	1	593/618 (96%)	567 (96%)	26 (4%)	0	100	100
3	2	439/441 (100%)	418 (95%)	20 (5%)	1 (0%)	47	78
4	3	243/325 (75%)	235 (97%)	8 (3%)	0	100	100
5	4	288/294 (98%)	276 (96%)	12 (4%)	0	100	100
6	5	121/123 (98%)	113 (93%)	7 (6%)	1 (1%)	19	56
7	6	122/151 (81%)	109 (89%)	13 (11%)	0	100	100
8	7	174/190 (92%)	169 (97%)	5 (3%)	0	100	100
9	8	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
10	9	95/97 (98%)	83 (87%)	12 (13%)	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%)	70 (97%)	2 (3%)	0	100	100
11	F	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	G	72/127 (57%)	72 (100%)	0	0	100	100
11	H	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	I	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
12	M	213/327 (65%)	207 (97%)	6 (3%)	0	100	100
13	P	191/229 (83%)	174 (91%)	16 (8%)	1 (0%)	29	66
14	Q	70/74 (95%)	69 (99%)	1 (1%)	0	100	100
15	R	175/199 (88%)	164 (94%)	11 (6%)	0	100	100
16	S	275/317 (87%)	261 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	521/562 (93%)	494 (95%)	24 (5%)	3 (1%)	25	62
17	U	521/562 (93%)	494 (95%)	26 (5%)	1 (0%)	47	78
17	V	518/562 (92%)	496 (96%)	21 (4%)	1 (0%)	47	78
18	X	540/574 (94%)	498 (92%)	41 (8%)	1 (0%)	47	78
18	Y	519/574 (90%)	481 (93%)	35 (7%)	3 (1%)	25	62
18	Z	536/574 (93%)	510 (95%)	23 (4%)	3 (1%)	25	62
All	All	7038/8234 (86%)	6676 (95%)	347 (5%)	15 (0%)	50	78

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	383	PRO
17	T	493	PRO
18	Z	308	VAL
17	U	349	ALA
18	X	308	VAL
18	Z	307	ALA
17	T	56	LYS
17	T	349	ALA
17	V	349	ALA
18	Y	308	VAL
18	Z	306	SER
13	P	187	GLN
18	Y	148	PRO
18	Y	455	GLY
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

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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%)	95 (99%)	1 (1%)	76	86
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%)	49 (98%)	1 (2%)	55	74
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%)	49 (98%)	1 (2%)	55	74
11	H	50/86 (58%)	50 (100%)	0	100	100
11	I	50/86 (58%)	49 (98%)	1 (2%)	55	74
11	J	50/86 (58%)	49 (98%)	1 (2%)	55	74
12	M	178/272 (65%)	177 (99%)	1 (1%)	86	93
13	P	171/196 (87%)	171 (100%)	0	100	100
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%)	235 (100%)	0	100	100
17	T	419/448 (94%)	419 (100%)	0	100	100
17	U	419/448 (94%)	417 (100%)	2 (0%)	88	94
17	V	418/448 (93%)	418 (100%)	0	100	100
18	X	449/469 (96%)	447 (100%)	2 (0%)	91	95
18	Y	430/469 (92%)	428 (100%)	2 (0%)	88	94
18	Z	446/469 (95%)	446 (100%)	0	100	100
All	All	5631/6445 (87%)	5619 (100%)	12 (0%)	93	97

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

Mol	Chain	Res	Type
7	6	146	PHE
11	D	85	LEU
11	G	95	ILE
11	I	121	VAL
11	J	111	GLU
12	M	227	ILE
17	U	479	ARG
17	U	513	ARG
18	X	383	THR
18	X	521	LEU
18	Y	328	THR
18	Y	489	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	48	ASN
2	1	285	GLN
2	1	298	GLN
2	1	316	ASN
2	1	365	GLN
2	1	587	ASN
2	1	590	HIS
2	1	606	ASN
3	2	68	ASN
3	2	122	ASN
3	2	243	GLN
4	3	229	ASN
5	4	38	GLN
5	4	135	ASN
5	4	139	ASN
5	4	240	GLN
6	5	79	ASN
8	7	60	GLN
8	7	86	HIS
8	7	123	HIS
8	7	170	HIS
8	7	184	ASN
9	8	26	HIS
9	8	78	HIS
11	A	98	GLN
11	G	94	ASN
11	I	87	ASN

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Mol	Chain	Res	Type
11	J	87	ASN
11	J	98	GLN
12	M	120	GLN
12	M	163	ASN
13	P	76	GLN
13	P	223	ASN
14	Q	43	GLN
14	Q	49	GLN
15	R	38	ASN
15	R	66	HIS
15	R	85	GLN
15	R	178	GLN
16	S	52	ASN
16	S	96	ASN
16	S	174	GLN
16	S	186	ASN
16	S	219	GLN
16	S	250	HIS
16	S	257	ASN
16	S	262	ASN
16	S	293	ASN
16	S	297	GLN
17	T	64	GLN
17	T	139	HIS
17	T	228	GLN
17	T	241	HIS
17	T	253	GLN
17	T	271	GLN
17	T	386	GLN
17	U	134	ASN
17	U	242	GLN
17	U	248	GLN
17	U	330	GLN
17	U	386	GLN
17	U	497	GLN
17	V	152	ASN
17	V	196	GLN
17	V	241	HIS
17	V	244	ASN
17	V	271	GLN
17	V	278	GLN
17	V	497	GLN

