Full wwPDB EM Validation Report (i)

May 12, 2024 – 04:40 am BST

PDB ID	:	6RDO
EMDB ID	:	EMD-4825
Title	:	Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 1C, composite map
Authors	:	Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on	:	2019-04-12
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

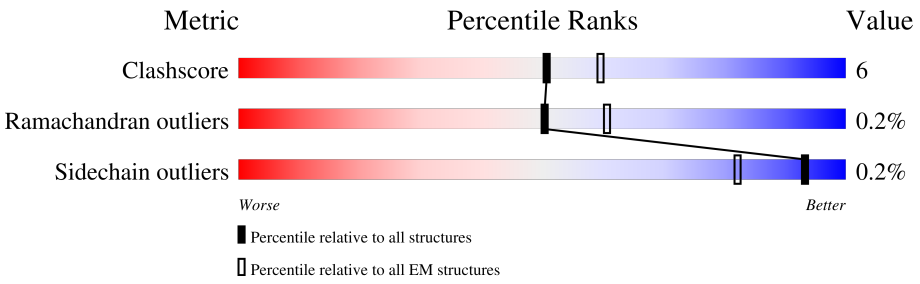
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	0	82	98% • •
2	1	618	85% 11% •
3	2	441	87% 13%
4	3	325	65% 11% 25%
5	4	294	89% 10% •
6	5	123	84% 15% •
7	6	151	69% 13% 18%
8	7	190	78% 14% 7%

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Mol	Chain	Length	Quality of chain
9	8	89	82% 17%
10	9	97	94% 6%
11	A	127	41% 17% 42%
11	B	127	39% 20% 42%
11	C	127	46% 13% 42%
11	D	127	53% 6% 42%
11	E	127	49% 9% 42%
11	F	127	47% 11% 42%
11	G	127	46% 13% 42%
11	H	127	41% 17% 42%
11	I	127	39% 19% 42%
11	J	127	46% 13% 42%
12	M	327	59% 7% 34%
13	P	229	69% 15% 16%
14	Q	74	82% 15%
15	R	199	73% 15% 11%
16	S	317	71% 16% 13%
17	T	562	80% 12% 7%
17	U	562	79% 14% 7%
17	V	562	80% 13% 7%
18	X	574	79% 15% 6%
18	Y	574	73% 17% 9%
18	Z	574	83% 10% 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 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	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

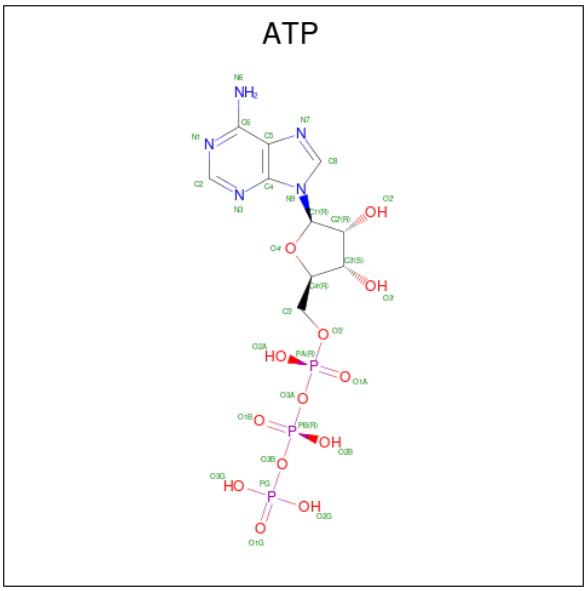
There are 6 discrepancies between the modelled and reference sequences:

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

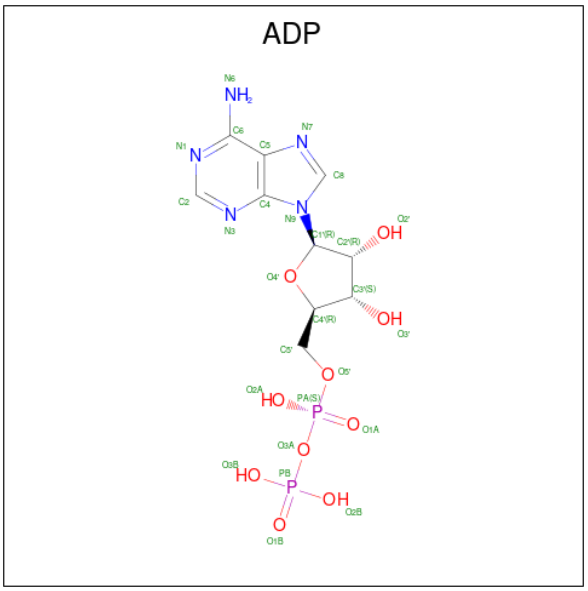


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

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



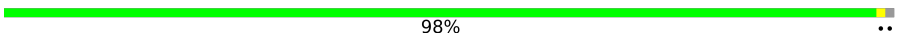
Mol	Chain	Residues	Atoms					AltConf
22	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

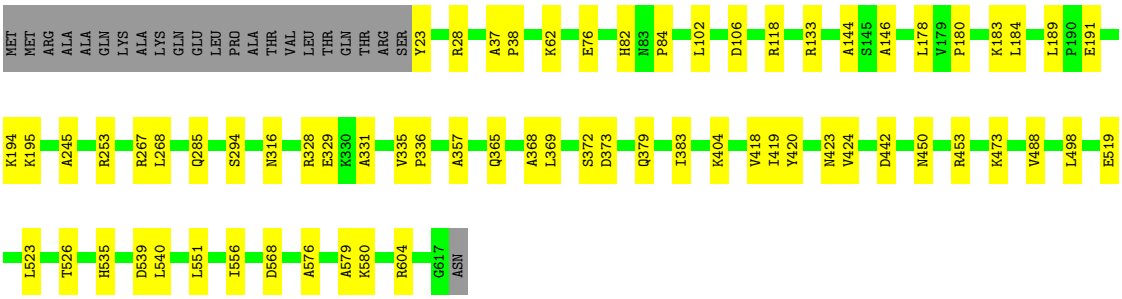
• Molecule 1: ASA-10: Polytomella F-ATP synthase associated subunit 10

Chain 0:



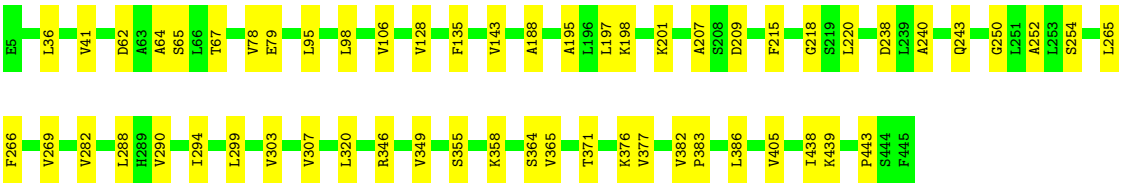
• Molecule 2: ATP synthase associated protein ASA1

Chain 1:



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

Chain 2:



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

Chain 3:

ALA LEU GLY ALA THR LYS LYS VAL VAL CYS GLY LEU ALA SER SER GLY P77 S78 Q79 V82 S83 N87 L110 F115 T116 S117 F121 F124 V132 V145 E162 A163 N164 T170 E173 L177 L178 Q179 S191 L195 D196 D197 V198 A199 D200

T203 N206 D217 T224 Y225 Y226 R233 A234 D235 L236 R242 S263 G321 ALA HIS GLY HIS

• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4: 89% 10%

ALA THR GLU PRO A5 V6 S7 K8 K9 E10 V11 L15 E40 S47 E48 L49 V63 L72 P73 L74 L92 P101 T118 V119 K120 D121 M124 V145 L154 F165 L178 P179 T182 I183 L184 S190 A196 D197 K198 V219 V292 A293

A294

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

Chain 5: 84% 15%

M1 P5 L26 D27 M35 R36 E37 H38 K39 W44 A47 Y51 L58 Y62 A70 V71 E78 K86 H91 L92 K119 P120 F123

• Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6: 69% 13% 18%

MET MET LEU ARG THR LEU THR ARG SER SER ALA VAL ALA GLY GLN ALA VAL ARG LEU PHE LYS THR SER ALA ALA ALA ALA E28 S31 V32 K37 E41 L51 A58 A59 P60 T73 K76 R89 Q93 S94 K95 L105 N106 V107 L108 R123 G142

L143 F146 S150 L151

• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7: 78% 14% 7%

MET SER SER VAL ARG ALA GLY VAL GLU ALA GLY ARG ARG ASP L15 L23 L31 A40 E47 V50 A57 Q60 A63 R67 I74 V79 A80 Y120 H123 P124 E125 D135 Y138 S155 N160 R165 H170 P171 A172 I173

T183 L187 Q190

• Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8: 82% 17%

MET V2 K9 D10 I11 L12 R13 T14 P15 H26 P27 F28 Q29 A36 L40 H44 R65 T82 P83 H89

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

Chain 9: 94% 6%

M1 A2 V3 T4 E12 G48 L53 N56 N97

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain A: 41% 17% 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 A58 I69 A70 L71

A72 G73 V74 G75 V80 S84 L85 I86 A90 R91 N92 I95 A96 K97 A108 E111 A114 L115 L119 L125 F126 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain B: 39% 20% 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 S59 V62

G63 A67 A70 L71 A72 G73 V74 V80 L85 I86 A90 R91 N92 P93 N94 I95 A96 K97 Q98 L99 I113 A114 L115 L118 V121 I124 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain C: 46% 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 I69 A70 L71 A72 G73

V74 L85 A90 R91 N92 L99 Y102 A103 E111 A114 L115 F116 S117 L118 L123 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

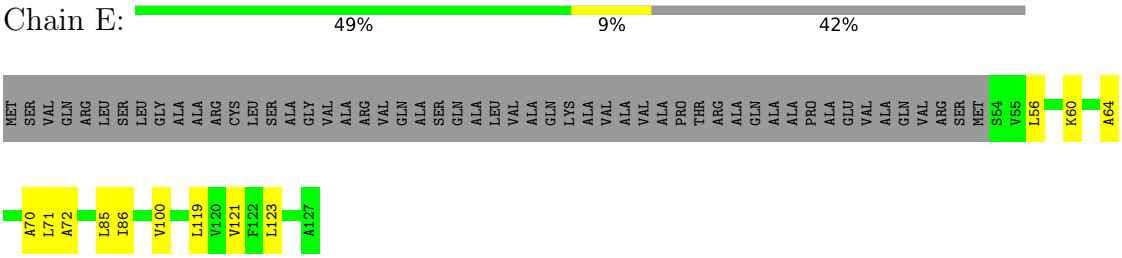
Chain D: 53% 6% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 A70 L71 A72 I86

N92 I113 L118 V121 A127

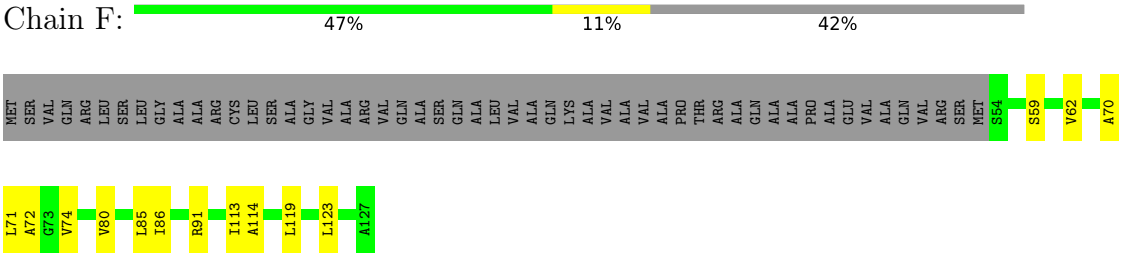
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain E:



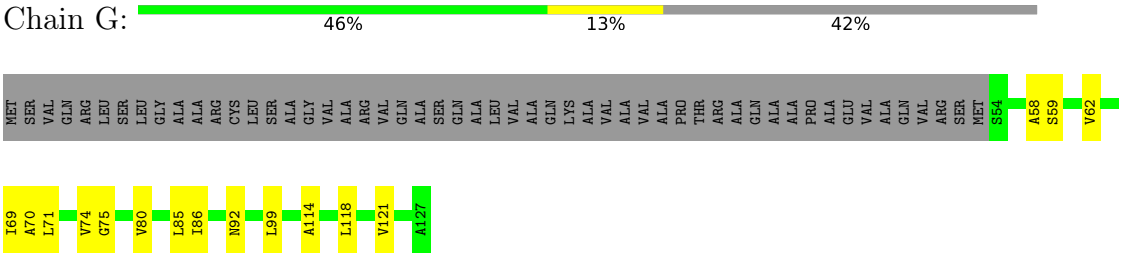
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain F:



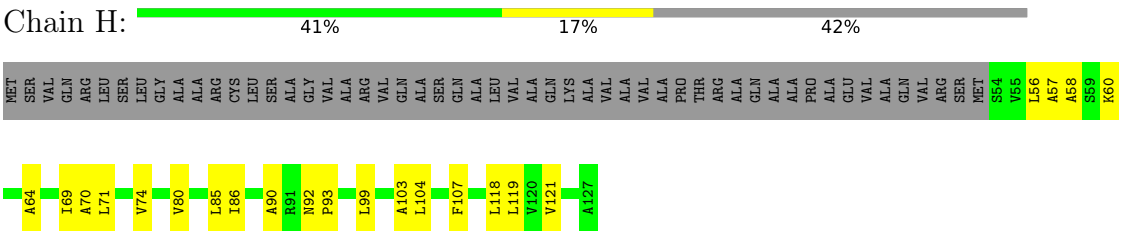
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain G:



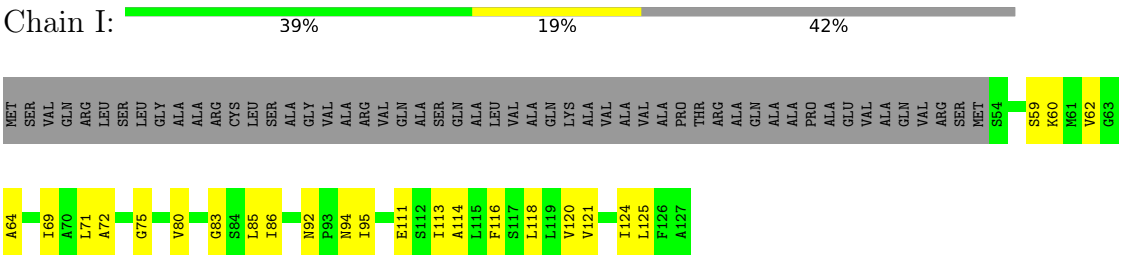
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain H:



• Molecule 11: Mitochondrial ATP synthase subunit c

Chain I:



• Molecule 11: Mitochondrial ATP synthase subunit c

Chain J: 46% 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 A70 L71 A72 G73 V74

V80 G83 S84 L85 I86 N92 P93 L99 A103 I113 A114 L123 I124 A127

• Molecule 12: Mitochondrial ATP synthase subunit 6

Chain M: 59% 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 ASN GLN THR MET ALA MET S95 T107 T111 K125 P126 D132 T153 A181 T200 G201 P205 GLY HIS PHE ILE PRO GLY GLY

THR PRO TRP PRO MET ALA F219 V234 V238 W241 L250 L251 P262 V271 F275 L281 L284 V285 L302 G308 N311 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 P40 L46 Q59 K69 F77 L87 V108 L109 K119 K120 L121 E136 N140

C154 T155 V156 I157 L162 L170 T171 A174 A180 G181 F182 K183 L184 V185 M186 Q187 E188 K189 K193 L194 L195 V199 I200 E201 R206 M209 S210 T211 V215 I229

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

Chain Q: 82% 15% •

MET CYS A3 P4 R10 L17 R18 K32 E33 P34 F35 K36 R48 Q49 Y52 K56 N74

• Molecule 15: Mitochondrial ATP synthase subunit delta

Chain R: 73% 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 F33 W37 L45 T55 K58 P71 V72 N73 F74 Y75 T76 P77 H78 K86 V90 G99 V116 E117 L118 E125 V136 N139 G140 V141

T142 D143 T144 T151 L152 D153 Q154 V155 E175 Q178 L191 V195 K198 A199

• Molecule 16: ATP synthase gamma chain, mitochondrial

Chain S: 71% 16% 13%

MET ALA LEU ARG LYS ALA VAL LEU SER LEU GLY LEU SER GLN GLY VAL ALA ALA GLU ALA VAL LEU GLY SER GLY MET PHE ASN ALA VAL GLN HIS GLU SER VAL ARG TYR ALA S39 R46 S66 N70 R79 F92 P93 A94 S97 N98 K99 S100 V101 C112

T120 K121 Y122 T123 L127 A128 T129 V138 V139 V140 D144 S148 Q149 L150 T151 R152 Q159 L160 A163 K167 E180 E181 L182 N186 P187 Q188 S189 Y190 F197 F203 K204 P205 I210 L211 L215 L216 E217 T224 G225 E238 R239 V242 D245

