



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:35 PM UTC

PDB ID : 7P2Y / pdb_00007p2y
EMDB ID : EMD-13174
Title : F1Fo-ATP synthase from *Acinetobacter baumannii* (state 1)
Authors : Demmer, J.K.; Phillips, B.P.; Uhrig, O.L.; Filloux, A.; Allsopp, L.P.; Bubltz, M.; Meier, T.
Deposited on : 2021-07-06
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

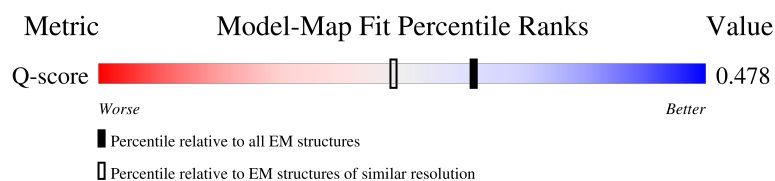
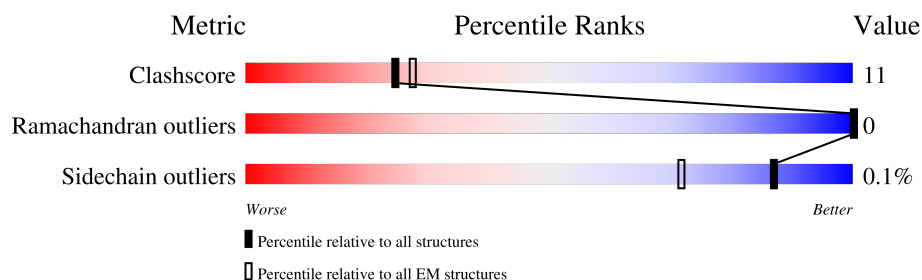
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	
1	C	514	
2	D	464	

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Mol	Chain	Length	Quality of chain
2	E	464	 5% 85% 15%
2	F	464	 83% 17%
3	G	81	 72% 26% .
3	H	81	 69% 28% .
3	J	81	 73% 26% .
3	K	81	 75% 23% .
3	L	81	 80% 19% .
3	O	81	 72% 27% .
3	P	81	 77% 21% .
3	Q	81	 75% 22% .
3	R	81	 74% 25% .
3	S	81	 68% 31% .
4	a	291	 19% 53% 42% 5%
5	b	156	 19% 54% 44% ..
5	p	156	 63% 36% .
6	d	178	 80% 17% ..
7	e	139	 78% 22% .
8	g	289	 86% 14%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 37172 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	509	Total	C	N	O	S	0	0
			3846	2420	661	750	15		
1	B	514	Total	C	N	O	S	0	0
			3892	2448	668	760	16		
1	C	509	Total	C	N	O	S	0	0
			3850	2423	660	752	15		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	463	Total	C	N	O	S	0	0
			3525	2223	602	687	13		
2	E	463	Total	C	N	O	S	0	0
			3525	2223	602	687	13		
2	F	464	Total	C	N	O	S	0	0
			3533	2228	603	688	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	79	Total	C	N	O	S	0	0
			577	388	92	95	2		
3	H	79	Total	C	N	O	S	0	0
			577	388	92	95	2		
3	J	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	K	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	L	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	O	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	P	79	Total	C	N	O	S	0	0
			577	388	92	95	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	79	Total	C	N	O	S	0	0
			577	388	92	95	2		
3	R	80	Total	C	N	O	S	0	0
			585	393	93	96	3		
3	S	80	Total	C	N	O	S	0	0
			585	393	93	96	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	277	Total	C	N	O	S	0	0
			2104	1405	336	350	13		

- Molecule 5 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	154	Total	C	N	O	S	0	0
			1162	719	217	223	3		
5	p	155	Total	C	N	O	S	0	0
			1185	734	220	228	3		

- Molecule 6 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	174	Total	C	N	O	S	0	0
			1347	849	227	270	1		

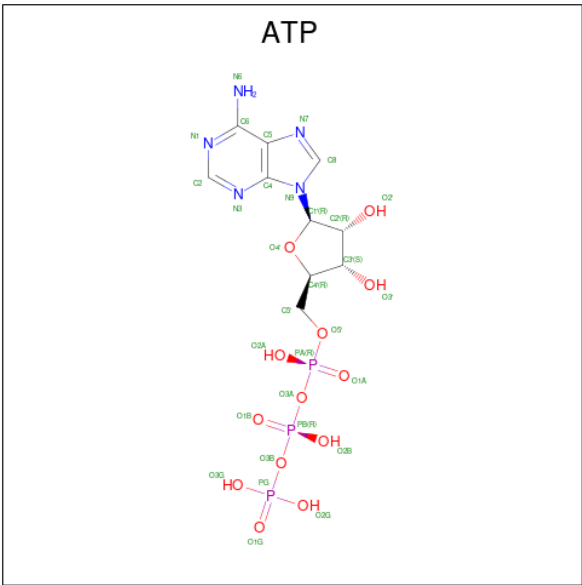
- Molecule 7 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	138	Total	C	N	O	S	0	0
			1010	631	175	201	3		

- Molecule 8 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	288	Total	C	N	O	S	0	0
			2243	1411	400	420	12		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

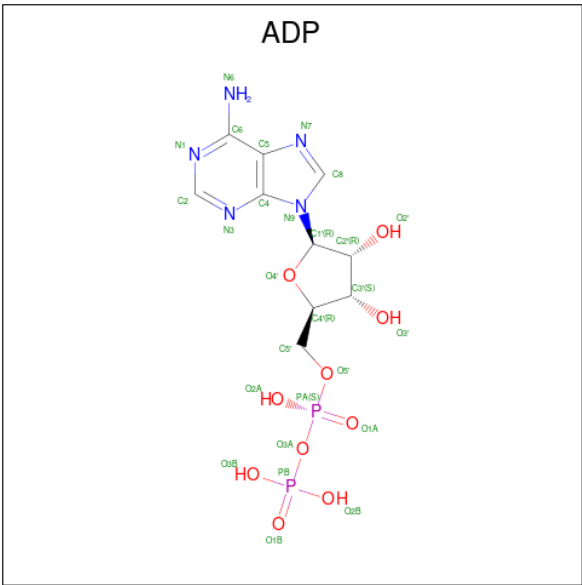


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

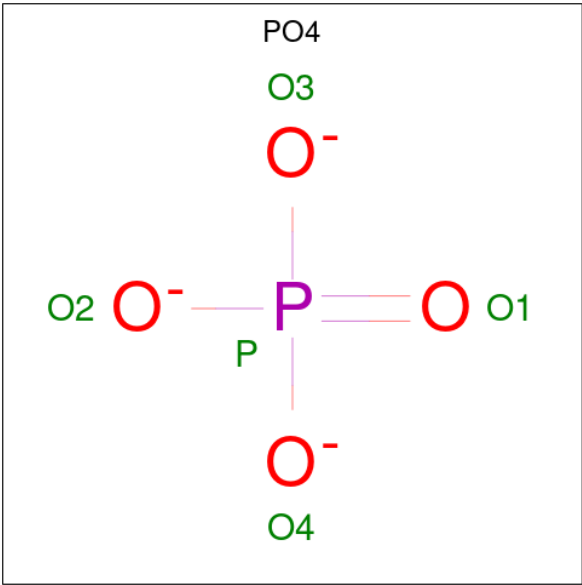
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
12	E	1	Total	O	P	0
			5	4	1	

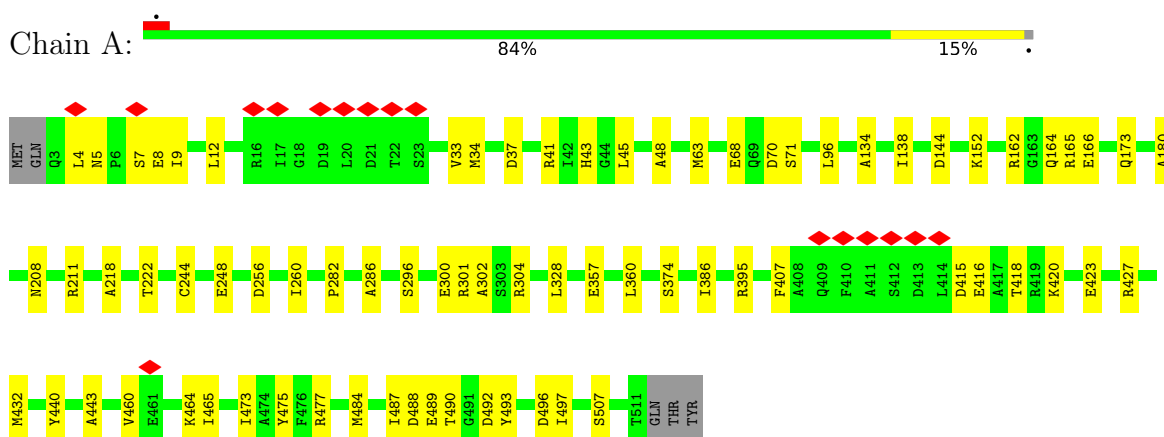
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 1	O 1	0
13	B	1	Total 1	O 1	0
13	C	1	Total 1	O 1	0

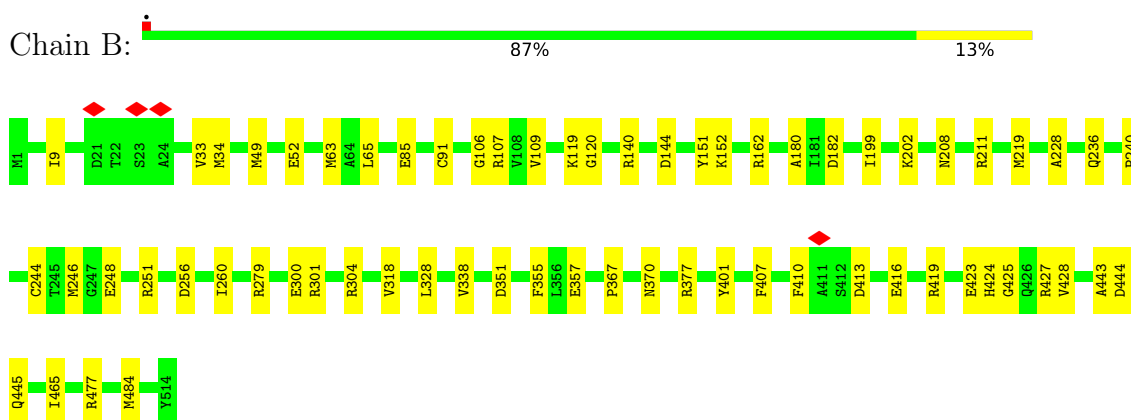
3 Residue-property plots

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

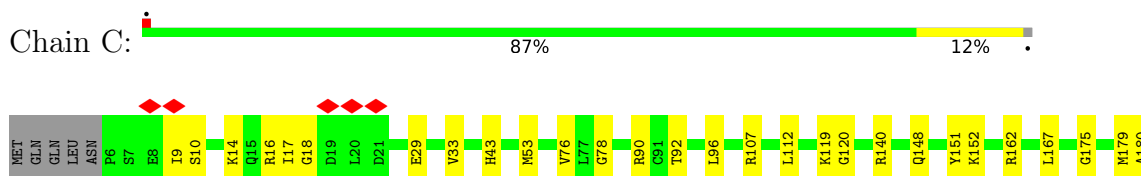
- Molecule 1: ATP synthase subunit alpha

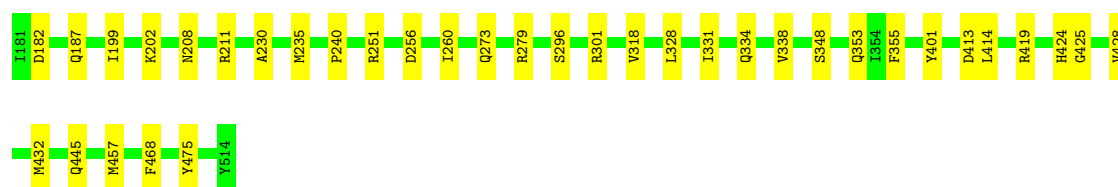


- Molecule 1: ATP synthase subunit alpha

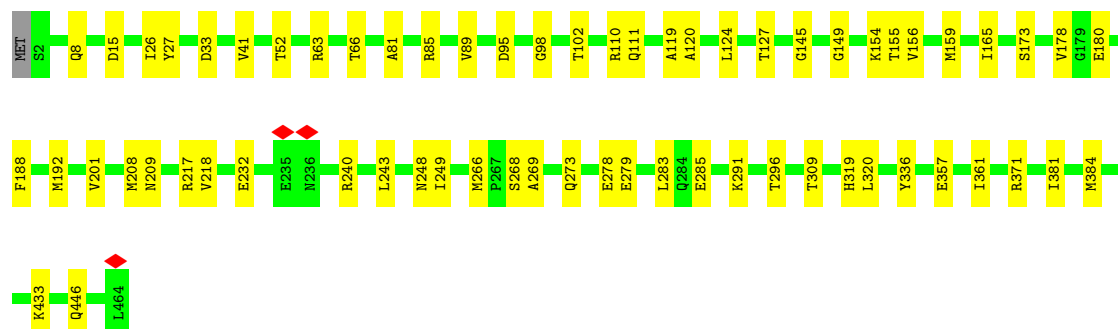
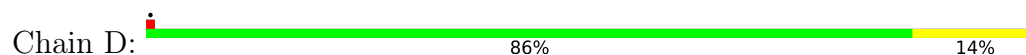


- Molecule 1: ATP synthase subunit alpha

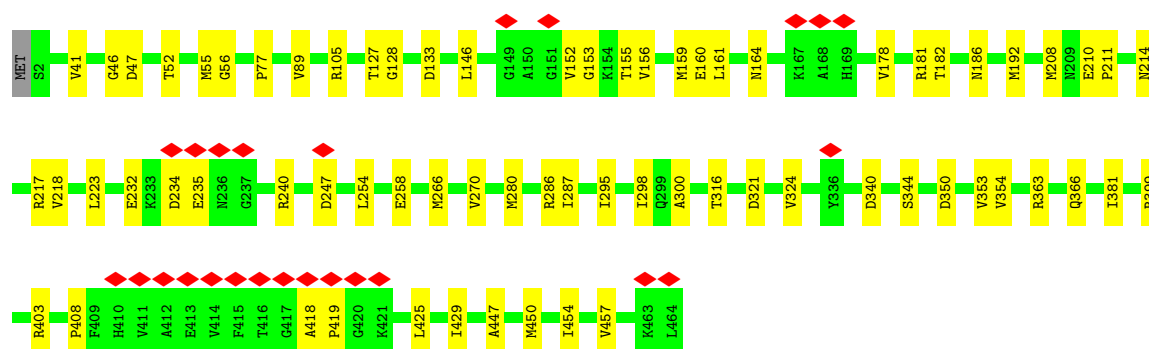
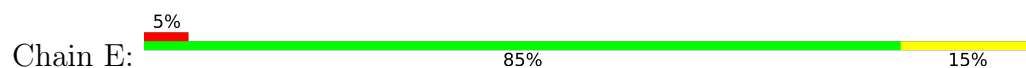




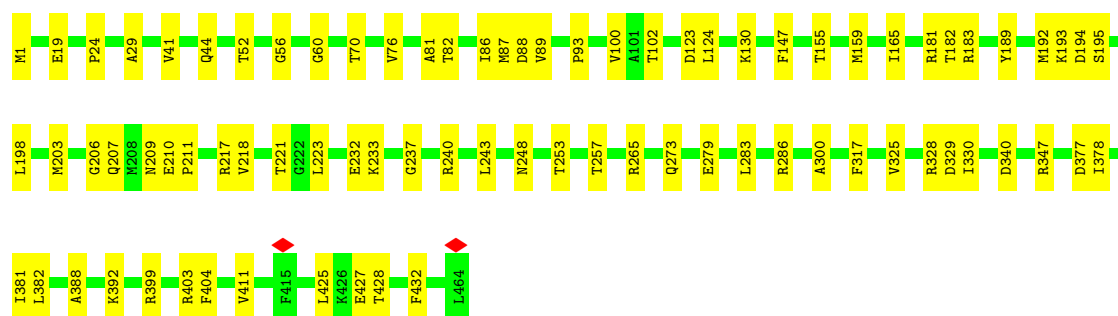
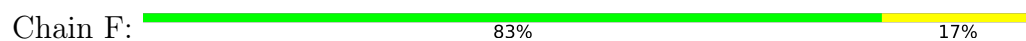
• Molecule 2: ATP synthase subunit beta



• Molecule 2: ATP synthase subunit beta



• Molecule 2: ATP synthase subunit beta



• Molecule 3: ATP synthase subunit c

Chain G:  72% 26%



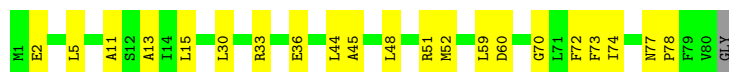
- Molecule 3: ATP synthase subunit c

Chain H:  69% 28%



- Molecule 3: ATP synthase subunit c

Chain J:  73% 26%



- Molecule 3: ATP synthase subunit c

Chain K:  75% 23%



- Molecule 3: ATP synthase subunit c

Chain L:  80% 19%



- Molecule 3: ATP synthase subunit c

Chain O:  72% 27%



- Molecule 3: ATP synthase subunit c

Chain P:  77% 21%



- Molecule 3: ATP synthase subunit c

Chain Q: 



- Molecule 3: ATP synthase subunit c

Chain R: 