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Mol	Chain	Res	Type
18	X	198	ASN
18	X	199	ASN
18	X	278	GLN
18	X	322	GLN
18	X	337	GLN
18	X	408	GLN
18	X	448	GLN
18	X	471	GLN
18	Y	174	GLN
18	Y	221	ASN
18	Z	42	GLN
18	Z	100	GLN
18	Z	199	ASN
18	Z	241	ASN
18	Z	250	GLN
18	Z	278	GLN
18	Z	322	GLN
18	Z	337	GLN
18	Z	404	GLN
18	Z	440	GLN
18	Z	471	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	$\#\|Z\| > 2$
20	ATP	T	1001	21	26,33,33	0.91	1 (3%)	31,52,52	1.58	5 (16%)
22	ADP	Y	601	21	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
20	ATP	V	1001	21	26,33,33	0.90	1 (3%)	31,52,52	1.53	5 (16%)
22	ADP	X	601	21	24,29,29	0.95	1 (4%)	29,45,45	1.57	4 (13%)
20	ATP	U	1001	21	26,33,33	0.89	1 (3%)	31,52,52	1.60	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
20	ATP	T	1001	21	-	4/18/38/38	0/3/3/3
22	ADP	Y	601	21	-	3/12/32/32	0/3/3/3
20	ATP	V	1001	21	-	2/18/38/38	0/3/3/3
22	ADP	X	601	21	-	5/12/32/32	0/3/3/3
20	ATP	U	1001	21	-	1/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	601	ADP	C5-C4	2.42	1.47	1.40
20	T	1001	ATP	C5-C4	2.35	1.47	1.40
20	V	1001	ATP	C5-C4	2.29	1.47	1.40
22	X	601	ADP	C5-C4	2.22	1.46	1.40
20	U	1001	ATP	C5-C4	2.22	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	1001	ATP	PB-O3B-PG	-4.54	117.26	132.83
20	T	1001	ATP	PB-O3B-PG	-3.97	119.22	132.83
22	X	601	ADP	PA-O3A-PB	-3.83	119.67	132.83
22	X	601	ADP	C3'-C2'-C1'	3.81	106.71	100.98
22	Y	601	ADP	C3'-C2'-C1'	3.73	106.59	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Y	601	ADP	PA-O3A-PB	-3.54	120.69	132.83
20	V	1001	ATP	PA-O3A-PB	-3.40	121.14	132.83
20	T	1001	ATP	PA-O3A-PB	-3.37	121.27	132.83
20	V	1001	ATP	N3-C2-N1	-3.22	123.64	128.68
20	U	1001	ATP	N3-C2-N1	-3.21	123.65	128.68
20	V	1001	ATP	PB-O3B-PG	-3.21	121.81	132.83
20	T	1001	ATP	N3-C2-N1	-3.20	123.67	128.68
22	X	601	ADP	N3-C2-N1	-3.13	123.78	128.68
20	V	1001	ATP	C3'-C2'-C1'	3.11	105.66	100.98
22	Y	601	ADP	N3-C2-N1	-3.10	123.83	128.68
20	U	1001	ATP	PA-O3A-PB	-2.73	123.47	132.83
20	T	1001	ATP	C3'-C2'-C1'	2.72	105.08	100.98
20	U	1001	ATP	C3'-C2'-C1'	2.70	105.05	100.98
20	U	1001	ATP	C4-C5-N7	-2.70	106.59	109.40
22	X	601	ADP	C4-C5-N7	-2.68	106.61	109.40
20	V	1001	ATP	C4-C5-N7	-2.55	106.75	109.40
20	T	1001	ATP	C4-C5-N7	-2.35	106.95	109.40
22	Y	601	ADP	C4-C5-N7	-2.33	106.97	109.40

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	T	1001	ATP	C5'-O5'-PA-O3A
22	X	601	ADP	C5'-O5'-PA-O1A
22	X	601	ADP	C5'-O5'-PA-O2A
22	X	601	ADP	O4'-C4'-C5'-O5'
22	Y	601	ADP	C5'-O5'-PA-O1A
22	X	601	ADP	C3'-C4'-C5'-O5'
22	Y	601	ADP	PA-O3A-PB-O1B
20	T	1001	ATP	C5'-O5'-PA-O1A
20	T	1001	ATP	C5'-O5'-PA-O2A
22	X	601	ADP	C5'-O5'-PA-O3A
22	Y	601	ADP	C5'-O5'-PA-O3A
20	T	1001	ATP	PG-O3B-PB-O1B
20	U	1001	ATP	PA-O3A-PB-O2B
20	V	1001	ATP	PG-O3B-PB-O2B
20	V	1001	ATP	PA-O3A-PB-O2B

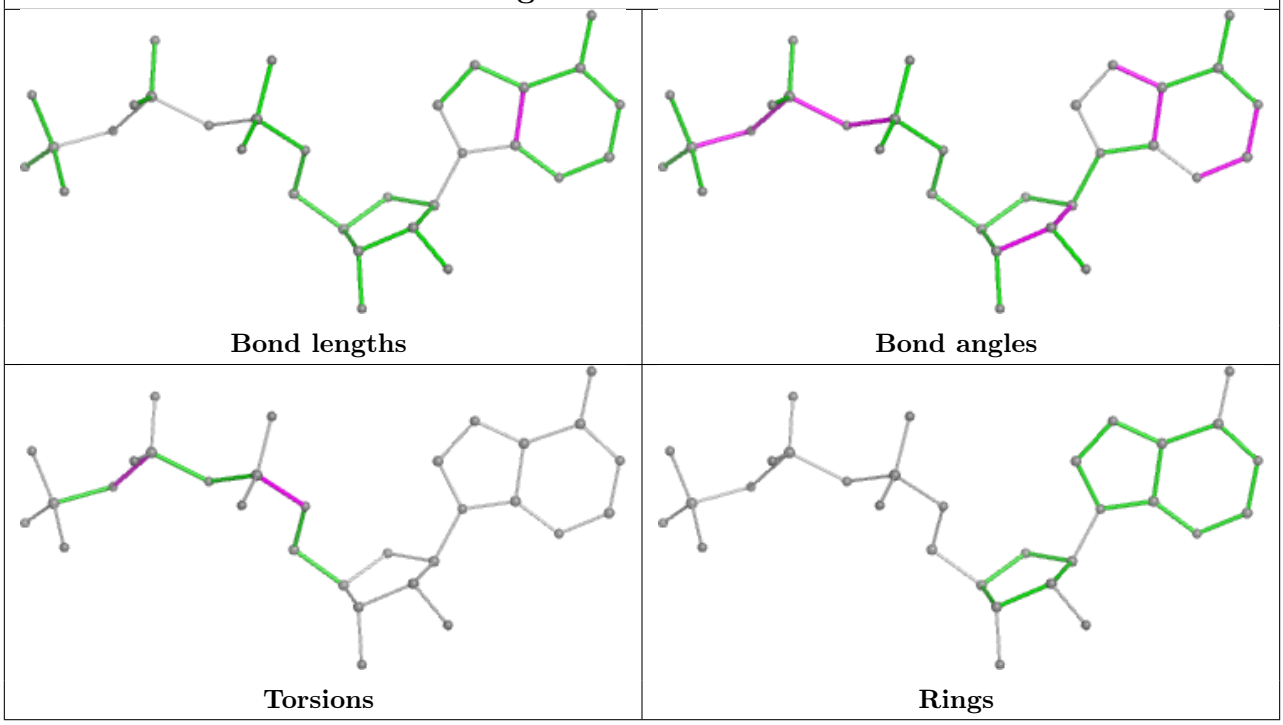
There are no ring outliers.

2 monomers are involved in 2 short contacts:

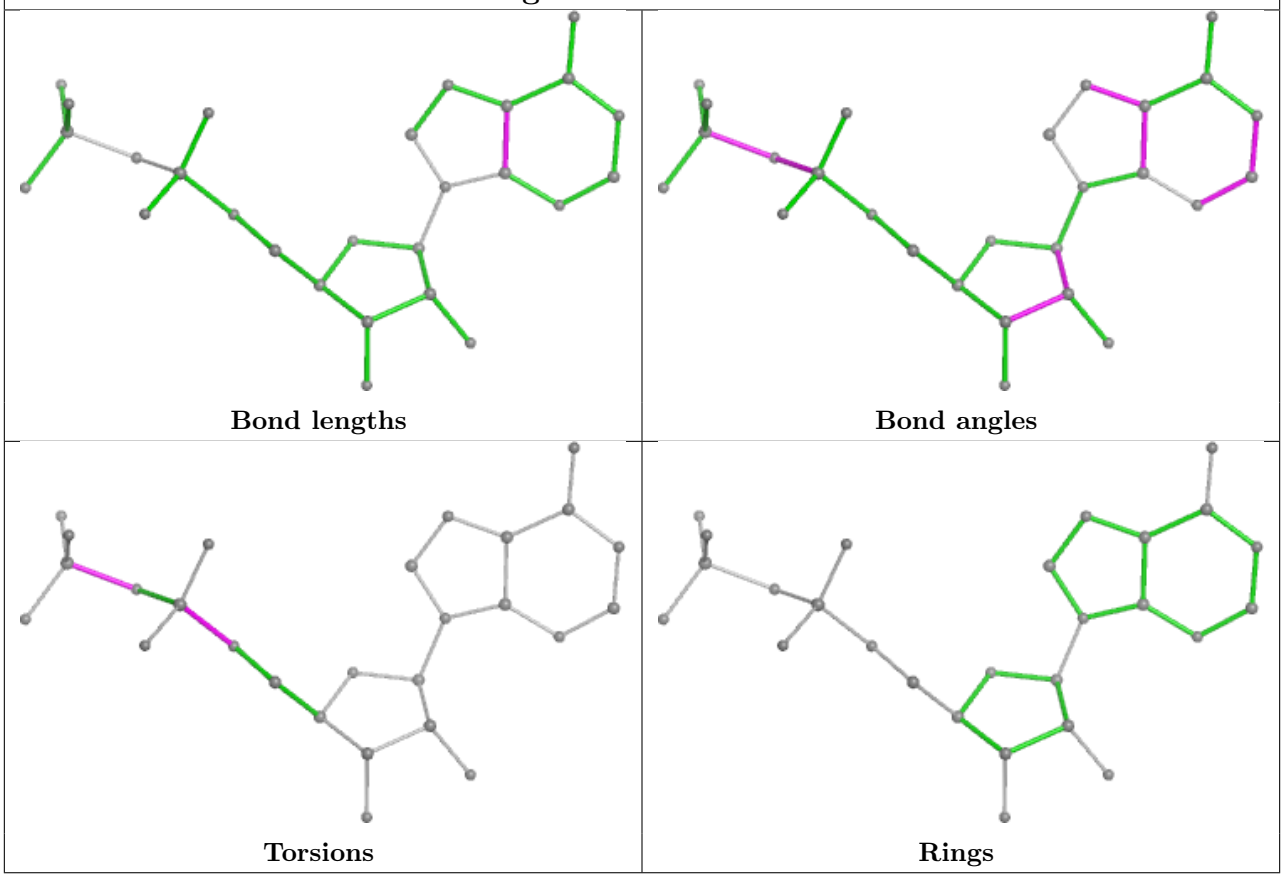
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	T	1001	ATP	1	0
22	X	601	ADP	1	0

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.