L246 L251 E261 S269 L314 M315 ASP GLU

- Molecule 17: ATP synthase subunit alpha

Chain T: 80% 12% 7%

MET ARG SER PRO ALA ALA PHE VAL ALA ARG SER GLY LEU PHE LYS ALA SER LEU GLY GLN SER ASN TRP ALA GLN LYS ALA GLU GLN MET MET ALA SER VAL THR ARG THR PHE ALA A40 L48 S55 K56 Y57 I67 V70 P79 V90 G91 D92 D112 L120

N121 D125 F132 I138 V151 T164 P170 I171 D172 V180 L202 Q219 R220 E221 A235 H241 R266 P297 F300 L301 Y304 R314 I323 D326 K329 R335 R343 R347 E348 A349 L357 R364 K370 T378

A379 F380 P381 V382 S400 D403 K415 R429 Y453 V456 A457 Y472 V473 L474 E475 R476 R479 P493 I494 E495 T498 V501 T505 V512 D516 A520 V528 A531 V532 F533 L554 A562

- Molecule 17: ATP synthase subunit alpha

Chain U: 79% 14% 7%

MET ARG SER PRO ALA ALA PHE VAL ALA ARG SER GLY LEU PHE LYS ALA SER LEU GLY GLN SER ASN TRP ALA GLN LYS ALA GLU GLN MET MET ALA SER VAL THR ARG THR PHE ALA A40 L45 Y57 L58 H61 V62 K65 L66 V70 Y77 L84 D92

E107 L108 D112 N121 S136 L143 R146 I150 V151 I155 G156 P157 L167 D172 G173 K174 V180 V198 L202 F203 T204 D210 R217 D226 K231 A235 A238 I239 N246 K251 V255 F300 P303 Y304 Y312 F313

R314 D315 T316 G317 K318 I323 D326 R335 L340 R347 E348 A349 L357 L361 R364 T378 A379 F380 P381 V382 V430 P437 Q441 V442 L446 E449 Q471 E475 R476 R479 Q497 V501 V512 R513 Q527 V532 I535

K541 L546 L550 K558 A562

- Molecule 17: ATP synthase subunit alpha

Chain V: 80% 13% 7%

MET ARG SER PRO ALA ALA PHE VAL ALA ARG SER GLY LEU PHE LYS ALA SER LEU GLY GLN SER ASN TRP ALA GLN LYS ALA GLU GLN MET MET ALA SER VAL THR ARG THR PHE ALA ALA ASP ALA K43 E47 L48 L66 E72 W73 E74 K75 L108 L122 D125

R146 T147 I150 V151 N152 V153 P154 I155 N179 R195 F203 K207 D210 D226 K231 T232 A235 Q242 K243 R266 A281 T291 Y304 S305 E311 Y312 F313 R314 I323 R335 E348 A349 L357 R360 E363 K367 L368

S376 F380 Q386 E411 K415 A443 L446 K447 Y453 L466 Q471 G477 E482 M483 L484 K485 Q486 Q497 A500 V501 Y502 F508 L509 I517 N529 T543 P544 A545 L546 D547 A548 H549 L550 K551 A562

• Molecule 18: ATP synthase subunit beta

Chain X: 79% 15% 6%

MET ALA LEU ARG TYR ALA ALA GLY LEU ALA LYS ASN VAL VAL GLN ARG GLN GLY ALA SER LEU ASN ILE ALA ARG ALA PHE ALA ALA GLU PRO ALA P33 D36 Q42 D49 L56 E66 N83 K101 P108 V111 L118 S142 P148 D168

P172 R175 G180 G184 A185 N199 R216 L223 E226 R239 G249 Q250 E253 R258 V261 T264 G265 L266 R273 V284 D285 N286 I287 F288 R289 E296 R303 S306 A307 V308 L321 I325 T326 T327 I333 T334 A338 V339

Y340 V341 P342 D348 P351 T354 L358 R366 I373 M386 K405 D415 L420 E424 S444 Q445 P446 F447 Q448 G458 K459 L463 V489 V495 K498 M502 A503 I506 R509 K516 V517 S518 D528 I534 E540

L545 D548 E557 L561 N562 E563 E564 P569 N574

• Molecule 18: ATP synthase subunit beta

Chain Y: 73% 17% 9%

MET ALA LEU ARG TYR ALA ALA GLY LEU ALA LYS ASN VAL VAL GLN ARG GLN GLY ALA SER LEU ASN ILE ALA ARG ALA PHE ALA ALA GLU PRO ALA PRO ALA ILE D36 Q42 Y43 I44 D49 F52 L56 Q78 H79 M80 G81 D82 N83 T84 K101 G116 R120

N123 E127 Q132 D136 S142 R145 E158 K165 V166 L170 R175 G180 G186 T190 I193 M194 E195 L196 I197 N198 N199 V200 A201 E215 R216 R225 E238 R239 G240 N241 G249 Q250 M251 N252 V261 L266 R273 E276

G277 Q278 N286 R289 F290 T291 Q292 A293 N294 L301 I304 P305 S306 A307 V308 L318 I325 T326 T327 S332 I333 T334 S335 V336 Q337 A338 V341 D344 D345 L346 T347 T354 L358 T361 R366 I373 A394 N398 I417 E424 L425

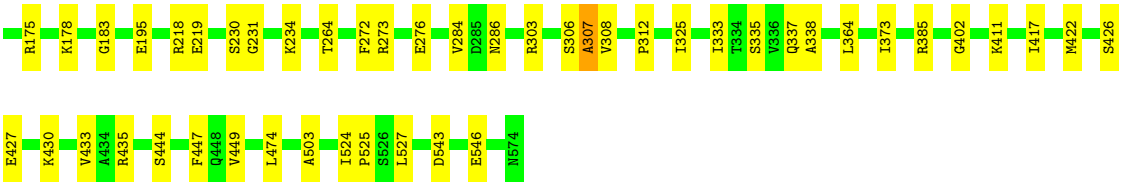
S444 Q445 Q448 G455 G458 K459 F470 L474 A485 F486 Y487 G490 D491 I492 K493 K498 A499 D500 K501 M502 A503 K504 S508 E511 D523 D528 V531 S555 S556 GLU THR VAL VAL LEU ASN GLU GLU GLY LYS SER VAL PRO LEU PRO LYS LYS

ASN

• Molecule 18: ATP synthase subunit beta

Chain Z: 83% 10% 6%

MET ALA LEU ARG TYR ALA ALA GLY LEU ALA LYS ASN VAL VAL GLN ARG GLN GLY ALA SER LEU ASN ILE ALA ARG ALA PHE ALA ALA GLU PRO ALA PRO ALA ILE ASP A37 Q42 D49 I59 V65 Q78 R86 L96 V97 R98 K110 V111 I140 E158


R175
K178
G183
E195
R218
E219
S230
G231
K234
T264
F272
R273
E276
V284
D285
N286
R303
S306
A307
V308
P312
I325
I333
T334
S335
V336
Q337
A338
L364
I373
R385
G402
K411
I417
M422
S426
E427
K430
V433
A434
R435
S444
F447
Q448
V449
L474
A503
I524
P525
S526
L527
D543
E546
N574

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112810	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	41.504	Depositor
Minimum map value	-23.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.038	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: ZN, MG, ATP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.47	0/628	0.49	0/856
2	1	0.47	0/4750	0.54	0/6434
3	2	0.38	0/3212	0.56	0/4371
4	3	0.44	0/1911	0.55	1/2601 (0.0%)
5	4	0.43	0/2216	0.52	0/3000
6	5	0.57	0/1011	0.62	0/1376
7	6	0.49	0/946	0.56	0/1287
8	7	0.52	0/1374	0.57	0/1865
9	8	0.52	0/715	0.60	0/974
10	9	0.38	0/802	0.52	0/1084
11	A	0.37	0/520	0.56	0/704
11	B	0.39	0/520	0.64	2/704 (0.3%)
11	C	0.35	0/519	0.61	0/701
11	D	0.32	0/520	0.58	0/704
11	E	0.32	0/520	0.63	0/704
11	F	0.34	0/520	0.55	0/704
11	G	0.35	0/520	0.56	0/704
11	H	0.35	0/520	0.66	0/704
11	I	0.33	0/520	0.60	0/704
11	J	0.35	0/520	0.56	1/704 (0.1%)
12	M	0.52	0/1683	0.62	0/2295
13	P	0.42	0/1553	0.60	1/2093 (0.0%)
14	Q	0.36	0/574	0.58	0/774
15	R	0.42	0/1336	0.57	1/1827 (0.1%)
16	S	0.42	0/2153	0.59	0/2901
17	T	0.55	0/4048	0.61	0/5481
17	U	0.59	0/4049	0.63	2/5481 (0.0%)
17	V	0.53	0/4031	0.61	0/5456
18	X	0.57	0/4176	0.61	1/5659 (0.0%)
18	Y	0.49	0/4015	0.58	0/5440
18	Z	0.53	0/4147	0.59	0/5619
All	All	0.49	0/54529	0.59	9/73911 (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
6	5	0	1
17	T	0	1
17	U	0	1
17	V	0	2
18	X	0	1
18	Y	0	4
18	Z	0	2
All	All	0	13

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	X	36	ASP	CB-CG-OD1	6.59	124.24	118.30
11	B	95	ILE	CG1-CB-CG2	-6.06	98.07	111.40
4	3	77	PRO	N-CA-CB	5.89	110.36	103.30
13	P	170	LEU	CA-CB-CG	5.49	127.92	115.30
11	J	123	LEU	CA-CB-CG	5.35	127.60	115.30
15	R	155	VAL	C-N-CA	-5.28	108.50	121.70
11	B	56	LEU	CA-CB-CG	5.11	127.05	115.30
17	U	347	ARG	C-N-CA	5.09	134.43	121.70
17	U	167	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	4	47	SER	Peptide
6	5	119	LYS	Peptide
17	T	348	GLU	Peptide
17	U	348	GLU	Peptide
17	V	348	GLU	Peptide
17	V	75	LYS	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Y	424	GLU	Peptide