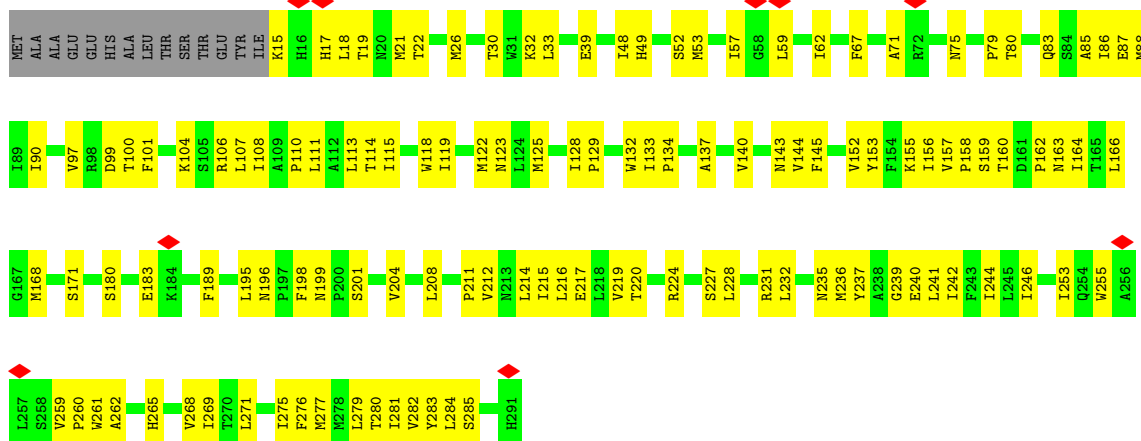
- Molecule 3: ATP synthase subunit c

Chain S: 



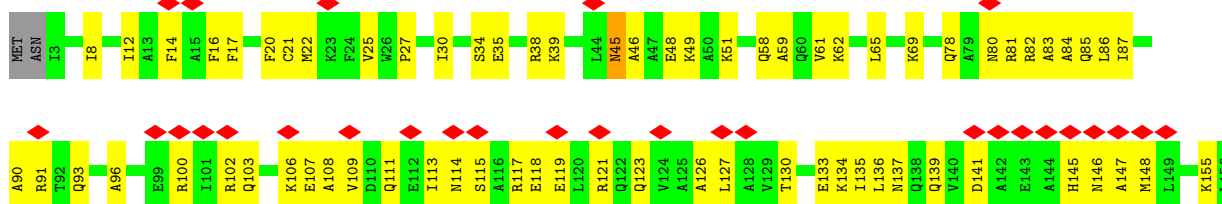
- Molecule 4: ATP synthase subunit a

Chain a: 



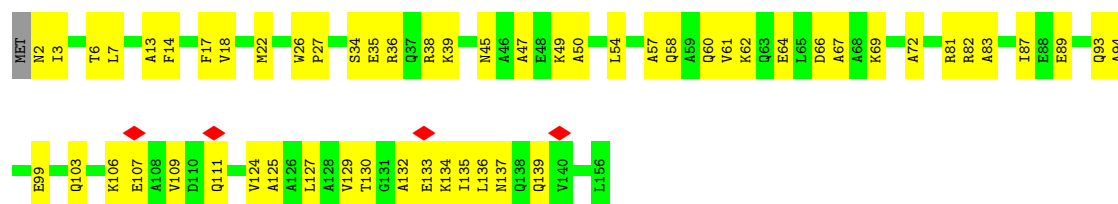
- Molecule 5: ATP synthase subunit b

Chain b: 



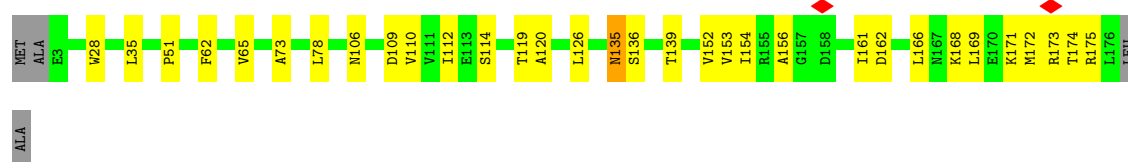
- Molecule 5: ATP synthase subunit b

Chain p:  63% 36%



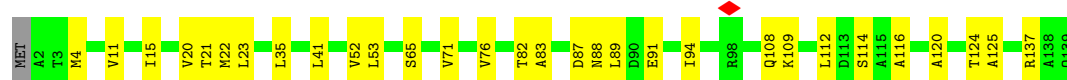
• Molecule 6: ATP synthase subunit delta

Chain d:  80% 17%



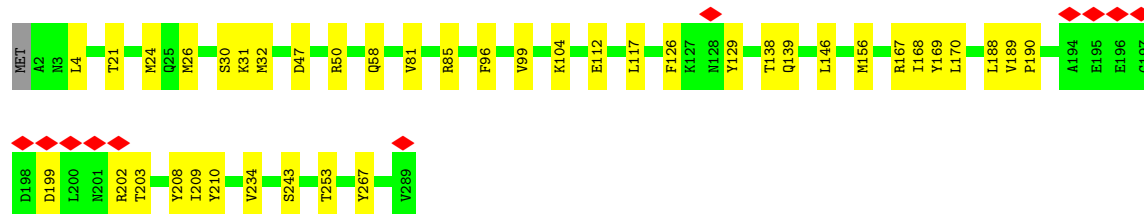
• Molecule 7: ATP synthase epsilon chain

Chain e:  78% 22%



• Molecule 8: ATP synthase gamma chain

Chain g:  86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	85000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	33.068	Depositor
Minimum map value	-13.075	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.066	Depositor
Recommended contour level	6.24	Depositor
Map size ($\text{\AA}$)	382.5, 382.5, 382.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ATP, PO4

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	A	0.19	0/3902	0.38	0/5281
1	B	0.19	0/3949	0.38	0/5343
1	C	0.19	0/3907	0.37	0/5286
2	D	0.20	0/3582	0.37	0/4854
2	E	0.18	0/3582	0.40	0/4854
2	F	0.19	0/3590	0.40	0/4864
3	G	0.18	0/588	0.41	0/798
3	H	0.17	0/588	0.40	0/798
3	J	0.17	0/596	0.39	0/808
3	K	0.17	0/596	0.39	0/808
3	L	0.18	0/596	0.39	0/808
3	O	0.16	0/596	0.37	0/808
3	P	0.18	0/588	0.40	0/798
3	Q	0.16	0/588	0.37	0/798
3	R	0.16	0/596	0.40	0/808
3	S	0.19	0/596	0.48	0/808
4	a	0.19	0/2162	0.50	0/2953
5	b	0.27	0/1171	0.56	0/1578
5	p	0.17	0/1194	0.39	0/1608
6	d	0.14	0/1364	0.34	0/1854
7	e	0.17	0/1018	0.42	0/1383
8	g	0.18	0/2273	0.39	0/3062
All	All	0.19	0/37622	0.40	0/50960

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	3846	0	3881	52	0
1	B	3892	0	3925	46	0
1	C	3850	0	3881	60	0
2	D	3525	0	3555	49	0
2	E	3525	0	3555	51	0
2	F	3533	0	3567	54	0
3	G	577	0	614	22	0
3	H	577	0	614	21	0
3	J	585	0	626	20	0
3	K	585	0	626	19	0
3	L	585	0	626	14	0
3	O	585	0	626	22	0
3	P	577	0	614	17	0
3	Q	577	0	614	16	0
3	R	585	0	626	20	0
3	S	585	0	626	24	0
4	a	2104	0	2124	132	0
5	b	1162	0	1161	175	0
5	p	1185	0	1203	124	0
6	d	1347	0	1355	33	0
7	e	1010	0	1048	27	0
8	g	2243	0	2294	34	0
9	A	31	0	12	2	0
9	B	31	0	12	6	0
9	C	31	0	12	3	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	D	27	0	12	6	0
12	E	5	0	0	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
All	All	37172	0	37809	792	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 11.