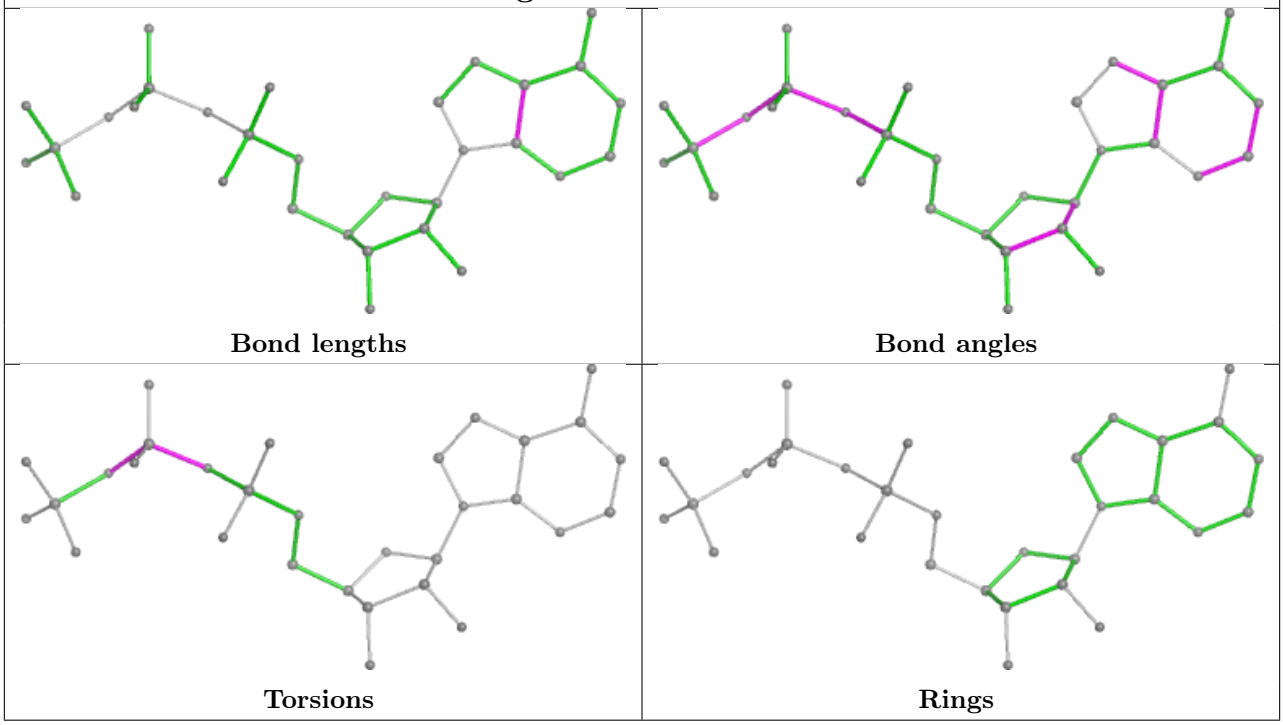
Ligand ATP T 1001



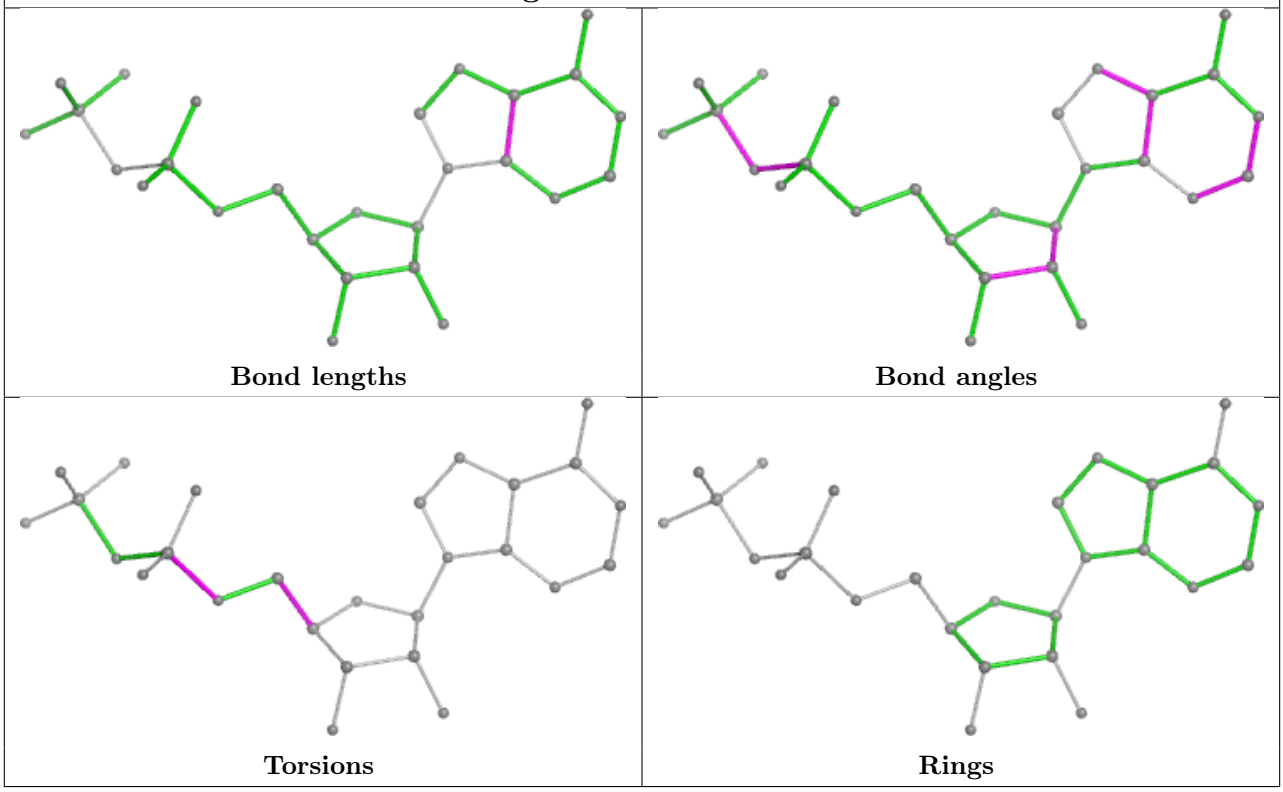
Ligand ADP Y 601



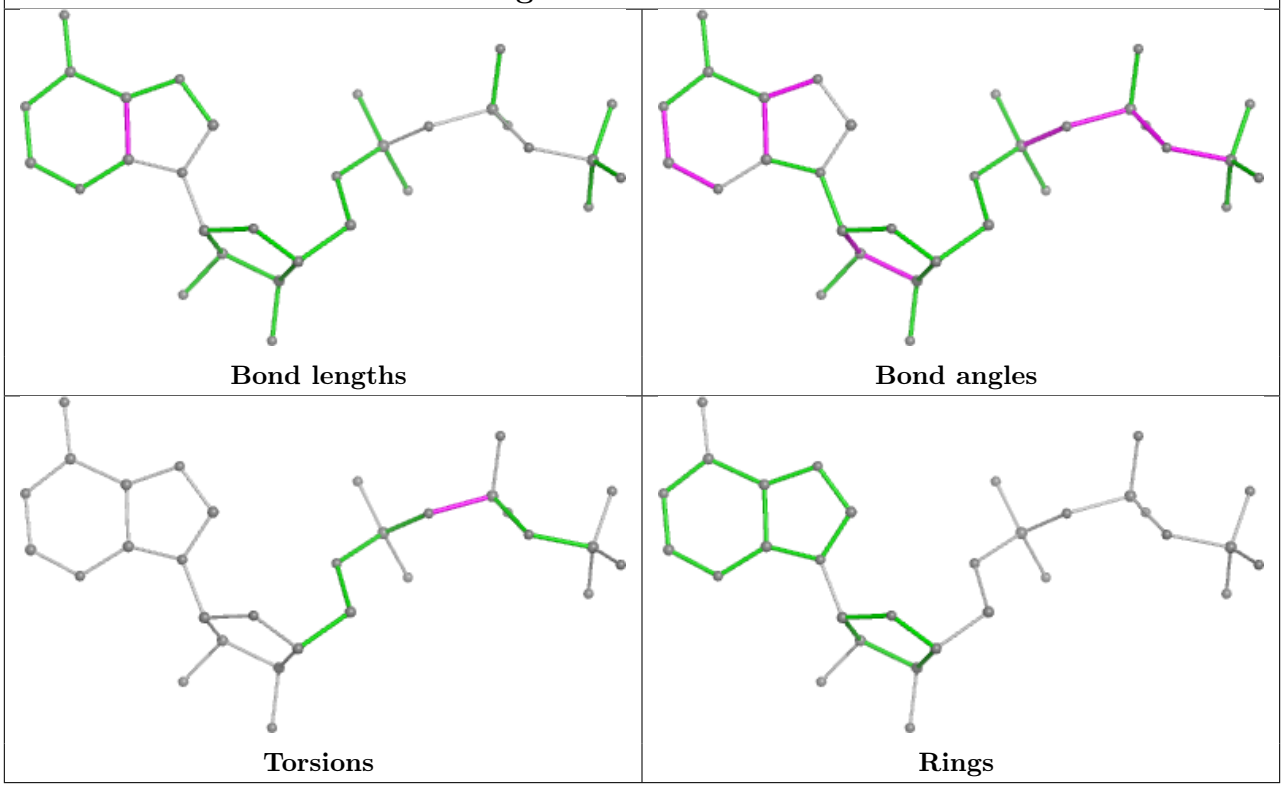
Ligand ATP V 1001



Ligand ADP X 601



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	3.89

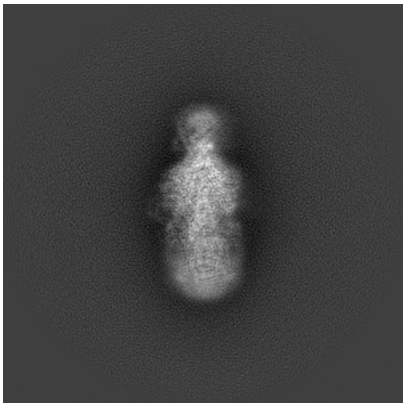
6 Map visualisation (i)

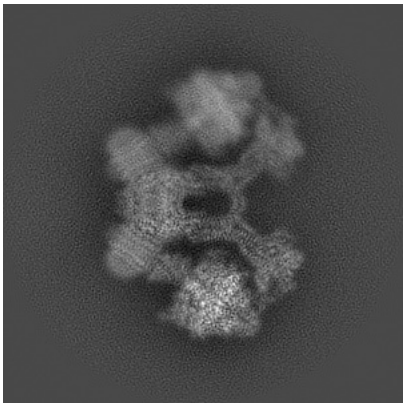
This section contains visualisations of the EMDB entry EMD-4821. These allow visual inspection of the internal detail of the map and identification of artifacts.