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Mol	Chain	Res	Type	Group
18	Y	425	LEU	Peptide
18	Y	455	GLY	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	1	0
2	1	4661	0	4695	45	0
3	2	3163	0	3262	33	0
4	3	1874	0	1826	20	0
5	4	2177	0	2169	18	0
6	5	986	0	1021	18	0
7	6	926	0	941	17	0
8	7	1347	0	1345	24	0
9	8	692	0	694	11	0
10	9	776	0	757	5	0
11	A	514	0	554	23	0
11	B	514	0	554	22	0
11	C	514	0	553	17	0
11	D	514	0	554	11	0
11	E	514	0	554	9	0
11	F	514	0	554	12	0
11	G	514	0	554	15	0
11	H	514	0	554	20	0
11	I	514	0	554	24	0
11	J	514	0	554	19	0
12	M	1640	0	1665	17	0
13	P	1532	0	1603	38	0
14	Q	561	0	565	13	0
15	R	1303	0	1266	21	0
16	S	2130	0	2180	39	0
17	T	3979	0	4119	52	0
17	U	3980	0	4119	53	0
17	V	3962	0	4105	45	0
18	X	4115	0	4137	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	3957	0	3966	62	0
18	Z	4087	0	4110	35	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	1	0
20	V	31	0	12	1	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	X	1	0	0	0	0
21	Y	1	0	0	0	0
22	X	27	0	12	0	0
22	Y	27	0	12	2	0
All	All	53748	0	54728	643	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 (643) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:180:ALA:HB3	13:P:182:PHE:CD2	1.59	1.35
17:T:453:TYR:CE1	17:T:474:LEU:HD12	1.63	1.32
13:P:171:THR:HA	13:P:186:MET:HE1	1.23	1.17
13:P:180:ALA:CB	13:P:182:PHE:CE2	2.35	1.10
18:X:498:LYS:O	18:X:502:MET:HG3	1.52	1.09
13:P:180:ALA:HB3	13:P:182:PHE:CE2	1.88	1.09
13:P:154:CYS:HB2	13:P:184:LEU:HD11	1.35	1.05
13:P:171:THR:HA	13:P:186:MET:CE	1.89	1.02
13:P:180:ALA:CB	13:P:182:PHE:CD2	2.44	0.99
17:T:453:TYR:CE1	17:T:474:LEU:CD1	2.50	0.93
13:P:180:ALA:HB2	13:P:182:PHE:CE2	2.03	0.90
7:6:89:ARG:O	7:6:93:GLN:HB2	1.71	0.90
13:P:154:CYS:HB2	13:P:184:LEU:CD1	2.02	0.89
17:T:453:TYR:HE1	17:T:474:LEU:HD12	1.29	0.88
13:P:154:CYS:CB	13:P:184:LEU:HD11	2.04	0.86
13:P:180:ALA:HB2	13:P:182:PHE:HE2	1.44	0.80
18:X:498:LYS:O	18:X:502:MET:CG	2.29	0.80
11:C:111:GLU:OE1	11:D:113:ILE:HD11	1.87	0.75
18:X:327:THR:HG22	18:X:333:ILE:H	1.51	0.74
18:X:503:ALA:O	18:X:506:ILE:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:154:CYS:HB3	13:P:186:MET:HA	1.70	0.71
11:J:85:LEU:CD1	11:J:99:LEU:HB3	2.19	0.71
18:Y:498:LYS:O	18:Y:502:MET:HG3	1.89	0.71
17:V:335:ARG:HD2	17:V:349:ALA:HB3	1.74	0.70
2:1:316:ASN:HD21	2:1:331:ALA:H	1.36	0.70
17:T:400:SER:HB3	18:Y:289:ARG:HH22	1.57	0.68
11:G:86:ILE:HG21	11:H:85:LEU:HA	1.76	0.68
11:I:75:GLY:HA3	11:J:74:VAL:HG12	1.76	0.68
13:P:154:CYS:SG	13:P:184:LEU:HD11	2.34	0.67
17:U:335:ARG:HD2	17:U:349:ALA:HB3	1.78	0.66
11:F:86:ILE:HG21	11:G:85:LEU:HA	1.78	0.66
18:Y:142:SER:O	18:Y:145:ARG:NH2	2.28	0.65
2:1:180:PRO:HG2	2:1:183:LYS:HB3	1.78	0.65
11:A:95:ILE:HD13	11:J:93:PRO:HG3	1.78	0.65
17:T:335:ARG:HD2	17:T:349:ALA:HB3	1.78	0.64
18:X:266:LEU:HD21	18:X:325:ILE:HG12	1.79	0.64
18:Y:197:ILE:O	18:Y:201:ALA:HB3	1.97	0.64
11:J:74:VAL:HG21	11:J:114:ALA:HB2	1.78	0.64
18:X:118:LEU:O	18:X:239:ARG:NH2	2.31	0.64
8:7:123:HIS:HD2	8:7:125:GLU:H	1.46	0.64
2:1:404:LYS:HZ1	6:5:78:GLU:HB3	1.62	0.63
17:U:479:ARG:NH2	17:U:512:VAL:O	2.31	0.63
17:U:479:ARG:NH2	17:U:513:ARG:O	2.32	0.62
17:T:202:LEU:HD22	17:T:378:THR:HG21	1.81	0.61
14:Q:32:LYS:HE3	15:R:154:GLN:HA	1.83	0.61
17:U:347:ARG:NH2	18:X:348:ASP:OD2	2.31	0.61
18:Z:417:ILE:HG23	18:Z:422:MET:HA	1.82	0.61
17:U:226:ASP:O	17:U:231:LYS:NZ	2.33	0.61
18:Y:238:GLU:OE1	18:Y:241:ASN:ND2	2.33	0.61
16:S:123:THR:O	16:S:127:LEU:HB2	2.01	0.61
18:Y:80:MET:HB2	18:Y:84:THR:HG23	1.83	0.61
17:V:153:VAL:HG21	17:V:305:SER:HB2	1.82	0.61
18:X:42:GLN:HG2	18:X:49:ASP:HB2	1.82	0.61
16:S:66:SER:O	16:S:70:ASN:ND2	2.34	0.60
17:T:323:ILE:HG12	17:T:380:PHE:HB2	1.83	0.60
13:P:171:THR:HG23	13:P:186:MET:HE3	1.84	0.60
18:Y:158:GLU:HG3	18:Y:175:ARG:HB3	1.83	0.60
17:U:155:ILE:HD12	17:U:312:TYR:HB2	1.84	0.60
13:P:185:VAL:HG12	13:P:185:VAL:O	2.02	0.60
17:T:479:ARG:NH1	17:T:512:VAL:O	2.35	0.59
17:V:207:LYS:HG3	17:V:486:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:449:GLU:OE1	17:U:476:ARG:NH1	2.35	0.59
2:1:267:ARG:NH1	2:1:519:GLU:OE1	2.35	0.59
11:A:70:ALA:HA	11:J:72:ALA:HB2	1.85	0.59
13:P:180:ALA:HB3	13:P:182:PHE:HD2	1.52	0.59
17:V:266:ARG:HG2	17:V:291:THR:HG21	1.84	0.59
17:U:246:ASN:HD21	17:U:255:VAL:H	1.51	0.59
17:V:155:ILE:HD12	17:V:312:TYR:HB2	1.85	0.59
18:X:373:ILE:HG23	18:X:444:SER:HB3	1.85	0.59
5:4:190:SER:HB3	5:4:196:ALA:HB2	1.85	0.59
11:G:59:SER:HA	11:G:62:VAL:HG12	1.84	0.59
11:I:71:LEU:HD11	11:I:118:LEU:HD21	1.84	0.59
16:S:148:SER:O	16:S:152:ARG:NH2	2.36	0.58
11:I:111:GLU:O	11:I:114:ALA:N	2.36	0.58
12:M:200:THR:OG1	12:M:201:GLY:N	2.36	0.58
17:T:326:ASP:H	17:T:382:VAL:HB	1.69	0.58
16:S:120:THR:HG23	16:S:150:LEU:HD23	1.85	0.58
17:V:210:ASP:HB2	17:V:497:GLN:HE22	1.68	0.58
11:F:72:ALA:HB2	11:G:70:ALA:HA	1.86	0.58
11:J:85:LEU:HD22	11:J:103:ALA:HB2	1.86	0.58
2:1:450:ASN:OD1	2:1:453:ARG:NH2	2.37	0.57
18:Z:231:GLY:O	18:Z:234:LYS:NZ	2.36	0.57
11:A:80:VAL:HG21	11:J:80:VAL:HG12	1.85	0.57
11:C:111:GLU:CD	11:D:113:ILE:HD11	2.23	0.57
18:Y:266:LEU:HD21	18:Y:325:ILE:HG12	1.87	0.57
18:Z:218:ARG:NH2	18:Z:219:GLU:OE2	2.37	0.57
17:V:529:ASN:HD21	18:Z:527:LEU:HD23	1.68	0.57
3:2:128:VAL:HG21	3:2:143:VAL:HG11	1.86	0.57
13:P:157:ILE:HG23	13:P:199:VAL:HG13	1.85	0.57
17:T:235:ALA:HB1	17:T:323:ILE:HD13	1.86	0.57
11:A:71:LEU:HD12	11:B:113:ILE:HG23	1.87	0.57
11:G:74:VAL:HG11	11:G:114:ALA:HB2	1.86	0.57
18:Y:165:LYS:HE2	18:Y:445:GLN:HB2	1.86	0.57
11:A:75:GLY:HA3	11:B:74:VAL:HG12	1.86	0.57
17:T:314:ARG:NH1	17:T:364:ARG:O	2.38	0.57
11:I:72:ALA:HB2	11:J:70:ALA:HA	1.87	0.56
17:U:210:ASP:HB2	17:U:497:GLN:HE22	1.69	0.56
3:2:197:LEU:O	3:2:201:LYS:NZ	2.38	0.56
11:G:75:GLY:HA3	11:H:74:VAL:HG22	1.87	0.56
17:V:179:ASN:ND2	18:Z:546:GLU:OE2	2.38	0.56
2:1:368:ALA:O	2:1:379:GLN:NE2	2.36	0.56
5:4:118:THR:HG23	5:4:121:ASP:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:60:PRO:HB3	9:8:15:PRO:HB2	1.87	0.56
9:8:36:ALA:HA	9:8:40:LEU:HB3	1.88	0.56
11:A:80:VAL:HG12	11:B:80:VAL:HG21	1.87	0.56
15:R:151:THR:HG22	15:R:153:ASP:H	1.70	0.56
18:X:446:PRO:HB2	18:X:458:GLY:HA2	1.87	0.56
18:Y:306:SER:OG	18:Y:307:ALA:N	2.39	0.56
3:2:382:VAL:HG13	3:2:386:LEU:HB2	1.88	0.56
11:E:72:ALA:HB2	11:F:70:ALA:HA	1.88	0.56
16:S:46:ARG:NH1	18:X:415:ASP:OD1	2.39	0.56
18:X:216:ARG:O	18:X:250:GLN:NE2	2.39	0.56
14:Q:32:LYS:O	14:Q:36:LYS:N	2.39	0.56
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.87	0.56
8:7:165:ARG:NH2	8:7:171:PRO:O	2.38	0.56
17:T:266:ARG:NH1	18:X:148:PRO:O	2.38	0.56
17:V:311:GLU:OE2	17:V:314:ARG:NH1	2.39	0.56
16:S:188:GLN:HG3	16:S:215:LEU:HB3	1.87	0.55
11:G:80:VAL:HG12	11:H:80:VAL:HG11	1.87	0.55
18:X:253:GLU:O	18:X:258:ARG:NH1	2.39	0.55
2:1:76:GLU:OE2	2:1:133:ARG:NH2	2.39	0.55
4:3:83:SER:O	4:3:87:ASN:ND2	2.39	0.55
17:U:235:ALA:HB1	17:U:323:ILE:HG12	1.88	0.55
18:X:287:ILE:HD11	18:X:321:LEU:HD21	1.89	0.55
11:E:71:LEU:HD12	11:F:113:ILE:HG23	1.87	0.55
17:T:121:ASN:HB3	17:T:343:ARG:HH21	1.71	0.55
18:Y:216:ARG:O	18:Y:250:GLN:NE2	2.40	0.55
2:1:539:ASP:N	2:1:539:ASP:OD1	2.39	0.55
11:I:59:SER:HA	11:I:62:VAL:HG12	1.89	0.55
11:B:90:ALA:O	11:C:92:ASN:ND2	2.39	0.54
5:4:8:LYS:HD2	5:4:40:GLU:HG2	1.88	0.54
12:M:308:GLY:HA2	12:M:311:ASN:HB2	1.90	0.54
3:2:371:THR:HG22	3:2:376:LYS:HG2	1.90	0.54
17:V:549:HIS:HE1	18:Z:524:ILE:HB	1.73	0.54
18:Y:485:ALA:HA	18:Y:498:LYS:HD3	1.90	0.54
18:Z:325:ILE:HG21	18:Z:335:SER:HB2	1.89	0.54
13:P:87:LEU:HB2	17:U:66:LEU:HD21	1.89	0.54
18:X:185:ALA:O	18:X:366:ARG:NH2	2.41	0.54
3:2:364:SER:OG	3:2:365:VAL:N	2.41	0.54
16:S:79:ARG:NH2	16:S:197:PHE:O	2.40	0.54
8:7:40:ALA:HB3	8:7:47:GLU:HB2	1.89	0.53
17:U:84:LEU:HD13	18:X:563:GLU:HG2	1.90	0.53
17:V:235:ALA:HB1	17:V:323:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:544:PRO:HA	17:V:547:ASP:HB3	1.89	0.53
4:3:242:ARG:NH2	12:M:132:ASP:OD2	2.41	0.53
18:Y:52:PHE:HB2	18:Y:56:LEU:HD23	1.90	0.53
11:I:94:ASN:ND2	16:S:224:THR:O	2.41	0.53
18:Z:65:VAL:HG11	18:Z:96:LEU:HD11	1.89	0.53
11:H:57:ALA:HA	11:H:60:LYS:HG2	1.91	0.53
18:X:249:GLY:HA3	18:X:261:VAL:HG11	1.90	0.53
11:C:123:LEU:O	11:C:127:ALA:N	2.42	0.53
17:V:72:GLU:OE1	17:V:73:TRP:NE1	2.41	0.53
4:3:203:THR:HG21	4:3:235:ASP:HB2	1.90	0.53
11:E:56:LEU:O	11:E:60:LYS:NZ	2.42	0.53
18:Z:111:VAL:HG11	18:Z:264:THR:HG23	1.89	0.53
2:1:420:TYR:HB2	2:1:424:VAL:HG23	1.91	0.53
17:U:475:GLU:HB3	17:U:479:ARG:HH11	1.74	0.53
11:B:94:ASN:ND2	14:Q:4:PRO:O	2.42	0.53
15:R:33:PHE:O	15:R:37:TRP:HB2	2.09	0.53
18:Y:136:ASP:OD2	18:Y:239:ARG:NH2	2.42	0.53
4:3:79:GLN:HA	4:3:82:VAL:HB	1.90	0.52
5:4:178:LEU:HD11	8:7:183:THR:HG21	1.91	0.52
16:S:79:ARG:NE	16:S:261:GLU:OE2	2.41	0.52
2:1:245:ALA:HB1	2:1:498:LEU:HD13	1.92	0.52
2:1:329:GLU:HG3	7:6:123:ARG:HB2	1.90	0.52
4:3:116:THR:OG1	4:3:117:SER:N	2.43	0.52
11:E:85:LEU:HD11	11:E:100:VAL:HG22	1.90	0.52
17:T:531:ALA:HB1	18:Y:531:VAL:HG11	1.91	0.52
4:3:145:VAL:HG11	4:3:179:GLN:HE21	1.73	0.52
17:U:314:ARG:NH2	17:U:364:ARG:O	2.42	0.52
17:V:150:ILE:O	17:V:152:ASN:ND2	2.42	0.52
11:C:111:GLU:OE2	11:D:113:ILE:HD11	2.08	0.52
11:E:119:LEU:O	11:E:123:LEU:HB2	2.08	0.52
17:T:516:ASP:O	17:T:520:ALA:N	2.43	0.52
17:V:125:ASP:OD1	17:V:125:ASP:N	2.43	0.52
3:2:36:LEU:HD22	3:2:41:VAL:HG21	1.90	0.52
3:2:355:SER:O	3:2:358:LYS:NZ	2.42	0.52
4:3:235:ASP:OD1	4:3:235:ASP:N	2.41	0.52
17:U:303:PRO:HB2	17:U:361:LEU:HD11	1.90	0.52
11:H:86:ILE:HG21	11:I:85:LEU:HA	1.91	0.52
18:Y:123:ASN:HD22	18:Y:127:GLU:HB2	1.75	0.52
13:P:194:LEU:HD21	13:P:199:VAL:HG12	1.91	0.52
17:U:136:SER:HA	18:Z:59:ILE:HB	1.91	0.52
18:X:172:PRO:HG2	18:X:386:MET:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:86:ILE:HG21	11:J:85:LEU:HD13	1.91	0.52
17:T:304:TYR:OH	17:T:357:LEU:O	2.28	0.52
6:5:27:ASP:OD2	9:8:44:HIS:NE2	2.43	0.52
11:A:85:LEU:HA	11:J:86:ILE:HG21	1.93	0.52
11:A:69:ILE:HA	11:B:70:ALA:HB2	1.92	0.51
18:X:506:ILE:O	18:X:509:ARG:NH2	2.42	0.51
17:T:472:TYR:OH	17:T:476:ARG:NH1	2.44	0.51
11:C:69:ILE:HA	11:D:70:ALA:HB2	1.91	0.51
17:U:92:ASP:HB3	17:U:340:LEU:HD13	1.91	0.51
2:1:84:PRO:HG2	6:5:71:VAL:HG11	1.92	0.51
11:A:72:ALA:HB2	11:B:70:ALA:HA	1.91	0.51
13:P:155:THR:HA	13:P:187:GLN:HB3	1.92	0.51
17:T:121:ASN:HB2	18:Y:44:ILE:HG12	1.92	0.51
18:Y:78:GLN:NE2	18:Y:301:LEU:O	2.40	0.51
18:Y:286:ASN:H	18:Y:338:ALA:HB3	1.75	0.51
18:Y:394:ALA:O	18:Y:398:ASN:ND2	2.44	0.51
11:H:90:ALA:HA	11:I:95:ILE:HD11	1.91	0.51
11:I:86:ILE:HG21	11:J:85:LEU:CD1	2.40	0.51
15:R:55:THR:O	15:R:58:LYS:NZ	2.43	0.51
11:B:115:LEU:HD22	12:M:250:LEU:HD22	1.93	0.51
17:U:437:PRO:HB2	17:U:541:LYS:HB3	1.93	0.51
15:R:86:LYS:HG3	15:R:118:LEU:HD12	1.91	0.51
18:Y:448:GLN:HG2	18:Y:458:GLY:HA3	1.93	0.51
2:1:28:ARG:NH2	8:7:160:ASN:OD1	2.43	0.51
11:E:86:ILE:HG21	11:F:85:LEU:HA	1.93	0.51
11:H:64:ALA:HB1	11:H:121:VAL:HG13	1.93	0.51
17:U:107:GLU:HA	17:U:150:ILE:HA	1.93	0.51
6:5:86:LYS:NZ	8:7:135:ASP:OD1	2.45	0.50
8:7:170:HIS:CD2	8:7:172:ALA:H	2.28	0.50
6:5:5:PRO:O	9:8:65:ARG:NH1	2.43	0.50
17:V:508:PHE:HZ	17:V:551:LYS:HG3	1.75	0.50
18:X:175:ARG:O	18:X:334:THR:OG1	2.23	0.50
18:Z:426:SER:OG	18:Z:427:GLU:N	2.44	0.50
3:2:266:PHE:HA	3:2:269:VAL:HG22	1.93	0.50
9:8:26:HIS:HD2	9:8:28:PHE:H	1.59	0.50
18:X:111:VAL:HG11	18:X:264:THR:HG23	1.94	0.50
18:X:557:GLU:HG2	18:X:569:PRO:HB3	1.94	0.50
18:X:284:VAL:HG11	18:X:287:ILE:HD13	1.94	0.50
17:V:243:LYS:HG3	17:V:281:ALA:HA	1.93	0.50
18:X:286:ASN:HB3	18:X:289:ARG:HG2	1.93	0.50
17:T:347:ARG:HD2	18:Y:308:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:555:SER:OG	18:Y:556:SER:N	2.45	0.50
4:3:195:LEU:O	4:3:226:TYR:OH	2.26	0.49
17:T:90:VAL:HG21	17:T:138:ILE:HB	1.93	0.49
18:Z:230:SER:HB3	18:Z:449:VAL:HB	1.93	0.49
3:2:377:VAL:HG11	3:2:438:ILE:HG23	1.94	0.49
11:C:111:GLU:OE1	11:D:113:ILE:CD1	2.60	0.49
5:4:63:VAL:HA	5:4:92:LEU:HD11	1.93	0.49
16:S:92:PHE:HB2	16:S:211:LEU:HD11	1.93	0.49
16:S:97:SER:OG	16:S:99:LYS:O	2.29	0.49
16:S:190:TYR:HB2	16:S:210:ILE:HB	1.94	0.49
17:T:151:VAL:HG11	17:T:301:LEU:HD21	1.94	0.49
5:4:6:VAL:HB	5:4:10:GLU:HB3	1.93	0.49
18:X:184:GLY:O	18:X:366:ARG:NH2	2.45	0.49
4:3:173:GLU:HA	4:3:206:ASN:HD21	1.77	0.49
13:P:69:LYS:NZ	17:U:57:TYR:OH	2.45	0.49
17:T:403:ASP:O	17:T:429:ARG:NH2	2.36	0.49
18:X:286:ASN:H	18:X:338:ALA:HB3	1.77	0.49
3:2:299:LEU:HD13	3:2:303:VAL:HG12	1.94	0.49
17:V:226:ASP:O	17:V:231:LYS:NZ	2.44	0.49
18:Z:195:GLU:HG3	18:Z:447:PHE:CG	2.48	0.49
17:V:47:GLU:HG2	17:V:48:LEU:HG	1.94	0.49
18:Y:42:GLN:HB3	18:Y:49:ASP:HB2	1.95	0.49
3:2:64:ALA:HB3	8:7:31:LEU:HD21	1.95	0.49
3:2:209:ASP:OD1	8:7:67:ARG:NH2	2.43	0.49
10:9:53:LEU:HD12	12:M:262:PRO:HB2	1.95	0.49
17:U:471:GLN:HE21	17:U:475:GLU:HG2	1.77	0.49
18:Y:318:LEU:HD21	18:Y:354:THR:HB	1.95	0.49
7:6:108:LEU:HD11	12:M:281:LEU:HD13	1.95	0.49
11:F:86:ILE:HG23	11:G:99:LEU:HD22	1.94	0.49
13:P:136:GLU:HG2	17:U:45:LEU:HD21	1.95	0.49
14:Q:48:ARG:HE	16:S:163:ALA:HB3	1.78	0.49
18:X:420:LEU:HD13	18:X:424:GLU:HG2	1.94	0.49
11:A:119:LEU:HD21	12:M:234:VAL:HG11	1.94	0.48
18:X:168:ASP:HB3	18:X:463:LEU:HD13	1.95	0.48
18:Z:178:LYS:HG3	18:Z:335:SER:HB3	1.95	0.48
18:Z:183:GLY:HA2	18:Z:364:LEU:HB2	1.95	0.48
18:Z:284:VAL:HB	18:Z:337:GLN:HG2	1.94	0.48
5:4:74:LEU:HD23	5:4:219:VAL:HG13	1.94	0.48
11:C:90:ALA:O	11:D:92:ASN:ND2	2.46	0.48
13:P:195:LEU:O	13:P:211:THR:OG1	2.31	0.48
17:T:241:HIS:CE1	17:T:493:PRO:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:457:ALA:HB2	17:T:474:LEU:HD13	1.95	0.48
17:U:535:ILE:HD13	18:X:534:ILE:HD11	1.95	0.48
17:V:203:PHE:O	17:V:242:GLN:NE2	2.35	0.48
3:2:240:ALA:H	3:2:243:GLN:HE21	1.61	0.48
9:8:9:LYS:NZ	9:8:10:ASP:OD2	2.44	0.48
11:A:115:LEU:HD22	12:M:238:VAL:HG12	1.95	0.48
11:B:92:ASN:OD1	11:B:92:ASN:N	2.46	0.48
18:X:185:ALA:HB2	18:X:340:TYR:HE1	1.77	0.48
11:G:86:ILE:HG23	11:H:99:LEU:HG	1.95	0.48
17:U:316:THR:OG1	17:U:318:LYS:NZ	2.45	0.48
17:V:314:ARG:HH21	17:V:368:LEU:HD21	1.78	0.48
18:Y:335:SER:OG	18:Y:337:GLN:NE2	2.45	0.48
2:1:253:ARG:HD3	2:1:369:LEU:HB3	1.95	0.48
2:1:365:GLN:HG2	2:1:383:ILE:HD12	1.95	0.48
3:2:282:VAL:HG21	5:4:15:LEU:HD22	1.95	0.48
4:3:199:ALA:HA	4:3:236:LEU:HD13	1.95	0.48
11:A:111:GLU:HG3	11:B:113:ILE:HD11	1.95	0.48
16:S:140:VAL:HG22	16:S:160:LEU:HB3	1.96	0.48
17:U:475:GLU:OE1	17:U:479:ARG:NH1	2.46	0.48
2:1:372:SER:OG	2:1:373:ASP:N	2.45	0.48
10:9:3:VAL:HG23	10:9:4:THR:HG23	1.95	0.48
11:C:74:VAL:HG21	11:C:114:ALA:HB2	1.96	0.48
11:I:92:ASN:OD1	11:I:92:ASN:N	2.46	0.48
17:U:204:THR:HG23	17:U:238:ALA:HB2	1.95	0.48
18:X:180:GLY:HA3	18:X:358:LEU:HD13	1.96	0.48
2:1:285:GLN:NE2	2:1:294:SER:OG	2.47	0.48
6:5:26:LEU:HD21	12:M:153:THR:HG23	1.95	0.48
15:R:90:VAL:HB	15:R:117:GLU:HB2	1.96	0.48
18:X:258:ARG:NH2	18:X:296:GLU:OE1	2.47	0.48
18:Z:373:ILE:HG23	18:Z:444:SER:HB3	1.96	0.48
3:2:439:LYS:HD3	3:2:443:PRO:HA	1.94	0.48
6:5:91:HIS:ND1	8:7:138:TYR:OH	2.33	0.48
12:M:271:VAL:O	12:M:275:PHE:HB2	2.13	0.48
3:2:67:THR:HG22	3:2:106:VAL:HG23	1.96	0.48
4:3:200:ASP:OD1	4:3:233:ARG:NH1	2.42	0.48
13:P:201:GLU:OE2	13:P:206:ARG:NE	2.42	0.48
17:T:55:SER:O	17:T:57:TYR:N	2.45	0.48
9:8:26:HIS:CD2	9:8:28:PHE:H	2.32	0.47
11:F:91:ARG:O	15:R:99:GLY:N	2.46	0.47
16:S:211:LEU:HB2	16:S:217:GLU:HB2	1.95	0.47
17:V:367:LYS:HD2	17:V:376:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:466:LEU:HG	17:V:471:GLN:HG3	1.96	0.47
17:V:509:LEU:HD23	17:V:517:ILE:HG23	1.95	0.47
18:Y:327:THR:HA	18:Y:332:SER:HA	1.95	0.47
11:H:93:PRO:HG3	11:I:95:ILE:HD13	1.95	0.47
17:T:164:THR:HA	17:T:170:PRO:HA	1.96	0.47
17:V:545:ALA:HA	18:Z:524:ILE:HG22	1.96	0.47
5:4:145:VAL:HG21	5:4:165:PHE:HA	1.96	0.47
17:T:456:VAL:HG21	17:T:473:VAL:HG23	1.96	0.47
17:V:323:ILE:HG12	17:V:380:PHE:HB2	1.95	0.47
3:2:215:PHE:HA	3:2:250:GLY:HA3	1.95	0.47
11:B:86:ILE:HG23	11:C:99:LEU:HB3	1.96	0.47
17:U:146:ARG:HG2	18:X:561:LEU:HD12	1.96	0.47
18:Y:166:VAL:HG23	18:Y:170:LEU:HD12	1.95	0.47
3:2:95:LEU:HD12	3:2:98:LEU:HD12	1.95	0.47
6:5:47:ALA:O	6:5:51:TYR:HB2	2.14	0.47
11:A:92:ASN:N	11:A:92:ASN:OD1	2.48	0.47
14:Q:32:LYS:HG2	14:Q:34:PRO:HD2	1.96	0.47