All (792) 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)
4:a:118:TRP:CZ3	5:b:17:PHE:HD1	1.34	1.44
5:b:12:ILE:HG23	5:b:16:PHE:CE2	1.54	1.42
4:a:118:TRP:HZ3	5:b:17:PHE:CD1	1.43	1.35
4:a:53:MET:SD	4:a:164:ILE:HG12	1.64	1.34
4:a:48:ILE:C	5:b:8:ILE:HD12	1.49	1.33
4:a:53:MET:SD	4:a:164:ILE:CG1	2.22	1.26
5:b:12:ILE:CG2	5:b:16:PHE:CE2	2.20	1.23
4:a:118:TRP:CZ3	5:b:17:PHE:CD1	2.23	1.22
5:b:135:ILE:CG2	5:p:132:ALA:HB1	1.73	1.19
4:a:48:ILE:O	5:b:8:ILE:HD12	1.38	1.18
6:d:168:LYS:HE2	5:p:136:LEU:HD12	1.19	1.18
5:b:135:ILE:HD11	5:p:135:ILE:CG2	1.78	1.13
4:a:49:HIS:HA	5:b:8:ILE:HD13	1.18	1.11
5:b:135:ILE:CD1	5:p:135:ILE:CG2	2.26	1.11
5:b:62:LYS:CE	5:p:64:GLU:HB3	1.78	1.11
4:a:48:ILE:C	5:b:8:ILE:CD1	2.26	1.09
5:b:135:ILE:HG22	5:p:132:ALA:HB1	1.18	1.08
5:b:135:ILE:CD1	5:p:135:ILE:HG21	1.82	1.08
4:a:49:HIS:HA	5:b:8:ILE:CD1	1.85	1.05
5:b:45:ASN:OD1	5:p:47:ALA:HB2	1.56	1.05
5:b:48:GLU:HG2	5:p:54:LEU:HB2	1.38	1.05
5:b:106:LYS:HD2	5:p:109:VAL:HG22	1.36	1.05
5:b:48:GLU:CG	5:p:54:LEU:HB2	1.87	1.04
5:b:135:ILE:HD11	5:p:135:ILE:HG21	1.05	1.03
5:b:16:PHE:O	5:b:20:PHE:HD2	1.41	1.03
5:b:62:LYS:HE2	5:p:64:GLU:HB3	1.04	1.03
4:a:110:PRO:HB3	5:b:25:VAL:HG23	1.42	1.01
5:b:80:ASN:HD21	5:p:83:ALA:CB	1.75	1.00
6:d:119:THR:HG22	6:d:120:ALA:H	1.26	1.00
5:b:135:ILE:CG2	5:p:132:ALA:CB	2.41	0.99
5:b:12:ILE:HG23	5:b:16:PHE:CZ	1.98	0.98
5:b:80:ASN:ND2	5:p:83:ALA:CB	2.27	0.98
4:a:53:MET:SD	4:a:164:ILE:HG13	2.01	0.98
5:p:58:GLN:O	5:p:61:VAL:HG22	1.62	0.97
5:b:102:ARG:HH12	5:p:106:LYS:NZ	1.64	0.96
5:b:80:ASN:ND2	5:p:83:ALA:HB1	1.81	0.96
5:b:62:LYS:HE2	5:p:64:GLU:CB	1.95	0.95
4:a:144:VAL:HG23	4:a:145:PHE:HD2	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:110:PRO:CB	5:b:25:VAL:HG23	1.98	0.93
6:d:168:LYS:CE	5:p:136:LEU:HD12	1.99	0.92
5:b:16:PHE:HB3	5:b:20:PHE:HE2	1.35	0.91
4:a:49:HIS:CA	5:b:8:ILE:HD13	2.01	0.91
4:a:171:SER:HB2	5:b:14:PHE:CD1	2.05	0.91
6:d:168:LYS:HE2	5:p:136:LEU:CD1	2.01	0.91
11:D:502:ADP:H8	11:D:502:ADP:H5'1	1.35	0.90
4:a:57:ILE:HG23	5:b:20:PHE:CZ	2.06	0.90
4:a:171:SER:HB2	5:b:14:PHE:HD1	1.34	0.90
4:a:49:HIS:CA	5:b:8:ILE:CD1	2.51	0.88
5:b:91:ARG:HD2	5:p:94:ALA:CB	2.03	0.88
5:b:135:ILE:HD13	5:p:135:ILE:HB	1.55	0.88
5:b:16:PHE:O	5:b:20:PHE:CD2	2.25	0.87
5:b:96:ALA:HB1	5:b:100:ARG:HH12	1.38	0.87
1:C:18:GLY:HA2	5:b:137:ASN:HD21	1.40	0.86
4:a:168:MET:HE1	5:b:17:PHE:CE1	2.11	0.86
5:b:106:LYS:NZ	5:p:109:VAL:HA	1.93	0.84
5:b:45:ASN:HD22	5:b:46:ALA:N	1.76	0.84
2:E:408:PRO:HB2	2:E:419:PRO:HG2	1.61	0.83
5:p:58:GLN:O	5:p:61:VAL:CG2	2.26	0.83
2:D:156:VAL:HG23	11:D:502:ADP:O2A	1.79	0.83
5:b:16:PHE:HB3	5:b:20:PHE:CE2	2.13	0.83
5:b:146:ASN:HD21	5:p:139:GLN:HB3	1.43	0.82
4:a:88:MET:HE2	5:p:36:ARG:HD2	1.62	0.81
9:C:602:ATP:O1A	9:C:602:ATP:H3'	1.80	0.81
5:b:12:ILE:HG23	5:b:16:PHE:CD2	2.14	0.81
5:b:12:ILE:CG2	5:b:16:PHE:CD2	2.64	0.81
5:p:136:LEU:HD22	5:p:139:GLN:NE2	1.96	0.80
5:b:45:ASN:HB2	5:p:47:ALA:HA	1.61	0.80
6:d:119:THR:HG22	6:d:120:ALA:N	1.93	0.79
5:p:58:GLN:C	5:p:61:VAL:HG22	2.06	0.79
4:a:49:HIS:N	5:b:8:ILE:CD1	2.45	0.79
4:a:49:HIS:N	5:b:8:ILE:HD12	1.98	0.77
5:b:106:LYS:CD	5:p:109:VAL:HG22	2.12	0.77
6:d:119:THR:CG2	6:d:120:ALA:H	1.97	0.76
1:A:300:GLU:HG2	2:D:209:ASN:HB3	1.66	0.76
5:b:45:ASN:CB	5:p:47:ALA:HA	2.15	0.76
5:b:155:LYS:CE	5:p:127:LEU:HB2	2.15	0.76
5:p:136:LEU:CD2	5:p:139:GLN:NE2	2.49	0.76
4:a:57:ILE:CG2	5:b:20:PHE:CZ	2.69	0.76
7:e:20:VAL:HG21	7:e:52:VAL:HB	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:MET:HE3	2:F:60:GLY:HA2	1.69	0.75
5:b:78:GLN:OE1	5:b:81:ARG:NH2	2.21	0.74
5:b:80:ASN:CG	5:p:83:ALA:HB1	2.12	0.74
5:b:106:LYS:CE	5:p:109:VAL:HA	2.17	0.74
4:a:228:LEU:HD21	4:a:279:LEU:HD22	1.70	0.74
5:b:102:ARG:HH12	5:p:106:LYS:HZ1	1.34	0.73
2:F:232:GLU:OE2	2:F:240:ARG:NH2	2.20	0.73
4:a:144:VAL:HG23	4:a:145:PHE:CD2	2.21	0.73
5:b:91:ARG:HD2	5:p:94:ALA:HB1	1.69	0.73
1:C:16:ARG:HB3	6:d:175:ARG:HH22	1.52	0.72
2:D:309:THR:HG21	7:e:137:ARG:HE	1.54	0.72
5:b:135:ILE:CD1	5:p:135:ILE:HG22	2.18	0.72
1:C:10:SER:OG	5:b:127:LEU:HD11	1.89	0.71
5:b:91:ARG:HD2	5:p:94:ALA:HB3	1.72	0.71
5:b:106:LYS:HE3	5:p:109:VAL:HA	1.73	0.71
2:D:273:GLN:NE2	2:D:279:GLU:OE2	2.23	0.71
8:g:199:ASP:OD1	8:g:202:ARG:NH1	2.23	0.71
1:B:407:PHE:HZ	8:g:26:MET:HG3	1.56	0.71
5:b:135:ILE:HG21	5:p:132:ALA:CA	2.21	0.71
1:C:53:MET:HE1	1:C:96:LEU:HD13	1.73	0.71
2:D:119:ALA:HB2	2:D:291:LYS:HD3	1.71	0.71
5:b:135:ILE:HD13	5:p:135:ILE:CB	2.20	0.71
1:C:211:ARG:HH22	2:D:120:ALA:HB3	1.55	0.70
5:b:146:ASN:ND2	5:p:139:GLN:HB3	2.07	0.70
2:D:149:GLY:O	2:D:154:LYS:NZ	2.25	0.70
5:p:58:GLN:HA	5:p:61:VAL:HG22	1.73	0.70
6:d:168:LYS:CE	5:p:136:LEU:CD1	2.66	0.69
6:d:112:ILE:HG12	6:d:154:ILE:HG22	1.73	0.69
3:G:65:ILE:HD11	4:a:219:VAL:HB	1.74	0.69
3:G:10:ILE:HD13	3:S:11:ALA:HB2	1.75	0.69
5:b:48:GLU:OE2	5:p:54:LEU:N	2.26	0.69
5:b:135:ILE:HG21	5:p:132:ALA:HA	1.75	0.69
1:C:96:LEU:HD11	1:C:112:LEU:HD22	1.76	0.68
5:b:69:LYS:HE3	5:p:72:ALA:CB	2.23	0.68
2:D:232:GLU:OE1	2:D:240:ARG:NH1	2.26	0.68
5:b:45:ASN:HD22	5:b:45:ASN:C	2.00	0.68
1:C:17:ILE:HG22	5:b:137:ASN:HD22	1.59	0.67
4:a:253:ILE:HG12	4:a:255:TRP:H	1.58	0.67
5:b:135:ILE:CD1	5:p:135:ILE:CB	2.71	0.67
3:R:59:LEU:HA	3:S:27:PHE:HD2	1.57	0.67
5:b:102:ARG:NH1	5:p:106:LYS:NZ	2.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:228:LEU:HA	4:a:231:ARG:HH12	1.59	0.67
1:B:63:MET:HE3	1:B:65:LEU:HD21	1.76	0.67
2:F:273:GLN:NE2	2:F:279:GLU:OE1	2.28	0.67
4:a:22:THR:HB	4:a:26:MET:HE1	1.77	0.66
6:d:154:ILE:HD11	6:d:161:ILE:HD12	1.77	0.66
1:C:10:SER:OG	5:b:127:LEU:CD1	2.44	0.66
8:g:168:ILE:HD12	8:g:189:VAL:HG21	1.76	0.66
7:e:4:MET:HE2	7:e:76:VAL:HG23	1.78	0.65
2:F:248:ASN:H	2:F:300:ALA:HB3	1.60	0.65
5:b:102:ARG:HH22	5:p:106:LYS:HZ3	1.44	0.65
3:S:57:GLY:HA3	4:a:275:ILE:HG13	1.79	0.65
4:a:79:PRO:HG3	5:b:38:ARG:HH12	1.62	0.65
2:F:182:THR:HG22	2:F:207:GLN:HG2	1.78	0.65
8:g:21:THR:HG1	8:g:253:THR:HG1	1.40	0.65
5:p:58:GLN:CA	5:p:61:VAL:HG22	2.27	0.65
8:g:156:MET:HB3	8:g:168:ILE:HD13	1.79	0.65
4:a:137:ALA:HB1	4:a:155:LYS:HE3	1.79	0.65
5:b:12:ILE:HG21	5:b:16:PHE:CE2	2.27	0.65
1:B:144:ASP:OD1	1:B:304:ARG:NH1	2.30	0.64
2:E:156:VAL:O	2:E:160:GLU:HG2	1.97	0.64
3:G:74:ILE:HD12	3:S:73:PHE:HZ	1.61	0.64
5:b:65:LEU:O	5:b:69:LYS:HG2	1.97	0.64
5:p:136:LEU:HD22	5:p:139:GLN:HE22	1.62	0.64
1:A:162:ARG:NH1	1:A:256:ASP:OD2	2.30	0.64
2:D:371:ARG:HH22	2:D:394:VAL:HG21	1.62	0.64
1:A:208:ASN:OD1	1:A:211:ARG:NH2	2.30	0.64
1:A:68:GLU:O	2:D:63:ARG:NH1	2.31	0.64
4:a:195:LEU:HD22	4:a:216:LEU:HD13	1.78	0.64
5:b:69:LYS:HE3	5:p:72:ALA:HB1	1.78	0.63
2:F:194:ASP:OD1	2:F:195:SER:N	2.30	0.63
5:b:106:LYS:HZ1	5:p:109:VAL:HA	1.61	0.63
1:B:162:ARG:NH1	1:B:256:ASP:OD2	2.30	0.63
4:a:162:PRO:O	4:a:166:LEU:HG	1.99	0.63
3:L:11:ALA:HB2	3:O:10:ILE:HD13	1.81	0.63
3:Q:11:ALA:HB2	3:R:10:ILE:HD13	1.80	0.63
8:g:170:LEU:HB2	8:g:188:LEU:HD23	1.80	0.62
1:A:165:ARG:NH2	1:A:302:ALA:O	2.30	0.62
4:a:228:LEU:HD23	4:a:231:ARG:HH12	1.63	0.62
5:p:58:GLN:HA	5:p:61:VAL:CG2	2.29	0.62
2:E:223:LEU:HD21	2:E:286:ARG:HB2	1.81	0.62
1:A:473:ILE:O	1:A:477:ARG:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:43:GLU:OE2	7:e:22:MET:HE1	2.00	0.62
4:a:129:PRO:HG2	4:a:132:TRP:CD2	2.34	0.61
4:a:57:ILE:HG13	5:b:16:PHE:CD2	2.35	0.61
2:E:178:VAL:HG22	2:E:218:VAL:HG23	1.82	0.61
2:F:381:ILE:HD13	8:g:26:MET:HE2	1.81	0.61
4:a:49:HIS:CA	5:b:8:ILE:HD12	2.25	0.61
5:b:135:ILE:CD1	5:p:135:ILE:HB	2.27	0.61
1:C:10:SER:CB	5:b:127:LEU:HD11	2.31	0.61
9:B:601:ATP:H8	9:B:601:ATP:C5'	2.13	0.61
5:b:102:ARG:NH1	5:p:106:LYS:HZ1	1.98	0.61
1:C:152:LYS:HG2	1:C:445:GLN:HG2	1.82	0.61
2:E:232:GLU:OE1	2:E:240:ARG:NH2	2.24	0.61
2:F:24:PRO:O	2:F:44:GLN:NE2	2.34	0.61
4:a:57:ILE:HD12	5:b:20:PHE:CE2	2.36	0.61
9:B:601:ATP:H8	9:B:601:ATP:O5'	1.84	0.60
11:D:502:ADP:H5'1	11:D:502:ADP:C8	2.28	0.60
1:C:175:GLY:HA2	9:C:602:ATP:O2A	2.01	0.60
2:E:353:VAL:HG23	2:E:354:VAL:HG13	1.82	0.60
3:G:11:ALA:HB2	3:H:10:ILE:HD13	1.83	0.60
5:p:35:GLU:O	5:p:39:LYS:HE3	2.01	0.60
3:S:19:GLY:HA2	3:S:63:PRO:HB3	1.83	0.60
5:b:35:GLU:OE1	5:b:35:GLU:N	2.28	0.60
5:b:114:ASN:OD1	5:b:115:SER:N	2.36	0.59
9:B:601:ATP:C5'	9:B:601:ATP:C8	2.86	0.59
4:a:152:VAL:HG13	4:a:153:TYR:H	1.66	0.59
5:b:90:ALA:O	5:b:93:GLN:NE2	2.35	0.59
1:A:41:ARG:NH2	1:A:71:SER:OG	2.34	0.59
2:D:243:LEU:HD23	2:D:296:THR:HB	1.85	0.59
5:p:136:LEU:HA	5:p:139:GLN:HG2	1.84	0.59
1:A:357:GLU:HG2	1:A:360:LEU:HD13	1.84	0.59
4:a:231:ARG:O	4:a:235:ASN:ND2	2.36	0.59
1:A:33:VAL:HG12	1:A:34:MET:HG3	1.84	0.59
1:B:208:ASN:OD1	1:B:211:ARG:NH2	2.36	0.59
9:B:601:ATP:C8	9:B:601:ATP:H5'1	2.38	0.59
4:a:240:GLU:O	4:a:244:ILE:HD12	2.03	0.59
8:g:47:ASP:OD1	8:g:50:ARG:NH2	2.35	0.58
1:C:334:GLN:HB3	2:D:309:THR:HG23	1.85	0.58
2:F:223:LEU:HD21	2:F:286:ARG:HB2	1.85	0.58
3:H:51:ARG:HH21	3:J:45:ALA:HB1	1.69	0.58
4:a:239:GLY:HA2	4:a:261:TRP:HH2	1.69	0.58
5:b:96:ALA:HB1	5:b:100:ARG:NH1	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ALA:HB1	1:A:260:ILE:HD13	1.86	0.58
4:a:118:TRP:CE3	5:b:17:PHE:CD1	2.88	0.58
3:G:40:ARG:HH22	3:H:40:ARG:HD2	1.67	0.58
4:a:15:LYS:HE3	4:a:15:LYS:HA	1.83	0.58
5:b:48:GLU:HG3	5:p:54:LEU:HB2	1.79	0.58
8:g:138:THR:HG22	8:g:139:GLN:HG2	1.85	0.58
2:D:336:TYR:CG	11:D:502:ADP:C2	2.91	0.58
6:d:135:ASN:C	6:d:135:ASN:HD22	2.11	0.58
5:b:83:ALA:HA	5:b:86:LEU:HD12	1.86	0.58
5:b:81:ARG:NH1	5:b:85:GLN:OE1	2.35	0.57
2:E:55:MET:HE1	2:E:217:ARG:HG3	1.85	0.57
5:p:89:GLU:OE2	5:p:93:GLN:NE2	2.37	0.57
3:S:44:LEU:HG	3:S:47:GLN:HE21	1.67	0.57
3:Q:36:GLU:OE2	3:Q:40:ARG:NH2	2.37	0.57
3:G:53:PHE:CE2	4:a:282:VAL:HG11	2.40	0.57
3:P:43:GLU:OE2	7:e:22:MET:CE	2.52	0.57
5:b:135:ILE:HD12	5:p:135:ILE:HG22	1.85	0.57
4:a:57:ILE:HG13	5:b:16:PHE:HD2	1.69	0.57
1:B:180:ALA:HB1	1:B:260:ILE:HD13	1.87	0.57
1:C:413:ASP:OD1	8:g:85:ARG:NH2	2.37	0.57
5:b:62:LYS:CD	5:p:64:GLU:HB3	2.35	0.57
8:g:104:LYS:NZ	8:g:129:TYR:OH	2.38	0.57
5:b:35:GLU:H	5:b:35:GLU:CD	2.13	0.56
3:L:59:LEU:HA	3:O:27:PHE:HD2	1.69	0.56
1:B:427:ARG:HG2	1:B:465:ILE:HD11	1.87	0.56
1:C:230:ALA:HB2	2:D:285:GLU:HG3	1.87	0.56
3:O:44:LEU:HD21	3:P:42:PRO:HB3	1.88	0.56
1:B:401:TYR:HB2	1:B:425:GLY:HA3	1.88	0.56
5:b:118:GLU:O	5:b:121:ARG:HG2	2.05	0.56
8:g:96:PHE:HA	8:g:99:VAL:HG12	1.87	0.56
1:B:279:ARG:HA	2:E:266:MET:HE3	1.87	0.56
1:C:17:ILE:HG22	5:b:137:ASN:ND2	2.19	0.56
1:B:416:GLU:OE1	1:B:419:ARG:NH2	2.38	0.56
4:a:115:ILE:HG22	5:b:17:PHE:CZ	2.41	0.56
2:F:82:THR:HG22	2:F:87:MET:HE1	1.88	0.56
4:a:228:LEU:HA	4:a:231:ARG:NH1	2.20	0.56
7:e:71:VAL:HG23	7:e:76:VAL:HG22	1.87	0.55
3:S:70:GLY:O	3:S:74:ILE:HG12	2.06	0.55
6:d:109:ASP:OD1	6:d:139:THR:OG1	2.20	0.55
1:A:386:ILE:HD11	1:A:492:ASP:N	2.22	0.55
1:C:107:ARG:NH1	1:C:119:LYS:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:41:GLN:HB3	3:K:44:LEU:HD13	1.87	0.55
1:A:134:ALA:HB3	2:D:209:ASN:HD22	1.70	0.55
1:B:33:VAL:HG12	1:B:34:MET:HG3	1.89	0.55
1:C:208:ASN:OD1	1:C:211:ARG:NH2	2.39	0.55
4:a:129:PRO:HG3	5:p:14:PHE:HE1	1.72	0.55
1:C:180:ALA:HB1	1:C:260:ILE:HD13	1.88	0.55
3:S:11:ALA:HA	3:S:14:ILE:HD12	1.89	0.55
2:D:127:THR:HG22	2:D:165:ILE:HD11	1.88	0.55
5:p:136:LEU:HD23	5:p:139:GLN:NE2	2.22	0.55
1:C:162:ARG:NH1	1:C:256:ASP:OD2	2.38	0.55
3:G:55:ILE:HD11	3:H:52:MET:HE2	1.88	0.55
4:a:71:ALA:CB	5:b:27:PRO:HB3	2.36	0.55
5:b:106:LYS:HD2	5:p:109:VAL:CG2	2.25	0.55
1:A:489:GLU:HG3	1:A:490:THR:HG23	1.89	0.55
5:b:21:CYS:SG	5:b:22:MET:N	2.79	0.55
4:a:119:ILE:HA	4:a:122:MET:HE3	1.89	0.54
5:b:127:LEU:O	5:b:130:THR:OG1	2.21	0.54
2:E:41:VAL:HA	2:E:52:THR:HG22	1.90	0.54
5:b:113:ILE:HG23	5:b:117:ARG:NH2	2.23	0.54
1:C:140:ARG:NH1	2:E:182:THR:OG1	2.40	0.54
2:E:161:LEU:HD13	2:E:298:ILE:HD13	1.89	0.54
5:b:135:ILE:HG21	5:p:132:ALA:CB	2.33	0.54
5:p:22:MET:HA	5:p:26:TRP:CD1	2.43	0.54
1:B:338:VAL:HG11	1:B:355:PHE:HE1	1.72	0.54
4:a:183:GLU:OE1	4:a:183:GLU:N	2.38	0.54
3:K:11:ALA:HB2	3:L:10:ILE:HD13	1.90	0.54
4:a:101:PHE:HD2	4:a:281:ILE:HG22	1.73	0.54
5:p:45:ASN:HB3	5:p:49:LYS:NZ	2.22	0.54
1:A:43:HIS:CE1	6:d:51:PRO:HD3	2.43	0.54
5:b:102:ARG:HH12	5:p:106:LYS:HZ3	1.50	0.54
1:A:63:MET:HE3	1:A:96:LEU:HD22	1.89	0.54
3:H:70:GLY:O	3:H:74:ILE:HG12	2.08	0.53
8:g:32:MET:SD	8:g:243:SER:OG	2.61	0.53
5:p:22:MET:HA	5:p:26:TRP:HD1	1.73	0.53
1:B:260:ILE:HG12	1:B:328:LEU:HB2	1.89	0.53
4:a:101:PHE:HZ	4:a:282:VAL:HG22	1.73	0.53
4:a:118:TRP:CD1	4:a:122:MET:HE2	2.43	0.53
5:p:18:VAL:O	5:p:22:MET:HG2	2.09	0.53
2:E:454:ILE:HA	2:E:457:VAL:HG12	1.91	0.53
3:R:33:ARG:NH1	3:S:36:GLU:OE1	2.42	0.53
3:R:44:LEU:HB3	3:R:48:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:277:MET:O	4:a:281:ILE:HG13	2.09	0.53
5:b:81:ARG:HH11	5:b:85:GLN:CD	2.15	0.53
7:e:88:ASN:OD1	7:e:89:LEU:N	2.34	0.53
1:A:386:ILE:H	1:A:386:ILE:HD12	1.74	0.53
1:C:18:GLY:HA2	5:b:137:ASN:ND2	2.18	0.53
2:E:270:VAL:HG12	2:E:270:VAL:O	2.08	0.53
3:O:79:PHE:HD1	3:P:5:LEU:HB3	1.73	0.53
1:B:351:ASP:OD2	2:F:183:ARG:NE	2.42	0.53
3:H:61:ALA:O	3:H:65:ILE:HG12	2.09	0.53
2:D:159:MET:HE1	2:D:188:PHE:HD1	1.73	0.53
1:C:251:ARG:NH1	1:C:301:ARG:O	2.41	0.53
5:b:155:LYS:HE3	5:p:127:LEU:HB2	1.90	0.53
5:p:66:ASP:OD1	5:p:67:ALA:N	2.42	0.53
3:J:70:GLY:O	3:J:74:ILE:HG12	2.09	0.53
6:d:135:ASN:C	6:d:135:ASN:ND2	2.66	0.52
3:G:79:PHE:HE2	3:H:9:ALA:HB2	1.74	0.52
3:S:44:LEU:HB3	3:S:48:LEU:HD13	1.90	0.52
1:B:377:ARG:HH21	2:F:181:ARG:HH22	1.57	0.52
4:a:265:HIS:HA	4:a:268:VAL:HG12	1.91	0.52
1:A:152:LYS:HE3	1:A:432:MET:HA	1.92	0.52
1:A:173:GLN:HA	9:A:601:ATP:PB	2.49	0.52
3:Q:79:PHE:CD1	3:R:5:LEU:HB3	2.44	0.52
4:a:163:ASN:OD1	4:a:164:ILE:HD12	2.10	0.52
2:E:155:THR:HG22	2:E:159:MET:HE2	1.90	0.52
2:F:165:ILE:HG12	2:F:243:LEU:HD13	1.91	0.52
5:b:103:GLN:O	5:b:107:GLU:HG2	2.09	0.52
1:C:16:ARG:HB2	6:d:175:ARG:HH12	1.74	0.52
3:G:15:LEU:HD21	3:H:13:ALA:HA	1.91	0.52
1:C:296:SER:OG	2:E:208:MET:O	2.21	0.52
2:E:89:VAL:HG21	2:E:214:ASN:HA	1.91	0.52
3:G:65:ILE:HD12	4:a:215:ILE:HG23	1.91	0.52
5:b:58:GLN:O	5:b:61:VAL:HG12	2.10	0.52
5:b:106:LYS:HA	5:b:109:VAL:HG12	1.92	0.52
1:A:144:ASP:OD1	1:A:304:ARG:NH1	2.36	0.52
1:A:423:GLU:O	1:A:427:ARG:HG2	2.10	0.52
1:B:407:PHE:CZ	8:g:26:MET:HG3	2.43	0.52
2:D:381:ILE:HD12	7:e:125:ALA:HB2	1.92	0.52
3:O:1:MET:O	3:O:4:THR:OG1	2.20	0.52
4:a:99:ASP:OD1	4:a:100:THR:N	2.42	0.52
2:E:210:GLU:HB3	2:E:214:ASN:HD22	1.74	0.52
2:F:189:TYR:HD1	2:F:203:MET:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:133:GLU:HG3	5:b:147:ALA:HB3	1.91	0.52
8:g:126:PHE:HA	8:g:129:TYR:HB3	1.91	0.52
1:A:296:SER:HB2	2:D:208:MET:HG2	1.92	0.51
1:A:138:ILE:HG21	2:D:95:ASP:HA	1.92	0.51
1:C:175:GLY:N	9:C:602:ATP:O1B	2.35	0.51
3:L:73:PHE:O	3:L:77:ASN:HB3	2.09	0.51
1:C:140:ARG:HB2	2:E:186:ASN:HD22	1.75	0.51
4:a:53:MET:CE	4:a:164:ILE:HG23	2.41	0.51
1:A:45:LEU:HB3	1:A:48:ALA:HB2	1.92	0.51
2:D:180:GLU:OE2	2:D:248:ASN:ND2	2.26	0.51
2:E:254:LEU:O	2:E:258:GLU:HG3	2.10	0.51
3:K:44:LEU:HB3	3:K:48:LEU:HD13	1.90	0.51
3:O:51:ARG:HH21	3:P:45:ALA:HB1	1.75	0.51
4:a:115:ILE:HG22	5:b:17:PHE:CE1	2.45	0.51
4:a:196:ASN:HD22	4:a:212:VAL:HG12	1.76	0.51
5:b:12:ILE:HG22	5:b:16:PHE:CD2	2.44	0.51
5:b:59:ALA:O	5:b:62:LYS:HG2	2.11	0.51
1:B:107:ARG:NH1	1:B:119:LYS:HB2	2.25	0.51
4:a:97:VAL:HG22	4:a:281:ILE:HD13	1.93	0.51
4:a:144:VAL:CG2	4:a:145:PHE:CD2	2.93	0.51
4:a:171:SER:HB2	5:b:14:PHE:CE1	2.44	0.51
5:b:136:LEU:HD21	5:b:146:ASN:H	1.75	0.51
3:L:59:LEU:HA	3:O:27:PHE:CD2	2.46	0.51
3:Q:10:ILE:O	3:Q:14:ILE:HG12	2.11	0.51
5:b:69:LYS:HE3	5:p:72:ALA:HB2	1.93	0.51
1:B:144:ASP:OD1	1:B:144:ASP:N	2.44	0.51
5:p:60:GLN:O	5:p:64:GLU:HG2	2.11	0.51
2:E:156:VAL:HA	2:E:159:MET:HE3	1.93	0.50
3:P:70:GLY:O	3:P:74:ILE:HG12	2.10	0.50
5:b:22:MET:O	5:b:25:VAL:HG12	2.11	0.50
5:b:135:ILE:CG2	5:p:132:ALA:CA	2.83	0.50
2:F:93:PRO:HG3	2:F:100:VAL:HG23	1.93	0.50
5:p:133:GLU:OE2	5:p:137:ASN:ND2	2.45	0.50
2:E:363:ARG:NH1	2:E:366:GLN:OE1	2.34	0.50
3:O:79:PHE:CD1	3:P:5:LEU:HB3	2.46	0.50
4:a:53:MET:CG	4:a:164:ILE:HG13	2.40	0.50
7:e:11:VAL:HG11	8:g:146:LEU:HD22	1.93	0.50
2:E:350:ASP:HB3	2:E:353:VAL:HG22	1.93	0.50
3:H:4:THR:HG23	3:J:2:GLU:HB3	1.94	0.50
3:Q:70:GLY:O	3:Q:74:ILE:HG12	2.10	0.50
5:b:34:SER:O	5:b:38:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:ILE:HD11	2:D:283:LEU:HD21	1.93	0.50
2:E:127:THR:C	2:E:164:ASN:HD21	2.19	0.50
4:a:160:THR:HB	4:a:236:MET:HB3	1.93	0.50
2:F:76:VAL:HG11	2:F:221:THR:HG23	1.92	0.50
2:F:159:MET:HB3	2:F:411:VAL:HG11	1.94	0.50
8:g:81:VAL:HG11	8:g:234:VAL:HG22	1.94	0.50
5:p:107:GLU:O	5:p:111:GLN:HG2	2.12	0.50
6:d:169:LEU:O	6:d:173:ARG:HG3	2.11	0.50
1:A:282:PRO:HB2	1:A:286:ALA:HA	1.94	0.50
1:A:443:ALA:HB2	1:A:487:ILE:HG13	1.94	0.50
1:C:53:MET:O	1:C:92:THR:OG1	2.26	0.50
5:p:3:ILE:O	5:p:6:THR:OG1	2.27	0.50
5:p:13:ALA:HB1	5:p:17:PHE:HE2	1.77	0.50
1:C:273:GLN:NE2	2:D:278:GLU:OE1	2.35	0.49
3:S:64:MET:HE1	4:a:235:ASN:HA	1.93	0.49
5:b:27:PRO:HA	5:b:30:ILE:HD12	1.94	0.49
4:a:201:SER:HB3	4:a:204:VAL:HB	1.94	0.49
7:e:23:LEU:HD13	7:e:76:VAL:HG11	1.94	0.49
3:R:73:PHE:HZ	3:S:74:ILE:HD12	1.77	0.49
4:a:57:ILE:CG2	5:b:20:PHE:HZ	2.24	0.49
3:P:47:GLN:HE21	3:P:51:ARG:CZ	2.26	0.49
4:a:276:PHE:O	4:a:280:THR:HG23	2.12	0.49
1:C:348:SER:O	2:E:181:ARG:NH2	2.45	0.49
4:a:108:ILE:O	4:a:111:LEU:HG	2.13	0.49
8:g:4:LEU:HB3	8:g:267:TYR:HE1	1.77	0.49
1:C:353:GLN:HG3	1:C:355:PHE:CE2	2.48	0.49
4:a:157:VAL:HB	4:a:158:PRO:HD2	1.95	0.49
5:b:139:GLN:HG2	5:b:141:ASP:H	1.78	0.49
3:K:70:GLY:O	3:K:74:ILE:HG12	2.12	0.49
5:p:34:SER:O	5:p:38:ARG:HG2	2.13	0.49
5:p:139:GLN:O	5:p:139:GLN:HG3	2.13	0.49
2:E:89:VAL:HG22	2:E:218:VAL:HG12	1.94	0.49
2:F:253:THR:O	2:F:257:THR:HG23	2.12	0.48
5:p:45:ASN:HB3	5:p:49:LYS:HZ3	1.77	0.48
2:F:147:PHE:HZ	2:F:317:PHE:HE1	1.61	0.48
4:a:80:THR:HG22	4:a:83:GLN:HG2	1.95	0.48
4:a:83:GLN:HA	4:a:86:ILE:HG22	1.95	0.48
5:b:45:ASN:HB3	5:p:47:ALA:CB	2.43	0.48
5:b:80:ASN:ND2	5:p:83:ALA:HB3	2.26	0.48
5:b:145:HIS:NE2	5:b:148:MET:HB2	2.29	0.48
2:F:329:ASP:OD1	2:F:330:ILE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:87:GLU:OE2	5:b:35:GLU:HB3	2.13	0.48
5:b:80:ASN:O	5:p:87:ILE:HD11	2.13	0.48
2:D:173:SER:HB2	2:D:201:VAL:HG12	1.96	0.48
2:F:377:ASP:OD1	2:F:378:ILE:N	2.46	0.48
2:F:382:LEU:HD11	8:g:32:MET:HE1	1.95	0.48
2:D:371:ARG:NH2	2:D:394:VAL:HG21	2.29	0.48
3:H:11:ALA:HB1	3:J:13:ALA:HB2	1.95	0.48
7:e:65:SER:OG	7:e:82:THR:OG1	2.31	0.48
1:B:202:LYS:NZ	2:E:321:ASP:OD1	2.47	0.48
3:J:59:LEU:HA	3:K:27:PHE:CD2	2.49	0.48
3:O:18:PHE:HB2	3:P:17:ALA:HB1	1.96	0.48
5:b:139:GLN:C	5:b:141:ASP:H	2.21	0.48
1:A:418:THR:HG22	2:D:446:GLN:HE22	1.78	0.48
1:B:107:ARG:NH2	1:B:120:GLY:O	2.47	0.48
6:d:172:MET:HE2	5:p:129:VAL:HG11	1.95	0.48
3:K:15:LEU:HD21	3:L:13:ALA:HA	1.95	0.48
3:R:71:LEU:HA	3:R:74:ILE:HG22	1.95	0.48
1:B:152:LYS:HG2	1:B:445:GLN:HG2	1.96	0.48
3:R:1:MET:HE2	3:R:1:MET:HA	1.96	0.48
5:b:108:ALA:O	5:b:111:GLN:HG2	2.14	0.48
1:A:460:VAL:HB	1:A:464:LYS:HE2	1.96	0.47
2:F:257:THR:HG22	2:F:273:GLN:OE1	2.14	0.47
3:Q:79:PHE:HD1	3:R:5:LEU:HB3	1.79	0.47
4:a:132:TRP:CD1	5:p:7:LEU:HD22	2.48	0.47
1:B:199:ILE:HD11	1:B:240:PRO:HG3	1.95	0.47
1:B:357:GLU:HG2	1:B:370:ASN:HB2	1.95	0.47
1:C:107:ARG:NH2	1:C:120:GLY:O	2.47	0.47
4:a:79:PRO:HG3	5:b:38:ARG:NH1	2.28	0.47
5:b:48:GLU:OE2	5:p:54:LEU:CA	2.62	0.47
5:b:119:GLU:O	5:b:123:GLN:HG3	2.14	0.47
5:p:136:LEU:CD2	5:p:139:GLN:HE22	2.23	0.47
1:C:10:SER:HB3	5:b:127:LEU:HD21	1.96	0.47
3:J:11:ALA:HB2	3:K:10:ILE:HD13	1.96	0.47
3:O:44:LEU:HB3	3:O:48:LEU:HD13	1.96	0.47
5:b:46:ALA:HA	5:b:49:LYS:NZ	2.29	0.47
2:E:133:ASP:HB3	2:E:425:LEU:HD13	1.96	0.47
3:G:47:GLN:O	3:G:51:ARG:HG2	2.15	0.47
4:a:259:VAL:HB	4:a:260:PRO:HD3	1.96	0.47
1:A:374:SER:O	1:A:395:ARG:HD2	2.14	0.47
1:A:477:ARG:HG3	1:A:477:ARG:HH11	1.79	0.47
3:O:44:LEU:HD11	7:e:35:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:73:PHE:O	3:P:77:ASN:HB3	2.15	0.47
1:B:423:GLU:OE1	1:B:427:ARG:NH1	2.38	0.47
3:Q:15:LEU:HD21	3:R:13:ALA:HA	1.97	0.47
4:a:67:PHE:CD2	4:a:86:ILE:HD11	2.50	0.47
4:a:271:LEU:O	4:a:275:ILE:HG12	2.15	0.47
4:a:282:VAL:O	4:a:285:SER:OG	2.32	0.47
5:b:80:ASN:HD21	5:p:83:ALA:HB2	1.69	0.47
2:E:156:VAL:HA	2:E:159:MET:CE	2.44	0.47
2:F:328:ARG:HG2	2:F:328:ARG:HH11	1.80	0.47
3:K:11:ALA:HB1	3:L:13:ALA:HB2	1.97	0.47
1:A:218:ALA:O	1:A:222:THR:OG1	2.23	0.47
1:C:16:ARG:NH2	6:d:174:THR:O	2.48	0.47
4:a:110:PRO:O	4:a:113:LEU:HG	2.15	0.47
5:b:146:ASN:HD21	5:p:139:GLN:CB	2.21	0.47
1:A:386:ILE:HG13	1:A:493:TYR:HB2	1.97	0.47
2:E:146:LEU:HD23	2:E:324:VAL:HB	1.97	0.47
6:d:110:VAL:HG12	6:d:156:ALA:HB2	1.97	0.47
2:D:8:GLN:HB2	2:D:15:ASP:OD1	2.15	0.46
2:E:56:GLY:O	2:E:211:PRO:HG2	2.15	0.46
2:F:123:ASP:O	2:F:124:LEU:HG	2.15	0.46
3:Q:63:PRO:O	3:Q:67:VAL:HG23	2.15	0.46
1:A:164:GLN:NE2	1:A:166:GLU:OE1	2.48	0.46
1:B:9:ILE:HD11	1:B:33:VAL:HG13	1.96	0.46
3:R:11:ALA:HB1	3:S:13:ALA:HB2	1.97	0.46
1:A:260:ILE:HG12	1:A:328:LEU:HB2	1.97	0.46
9:B:601:ATP:H8	9:B:601:ATP:H5'1	1.77	0.46
3:G:70:GLY:O	3:G:74:ILE:HG12	2.15	0.46
2:D:155:THR:O	2:D:159:MET:HG2	2.15	0.46
4:a:140:VAL:HA	4:a:143:ASN:ND2	2.31	0.46
5:b:102:ARG:NH2	5:p:106:LYS:HZ3	2.10	0.46
3:S:27:PHE:CE1	3:S:59:LEU:HD22	2.50	0.46
2:D:85:ARG:NH2	2:D:98:GLY:O	2.42	0.46
7:e:109:LYS:HE3	8:g:31:LYS:HE2	1.96	0.46
1:C:112:LEU:HD11	1:C:235:MET:HE1	1.98	0.46
2:D:336:TYR:HB3	11:D:502:ADP:N1	2.31	0.46
2:E:234:ASP:O	2:E:235:GLU:HG2	2.15	0.46
2:F:381:ILE:HD13	8:g:26:MET:CE	2.44	0.46
5:b:45:ASN:CB	5:p:47:ALA:CA	2.92	0.46
3:H:33:ARG:HB3	3:J:36:GLU:OE2	2.15	0.46
5:b:155:LYS:NZ	5:p:127:LEU:HB2	2.30	0.46
1:B:52:GLU:OE2	1:B:91:CYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:502:ADP:H8	11:D:502:ADP:C5'	2.18	0.46
2:E:152:VAL:HG22	2:E:153:GLY:H	1.81	0.46
7:e:109:LYS:HE3	8:g:31:LYS:CE	2.46	0.46
2:D:192:MET:HA	2:D:192:MET:HE2	1.97	0.46
3:H:10:ILE:O	3:H:14:ILE:HG12	2.15	0.46
3:Q:7:LEU:HA	3:Q:10:ILE:HG22	1.98	0.46
3:Q:8:VAL:HG11	3:Q:77:ASN:HD22	1.81	0.46
5:b:117:ARG:HA	5:b:117:ARG:HD3	1.55	0.46
1:A:37:ASP:OD2	2:F:265:ARG:NH1	2.46	0.45
4:a:159:SER:HB2	4:a:164:ILE:HG12	1.97	0.45
1:B:106:GLY:HA2	1:B:219:MET:HG3	1.98	0.45
3:J:51:ARG:HH12	3:K:45:ALA:HB1	1.81	0.45
3:O:11:ALA:HB1	3:P:13:ALA:HB2	1.97	0.45
3:R:21:LEU:O	3:R:25:ILE:HG12	2.16	0.45
3:R:72:PHE:CE2	3:R:78:PRO:HD3	2.51	0.45
8:g:58:GLN:HE22	8:g:199:ASP:HB3	1.81	0.45
1:A:407:PHE:CZ	2:D:384:MET:HE1	2.52	0.45
1:C:18:GLY:CA	5:b:137:ASN:HD21	2.22	0.45
1:C:457:MET:HE2	1:C:468:PHE:CD2	2.52	0.45
3:G:13:ALA:HA	3:S:15:LEU:HD21	1.98	0.45
3:G:73:PHE:HZ	3:H:74:ILE:HD12	1.80	0.45
3:R:6:GLY:O	3:R:10:ILE:HG12	2.16	0.45
4:a:214:LEU:HA	4:a:217:GLU:OE1	2.16	0.45
5:p:130:THR:O	5:p:134:LYS:HG2	2.15	0.45
1:B:443:ALA:HB1	1:B:484:MET:SD	2.56	0.45
3:J:15:LEU:HD21	3:K:13:ALA:HA	1.97	0.45
3:L:47:GLN:O	3:L:51:ARG:HG2	2.17	0.45
3:O:73:PHE:O	3:O:77:ASN:HB3	2.16	0.45
4:a:125:MET:HE2	4:a:125:MET:HA	1.98	0.45
8:g:58:GLN:NE2	8:g:199:ASP:O	2.48	0.45
2:E:155:THR:O	2:E:159:MET:HE2	2.17	0.45
3:S:43:GLU:HG2	3:S:44:LEU:HD12	1.97	0.45
4:a:85:ALA:HA	4:a:88:MET:HG3	1.98	0.45
4:a:104:LYS:HE2	4:a:106:ARG:HG2	1.99	0.45
4:a:110:PRO:O	4:a:114:THR:HG23	2.16	0.45
1:C:33:VAL:HG21	1:C:43:HIS:ND1	2.31	0.45
1:C:260:ILE:HG12	1:C:328:LEU:HB2	1.98	0.45
2:D:41:VAL:HA	2:D:52:THR:HG22	1.99	0.45
2:F:123:ASP:OD1	2:F:124:LEU:N	2.40	0.45
3:J:44:LEU:HB3	3:J:48:LEU:HD13	1.98	0.45
4:a:48:ILE:C	5:b:8:ILE:HD11	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:59:ALA:HA	5:b:62:LYS:HE3	1.98	0.45
1:B:318:VAL:HG12	1:B:318:VAL:O	2.17	0.45
2:F:41:VAL:HA	2:F:52:THR:HG22	1.99	0.45
3:G:73:PHE:O	3:G:77:ASN:HB3	2.17	0.45
3:R:71:LEU:O	3:R:74:ILE:HG22	2.17	0.45
5:b:106:LYS:NZ	5:p:109:VAL:CA	2.72	0.45
7:e:41:LEU:HA	8:g:209:ILE:H	1.81	0.45
5:p:58:GLN:O	5:p:61:VAL:HG23	2.15	0.45
1:A:70:ASP:OD1	1:A:70:ASP:N	2.50	0.45
1:B:109:VAL:HG21	1:B:246:MET:HE1	1.98	0.45
2:E:425:LEU:O	2:E:429:ILE:HG12	2.17	0.45
1:C:9:ILE:HG13	1:C:10:SER:N	2.32	0.45
1:C:10:SER:O	1:C:14:LYS:HG2	2.16	0.45
2:E:127:THR:O	2:E:164:ASN:ND2	2.42	0.45
3:L:51:ARG:HH21	3:O:45:ALA:HB1	1.82	0.45
5:b:100:ARG:HA	5:b:103:GLN:HG2	1.98	0.45
1:A:173:GLN:HA	9:A:601:ATP:O3B	2.17	0.44
2:E:418:ALA:N	2:E:419:PRO:HD3	2.33	0.44
3:Q:73:PHE:O	3:Q:77:ASN:HB3	2.16	0.44
4:a:152:VAL:HG13	4:a:153:TYR:N	2.31	0.44
4:a:198:PHE:O	4:a:199:ASN:ND2	2.50	0.44
5:p:124:VAL:O	5:p:127:LEU:HG	2.17	0.44
2:E:214:ASN:O	2:E:218:VAL:HG13	2.17	0.44
3:J:60:ASP:OD1	3:J:60:ASP:N	2.49	0.44
4:a:53:MET:O	4:a:57:ILE:HG12	2.17	0.44
6:d:28:TRP:HZ2	6:d:73:ALA:HB1	1.82	0.44
7:e:91:GLU:OE1	7:e:94:ILE:HD13	2.17	0.44
7:e:116:ALA:HB3	8:g:24:MET:HE3	1.99	0.44
1:B:107:ARG:HH12	1:B:119:LYS:HB2	1.82	0.44
4:a:128:ILE:HA	5:p:14:PHE:HZ	1.81	0.44
5:b:84:ALA:HB2	5:p:87:ILE:HD13	2.00	0.44
1:C:432:MET:HA	1:C:432:MET:HE2	1.99	0.44
2:F:404:PHE:HD2	2:F:432:PHE:CZ	2.35	0.44
3:K:35:LEU:HA	3:K:38:VAL:HG12	1.98	0.44
5:p:81:ARG:HG2	5:p:81:ARG:HH11	1.82	0.44
1:A:415:ASP:OD1	1:A:415:ASP:N	2.51	0.44
2:D:285:GLU:OE1	2:D:285:GLU:HA	2.18	0.44
2:E:159:MET:HG2	2:E:192:MET:HE3	1.99	0.44
2:F:159:MET:HE1	2:F:192:MET:HA	1.99	0.44
3:K:3:LEU:HD23	3:L:3:LEU:HD22	1.99	0.44
3:R:63:PRO:O	3:R:67:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:224:ARG:HB3	4:a:283:TYR:HE2	1.82	0.44
5:b:108:ALA:HA	5:b:111:GLN:NE2	2.33	0.44
7:e:120:ALA:O	7:e:124:THR:HG23	2.18	0.44
1:C:279:ARG:HA	2:D:266:MET:HE3	2.00	0.44
2:D:81:ALA:HB3	2:D:102:THR:HB	1.98	0.44
2:E:128:GLY:N	2:E:133:ASP:OD2	2.49	0.44
4:a:57:ILE:HG23	5:b:20:PHE:CE2	2.52	0.44
4:a:216:LEU:O	4:a:220:THR:OG1	2.34	0.44
1:B:413:ASP:OD2	8:g:30:SER:OG	2.35	0.44
5:b:81:ARG:NH1	5:b:82:ARG:HA	2.33	0.44
5:b:100:ARG:O	5:b:103:GLN:HG2	2.17	0.44
6:d:119:THR:CG2	6:d:120:ALA:N	2.61	0.44
8:g:189:VAL:HB	8:g:190:PRO:HD3	2.00	0.44
1:A:5:ASN:O	1:A:9:ILE:HG12	2.18	0.44
1:A:420:LYS:O	1:A:423:GLU:HG2	2.18	0.44
1:C:475:TYR:HD1	5:p:82:ARG:HH22	1.65	0.44
1:B:140:ARG:NH1	2:F:182:THR:OG1	2.51	0.44
1:C:318:VAL:HG12	1:C:318:VAL:O	2.18	0.44
4:a:107:LEU:C	4:a:110:PRO:HD2	2.43	0.44
4:a:242:ILE:HG21	4:a:261:TRP:CE2	2.52	0.44
5:b:100:ARG:HG3	5:b:103:GLN:NE2	2.33	0.44
8:g:112:GLU:OE1	8:g:112:GLU:N	2.49	0.44
1:C:14:LYS:HD2	5:b:134:LYS:HE2	2.00	0.43
1:C:401:TYR:HB2	1:C:425:GLY:HA3	1.99	0.43
2:E:280:MET:HE3	2:E:316:THR:HG22	1.99	0.43
4:a:30:THR:C	4:a:32:LYS:H	2.26	0.43
4:a:262:ALA:HB3	5:p:17:PHE:CE1	2.53	0.43
1:A:496:ASP:OD1	1:A:497:ILE:N	2.51	0.43
2:D:124:LEU:HD23	2:D:124:LEU:HA	1.85	0.43
3:O:11:ALA:HB2	3:P:10:ILE:HD13	2.00	0.43
3:O:15:LEU:HD21	3:P:13:ALA:HA	1.99	0.43
5:b:58:GLN:HA	5:b:61:VAL:HG12	1.99	0.43
6:d:171:LYS:HE3	5:p:129:VAL:HG22	2.00	0.43
1:A:416:GLU:HG3	1:A:420:LYS:HE2	2.00	0.43
9:B:601:ATP:O5'	9:B:601:ATP:C8	2.70	0.43
2:F:56:GLY:H	2:F:211:PRO:HG2	1.83	0.43
3:G:11:ALA:HB1	3:H:13:ALA:HB2	2.00	0.43
3:G:32:GLY:HA3	3:S:33:ARG:HG3	2.01	0.43
3:J:59:LEU:HA	3:K:27:PHE:HD2	1.83	0.43
3:K:47:GLN:HG2	3:K:48:LEU:HD12	2.01	0.43
4:a:15:LYS:O	4:a:19:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:52:SER:HB3	4:a:156:ILE:HG12	2.00	0.43
5:b:135:ILE:HG23	5:p:132:ALA:CB	2.43	0.43
1:C:167:LEU:HD11	1:C:331:ILE:HG12	2.00	0.43
2:F:81:ALA:HB3	2:F:102:THR:HB	1.99	0.43
3:Q:11:ALA:HB1	3:R:13:ALA:HB2	2.01	0.43
4:a:280:THR:O	4:a:284:LEU:HD23	2.17	0.43
2:F:425:LEU:C	2:F:427:GLU:H	2.26	0.43
3:J:44:LEU:HD21	3:K:42:PRO:HB3	2.01	0.43
3:L:15:LEU:HD21	3:O:13:ALA:HA	1.99	0.43
1:C:29:GLU:HG2	1:C:90:ARG:HG2	2.00	0.43
4:a:171:SER:CB	5:b:14:PHE:CE1	3.01	0.43
6:d:112:ILE:HD13	6:d:126:LEU:HD13	1.99	0.43
1:C:16:ARG:CB	6:d:175:ARG:HH22	2.25	0.43
3:H:6:GLY:O	3:H:10:ILE:HG12	2.19	0.43
3:P:6:GLY:O	3:P:10:ILE:HG12	2.19	0.43
7:e:109:LYS:HE3	8:g:31:LYS:NZ	2.34	0.43
2:F:193:LYS:HB2	2:F:198:LEU:HD13	2.00	0.43
4:a:83:GLN:O	4:a:86:ILE:HG22	2.18	0.43
5:p:61:VAL:HG23	5:p:62:LYS:N	2.33	0.43
1:B:9:ILE:HG23	2:E:47:ASP:OD1	2.19	0.43
1:B:251:ARG:NH1	1:B:301:ARG:O	2.51	0.43
1:B:444:ASP:OD2	1:B:477:ARG:NH1	2.52	0.43
2:E:247:ASP:O	2:E:300:ALA:HB3	2.18	0.43
2:F:1:MET:N	2:F:19:GLU:OE2	2.52	0.43
2:F:223:LEU:HD22	2:F:283:LEU:HD12	2.00	0.43
3:P:15:LEU:HD21	3:Q:13:ALA:HA	2.00	0.43
3:R:11:ALA:HB2	3:S:10:ILE:HD13	2.01	0.43
5:b:80:ASN:HD21	5:p:83:ALA:HB3	1.72	0.43
3:H:15:LEU:HD21	3:J:13:ALA:HA	2.01	0.43
3:K:44:LEU:O	3:K:48:LEU:HD13	2.18	0.43
2:D:89:VAL:HG13	2:D:217:ARG:O	2.19	0.42
2:D:159:MET:HE1	2:D:188:PHE:CD1	2.53	0.42
2:F:192:MET:O	2:F:198:LEU:HB2	2.19	0.42
3:H:73:PHE:O	3:H:77:ASN:HB3	2.19	0.42
4:a:196:ASN:ND2	4:a:212:VAL:HG12	2.33	0.42
8:g:199:ASP:O	8:g:203:THR:HB	2.19	0.42
1:A:173:GLN:OE1	2:F:347:ARG:NH2	2.52	0.42
2:D:145:GLY:HA3	2:D:320:LEU:HD13	1.99	0.42
3:L:70:GLY:O	3:L:74:ILE:HG12	2.20	0.42
3:P:79:PHE:CD1	3:Q:5:LEU:HB3	2.54	0.42
1:A:4:LEU:O	1:A:7:SER:OG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:MET:O	1:A:488:ASP:HB2	2.18	0.42
3:O:2:GLU:H	3:O:2:GLU:CD	2.24	0.42
3:O:63:PRO:O	3:O:67:VAL:HG23	2.19	0.42
3:S:47:GLN:H	3:S:47:GLN:CD	2.27	0.42
6:d:62:PHE:HA	6:d:65:VAL:HG12	2.00	0.42
5:p:26:TRP:N	5:p:27:PRO:HD2	2.34	0.42
1:B:248:GLU:OE2	1:B:301:ARG:NE	2.51	0.42
2:E:381:ILE:HG21	7:e:114:SER:HB2	2.00	0.42
3:G:18:PHE:HB2	3:H:17:ALA:HB1	2.01	0.42
3:H:79:PHE:CD1	3:J:5:LEU:HB3	2.53	0.42
3:S:60:ASP:OD1	3:S:60:ASP:N	2.50	0.42
4:a:211:PRO:O	4:a:215:ILE:HG12	2.18	0.42
2:D:357:GLU:O	2:D:361:ILE:HG12	2.20	0.42
4:a:17:HIS:O	4:a:21:MET:HG2	2.20	0.42
5:b:83:ALA:O	5:b:87:ILE:HG12	2.19	0.42
5:p:57:ALA:O	5:p:61:VAL:HG13	2.19	0.42
3:G:36:GLU:OE1	3:S:33:ARG:HD2	2.20	0.42
3:H:8:VAL:HG11	3:H:77:ASN:HD22	1.85	0.42
3:L:79:PHE:CD1	3:O:5:LEU:HB3	2.55	0.42
5:b:51:LYS:HA	5:b:51:LYS:HE3	2.02	0.42
5:b:135:ILE:CG2	5:p:132:ALA:HA	2.46	0.42
5:b:145:HIS:CD2	5:b:148:MET:H	2.38	0.42
6:d:153:VAL:HG12	6:d:162:ASP:HA	2.02	0.42
1:C:17:ILE:HG13	6:d:175:ARG:NH1	2.35	0.42
1:C:148:GLN:O	1:C:187:GLN:NE2	2.52	0.42
2:D:110:ARG:HG2	2:D:111:GLN:N	2.34	0.42
3:Q:59:LEU:HA	3:R:27:PHE:HD2	1.85	0.42
4:a:33:LEU:HA	4:a:39:GLU:O	2.20	0.42
4:a:180:SER:HB2	4:a:189:PHE:CE1	2.55	0.42
4:a:208:LEU:HD12	4:a:212:VAL:HB	2.02	0.42
4:a:237:TYR:O	4:a:241:LEU:HD23	2.19	0.42
5:b:126:ALA:O	5:b:130:THR:HG23	2.19	0.42
6:d:35:LEU:HD13	6:d:78:LEU:HD21	2.02	0.42
1:A:8:GLU:O	1:A:12:LEU:HG	2.19	0.42
1:A:248:GLU:OE2	1:A:301:ARG:HB3	2.20	0.42
1:C:414:LEU:O	1:C:419:ARG:NH2	2.50	0.42
1:C:424:HIS:O	1:C:428:VAL:HG23	2.20	0.42
2:F:130:LYS:HG3	2:F:428:THR:HG22	2.02	0.42
5:p:2:ASN:O	5:p:6:THR:HG23	2.20	0.42
5:p:136:LEU:O	5:p:139:GLN:HG2	2.19	0.42
1:C:179:MET:HE3	1:C:179:MET:HB2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:155:THR:O	2:F:159:MET:HG3	2.19	0.42
6:d:114:SER:HB3	6:d:152:VAL:HG12	2.01	0.42
7:e:22:MET:SD	7:e:23:LEU:N	2.93	0.42
1:B:228:ALA:O	1:B:236:GLN:NE2	2.45	0.41
2:E:155:THR:C	2:E:159:MET:HE2	2.45	0.41
2:F:86:ILE:HD11	2:F:189:TYR:CD1	2.54	0.41
8:g:208:TYR:HB2	8:g:210:TYR:CE1	2.54	0.41
3:J:30:LEU:HD21	3:J:52:MET:HG2	2.01	0.41
4:a:123:ASN:CG	4:a:269:ILE:HG12	2.45	0.41
8:g:167:ARG:NH1	8:g:169:TYR:OH	2.53	0.41
5:p:99:GLU:O	5:p:103:GLN:HG2	2.19	0.41
1:B:424:HIS:O	1:B:428:VAL:HG23	2.20	0.41
2:D:33:ASP:OD2	2:D:66:THR:OG1	2.36	0.41
5:b:16:PHE:N	5:b:16:PHE:CD1	2.86	0.41
1:A:244:CYS:SG	1:A:301:ARG:HD2	2.60	0.41
1:B:151:TYR:CD2	1:B:367:PRO:HG3	2.56	0.41
3:O:16:ILE:HG22	3:O:67:VAL:HA	2.03	0.41
4:a:242:ILE:HD13	4:a:242:ILE:HA	1.92	0.41
6:d:175:ARG:HB3	5:p:125:ALA:HB1	2.01	0.41
1:B:300:GLU:HG3	2:F:209:ASN:HB3	2.02	0.41
1:C:199:ILE:HD11	1:C:240:PRO:HG3	2.01	0.41
3:H:44:LEU:HD22	3:H:47:GLN:NE2	2.35	0.41
3:J:11:ALA:HB1	3:K:13:ALA:HB2	2.03	0.41
3:P:78:PRO:HG2	3:P:79:PHE:CD2	2.56	0.41
4:a:125:MET:O	4:a:128:ILE:HG12	2.21	0.41
7:e:22:MET:HE3	7:e:53:LEU:HD13	2.01	0.41
7:e:87:ASP:OD1	7:e:88:ASN:N	2.52	0.41
1:B:85:GLU:OE1	2:E:46:GLY:HA2	2.21	0.41
4:a:59:LEU:O	4:a:62:ILE:HG22	2.19	0.41
4:a:87:GLU:HA	4:a:90:ILE:HG22	2.03	0.41
4:a:143:ASN:OD1	4:a:144:VAL:N	2.53	0.41
5:b:45:ASN:CG	5:p:47:ALA:HB2	2.38	0.41
7:e:108:GLN:HE22	7:e:112:LEU:HD11	1.85	0.41
1:A:138:ILE:HD13	2:D:95:ASP:HA	2.03	0.41
1:C:180:ALA:HB1	1:C:260:ILE:HG21	2.02	0.41
1:C:202:LYS:HD3	2:D:319:HIS:HA	2.02	0.41
2:F:325:VAL:HG13	2:F:340:ASP:HB3	2.02	0.41
4:a:242:ILE:O	4:a:246:ILE:HG13	2.20	0.41
5:b:108:ALA:HA	5:b:111:GLN:CD	2.46	0.41
2:E:77:PRO:HG3	2:E:105:ARG:NH2	2.35	0.41
3:G:65:ILE:O	3:G:69:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:MET:O	3:L:4:THR:OG1	2.23	0.41
3:S:61:ALA:O	3:S:65:ILE:HG13	2.20	0.41
6:d:162:ASP:OD1	6:d:166:LEU:HB3	2.20	0.41
1:A:427:ARG:HA	1:A:465:ILE:CD1	2.51	0.41
1:A:475:TYR:OH	1:A:507:SER:OG	2.34	0.41
1:B:410:PHE:HD1	7:e:112:LEU:HD22	1.86	0.41
2:D:26:ILE:HG22	2:D:27:TYR:CD1	2.56	0.41
2:D:357:GLU:OE2	2:D:433:LYS:NZ	2.38	0.41
2:E:399:ARG:O	2:E:403:ARG:HG2	2.21	0.41
2:F:130:LYS:O	2:F:130:LYS:HG2	2.20	0.41
2:F:206:GLY:HA3	2:F:218:VAL:HG11	2.03	0.41
2:F:388:ALA:O	2:F:392:LYS:HG2	2.21	0.41
3:G:20:ALA:HB1	3:S:63:PRO:HA	2.02	0.41
3:O:72:PHE:CE2	3:O:78:PRO:HD3	2.56	0.41
4:a:18:LEU:O	4:a:22:THR:HG23	2.21	0.41
4:a:224:ARG:O	4:a:227:SER:OG	2.24	0.41
4:a:232:LEU:HD23	4:a:236:MET:HG2	2.02	0.41
4:a:239:GLY:HA2	4:a:261:TRP:CH2	2.51	0.41
7:e:21:THR:OG1	7:e:53:LEU:O	2.32	0.41
1:C:151:TYR:OH	1:C:182:ASP:OD2	2.25	0.41
1:C:338:VAL:HG11	1:C:355:PHE:HE1	1.85	0.41
2:F:29:ALA:O	2:F:70:THR:OG1	2.24	0.41
2:F:88:ASP:N	2:F:88:ASP:OD1	2.48	0.41
3:J:33:ARG:HD2	3:K:36:GLU:OE2	2.20	0.41
5:b:48:GLU:CD	5:p:50:ALA:O	2.64	0.41
5:p:69:LYS:HD2	5:p:69:LYS:HA	1.92	0.41
2:F:147:PHE:HZ	2:F:317:PHE:CE1	2.38	0.40
3:G:14:ILE:HG23	3:G:18:PHE:CD1	2.56	0.40
4:a:224:ARG:HD2	4:a:283:TYR:CE2	2.56	0.40
5:b:145:HIS:CE1	5:b:148:MET:HB2	2.56	0.40
2:E:287:ILE:HG23	2:E:295:ILE:HG22	2.03	0.40
2:E:447:ALA:O	2:E:457:VAL:HG23	2.21	0.40
2:F:233:LYS:HD2	2:F:237:GLY:HA2	2.03	0.40
3:J:72:PHE:CE2	3:J:78:PRO:HD3	2.55	0.40
3:K:63:PRO:O	3:K:67:VAL:HG23	2.22	0.40
3:Q:59:LEU:HA	3:R:27:PHE:CD2	2.55	0.40
4:a:133:ILE:HB	4:a:134:PRO:HD3	2.04	0.40
7:e:15:ILE:HG13	7:e:83:ALA:HB3	2.02	0.40
1:A:152:LYS:HB2	1:A:440:TYR:CD2	2.57	0.40
1:B:244:CYS:O	1:B:248:GLU:HG3	2.20	0.40
2:F:89:VAL:HG21	2:F:217:ARG:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:399:ARG:O	2:F:403:ARG:HG2	2.21	0.40
3:J:73:PHE:O	3:J:77:ASN:HB3	2.21	0.40
3:S:35:LEU:HA	3:S:38:VAL:HG12	2.03	0.40
4:a:75:ASN:OD1	4:a:75:ASN:N	2.54	0.40
5:b:35:GLU:O	5:b:39:LYS:HG2	2.22	0.40
6:d:172:MET:HG3	5:p:129:VAL:HG11	2.03	0.40
1:B:151:TYR:OH	1:B:182:ASP:OD2	2.33	0.40
1:C:76:VAL:HG12	1:C:78:GLY:H	1.86	0.40
2:D:178:VAL:HG22	2:D:218:VAL:HG13	2.02	0.40
2:D:268:SER:OG	2:D:269:ALA:N	2.53	0.40
2:E:450:MET:HE3	2:E:450:MET:HB3	1.87	0.40
6:d:106:ASN:HB3	6:d:136:SER:OG	2.21	0.40
5:p:3:ILE:O	5:p:7:LEU:HG	2.21	0.40
2:E:340:ASP:O	2:E:344:SER:OG	2.23	0.40
4:a:195:LEU:CD2	4:a:216:LEU:HD13	2.48	0.40
8:g:117:LEU:HD11	8:g:126:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	507/514 (99%)	490 (97%)	17 (3%)	0	100	100
1	B	512/514 (100%)	492 (96%)	20 (4%)	0	100	100
1	C	507/514 (99%)	494 (97%)	13 (3%)	0	100	100
2	D	461/464 (99%)	445 (96%)	16 (4%)	0	100	100
2	E	461/464 (99%)	441 (96%)	20 (4%)	0	100	100
2	F	462/464 (100%)	446 (96%)	16 (4%)	0	100	100
3	G	77/81 (95%)	73 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	77/81 (95%)	73 (95%)	4 (5%)	0	100	100
3	J	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	K	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	L	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	O	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	P	77/81 (95%)	71 (92%)	6 (8%)	0	100	100
3	Q	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
3	R	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	S	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	a	275/291 (94%)	254 (92%)	21 (8%)	0	100	100
5	b	152/156 (97%)	146 (96%)	6 (4%)	0	100	100
5	p	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
6	d	172/178 (97%)	168 (98%)	4 (2%)	0	100	100
7	e	136/139 (98%)	128 (94%)	8 (6%)	0	100	100
8	g	286/289 (99%)	278 (97%)	8 (3%)	0	100	100
All	All	4860/4953 (98%)	4674 (96%)	186 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/406 (99%)	401 (100%)	0	100	100
1	B	406/406 (100%)	406 (100%)	0	100	100
1	C	401/406 (99%)	401 (100%)	0	100	100
2	D	378/379 (100%)	378 (100%)	0	100	100
2	E	378/379 (100%)	378 (100%)	0	100	100
2	F	379/379 (100%)	378 (100%)	1 (0%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	56/57 (98%)	56 (100%)	0	100	100
3	H	56/57 (98%)	56 (100%)	0	100	100
3	J	57/57 (100%)	57 (100%)	0	100	100
3	K	57/57 (100%)	57 (100%)	0	100	100
3	L	57/57 (100%)	57 (100%)	0	100	100
3	O	57/57 (100%)	57 (100%)	0	100	100
3	P	56/57 (98%)	56 (100%)	0	100	100
3	Q	56/57 (98%)	56 (100%)	0	100	100
3	R	57/57 (100%)	57 (100%)	0	100	100
3	S	57/57 (100%)	57 (100%)	0	100	100
4	a	216/246 (88%)	216 (100%)	0	100	100
5	b	108/115 (94%)	107 (99%)	1 (1%)	70	80
5	p	114/115 (99%)	114 (100%)	0	100	100
6	d	146/148 (99%)	145 (99%)	1 (1%)	76	82
7	e	106/107 (99%)	106 (100%)	0	100	100
8	g	235/236 (100%)	235 (100%)	0	100	100
All	All	3834/3892 (98%)	3831 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	210	GLU
5	b	45	ASN
6	d	135	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	87	GLN
1	A	164	GLN
1	A	421	GLN
1	A	424	HIS
1	B	201	GLN
1	B	203	GLN