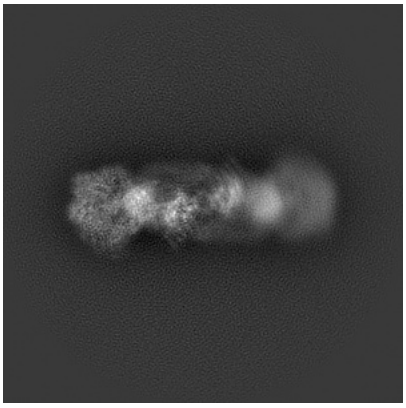
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

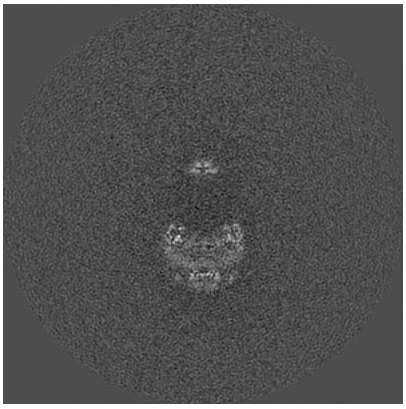

Y

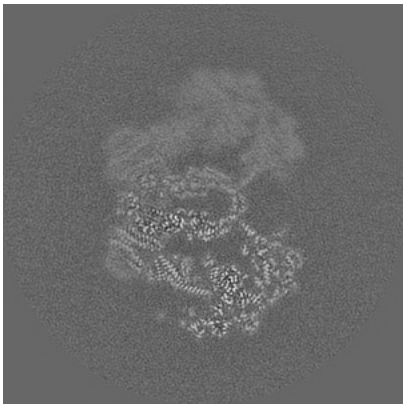

Z

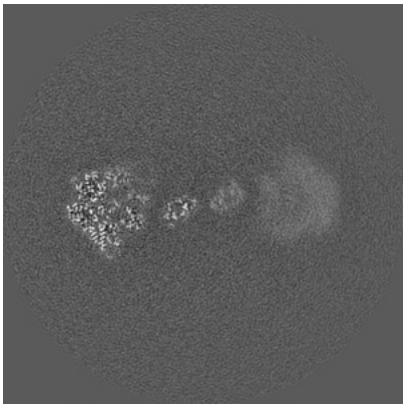
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 240

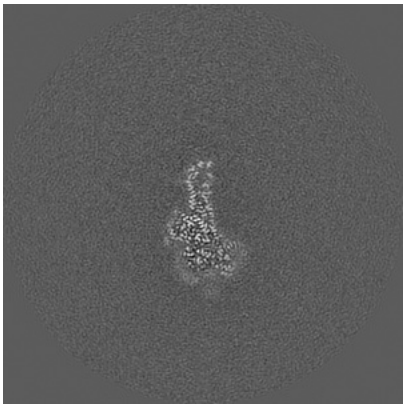

Y Index: 240


Z Index: 240

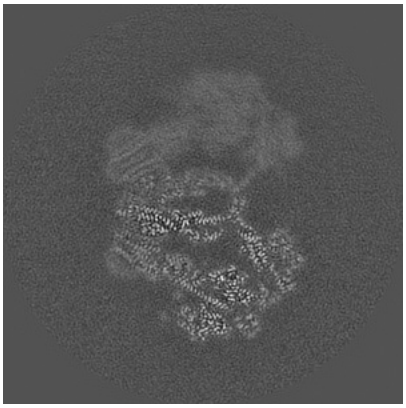
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

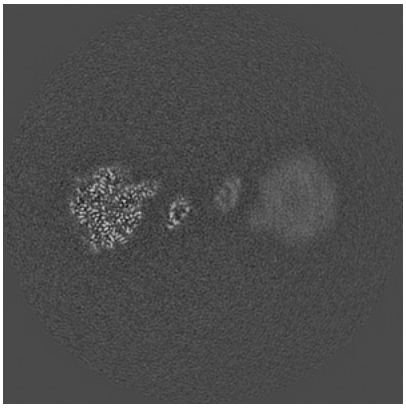
6.3.1 Primary map



X Index: 216



Y Index: 235

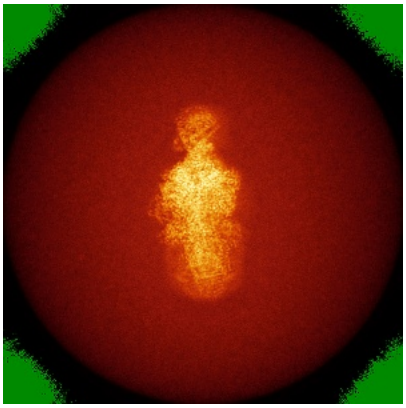


Z Index: 260

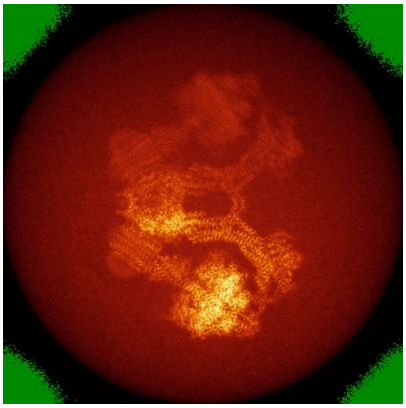
The images above show the largest variance slices of the map in three orthogonal directions.

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

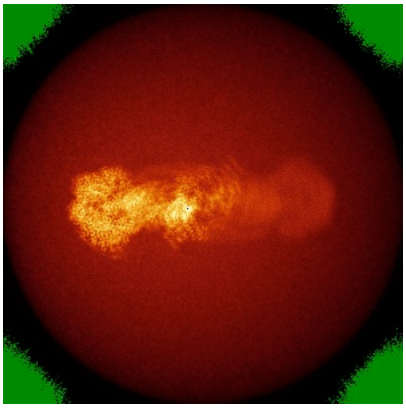
6.4.1 Primary map



X



Y

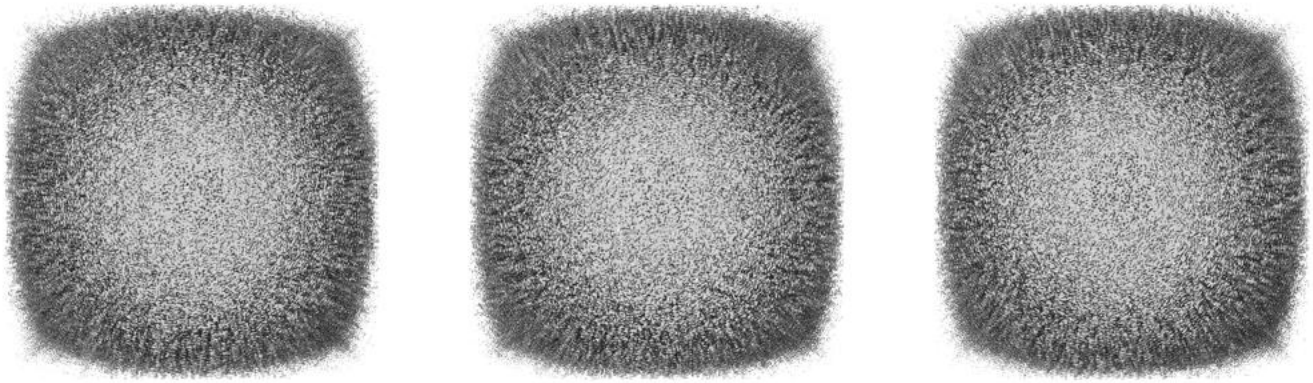


Z

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.