17:T:498:THR:HA	17:T:501:VAL:HG12	1.96	0.47
17:U:62:VAL:O	17:U:66:LEU:N	2.47	0.47
18:Y:249:GLY:HA3	18:Y:261:VAL:HG11	1.97	0.47
18:Z:195:GLU:HG2	18:Z:449:VAL:HG22	1.96	0.47
2:1:191:GLU:HA	2:1:194:LYS:HG2	1.95	0.47
2:1:568:ASP:HB2	2:1:580:LYS:HE3	1.97	0.47
3:2:290:VAL:HG22	3:2:405:VAL:HG21	1.97	0.47
8:7:50:VAL:HG23	8:7:57:ALA:HB3	1.97	0.47
15:R:195:VAL:HA	15:R:198:LYS:HZ3	1.80	0.47
17:U:121:ASN:OD1	17:U:121:ASN:N	2.45	0.47
18:X:199:ASN:HD21	18:X:448:GLN:HE22	1.62	0.47
18:Z:402:GLY:HA3	18:Z:474:LEU:HD21	1.95	0.47
11:C:116:PHE:HZ	12:M:284:LEU:HD21	1.80	0.47
17:U:198:VAL:HG22	17:U:430:VAL:HG12	1.96	0.47
11:H:58:ALA:HB1	11:I:59:SER:HB2	1.97	0.47
14:Q:49:GLN:HB2	16:S:160:LEU:HD11	1.97	0.47
18:Y:165:LYS:NZ	18:Y:490:GLY:O	2.39	0.47
4:3:132:VAL:O	4:3:164:ASN:ND2	2.47	0.47
13:P:40:PRO:O	13:P:59:GLN:NE2	2.47	0.47
13:P:77:PHE:HZ	13:P:109:LEU:HD11	1.80	0.47
2:1:418:VAL:HG23	2:1:419:ILE:HG13	1.96	0.46
11:B:71:LEU:HD11	11:B:118:LEU:HD21	1.97	0.46
11:C:72:ALA:HB2	11:D:70:ALA:HA	1.96	0.46
11:I:80:VAL:HG12	11:J:80:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:209:MET:CE	17:T:79:PRO:HD2	2.45	0.46
17:U:527:GLN:OE1	17:U:558:LYS:N	2.45	0.46
18:X:528:ASP:OD2	18:X:528:ASP:N	2.49	0.46
18:Y:344:ASP:OD1	18:Y:366:ARG:NH1	2.45	0.46
5:4:101:PRO:HG3	8:7:170:HIS:CD2	2.50	0.46
18:Z:286:ASN:H	18:Z:338:ALA:HB3	1.80	0.46
11:G:58:ALA:HB2	11:H:56:LEU:HD23	1.97	0.46
18:Y:290:PHE:O	18:Y:294:ASN:ND2	2.49	0.46
12:M:251:LEU:HD21	12:M:285:VAL:HG22	1.96	0.46
13:P:109:LEU:HD23	13:P:119:LYS:HA	1.97	0.46
13:P:121:LEU:HD13	17:V:66:LEU:HD11	1.98	0.46
2:1:556:ILE:HG21	6:5:36:ARG:HA	1.97	0.46
5:4:120:LYS:HE2	5:4:124:ASN:HD21	1.80	0.46
7:6:143:LEU:HD12	7:6:143:LEU:HA	1.77	0.46
11:I:83:GLY:O	11:J:84:SER:OG	2.34	0.46
16:S:242:VAL:O	16:S:246:LEU:HB2	2.15	0.46
17:T:415:LYS:O	18:X:405:LYS:NZ	2.45	0.46
17:T:516:ASP:OD1	17:T:516:ASP:N	2.48	0.46
17:V:549:HIS:NE2	18:Z:525:PRO:O	2.48	0.46
11:A:90:ALA:O	11:B:92:ASN:ND2	2.39	0.46
15:R:33:PHE:HD2	16:S:94:ALA:HB2	1.80	0.46
17:T:67:ILE:HA	17:T:70:VAL:HG12	1.96	0.46
17:T:453:TYR:CZ	17:T:474:LEU:HD12	2.39	0.46
17:U:441:GLN:HE22	17:U:541:LYS:HD3	1.80	0.46
18:Y:487:TYR:O	18:Y:498:LYS:NZ	2.48	0.46
2:1:604:ARG:NH2	4:3:196:ASP:OD2	2.49	0.46
15:R:58:LYS:O	15:R:139:ASN:ND2	2.48	0.46
17:U:446:LEU:HD22	17:U:501:VAL:HG21	1.98	0.46
18:Y:289:ARG:NH1	18:Y:292:GLN:OE1	2.43	0.46
3:2:128:VAL:HG22	3:2:135:PHE:HE2	1.81	0.46
11:I:118:LEU:HA	11:I:121:VAL:HG22	1.97	0.46
18:Y:180:GLY:HA3	18:Y:358:LEU:HD13	1.97	0.46
18:Z:158:GLU:OE2	18:Z:175:ARG:NH1	2.49	0.46
3:2:195:ALA:HA	3:2:198:LYS:HE3	1.97	0.46
4:3:177:LEU:HD22	4:3:198:VAL:HG22	1.98	0.46
2:1:568:ASP:OD2	6:5:38:HIS:NE2	2.47	0.46
8:7:23:LEU:HD12	8:7:63:ALA:HA	1.98	0.46
11:C:85:LEU:HD13	11:C:103:ALA:HB2	1.98	0.46
13:P:184:LEU:HG	13:P:186:MET:HG3	1.98	0.46
16:S:101:VAL:HG11	16:S:182:LEU:HD22	1.98	0.46
17:T:429:ARG:NH1	22:Y:601:ADP:O2B	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:445:GLN:NE2	18:Y:459:LYS:O	2.48	0.46
3:2:218:GLY:HA2	3:2:254:SER:HB2	1.98	0.45
11:A:84:SER:OG	11:J:83:GLY:O	2.29	0.45
15:R:71:PRO:HG2	15:R:141:VAL:HG12	1.98	0.45
17:U:202:LEU:HD22	17:U:378:THR:HG21	1.98	0.45
4:3:121:PHE:HA	4:3:124:PHE:HB2	1.99	0.45
17:T:241:HIS:HE1	17:T:493:PRO:HA	1.80	0.45
17:U:532:VAL:HG21	17:U:550:LEU:HD13	1.98	0.45
18:Y:195:GLU:O	18:Y:199:ASN:HB2	2.16	0.45
11:J:85:LEU:HD22	11:J:103:ALA:CB	2.47	0.45
16:S:210:ILE:HD13	16:S:251:LEU:HA	1.98	0.45
16:S:314:LEU:HD12	18:Y:304:ILE:HG22	1.97	0.45
18:Y:528:ASP:HA	18:Y:531:VAL:HG22	1.97	0.45
2:1:118:ARG:HH21	6:5:70:ALA:HB2	1.81	0.45
18:Y:273:ARG:HD3	18:Y:333:ILE:HG13	1.98	0.45
18:Y:358:LEU:HB2	18:Y:361:THR:HG22	1.99	0.45
5:4:8:LYS:HA	5:4:11:VAL:HG12	1.98	0.45
11:H:85:LEU:HD13	11:H:103:ALA:HB2	1.98	0.45
17:V:122:LEU:HB3	18:Z:98:ARG:HD3	1.98	0.45
18:Y:186:GLY:HA2	22:Y:601:ADP:H5'1	1.98	0.45
2:1:267:ARG:NE	7:6:150:SER:O	2.43	0.45
10:9:56:ASN:OD1	10:9:56:ASN:N	2.50	0.45
11:B:72:ALA:HB2	11:C:70:ALA:HA	1.99	0.45
11:F:80:VAL:HG12	11:G:80:VAL:HG21	1.98	0.45
17:T:112:ASP:OD1	17:T:112:ASP:N	2.49	0.45
17:U:84:LEU:HD23	17:U:143:LEU:HD12	1.99	0.45
17:V:232:THR:OG1	20:V:1001:ATP:O2B	2.34	0.45
18:X:341:VAL:HA	18:X:342:PRO:HD3	1.78	0.45
18:Y:508:SER:OG	18:Y:511:GLU:OE1	2.34	0.45
2:1:189:LEU:HD12	2:1:189:LEU:HA	1.88	0.45
2:1:576:ALA:HB1	2:1:579:ALA:HB3	1.99	0.45
13:P:46:LEU:HD13	13:P:140:ASN:HB3	1.99	0.45
1:0:62:PRO:HG2	7:6:95:LYS:HD3	1.98	0.45
11:B:93:PRO:HA	11:B:96:ALA:HB2	1.99	0.45
11:G:71:LEU:HB2	11:H:70:ALA:HB1	1.98	0.45
17:U:323:ILE:HG13	17:U:380:PHE:HB2	1.98	0.45
5:4:49:LEU:HD21	13:P:215:VAL:HG22	1.99	0.44
5:4:184:LEU:HD21	8:7:187:LEU:HB2	1.99	0.44
11:D:118:LEU:HA	11:D:121:VAL:HB	1.99	0.44
11:F:119:LEU:HG	11:F:123:LEU:HD12	1.98	0.44
13:P:174:ALA:HB3	13:P:186:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:523:ASP:N	18:Y:523:ASP:OD1	2.51	0.44
2:1:184:LEU:HG	2:1:488:VAL:HG21	1.99	0.44
14:Q:52:TYR:N	16:S:159:GLN:O	2.43	0.44
16:S:167:LYS:HE2	16:S:167:LYS:HB3	1.85	0.44
17:T:92:ASP:OD1	18:X:303:ARG:NH2	2.50	0.44
17:U:108:LEU:HG	17:U:151:VAL:HA	1.99	0.44
18:Y:252:ASN:OD1	18:Y:252:ASN:N	2.46	0.44
2:1:62:LYS:HD2	2:1:144:ALA:HB3	1.99	0.44
2:1:102:LEU:HD12	2:1:106:ASP:HB3	1.99	0.44
2:1:523:LEU:HA	2:1:526:THR:HG22	1.99	0.44
18:Z:273:ARG:HD3	18:Z:333:ILE:HG13	1.98	0.44
8:7:47:GLU:OE1	8:7:60:GLN:NE2	2.46	0.44
11:D:72:ALA:HB2	11:E:70:ALA:HA	2.00	0.44
11:J:92:ASN:OD1	11:J:92:ASN:N	2.50	0.44
17:V:357:LEU:HA	17:V:360:ARG:HH11	1.82	0.44
18:X:562:ASN:ND2	18:X:564:GLU:OE1	2.50	0.44
18:Z:42:GLN:HB2	18:Z:49:ASP:HB2	1.98	0.44
3:2:78:VAL:HA	8:7:74:ILE:HB	1.99	0.44
5:4:292:VAL:HG22	17:T:48:LEU:HD12	2.00	0.44
8:7:79:VAL:HG13	17:T:48:LEU:HB3	2.00	0.44
11:G:92:ASN:OD1	11:G:92:ASN:N	2.46	0.44
14:Q:17:LEU:HD23	14:Q:17:LEU:HA	1.89	0.44
3:2:188:ALA:HB2	3:2:220:LEU:HD22	2.00	0.44
17:V:386:GLN:HB3	18:Y:347:THR:HB	1.99	0.44
3:2:62:ASP:OD1	3:2:62:ASP:N	2.46	0.44
16:S:112:CYS:O	16:S:269:SER:OG	2.26	0.44
17:T:476:ARG:NH2	17:T:505:THR:O	2.50	0.44
18:Y:116:GLY:HA3	18:Y:136:ASP:HB2	2.00	0.44
2:1:328:ARG:NH1	10:9:12:GLU:OE1	2.51	0.44
17:V:304:TYR:OH	17:V:357:LEU:O	2.34	0.44
17:U:172:ASP:OD1	17:U:172:ASP:N	2.51	0.44
18:X:273:ARG:HD3	18:X:333:ILE:HG13	2.00	0.44
18:X:516:LYS:HE2	18:X:518:SER:HB2	2.00	0.44
18:Y:286:ASN:HB3	18:Y:289:ARG:HG2	1.98	0.44
7:6:37:LYS:O	7:6:41:GLU:HG2	2.18	0.43
17:T:453:TYR:CZ	17:T:474:LEU:CD1	2.99	0.43
17:T:132:PHE:HE1	17:T:297:PRO:HB2	1.83	0.43
18:Y:215:GLU:OE1	18:Y:286:ASN:ND2	2.47	0.43
18:Y:470:PHE:O	18:Y:474:LEU:HB2	2.18	0.43
18:Z:78:GLN:HG3	18:Z:86:ARG:HB3	2.00	0.43
4:3:110:LEU:HB3	4:3:115:PHE:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:173:ILE:HD12	8:7:173:ILE:HA	1.88	0.43
11:A:91:ARG:NH1	16:S:238:GLU:OE1	2.46	0.43
18:Y:120:ARG:NH1	18:Y:132:GLN:O	2.51	0.43
11:H:104:LEU:HA	11:H:107:PHE:HB3	1.99	0.43
2:1:23:TYR:O	8:7:155:SER:OG	2.36	0.43
17:T:172:ASP:OD2	17:T:172:ASP:N	2.46	0.43
17:V:195:ARG:NH2	17:V:363:GLU:O	2.51	0.43
18:Y:276:GLU:OE1	18:Y:278:GLN:NE2	2.52	0.43
18:Y:361:THR:O	18:Y:361:THR:OG1	2.36	0.43
2:1:420:TYR:OH	2:1:442:ASP:OD2	2.28	0.43
17:U:239:ILE:HD11	17:U:323:ILE:HD13	2.00	0.43
2:1:195:LYS:HD2	2:1:195:LYS:HA	1.73	0.43
4:3:217:ASP:N	4:3:217:ASP:OD1	2.51	0.43
7:6:105:LEU:HA	7:6:105:LEU:HD23	1.75	0.43
9:8:11:ILE:HG22	9:8:12:LEU:HG	2.01	0.43
11:B:63:GLY:O	11:B:67:ALA:N	2.52	0.43
11:B:97:LYS:NZ	11:C:102:TYR:OH	2.35	0.43
11:E:64:ALA:HB1	11:E:121:VAL:HG13	2.01	0.43
11:F:71:LEU:HA	11:F:74:VAL:HG22	2.01	0.43
15:R:136:VAL:HG22	15:R:142:THR:HG22	2.01	0.43
2:1:268:LEU:HD22	2:1:357:ALA:HB1	2.00	0.43
3:2:207:ALA:HB3	3:2:238:ASP:HB3	2.00	0.43
9:8:26:HIS:HB3	9:8:29:GLN:HG3	2.01	0.43
11:H:92:ASN:N	11:H:92:ASN:OD1	2.51	0.43
15:R:37:TRP:HD1	16:S:129:THR:HG1	1.65	0.43
17:T:120:LEU:HD23	17:T:120:LEU:HA	1.79	0.43
17:T:125:ASP:OD1	17:T:125:ASP:N	2.40	0.43
17:T:220:ARG:H	17:T:220:ARG:HG2	1.65	0.43
17:V:483:MET:HE3	17:V:500:ALA:HB1	2.00	0.43
18:Y:500:ASP:O	18:Y:504:LYS:HG3	2.19	0.43
3:2:79:GLU:OE1	8:7:15:LEU:N	2.51	0.42
17:U:92:ASP:OD1	18:Z:303:ARG:NH2	2.43	0.42
18:X:66:GLU:HG3	18:X:101:LYS:HD3	2.01	0.42
11:A:86:ILE:HG21	11:B:85:LEU:HA	2.00	0.42
13:P:157:ILE:HB	13:P:189:LYS:HB2	2.01	0.42
14:Q:32:LYS:N	15:R:154:GLN:O	2.49	0.42
17:T:528:VAL:HG21	17:T:554:LEU:HD23	2.01	0.42
18:X:445:GLN:NE2	18:X:459:LYS:O	2.49	0.42
3:2:62:ASP:OD1	3:2:65:SER:OG	2.32	0.42
11:F:59:SER:HA	11:F:62:VAL:HG12	2.00	0.42
16:S:186:ASN:OD1	16:S:186:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:447:LYS:HE2	17:V:447:LYS:HB3	1.91	0.42
18:Z:272:PHE:HD1	18:Z:276:GLU:HG3	1.85	0.42
14:Q:48:ARG:NH1	16:S:144:ASP:OD1	2.52	0.42
17:U:304:TYR:OH	17:U:357:LEU:O	2.34	0.42
11:H:118:LEU:HD22	11:I:120:VAL:HG21	2.00	0.42
14:Q:10:ARG:NH2	16:S:245:ASP:OD1	2.50	0.42
15:R:76:THR:HG22	15:R:78:HIS:H	1.85	0.42
17:U:217:ARG:O	17:U:378:THR:OG1	2.36	0.42
17:V:543:THR:HG23	17:V:546:LEU:H	1.84	0.42
3:2:252:ALA:HB1	3:2:294:ILE:HB	2.00	0.42
5:4:179:PRO:HB2	5:4:182:THR:HG22	2.02	0.42
6:5:51:TYR:HE2	7:6:143:LEU:HD13	1.85	0.42
6:5:62:TYR:OH	7:6:146:PHE:O	2.27	0.42
18:Y:225:ARG:HA	18:Y:225:ARG:HD3	1.82	0.42
2:1:535:HIS:HB3	2:1:540:LEU:HB2	2.01	0.42
11:A:108:ALA:HB1	12:M:302:LEU:HD11	2.01	0.42
16:S:98:ASN:HB3	16:S:188:GLN:HE21	1.85	0.42
17:V:411:GLU:HG2	17:V:415:LYS:HE3	2.00	0.42
2:1:178:LEU:HD23	2:1:178:LEU:HA	1.88	0.42
4:3:224:THR:HG21	4:3:263:SER:HB2	2.01	0.42
8:7:170:HIS:HD2	8:7:172:ALA:H	1.65	0.42
17:U:251:LYS:HB2	18:X:540:GLU:HB2	2.00	0.42
18:Z:306:SER:HB3	18:Z:312:PRO:HA	2.01	0.42
5:4:118:THR:HA	5:4:154:LEU:HA	2.01	0.42
17:V:453:TYR:CG	17:V:477:GLY:HA3	2.54	0.42
4:3:162:GLU:OE2	4:3:191:SER:OG	2.31	0.42
11:A:74:VAL:HG11	11:A:114:ALA:HB2	2.02	0.42
15:R:175:GLU:HA	15:R:178:GLN:HB3	2.02	0.42
17:U:58:LEU:HA	17:U:61:HIS:HB3	2.02	0.42
18:Y:341:VAL:HG11	18:Y:346:LEU:HD23	2.02	0.42
5:4:72:LEU:HB3	5:4:74:LEU:HG	2.02	0.41
9:8:82:THR:HA	9:8:83:PRO:HD3	1.91	0.41
11:A:86:ILE:HG23	11:B:99:LEU:HB3	2.01	0.41
14:Q:18:ARG:NE	16:S:180:GLU:OE1	2.53	0.41
17:T:219:GLN:NE2	17:T:221:GLU:OE1	2.53	0.41
17:U:326:ASP:H	17:U:382:VAL:HB	1.83	0.41
3:2:346:ARG:HA	3:2:349:VAL:HG22	2.01	0.41
6:5:35:MET:O	6:5:39:LYS:HB2	2.21	0.41
11:G:69:ILE:HA	11:H:70:ALA:HB2	2.02	0.41
15:R:116:VAL:HG11	15:R:144:ILE:HD13	2.02	0.41
17:V:311:GLU:HG2	17:V:314:ARG:HE	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:430:LYS:HA	18:Z:433:VAL:HB	2.03	0.41
3:2:288:LEU:HD23	3:2:307:VAL:HG11	2.02	0.41
11:G:118:LEU:HA	11:G:121:VAL:HG12	2.02	0.41
15:R:118:LEU:HB2	15:R:125:GLU:HG2	2.01	0.41
16:S:204:LYS:HA	16:S:205:PRO:HD3	1.83	0.41
17:U:112:ASP:OD2	17:U:112:ASP:N	2.51	0.41
18:Z:110:LYS:HB3	18:Z:140:ILE:HG22	2.01	0.41
18:Z:435:ARG:NH2	18:Z:474:LEU:O	2.53	0.41
11:C:111:GLU:O	11:C:114:ALA:N	2.54	0.41
11:H:71:LEU:HD13	11:I:113:ILE:HG23	2.02	0.41
11:J:85:LEU:HD11	11:J:99:LEU:HB3	1.97	0.41
11:J:113:ILE:HD13	11:J:113:ILE:HA	1.95	0.41
13:P:193:LYS:HE3	13:P:193:LYS:HB3	1.92	0.41
18:Y:493:LYS:HE2	18:Y:493:LYS:HB2	1.89	0.41
6:5:44:TRP:CE3	7:6:142:GLY:HA3	2.55	0.41
11:C:118:LEU:HD23	11:C:118:LEU:HA	1.95	0.41
12:M:181:ALA:HB3	12:M:241:TRP:HB2	2.02	0.41
16:S:101:VAL:HG22	16:S:138:VAL:HB	2.02	0.41
18:X:489:VAL:HG21	18:X:495:VAL:HG22	2.02	0.41
11:D:92:ASN:OD1	11:D:92:ASN:N	2.53	0.41
12:M:324:LYS:HB3	12:M:324:LYS:HE2	1.76	0.41
13:P:162:LEU:HD21	13:P:170:LEU:HD21	2.03	0.41
6:5:58:LEU:HD23	6:5:58:LEU:HA	1.93	0.41
7:6:32:VAL:HG23	9:8:14:THR:HG21	2.02	0.41
7:6:51:LEU:HD23	7:6:51:LEU:HA	1.92	0.41
7:6:107:VAL:HG11	10:9:48:GLY:HA3	2.03	0.41
11:I:125:LEU:HD21	11:J:124:ILE:HG12	2.02	0.41
17:U:174:LYS:HE2	17:U:174:LYS:HB3	1.89	0.41
17:U:546:LEU:O	17:U:550:LEU:HB2	2.20	0.41
17:V:108:LEU:O	17:V:147:THR:OG1	2.29	0.41
17:V:502:TYR:OH	17:V:547:ASP:OD2	2.23	0.41
18:X:548:ASP:OD2	18:X:548:ASP:N	2.52	0.41
18:Z:543:ASP:OD1	18:Z:543:ASP:N	2.52	0.41
2:1:335:VAL:HA	2:1:336:PRO:HD3	1.91	0.41
7:6:31:SER:HB2	7:6:58:ALA:HB1	2.03	0.41
11:B:59:SER:HA	11:B:62:VAL:HG22	2.03	0.41
11:D:86:ILE:HG21	11:E:85:LEU:HA	2.02	0.41
18:X:223:LEU:HA	18:X:226:GLU:HG2	2.02	0.41
2:1:551:LEU:HD21	4:3:170:THR:HB	2.03	0.41
3:2:320:LEU:HD23	3:2:320:LEU:HA	1.92	0.41
11:A:125:LEU:HD21	11:B:124:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:74:VAL:HG21	11:F:114:ALA:HB2	2.02	0.41
13:P:108:VAL:HG23	13:P:109:LEU:HD12	2.03	0.41
13:P:184:LEU:HD12	13:P:185:VAL:H	1.85	0.41
17:V:360:ARG:HE	17:V:360:ARG:HB3	1.67	0.41
18:X:56:LEU:HD11	18:X:83:ASN:HA	2.02	0.41
18:X:108:PRO:HB2	18:X:142:SER:HB2	2.03	0.41
18:X:306:SER:OG	18:X:307:ALA:N	2.52	0.41
18:X:351:PRO:HA	18:X:354:THR:HG22	2.02	0.41
18:X:516:LYS:HB3	18:X:518:SER:H	1.86	0.41
11:I:60:LYS:NZ	11:I:125:LEU:O	2.42	0.41
11:I:64:ALA:HB2	11:I:124:ILE:HB	2.03	0.41
17:U:70:VAL:HG13	17:U:77:TYR:HE2	1.86	0.41
20:U:1001:ATP:PG	18:Z:385:ARG:HH12	2.44	0.41
18:Y:190:THR:HA	18:Y:193:ILE:HG22	2.03	0.41
2:1:37:ALA:HA	2:1:38:PRO:HD3	1.91	0.40
2:1:423:ASN:HD22	2:1:423:ASN:HA	1.67	0.40
11:H:118:LEU:HD11	11:I:116:PHE:HB3	2.03	0.40
15:R:45:LEU:HB3	16:S:122:TYR:HE1	1.86	0.40
17:T:326:ASP:HB3	17:T:329:LYS:HB2	2.03	0.40
17:V:482:GLU:HA	17:V:485:LYS:HD3	2.03	0.40
18:Y:492:ILE:HD12	18:Y:492:ILE:HA	1.92	0.40
3:2:265:LEU:HD23	3:2:265:LEU:HA	1.96	0.40
6:5:120:PRO:HB3	8:7:80:ALA:HA	2.03	0.40
14:Q:56:LYS:HE3	16:S:151:THR:HG21	2.04	0.40
15:R:73:ASN:HB3	15:R:75:TYR:CZ	2.56	0.40
16:S:239:ARG:HA	16:S:242:VAL:HG12	2.03	0.40
17:U:157:PRO:HB3	18:X:545:LEU:HB3	2.02	0.40
17:U:442:VAL:HG11	17:U:501:VAL:HG13	2.04	0.40
18:Y:101:LYS:HD3	18:Y:101:LYS:HA	1.93	0.40
18:Y:165:LYS:H	18:Y:165:LYS:HG2	1.71	0.40
8:7:170:HIS:HB3	8:7:173:ILE:HB	2.04	0.40
16:S:197:PHE:N	16:S:261:GLU:OE1	2.48	0.40
17:U:65:LYS:HE2	17:U:65:LYS:HB3	1.89	0.40
11:A:58:ALA:O	11:B:59:SER:OG	2.27	0.40
11:A:97:LYS:HD2	11:A:97:LYS:HA	1.94	0.40
11:I:94:ASN:HD21	16:S:225:GLY:HA3	1.85	0.40
16:S:127:LEU:HD12	16:S:127:LEU:HA	1.93	0.40
17:T:132:PHE:CE1	17:T:297:PRO:HB2	2.56	0.40
18:Y:373:ILE:HG23	18:Y:444:SER:HB2	2.03	0.40
2:1:82:HIS:NE2	8:7:120:TYR:O	2.52	0.40
2:1:473:LYS:HD3	6:5:92:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:73:THR:HA	7:6:76:LYS:HE2	2.04	0.40
11:H:69:ILE:HD12	11:I:69:ILE:HD11	2.02	0.40
12:M:107:THR:O	12:M:111:THR:OG1	2.34	0.40
12:M:125:LYS:HA	12:M:126:PRO:HD3	1.96	0.40
15:R:155:VAL:HG21	15:R:191:LEU:HD21	2.03	0.40
17:T:370:LYS:HE2	17:T:370:LYS:HB2	1.95	0.40
17:T:495:GLU:HG3	17:T:533:PHE:HB3	2.04	0.40
17:V:443:ALA:HA	17:V:446:LEU:HB3	2.03	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%)	574 (97%)	19 (3%)	0	100	100
3	2	439/441 (100%)	420 (96%)	18 (4%)	1 (0%)	47	79
4	3	243/325 (75%)	236 (97%)	7 (3%)	0	100	100
5	4	288/294 (98%)	281 (98%)	7 (2%)	0	100	100
6	5	121/123 (98%)	113 (93%)	7 (6%)	1 (1%)	19	54
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%)	77 (90%)	9 (10%)	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%)	69 (96%)	3 (4%)	0	100	100
11	C	71/127 (56%)	69 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	D	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	E	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	F	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	G	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	H	72/127 (57%)	72 (100%)	0	0	100	100
11	I	72/127 (57%)	66 (92%)	6 (8%)	0	100	100
11	J	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
12	M	213/327 (65%)	205 (96%)	8 (4%)	0	100	100
13	P	191/229 (83%)	174 (91%)	17 (9%)	0	100	100
14	Q	70/74 (95%)	67 (96%)	3 (4%)	0	100	100
15	R	175/199 (88%)	160 (91%)	15 (9%)	0	100	100
16	S	275/317 (87%)	262 (95%)	13 (5%)	0	100	100
17	T	521/562 (93%)	490 (94%)	27 (5%)	4 (1%)	19	54
17	U	521/562 (93%)	489 (94%)	31 (6%)	1 (0%)	47	79
17	V	518/562 (92%)	496 (96%)	21 (4%)	1 (0%)	47	79
18	X	540/574 (94%)	504 (93%)	35 (6%)	1 (0%)	47	79
18	Y	519/574 (90%)	478 (92%)	38 (7%)	3 (1%)	25	59
18	Z	536/574 (93%)	503 (94%)	31 (6%)	2 (0%)	34	69
All	All	7038/8234 (86%)	6659 (95%)	365 (5%)	14 (0%)	50	79