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Mol	Chain	Res	Type
1	B	295	HIS
1	B	424	HIS
1	B	426	GLN
1	C	187	GLN
1	C	295	HIS
2	D	71	ASN
2	D	169	HIS
2	E	111	GLN
2	E	190	HIS
2	E	214	ASN
2	E	319	HIS
2	E	356	GLN
2	E	410	HIS
2	F	169	HIS
2	F	190	HIS
2	F	284	GLN
2	F	299	GLN
2	F	319	HIS
2	F	356	GLN
2	F	407	GLN
2	F	410	HIS
2	F	446	GLN
3	G	49	GLN
3	P	41	GLN
4	a	123	ASN
5	b	45	ASN
5	b	137	ASN
5	b	139	GLN
5	b	146	ASN
6	d	49	ASN
6	d	159	GLN
7	e	5	GLN
7	e	136	ASN
8	g	58	GLN
8	g	154	GLN
5	p	10	GLN
5	p	104	GLN
5	p	138	GLN
5	p	139	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 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$
11	ADP	D	502	10	28,29,29	1.48	4 (14%)	43,45,45	2.44	9 (20%)
9	ATP	A	601	10	32,33,33	2.08	4 (12%)	48,52,52	1.51	7 (14%)
9	ATP	C	602	10	32,33,33	2.08	4 (12%)	48,52,52	1.50	8 (16%)
12	PO4	E	601	-	4,4,4	0.98	0	6,6,6	0.50	0
9	ATP	B	601	10	32,33,33	2.08	5 (15%)	48,52,52	1.47	7 (14%)