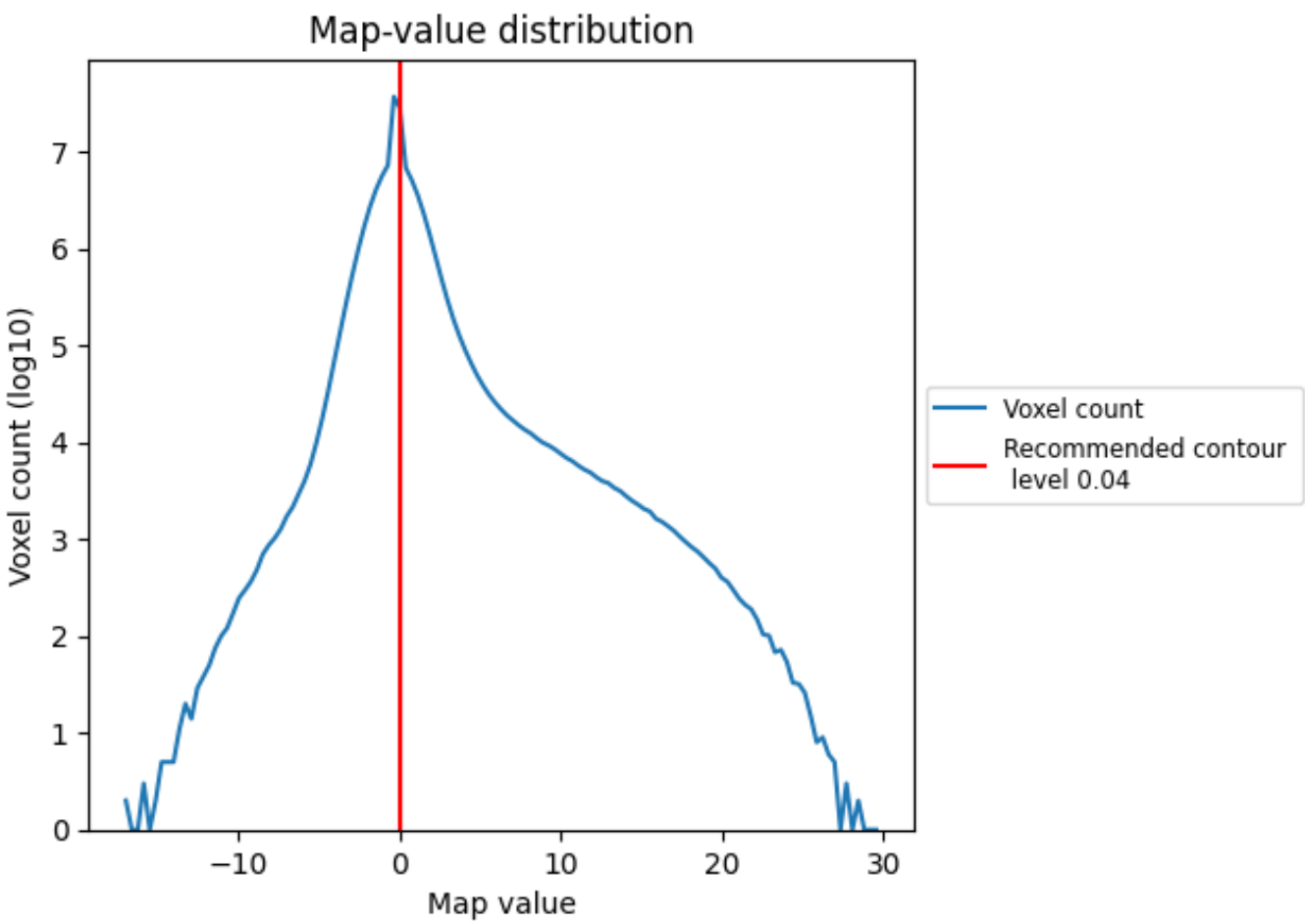
6.6 Mask visualisation (i)

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

7 Map analysis (i)

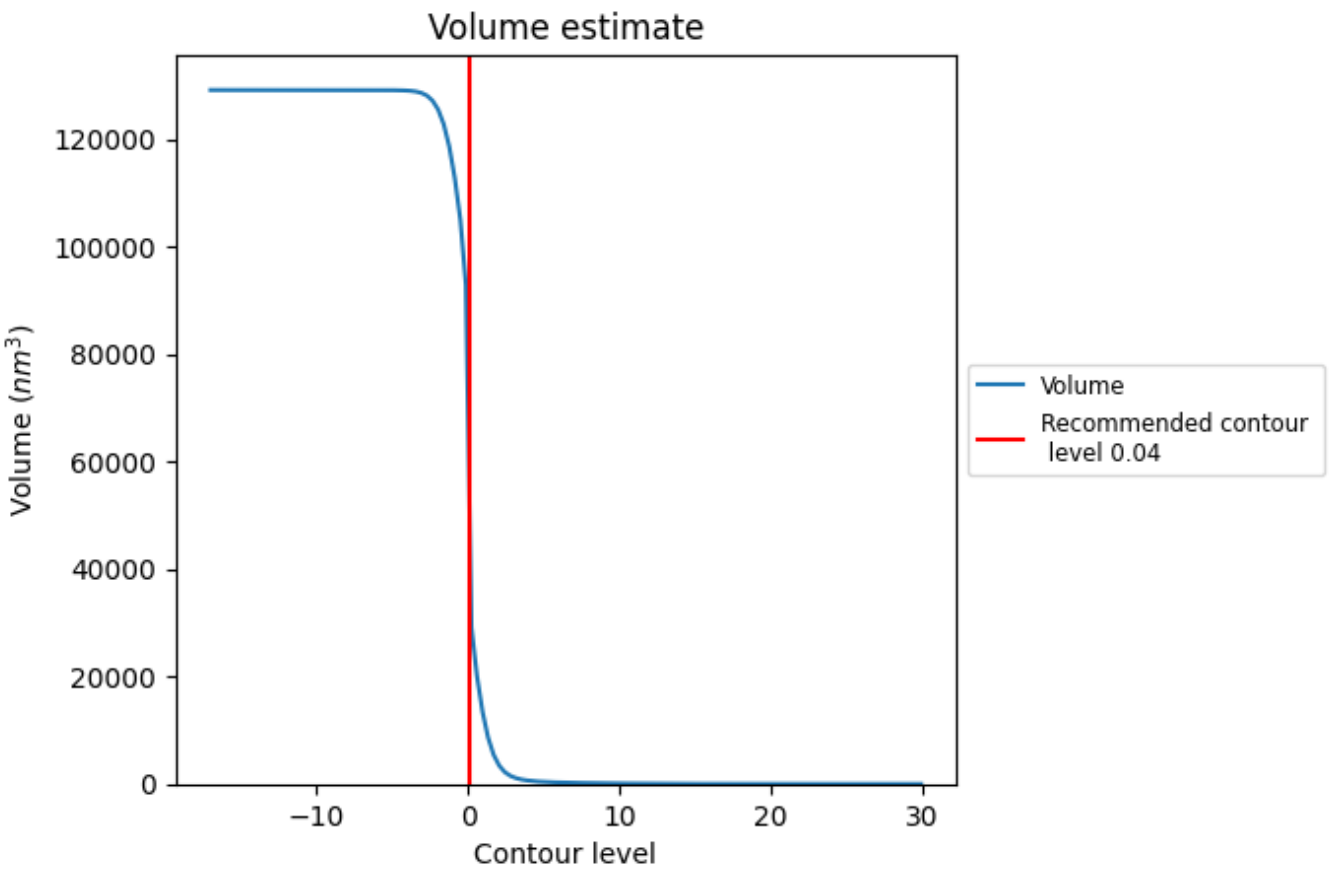
This section contains the results of statistical analysis of the map.