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	X	308	VAL
18	Z	308	VAL
3	2	383	PRO
17	T	493	PRO
17	U	349	ALA
17	V	349	ALA
18	Y	308	VAL
17	T	56	LYS
17	T	349	ALA
18	Z	307	ALA
18	Y	307	ALA
18	Y	455	GLY
17	T	494	ILE

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Mol	Chain	Res	Type
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%)	312 (100%)	0	100	100
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	219 (100%)	1 (0%)	88	94
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%)	49 (98%)	1 (2%)	55	80
11	C	50/86 (58%)	50 (100%)	0	100	100
11	D	50/86 (58%)	50 (100%)	0	100	100
11	E	50/86 (58%)	50 (100%)	0	100	100
11	F	50/86 (58%)	50 (100%)	0	100	100
11	G	50/86 (58%)	50 (100%)	0	100	100
11	H	50/86 (58%)	49 (98%)	1 (2%)	55	80
11	I	50/86 (58%)	50 (100%)	0	100	100
11	J	50/86 (58%)	50 (100%)	0	100	100
12	M	178/272 (65%)	178 (100%)	0	100	100
13	P	171/196 (87%)	171 (100%)	0	100	100
14	Q	56/58 (97%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	R	134/151 (89%)	134 (100%)	0	100	100
16	S	235/265 (89%)	234 (100%)	1 (0%)	91	96
17	T	419/448 (94%)	417 (100%)	2 (0%)	88	94
17	U	419/448 (94%)	417 (100%)	2 (0%)	88	94
17	V	418/448 (93%)	417 (100%)	1 (0%)	93	97
18	X	449/469 (96%)	449 (100%)	0	100	100
18	Y	430/469 (92%)	428 (100%)	2 (0%)	88	94
18	Z	446/469 (95%)	445 (100%)	1 (0%)	93	97
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
5	4	198	LYS
11	B	121	VAL
11	H	119	LEU
16	S	203	PHE
17	T	180	VAL
17	T	300	PHE
17	U	180	VAL
17	U	300	PHE
17	V	146	ARG
18	Y	82	ASP
18	Y	417	ILE
18	Z	411	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	48	ASN
1	0	60	GLN
2	1	65	GLN
2	1	257	HIS
2	1	285	GLN
2	1	313	GLN
2	1	316	ASN
2	1	346	GLN
2	1	365	GLN