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
9	ATP	A	601	10	-	7/22/38/38	0/3/3/3
11	ADP	D	502	10	-	8/16/32/32	0/3/3/3
9	ATP	C	602	10	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	B	601	10	-	7/22/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	ATP	PA-O3A	6.85	1.66	1.59
9	A	601	ATP	PA-O3A	6.83	1.66	1.59
9	C	602	ATP	PA-O3A	6.81	1.66	1.59
9	C	602	ATP	PB-O3A	6.73	1.66	1.59
9	A	601	ATP	PB-O3A	6.70	1.66	1.59
9	B	601	ATP	PB-O3A	6.65	1.66	1.59
11	D	502	ADP	C1'-N9	-4.36	1.34	1.46
9	A	601	ATP	PB-O3B	4.23	1.64	1.59
9	B	601	ATP	PB-O3B	4.22	1.64	1.59
9	C	602	ATP	PB-O3B	4.19	1.64	1.59
11	D	502	ADP	PA-O3A	3.72	1.63	1.59
9	B	601	ATP	C5-N7	-2.81	1.34	1.39
9	A	601	ATP	C5-N7	-2.80	1.34	1.39
9	C	602	ATP	C5-N7	-2.79	1.34	1.39
11	D	502	ADP	C8-N7	2.22	1.35	1.31
11	D	502	ADP	C5-N7	-2.04	1.35	1.39
9	B	601	ATP	C8-N9	-2.01	1.34	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	ADP	C1'-N9-C8	-8.19	108.92	127.09
11	D	502	ADP	C4-N9-C8	6.56	112.62	105.74
11	D	502	ADP	N9-C8-N7	-5.73	105.80	113.94
9	A	601	ATP	C5-C4-N3	-5.41	119.27	126.72
9	B	601	ATP	C5-C4-N3	-5.39	119.29	126.72
9	C	602	ATP	C5-C4-N3	-5.36	119.33	126.72
11	D	502	ADP	C4-N9-C1'	5.05	138.45	126.63
11	D	502	ADP	C5-C4-N3	-4.81	120.09	126.72
11	D	502	ADP	N3-C4-N9	4.80	135.33	127.17
11	D	502	ADP	C5-N7-C8	3.56	109.04	103.45
9	A	601	ATP	N3-C4-N9	3.41	132.97	127.17
9	B	601	ATP	N3-C4-N9	3.37	132.91	127.17
9	C	602	ATP	N3-C4-N9	3.37	132.90	127.17
9	A	601	ATP	C4'-O4'-C1'	-3.12	102.59	109.47
9	C	602	ATP	C4'-O4'-C1'	-3.06	102.70	109.47
9	A	601	ATP	C4-C5-N7	-2.88	107.29	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	601	ATP	C4-C5-N7	-2.87	107.30	110.58
9	C	602	ATP	C4-C5-N7	-2.85	107.32	110.58
9	A	601	ATP	C5-N7-C8	2.65	107.61	103.45
9	C	602	ATP	C5-N7-C8	2.62	107.58	103.45
9	B	601	ATP	C5-N7-C8	2.62	107.57	103.45
9	A	601	ATP	N9-C8-N7	-2.42	110.50	113.94
9	B	601	ATP	N9-C8-N7	-2.40	110.54	113.94
9	C	602	ATP	N9-C8-N7	-2.39	110.54	113.94
9	A	601	ATP	C2-N3-C4	2.32	117.50	111.83
9	B	601	ATP	C2-N3-C4	2.31	117.48	111.83
11	D	502	ADP	C4-C5-N7	-2.30	107.95	110.58
11	D	502	ADP	C2-N3-C4	2.29	117.43	111.83
9	C	602	ATP	C2-N3-C4	2.29	117.42	111.83
9	C	602	ATP	C6-C5-C4	2.02	119.94	117.18
9	B	601	ATP	C6-C5-C4	2.01	119.92	117.18