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.

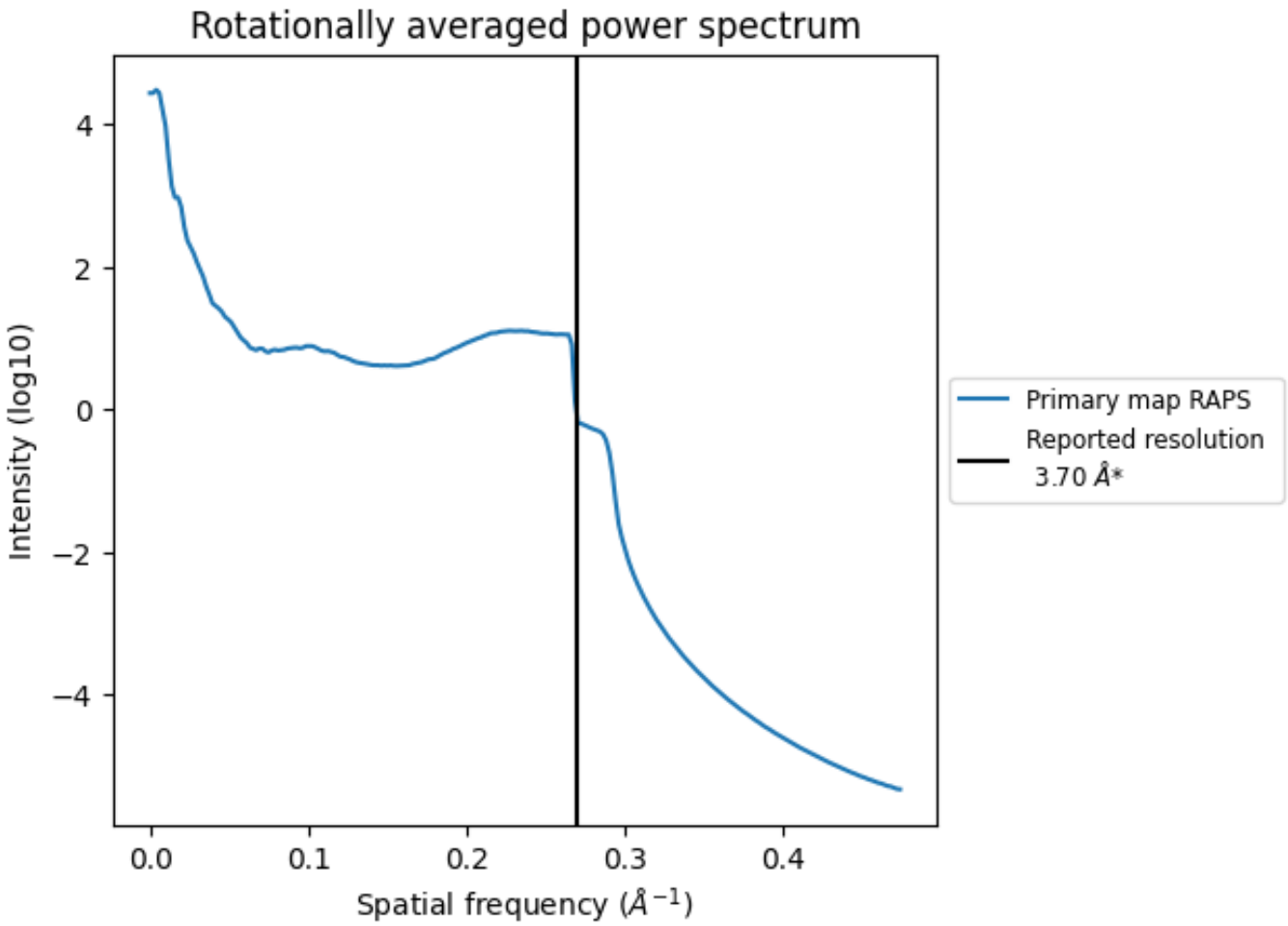
7.2 Volume estimate (i)



The volume at the recommended contour level is 62816 nm^3; this corresponds to an approximate mass of 56743 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 0.270 Å^{-1}

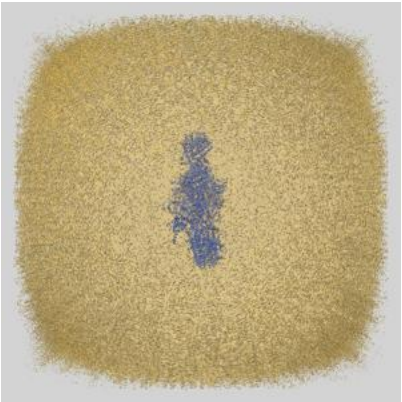
8 Fourier-Shell correlation (i)

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

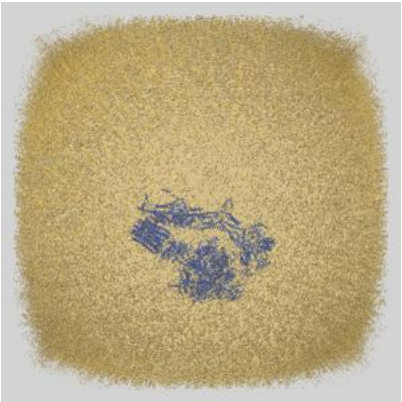
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4821 and PDB model 6RDK. Per-residue inclusion information can be found in section 3 on page 10.

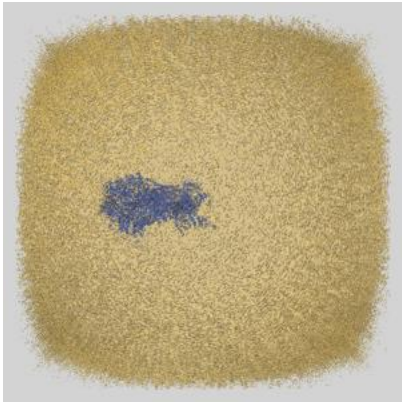
9.1 Map-model overlay (i)



X



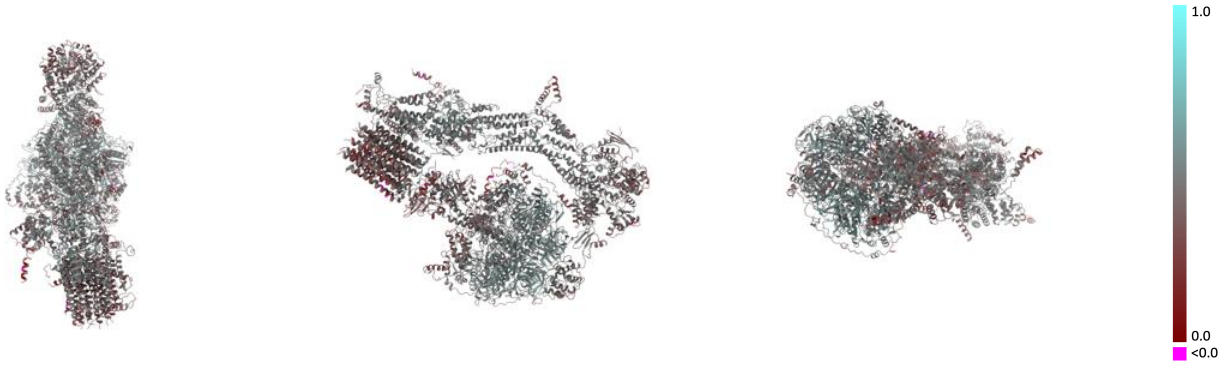
Y



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.