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Mol	Chain	Res	Type
2	1	423	ASN
2	1	482	ASN
2	1	587	ASN
2	1	590	HIS
3	2	40	GLN
3	2	68	ASN
3	2	122	ASN
3	2	243	GLN
3	2	289	HIS
3	2	427	GLN
4	3	97	ASN
4	3	179	GLN
4	3	206	ASN
5	4	38	GLN
5	4	124	ASN
5	4	135	ASN
5	4	240	GLN
6	5	29	GLN
6	5	107	ASN
7	6	40	ASN
7	6	74	GLN
8	7	86	HIS
8	7	98	ASN
8	7	123	HIS
8	7	170	HIS
8	7	184	ASN
8	7	190	GLN
9	8	26	HIS
10	9	80	GLN
11	D	94	ASN
11	G	87	ASN
11	I	94	ASN
12	M	108	ASN
12	M	163	ASN
13	P	220	ASN
13	P	223	ASN
15	R	38	ASN
15	R	73	ASN
15	R	85	GLN
15	R	171	GLN
15	R	178	GLN
16	S	70	ASN

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Mol	Chain	Res	Type
16	S	174	GLN
16	S	188	GLN
16	S	262	ASN
16	S	293	ASN
16	S	297	GLN
17	T	64	GLN
17	T	134	ASN
17	T	241	HIS
17	T	497	GLN
17	T	549	HIS
17	U	242	GLN
17	U	246	ASN
17	U	248	GLN
17	U	264	GLN
17	U	319	HIS
17	U	358	HIS
17	U	386	GLN
17	U	461	GLN
17	U	471	GLN
17	U	497	GLN
17	V	60	GLN
17	V	121	ASN
17	V	139	HIS
17	V	149	GLN
17	V	152	ASN
17	V	244	ASN
17	V	271	GLN
17	V	278	GLN
17	V	486	GLN
17	V	497	GLN
18	X	198	ASN
18	X	199	ASN
18	X	408	GLN
18	Y	123	ASN
18	Y	241	ASN
18	Y	398	ASN
18	Z	132	GLN
18	Z	199	ASN
18	Z	250	GLN
18	Z	278	GLN
18	Z	294	ASN
18	Z	398	ASN

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Mol	Chain	Res	Type
18	Z	414	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	U	1001	21	26,33,33	0.97	0	31,52,52	1.47	5 (16%)
22	ADP	X	601	21	24,29,29	0.99	0	29,45,45	1.36	4 (13%)
20	ATP	V	1001	21	26,33,33	0.97	1 (3%)	31,52,52	1.43	4 (12%)
22	ADP	Y	601	21	24,29,29	0.97	1 (4%)	29,45,45	1.39	4 (13%)
20	ATP	T	1001	21	26,33,33	0.99	1 (3%)	31,52,52	1.60	6 (19%)

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	U	1001	21	-	2/18/38/38	0/3/3/3
22	ADP	X	601	21	-	0/12/32/32	0/3/3/3
20	ATP	V	1001	21	-	2/18/38/38	0/3/3/3
22	ADP	Y	601	21	-	5/12/32/32	0/3/3/3
20	ATP	T	1001	21	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	601	ADP	C5-C4	2.26	1.46	1.40
20	T	1001	ATP	C2'-C1'	-2.14	1.50	1.53
20	V	1001	ATP	C5-C4	2.03	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	-3.50	120.81	132.83
20	V	1001	ATP	PB-O3B-PG	-3.49	120.86	132.83
20	T	1001	ATP	N3-C2-N1	-3.47	123.25	128.68
22	X	601	ADP	N3-C2-N1	-3.33	123.47	128.68
20	T	1001	ATP	C3'-C2'-C1'	3.32	105.98	100.98
20	U	1001	ATP	C3'-C2'-C1'	3.27	105.90	100.98
20	T	1001	ATP	PA-O3A-PB	-3.24	121.70	132.83
20	T	1001	ATP	PB-O3B-PG	-3.15	122.01	132.83
20	V	1001	ATP	N3-C2-N1	-3.13	123.79	128.68
20	U	1001	ATP	N3-C2-N1	-3.12	123.80	128.68
22	Y	601	ADP	N3-C2-N1	-3.08	123.86	128.68
22	X	601	ADP	C3'-C2'-C1'	3.07	105.59	100.98
22	Y	601	ADP	C3'-C2'-C1'	2.97	105.45	100.98
22	Y	601	ADP	PA-O3A-PB	-2.97	122.65	132.83
20	V	1001	ATP	C3'-C2'-C1'	2.75	105.12	100.98
20	U	1001	ATP	PA-O3A-PB	-2.69	123.59	132.83
22	Y	601	ADP	C4-C5-N7	-2.47	106.83	109.40
20	V	1001	ATP	C4-C5-N7	-2.36	106.94	109.40
22	X	601	ADP	C4-C5-N7	-2.35	106.95	109.40
20	T	1001	ATP	C4-C5-N7	-2.31	107.00	109.40
20	U	1001	ATP	C4-C5-N7	-2.14	107.17	109.40
22	X	601	ADP	PA-O3A-PB	-2.11	125.59	132.83
20	T	1001	ATP	C2-N1-C6	2.07	122.30	118.75

There are no chirality outliers.

All (13) torsion outliers are listed below:

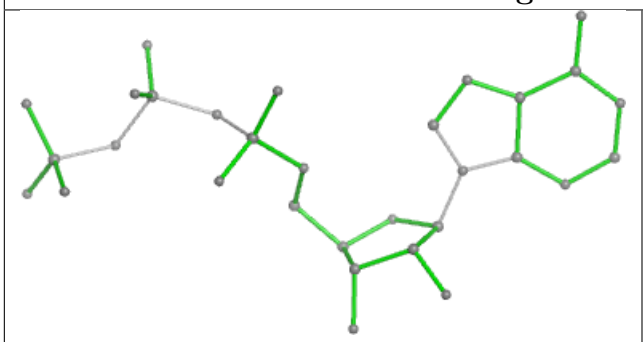
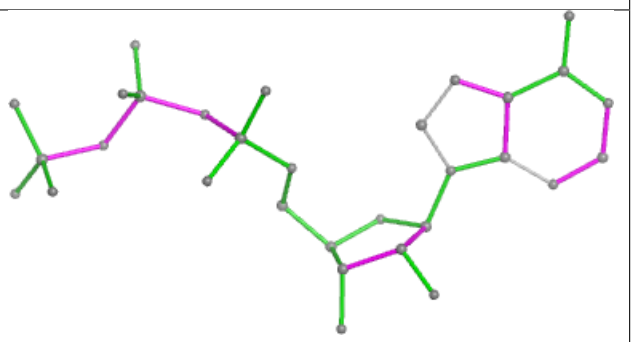
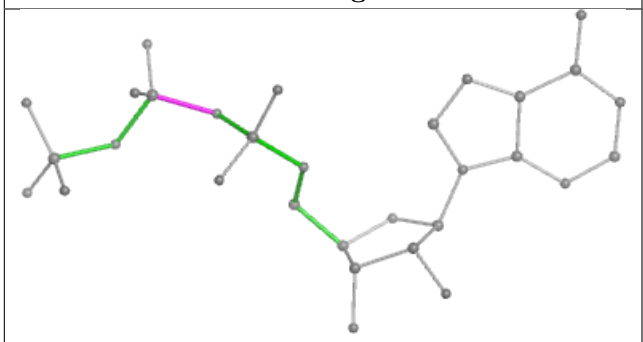
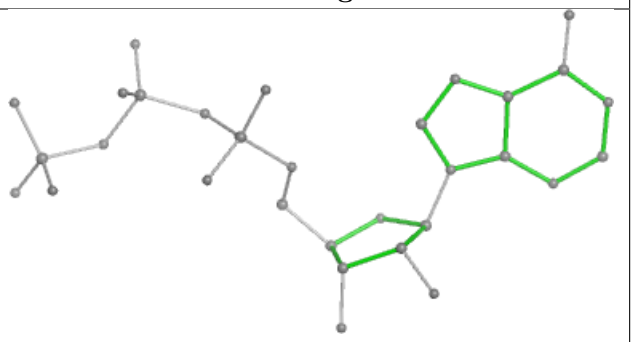
Mol	Chain	Res	Type	Atoms
22	Y	601	ADP	C5'-O5'-PA-O1A
22	Y	601	ADP	C5'-O5'-PA-O2A
20	U	1001	ATP	PA-O3A-PB-O1B
20	T	1001	ATP	C5'-O5'-PA-O3A
22	Y	601	ADP	C5'-O5'-PA-O3A
20	U	1001	ATP	PA-O3A-PB-O2B
20	T	1001	ATP	PG-O3B-PB-O1B
20	T	1001	ATP	PG-O3B-PB-O2B
20	V	1001	ATP	PB-O3A-PA-O1A
20	V	1001	ATP	PB-O3A-PA-O2A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

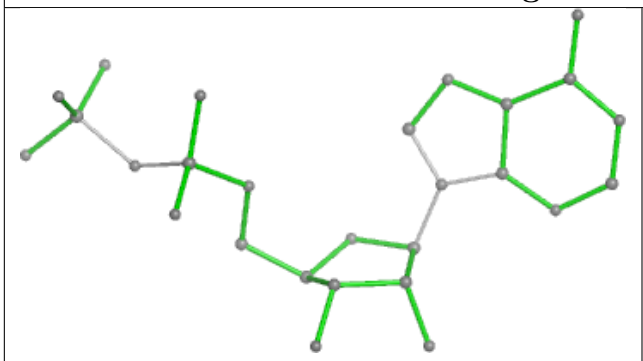
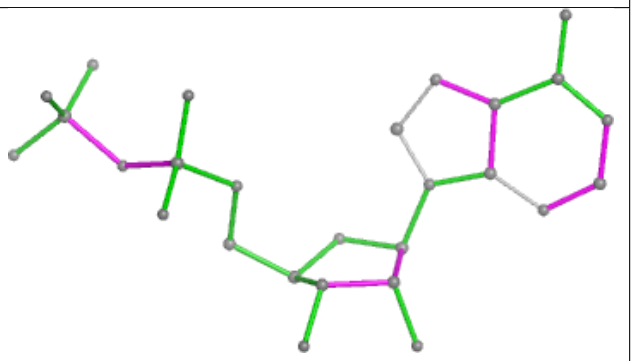
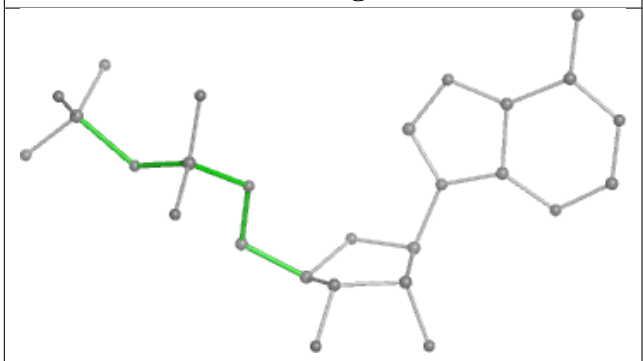
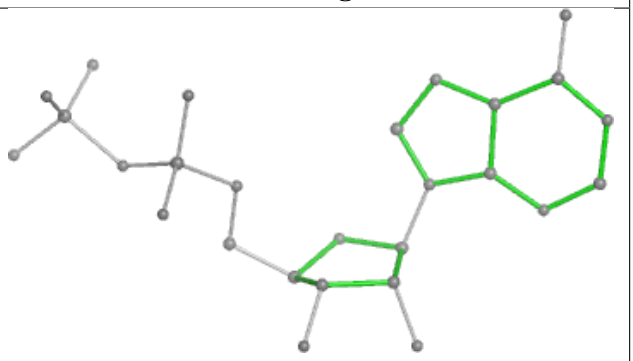
There are no ring outliers.

3 monomers are involved in 4 short contacts:

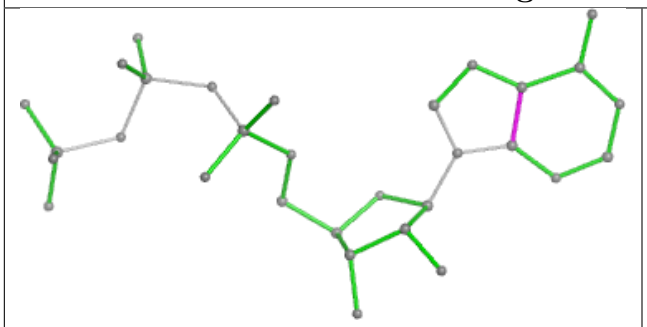
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	U	1001	ATP	1	0
20	V	1001	ATP	1	0
22	Y	601	ADP	2	0

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.

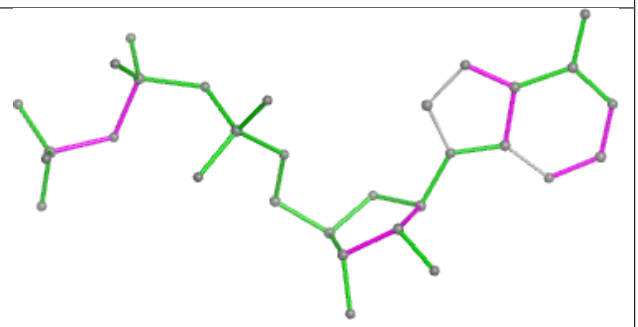
Ligand ATP U 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP X 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