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	ATP	C5'-O5'-PA-O1A
9	A	601	ATP	C5'-O5'-PA-O2A
11	D	502	ADP	C5'-O5'-PA-O1A
11	D	502	ADP	C5'-O5'-PA-O2A
11	D	502	ADP	C5'-O5'-PA-O3A
9	B	601	ATP	O4'-C4'-C5'-O5'
9	B	601	ATP	C3'-C4'-C5'-O5'
11	D	502	ADP	PA-O3A-PB-O1B
11	D	502	ADP	PB-O3A-PA-O5'
11	D	502	ADP	PA-O3A-PB-O3B
9	A	601	ATP	C5'-O5'-PA-O3A
9	B	601	ATP	C5'-O5'-PA-O1A
9	B	601	ATP	C5'-O5'-PA-O2A
9	B	601	ATP	C5'-O5'-PA-O3A
9	C	602	ATP	C5'-O5'-PA-O2A
9	C	602	ATP	C4'-C5'-O5'-PA
9	A	601	ATP	PG-O3B-PB-O2B
9	A	601	ATP	PA-O3A-PB-O1B
9	B	601	ATP	PA-O3A-PB-O2B
11	D	502	ADP	PB-O3A-PA-O1A
9	A	601	ATP	PG-O3B-PB-O1B
9	A	601	ATP	PA-O3A-PB-O2B