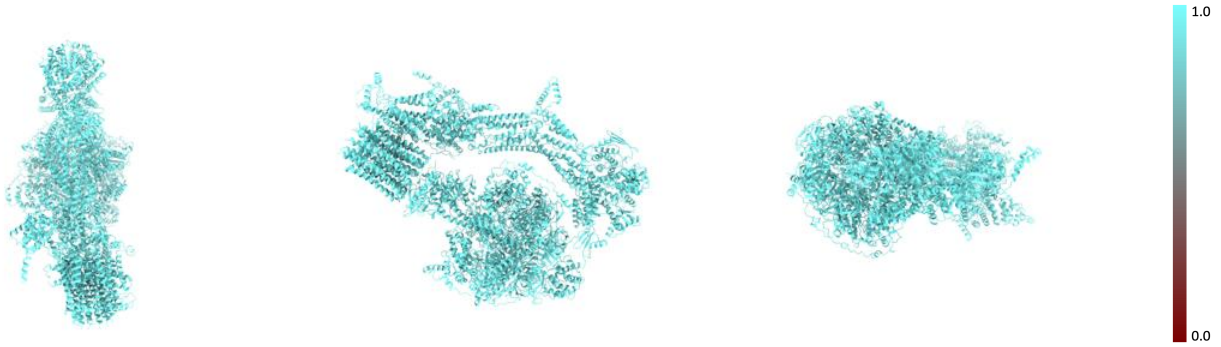
9.2 Q-score mapped to coordinate model (i)



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.

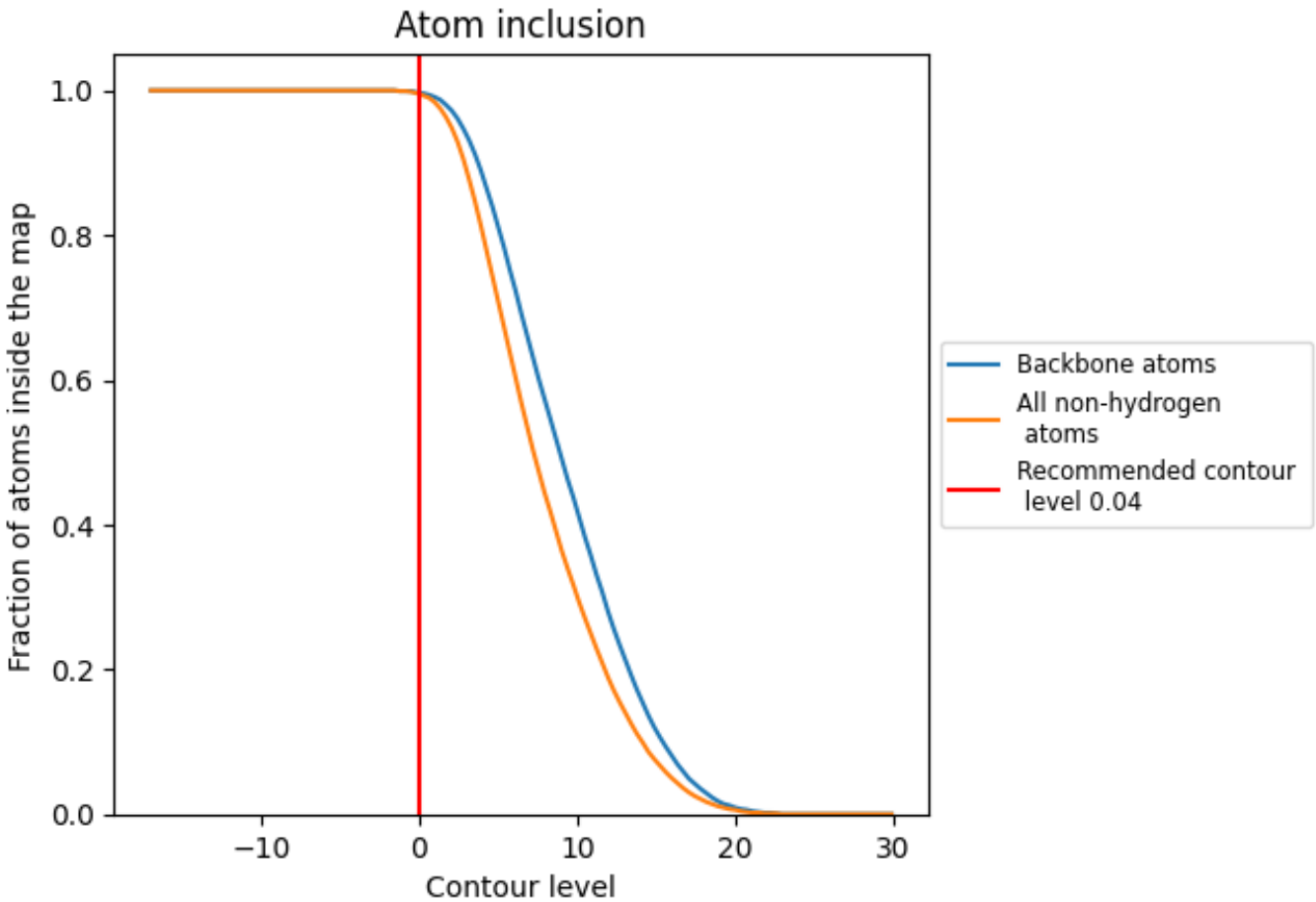
9.3 Atom inclusion mapped to coordinate model (i)



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	0.9950	0.4580
0	0.9950	0.4680
1	0.9970	0.4770
2	0.9970	0.4170
3	0.9960	0.4400
4	0.9980	0.4370
5	0.9900	0.5010
6	0.9910	0.4880
7	0.9960	0.4600
8	0.9970	0.4840
9	0.9870	0.4080
A	0.9800	0.4320
B	0.9770	0.4060
C	0.9770	0.3900
D	0.9880	0.3490
E	0.9940	0.3620
F	0.9900	0.3500
G	0.9900	0.3570
H	0.9880	0.3310
I	0.9940	0.3390
J	0.9920	0.3720
M	0.9940	0.4670
P	0.9960	0.4350
Q	0.9870	0.3600
R	0.9920	0.3630
S	0.9960	0.4340
T	0.9990	0.4990
U	0.9960	0.4930
V	0.9980	0.4920
X	0.9950	0.5040
Y	0.9910	0.4760
Z	0.9940	0.4720