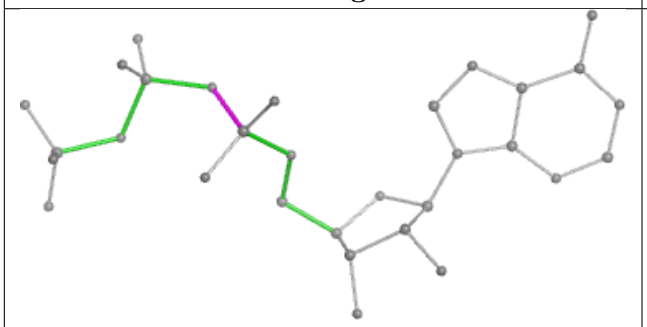
Ligand ATP V 1001



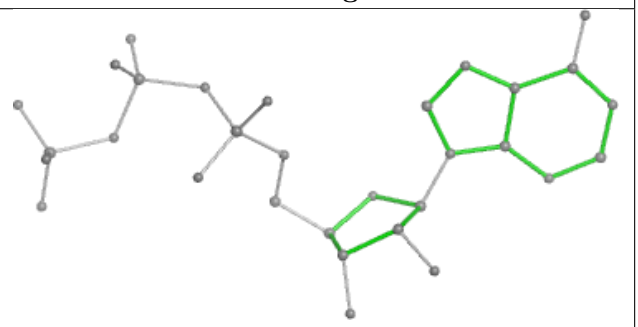
Bond lengths



Bond angles

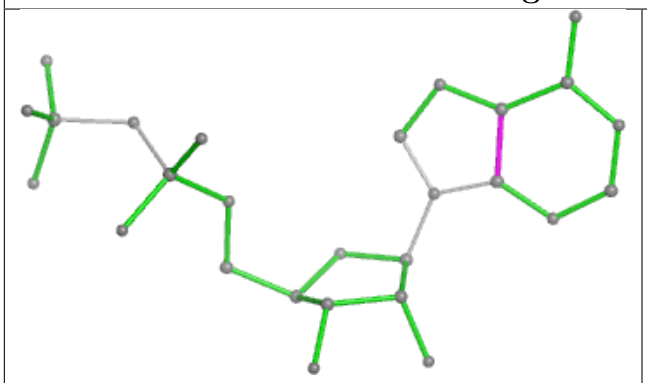


Torsions

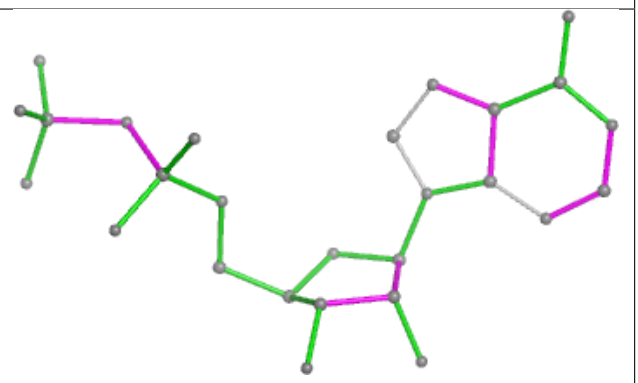


Rings

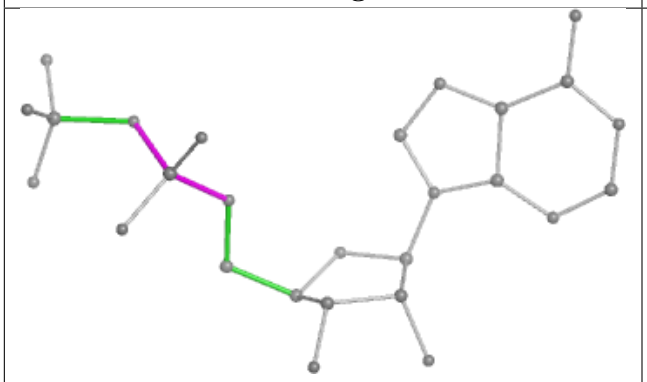
Ligand ADP Y 601



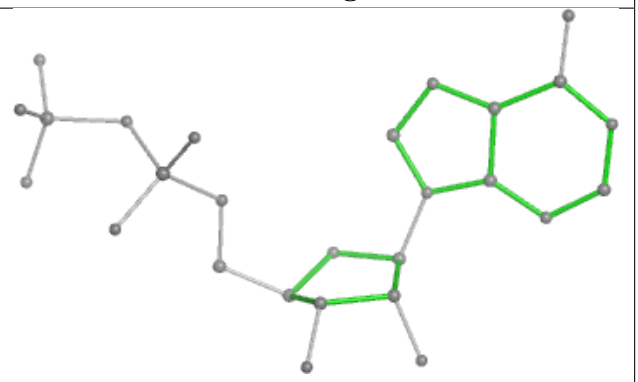
Bond lengths



Bond angles

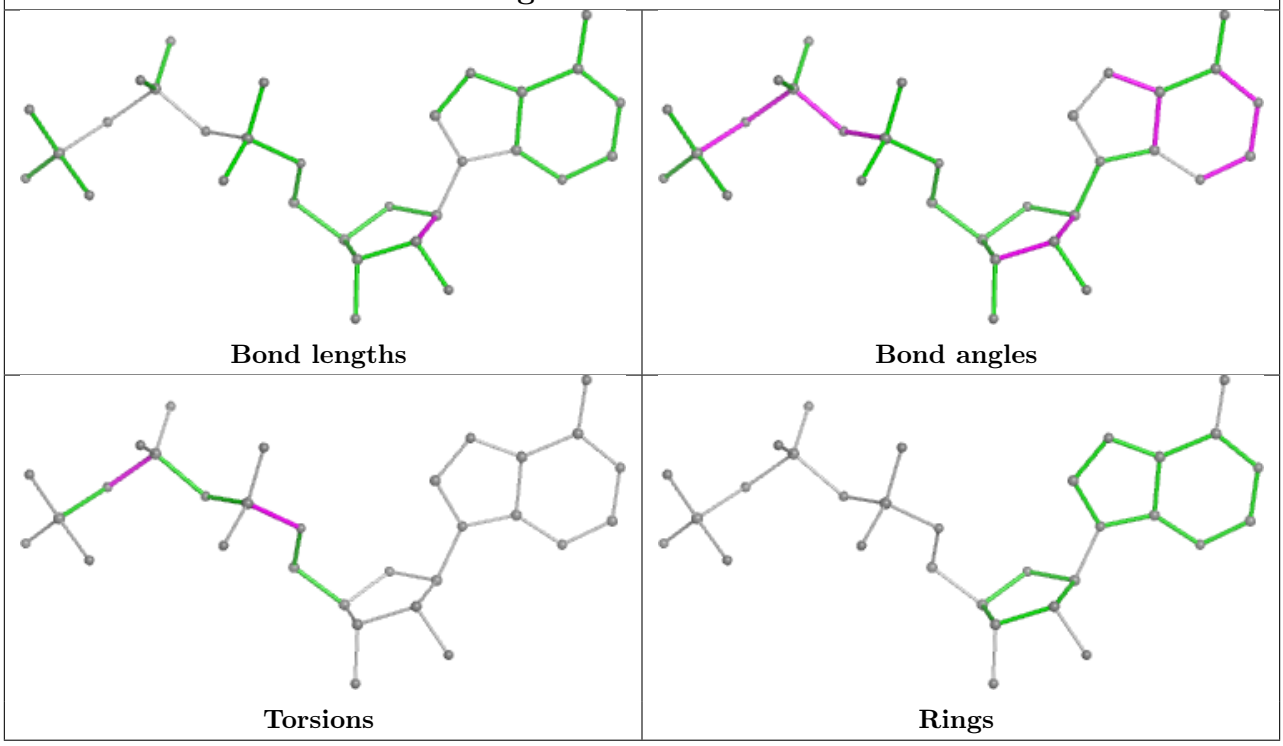


Torsions



Rings

Ligand ATP T 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	3.51

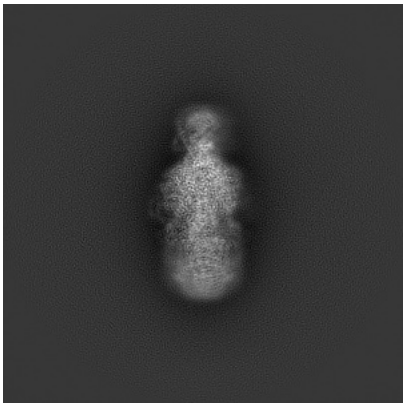
6 Map visualisation (i)

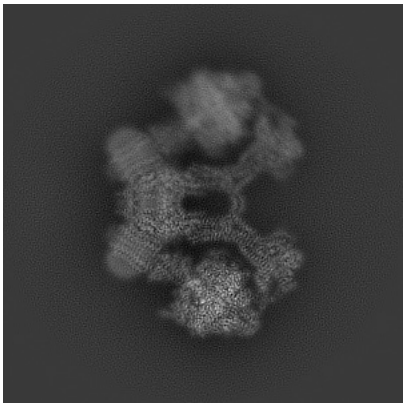
This section contains visualisations of the EMDB entry EMD-4825. These allow visual inspection of the internal detail of the map and identification of artifacts.

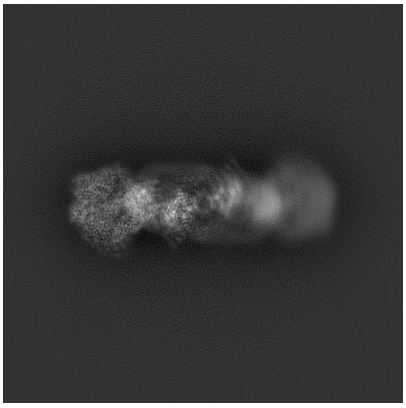
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

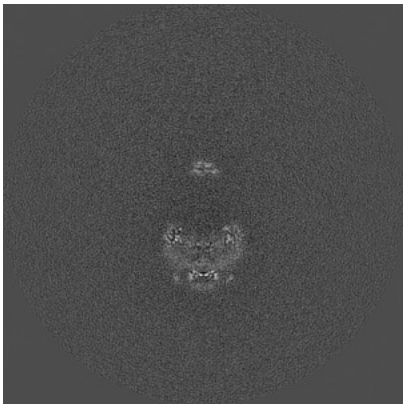

Y

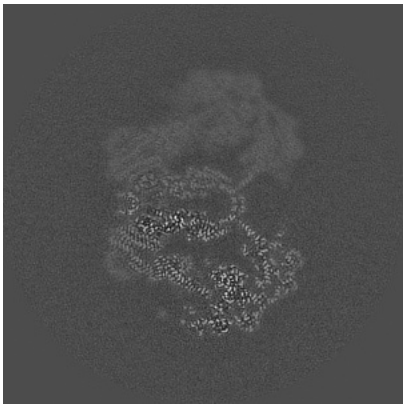

Z

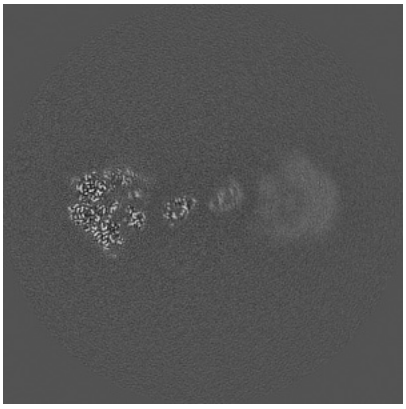
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 240

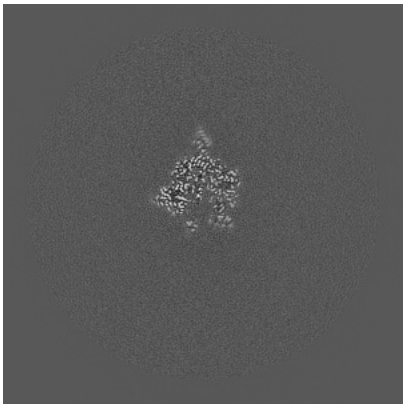

Y Index: 240


Z Index: 240

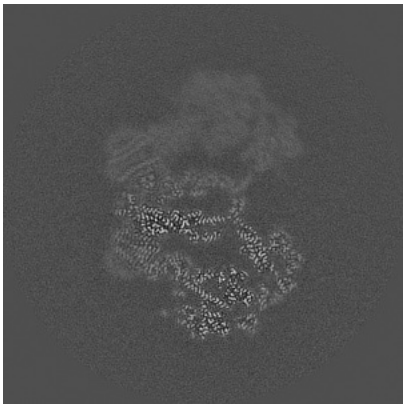
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

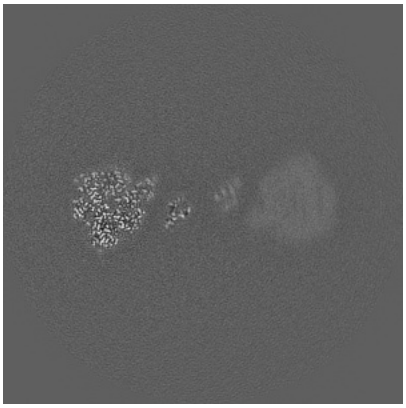
6.3.1 Primary map



X Index: 124



Y Index: 235

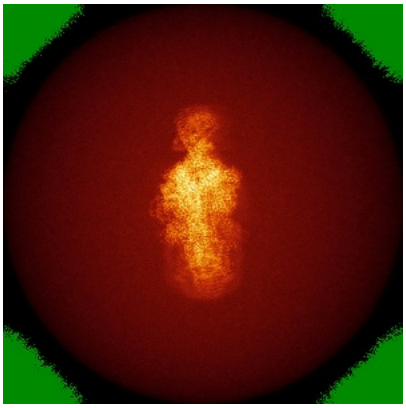


Z Index: 257

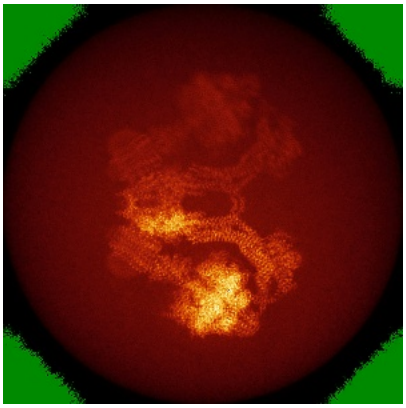
The images above show the largest variance slices of the map in three orthogonal directions.

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

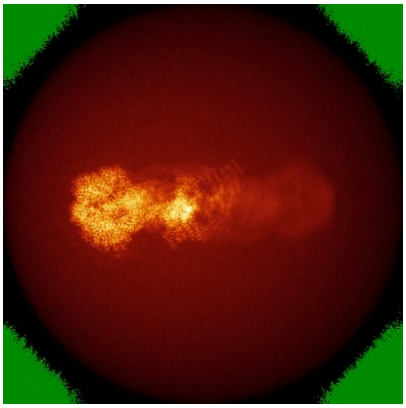
6.4.1 Primary map



X



Y

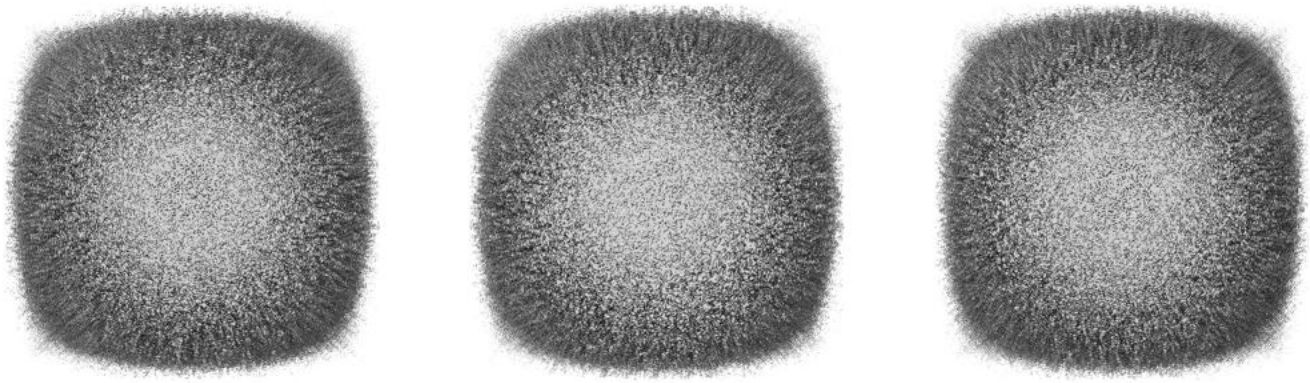


Z

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.

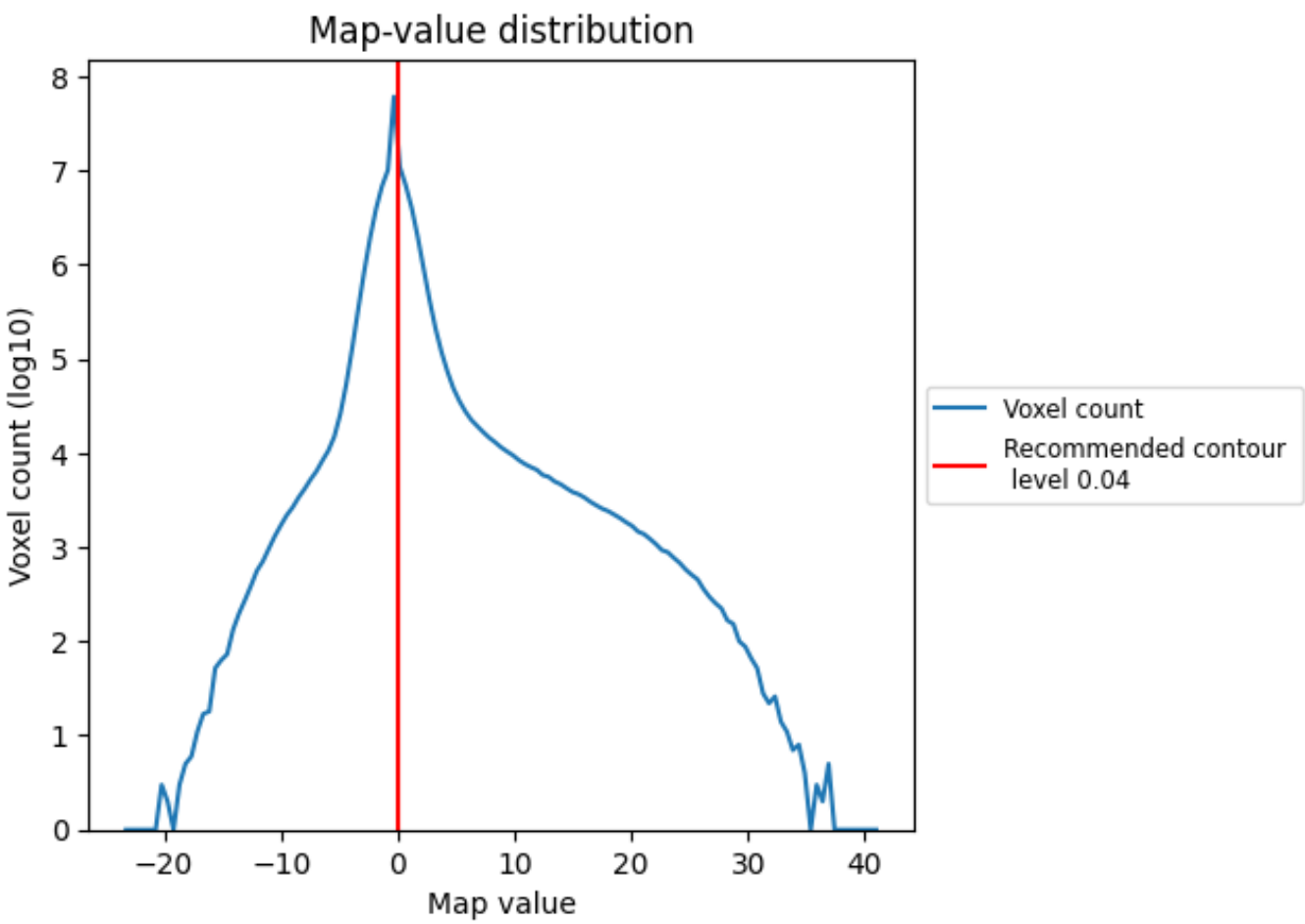
6.6 Mask visualisation (i)