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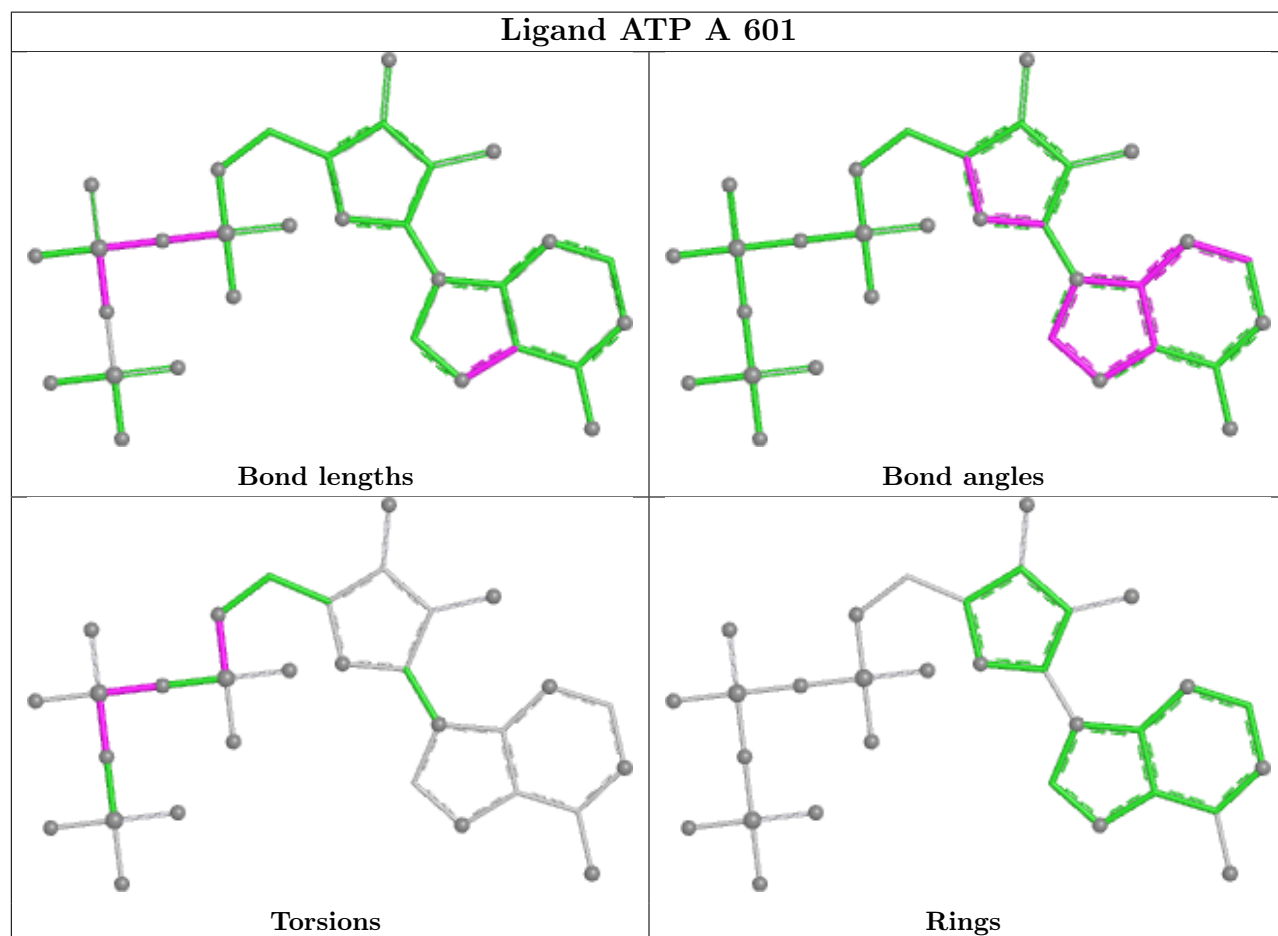
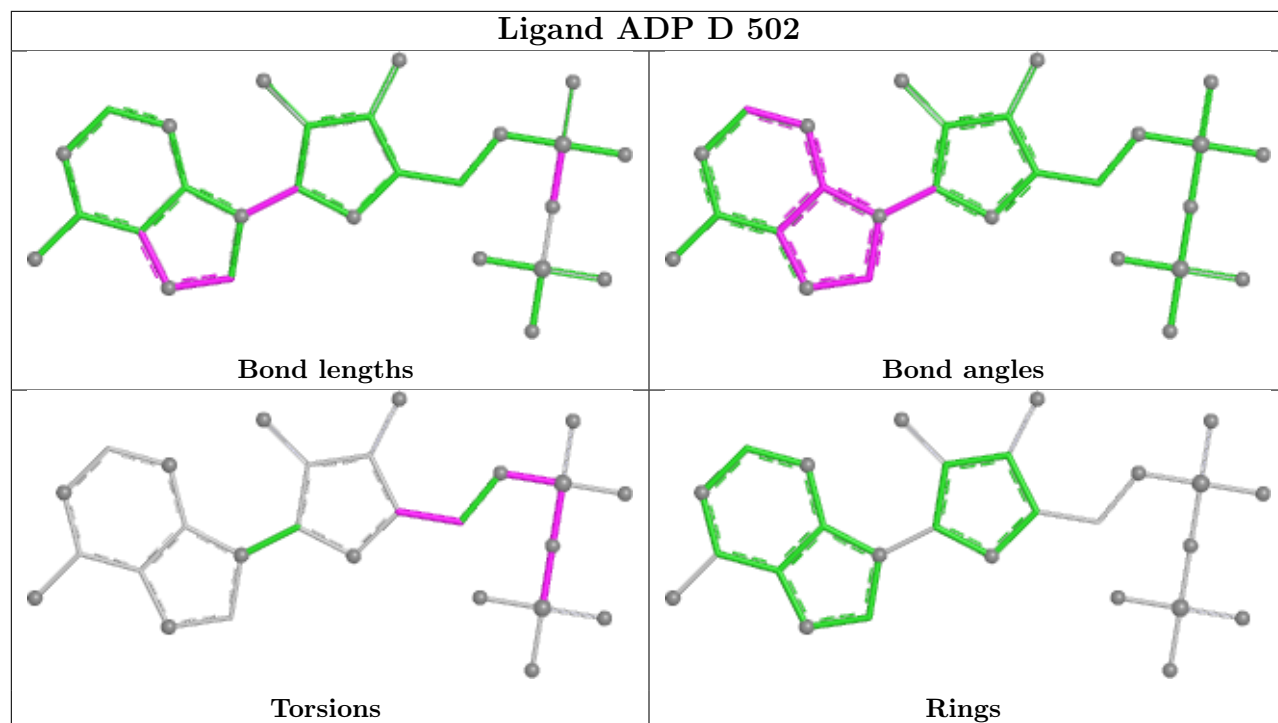
Mol	Chain	Res	Type	Atoms
9	B	601	ATP	PA-O3A-PB-O1B
11	D	502	ADP	O4'-C4'-C5'-O5'
9	C	602	ATP	O4'-C4'-C5'-O5'

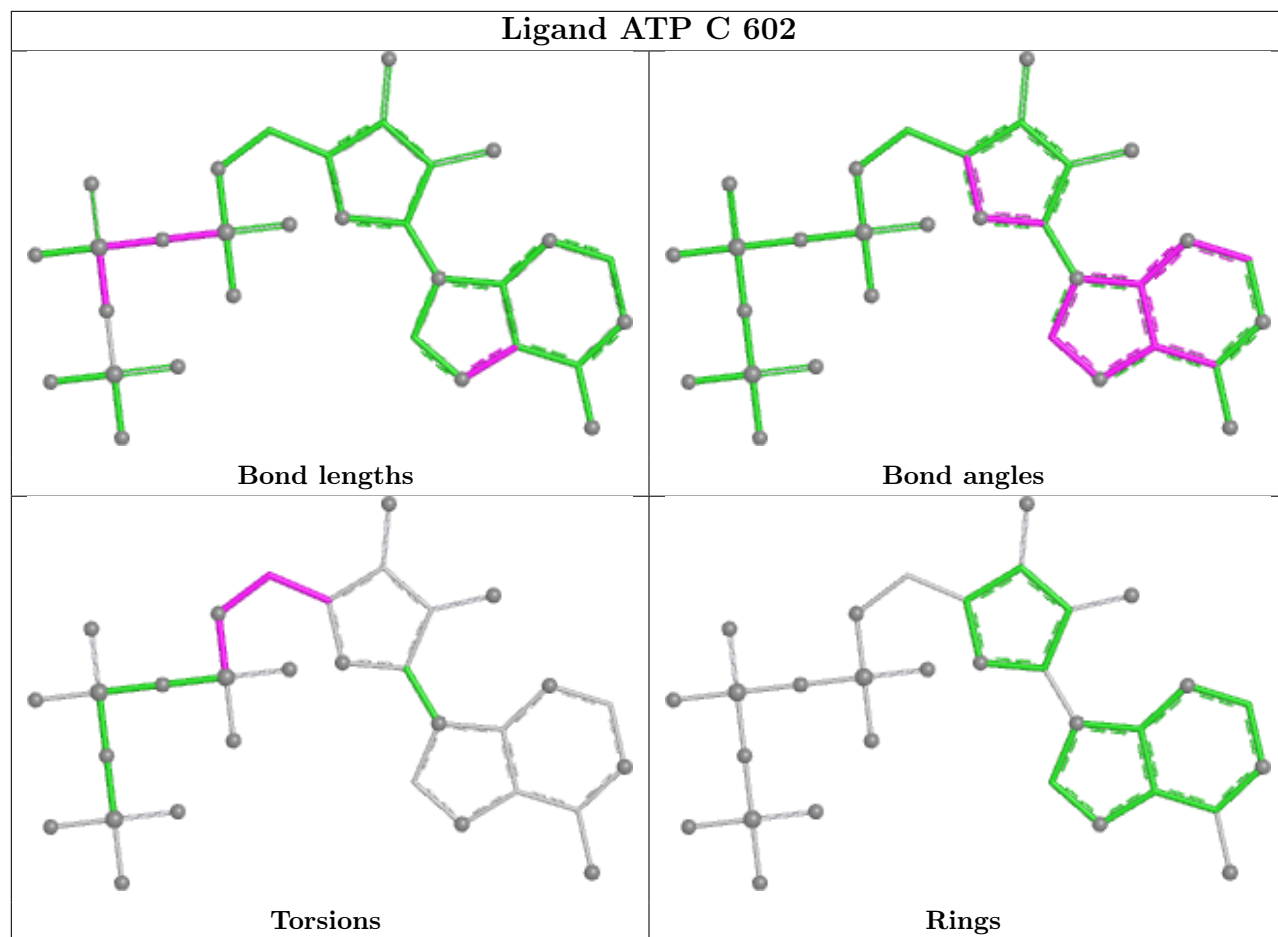
There are no ring outliers.

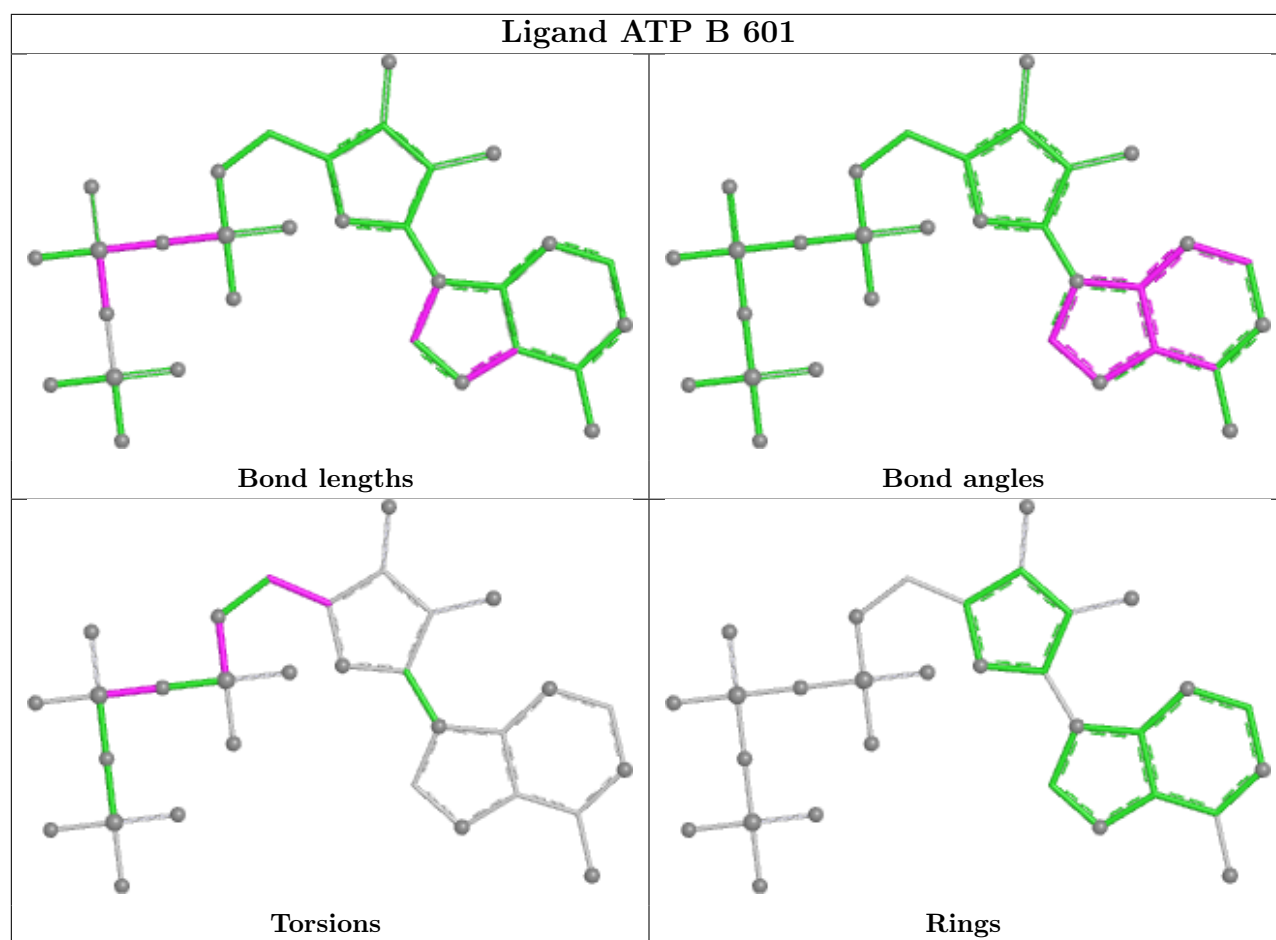
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	502	ADP	6	0
9	A	601	ATP	2	0
9	C	602	ATP	3	0
9	B	601	ATP	6	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

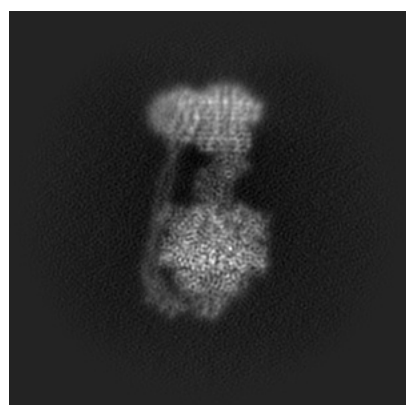
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13174. These allow visual inspection of the internal detail of the map and identification of artifacts.

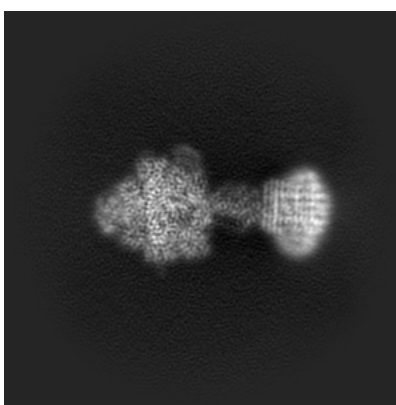
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

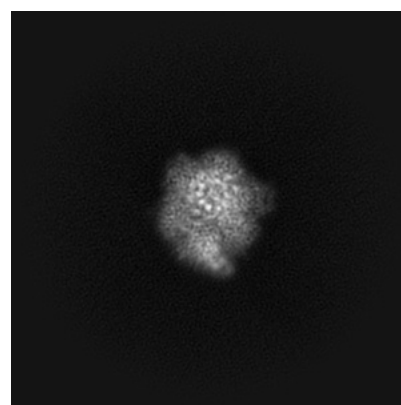
6.1.1 Primary map



X



Y

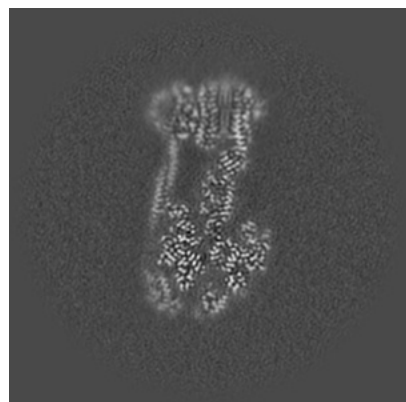


Z

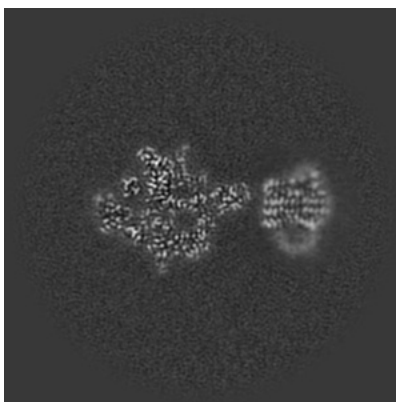
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

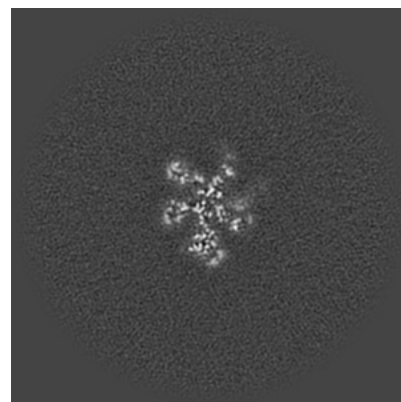
6.2.1 Primary map



X Index: 225



Y Index: 225

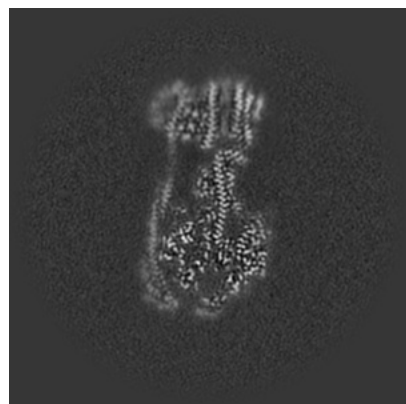


Z Index: 225

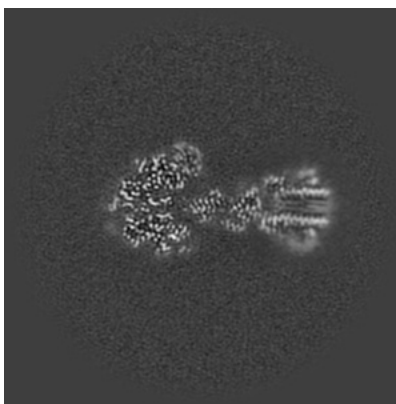
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

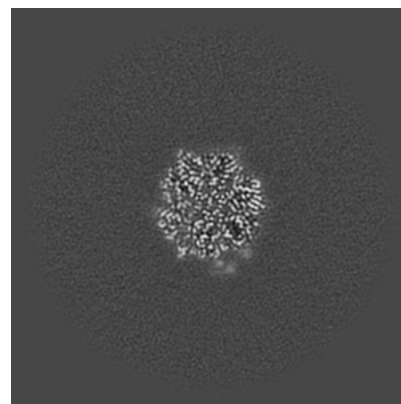
6.3.1 Primary map



X Index: 231



Y Index: 243

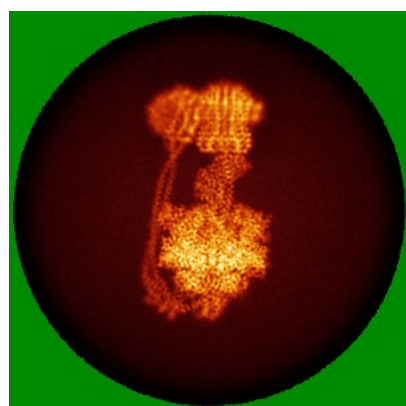


Z Index: 170

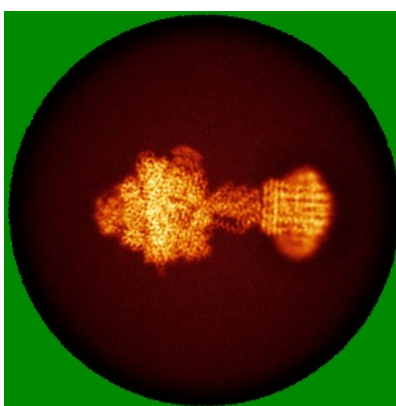
The images above show the largest variance slices of the map in three orthogonal directions.