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

7 Map analysis (i)

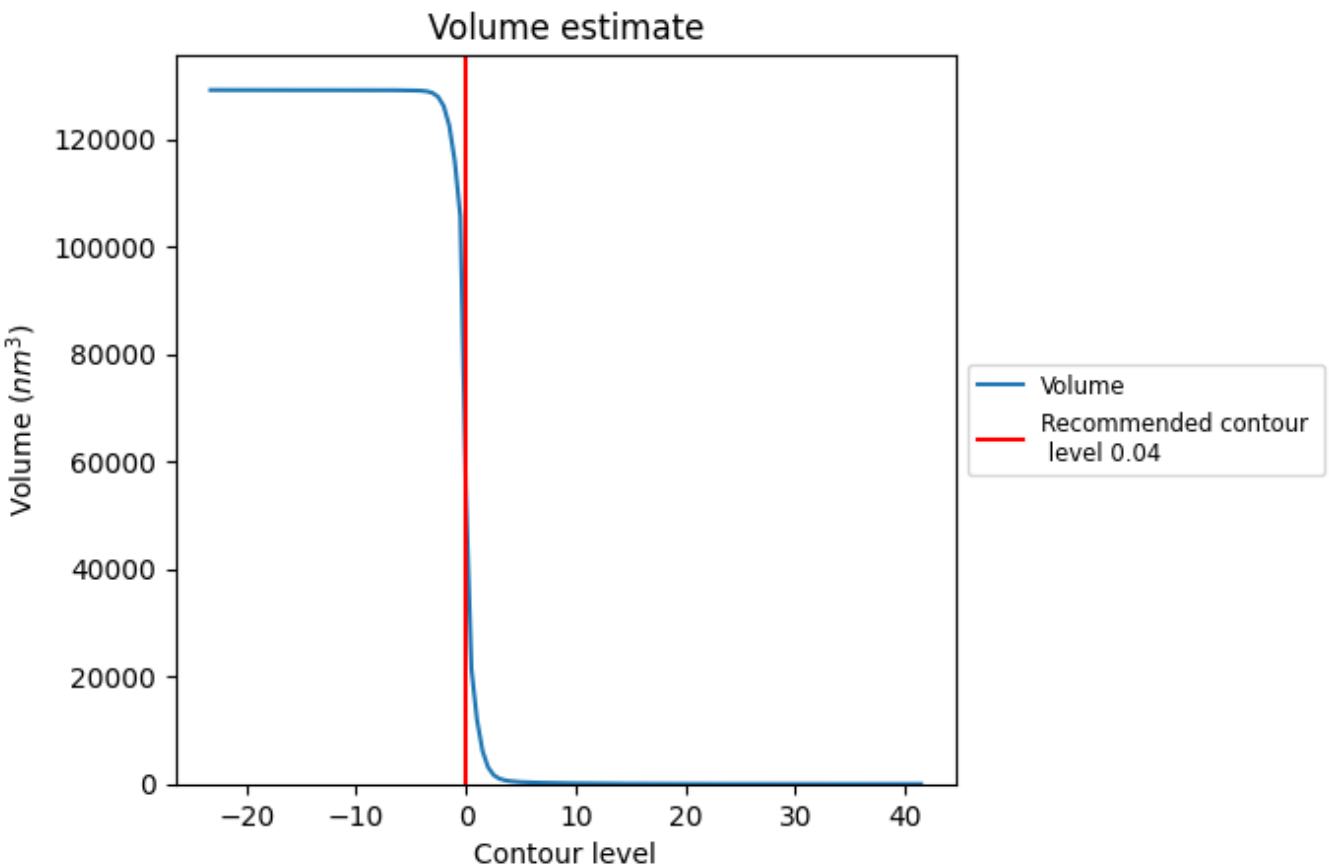
This section contains the results of statistical analysis of the map.

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.

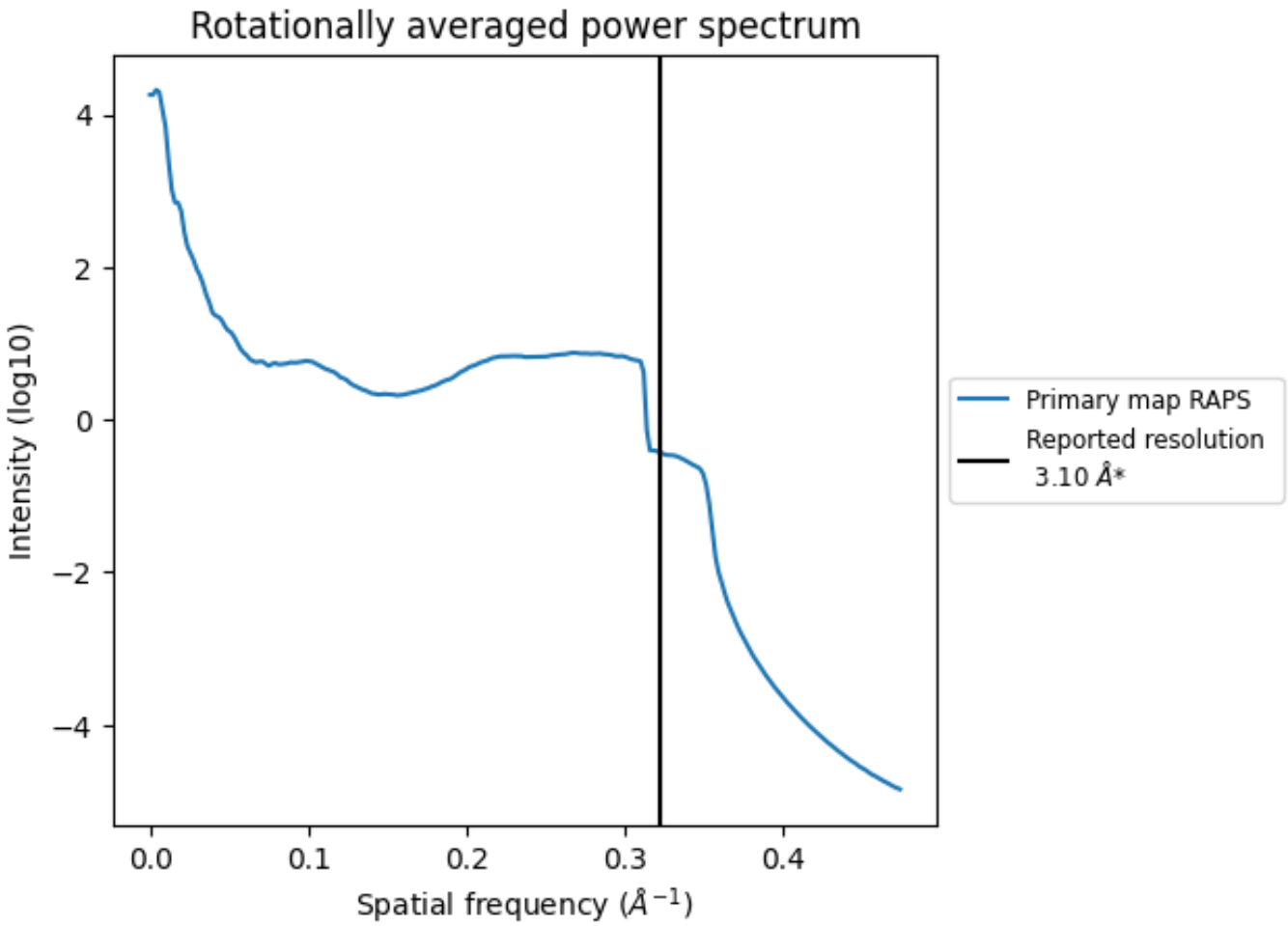
7.2 Volume estimate (i)



The volume at the recommended contour level is 52187 nm^3; this corresponds to an approximate mass of 47142 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

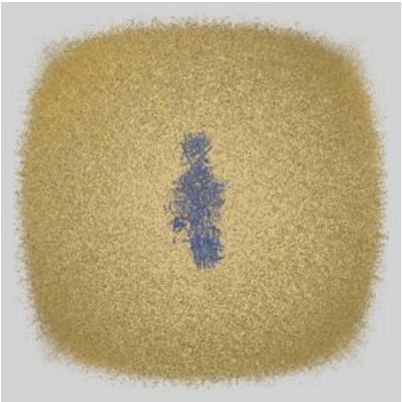
8 Fourier-Shell correlation (i)

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

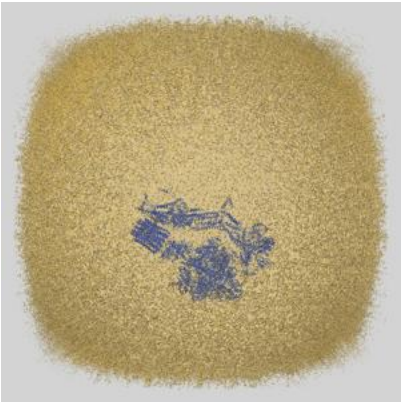
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4825 and PDB model 6RDO. Per-residue inclusion information can be found in section 3 on page 10.

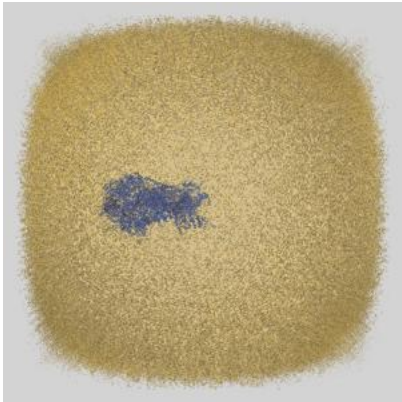
9.1 Map-model overlay (i)



X



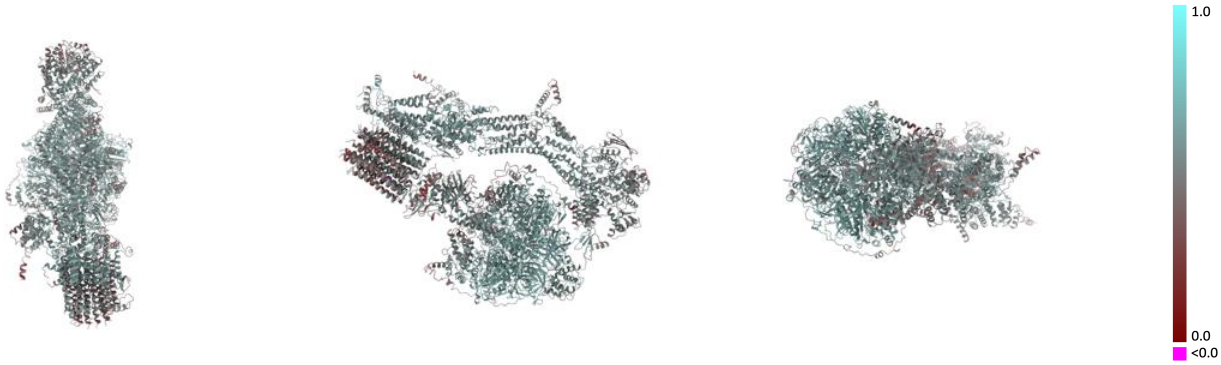
Y



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.

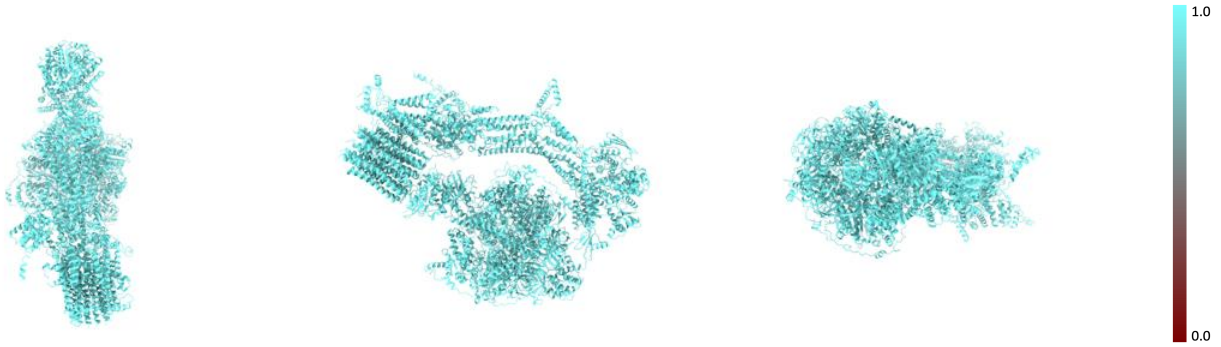
9.2 Q-score mapped to coordinate model (i)



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.

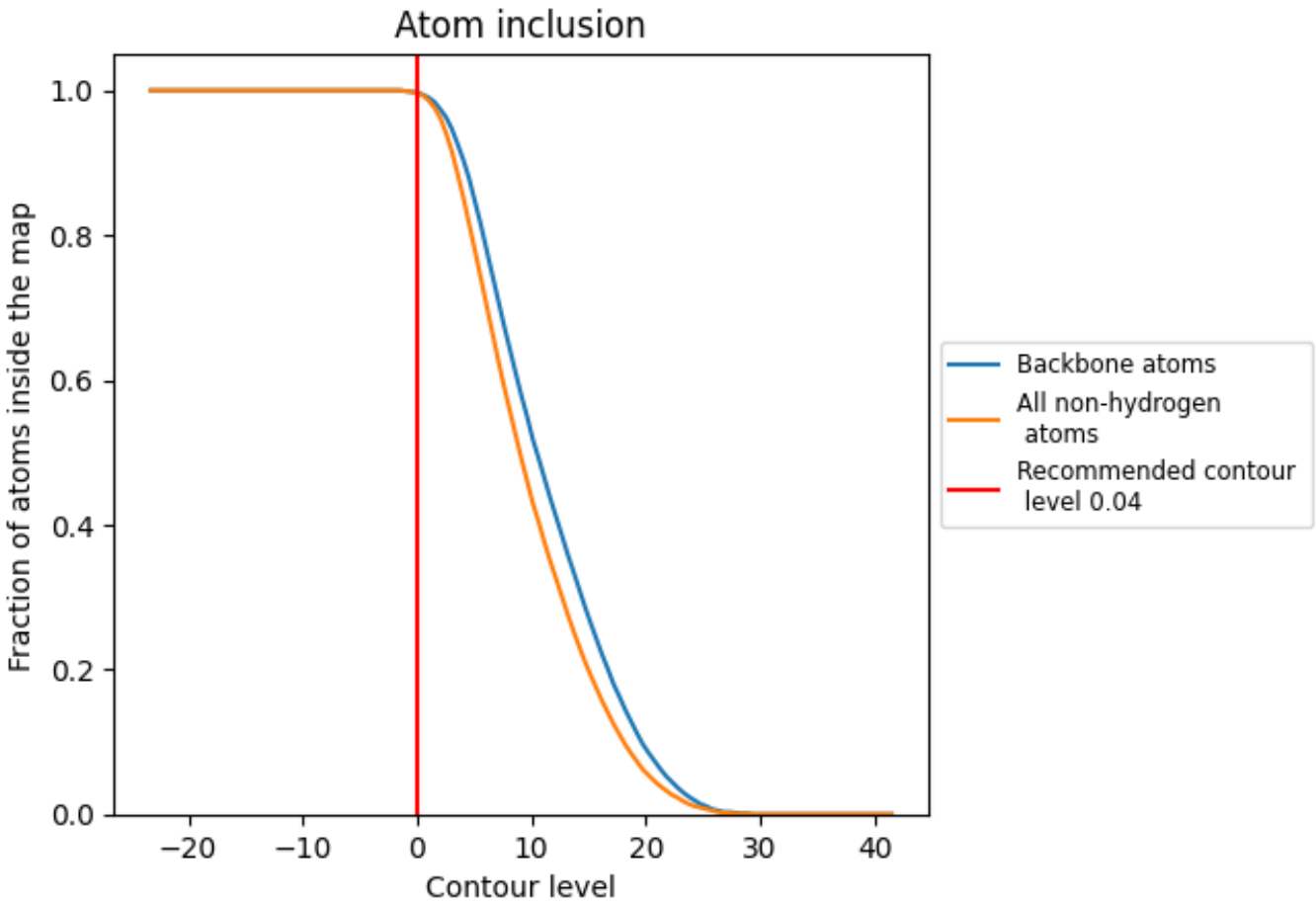
9.3 Atom inclusion mapped to coordinate model (i)



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	0.9960	0.5430
0	0.9930	0.5530
1	0.9970	0.5480
2	0.9990	0.5010
3	0.9990	0.5080
4	0.9990	0.5180
5	0.9980	0.5750
6	0.9950	0.5590
7	0.9980	0.5360
8	0.9990	0.5750
9	0.9970	0.4970
A	0.9820	0.4770
B	0.9800	0.4690
C	0.9860	0.4530
D	0.9820	0.4200
E	0.9940	0.4310
F	0.9940	0.4480
G	0.9900	0.4170
H	0.9860	0.3650
I	0.9880	0.3960
J	0.9730	0.4440
M	0.9960	0.5570
P	0.9940	0.5290
Q	0.9960	0.4640
R	0.9950	0.4490
S	0.9950	0.5230
T	0.9970	0.5840
U	0.9980	0.5920
V	0.9980	0.5830
X	0.9970	0.5940
Y	0.9960	0.5690
Z	0.9960	0.5730