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

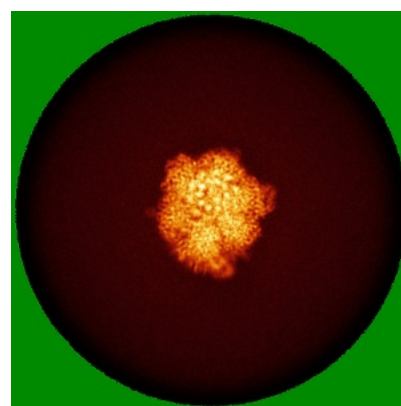
6.4.1 Primary map



X



Y

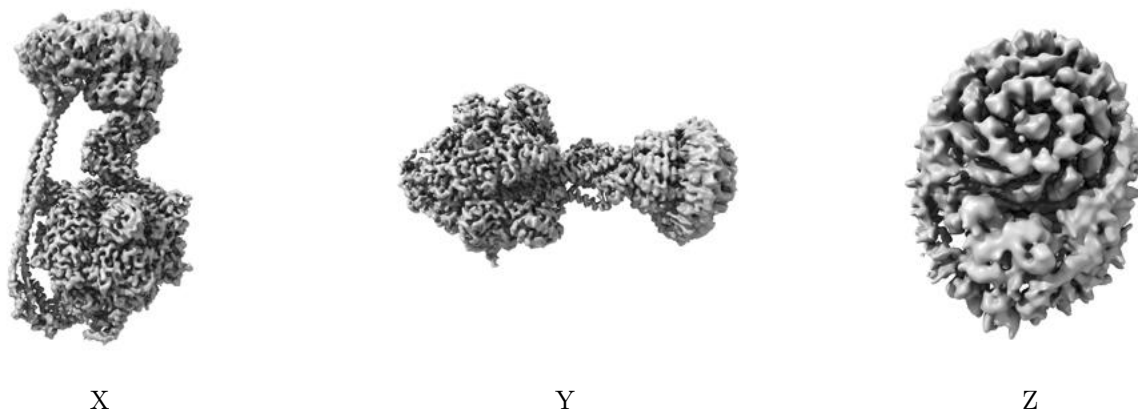


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

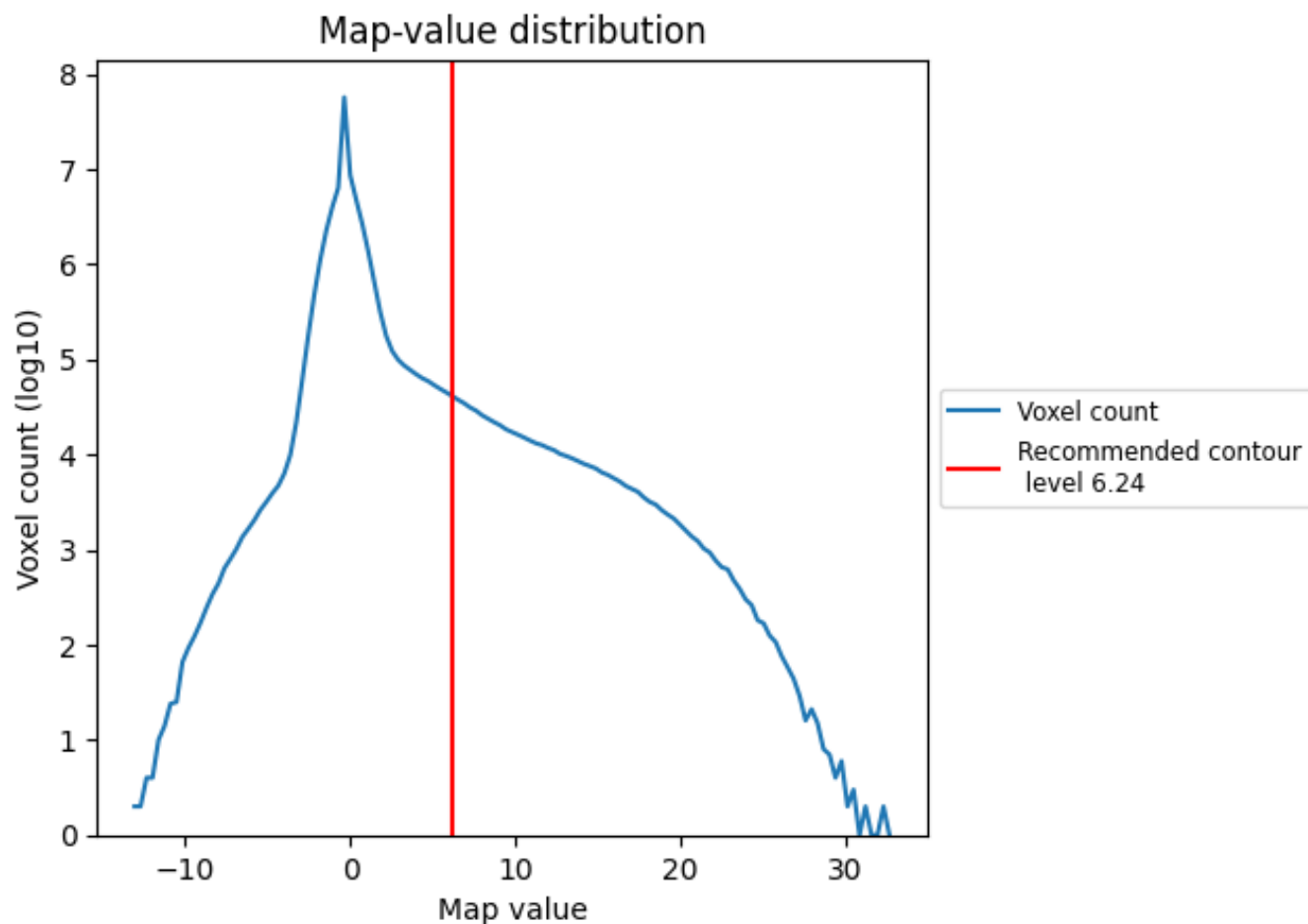
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

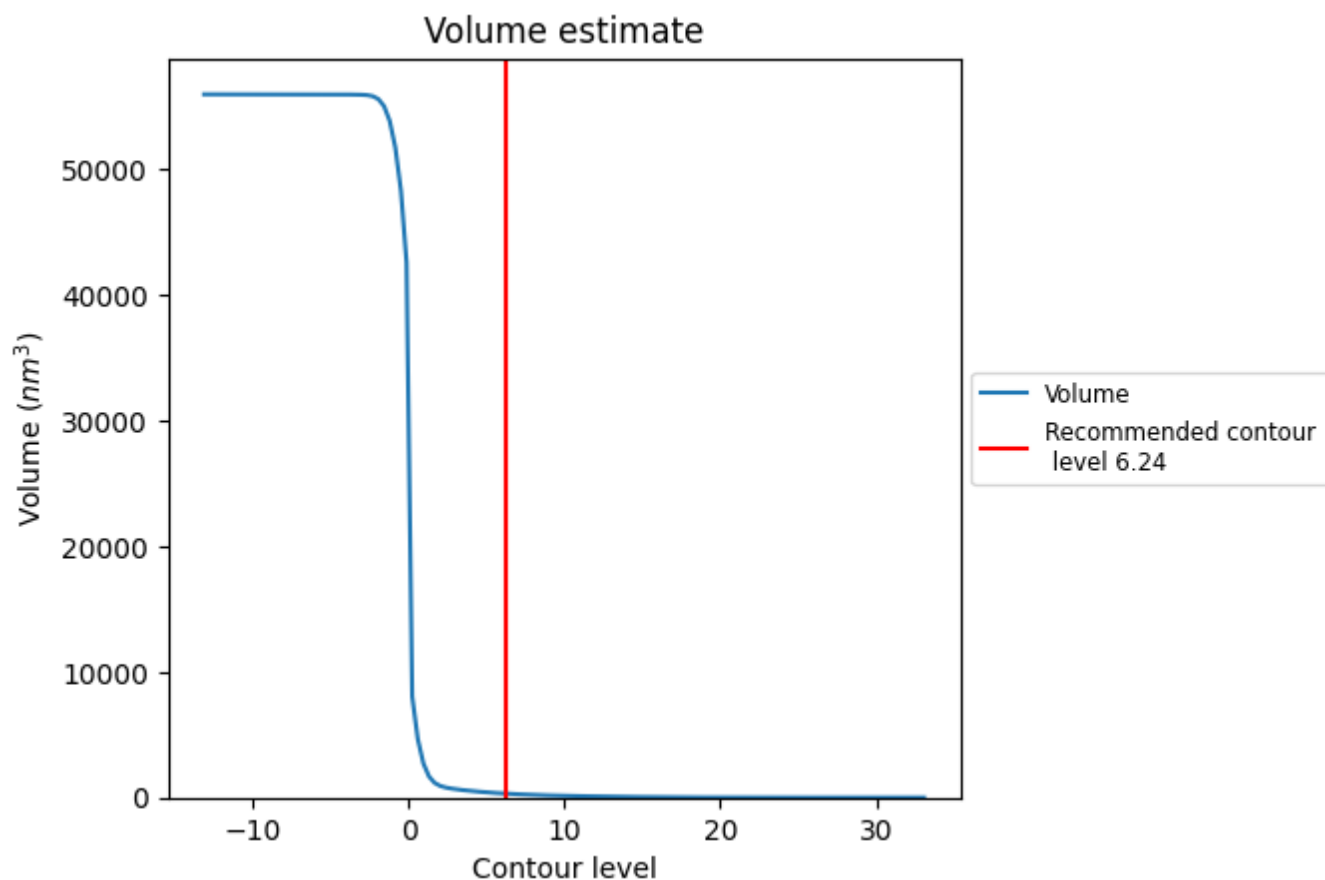
This section contains the results of statistical analysis of the map.

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.

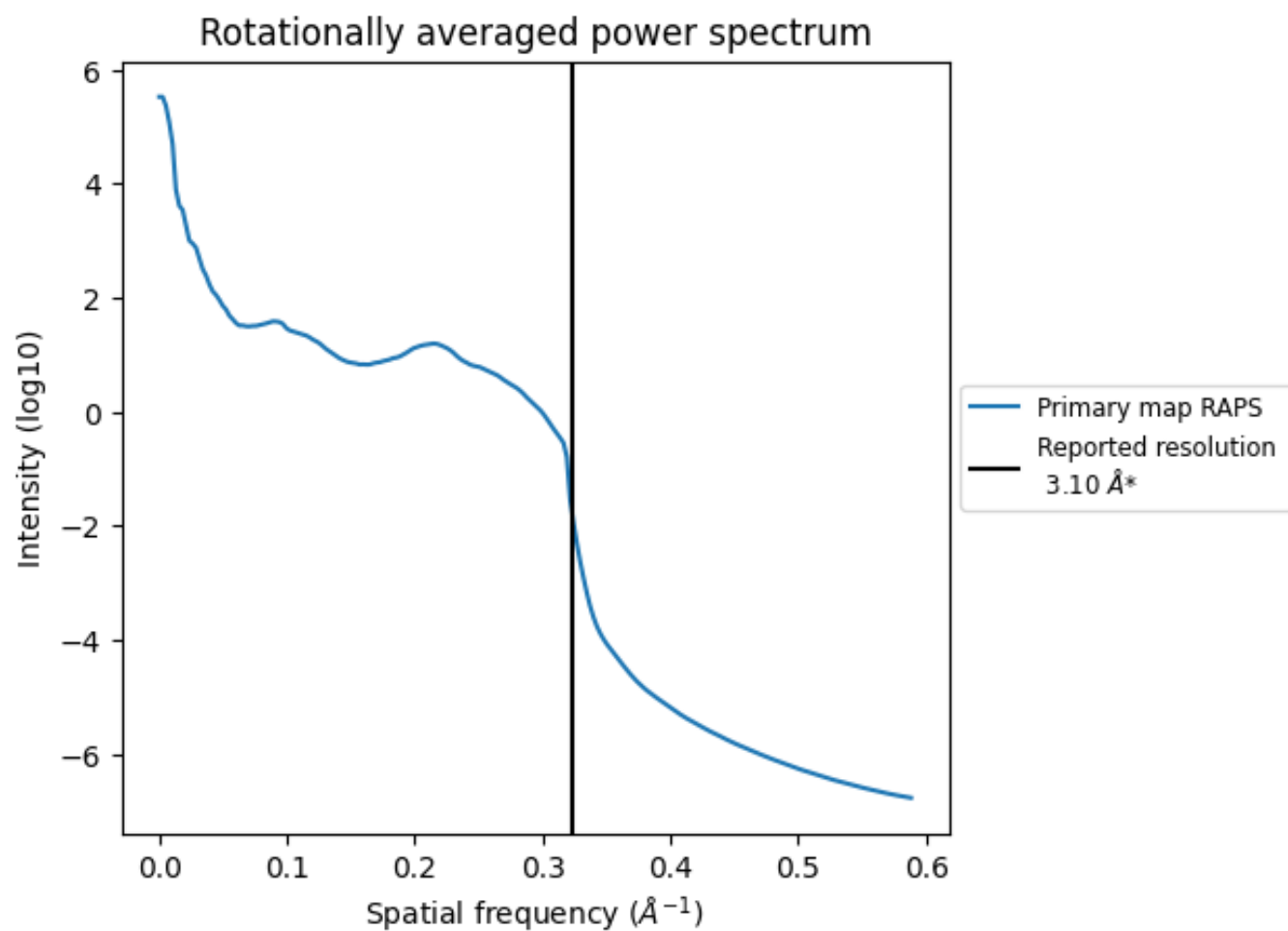
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 316 nm³; this corresponds to an approximate mass of 285 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

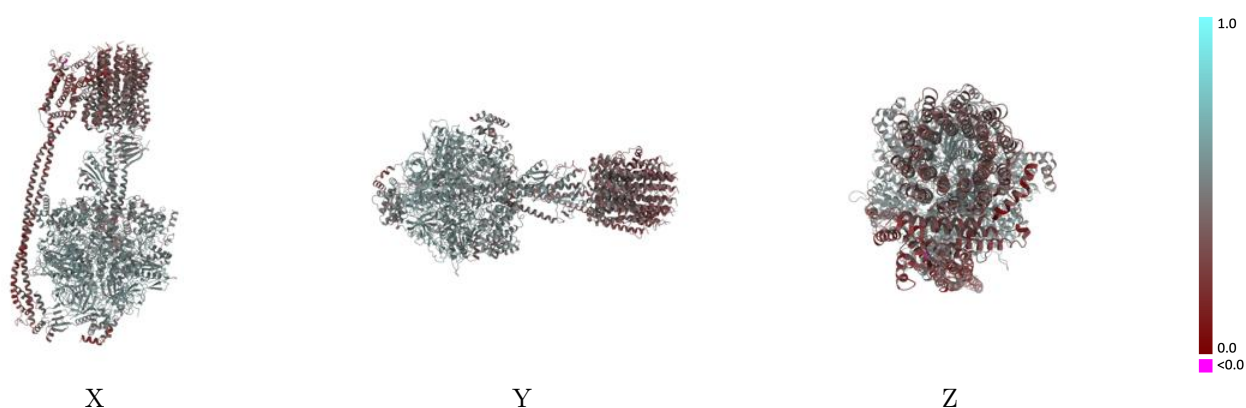
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13174 and PDB model 7P2Y. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

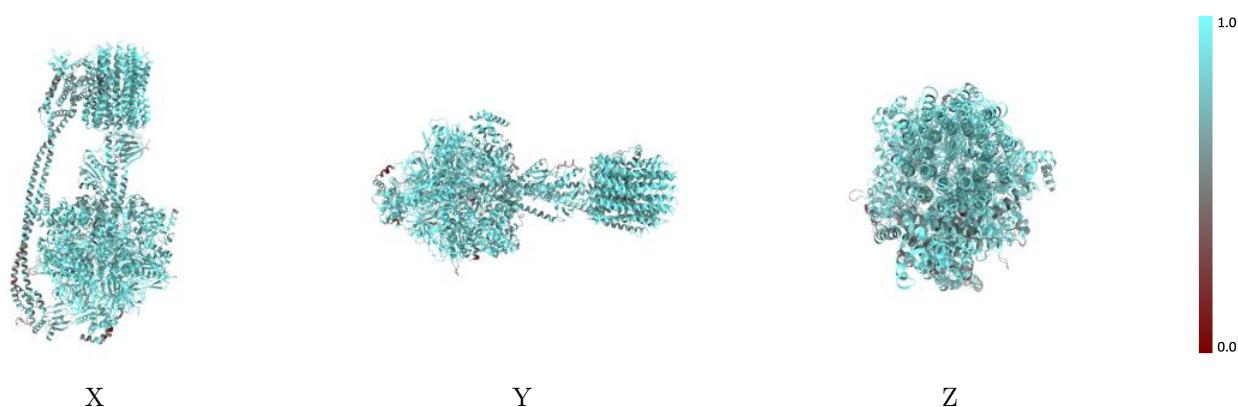
This section was not generated.

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



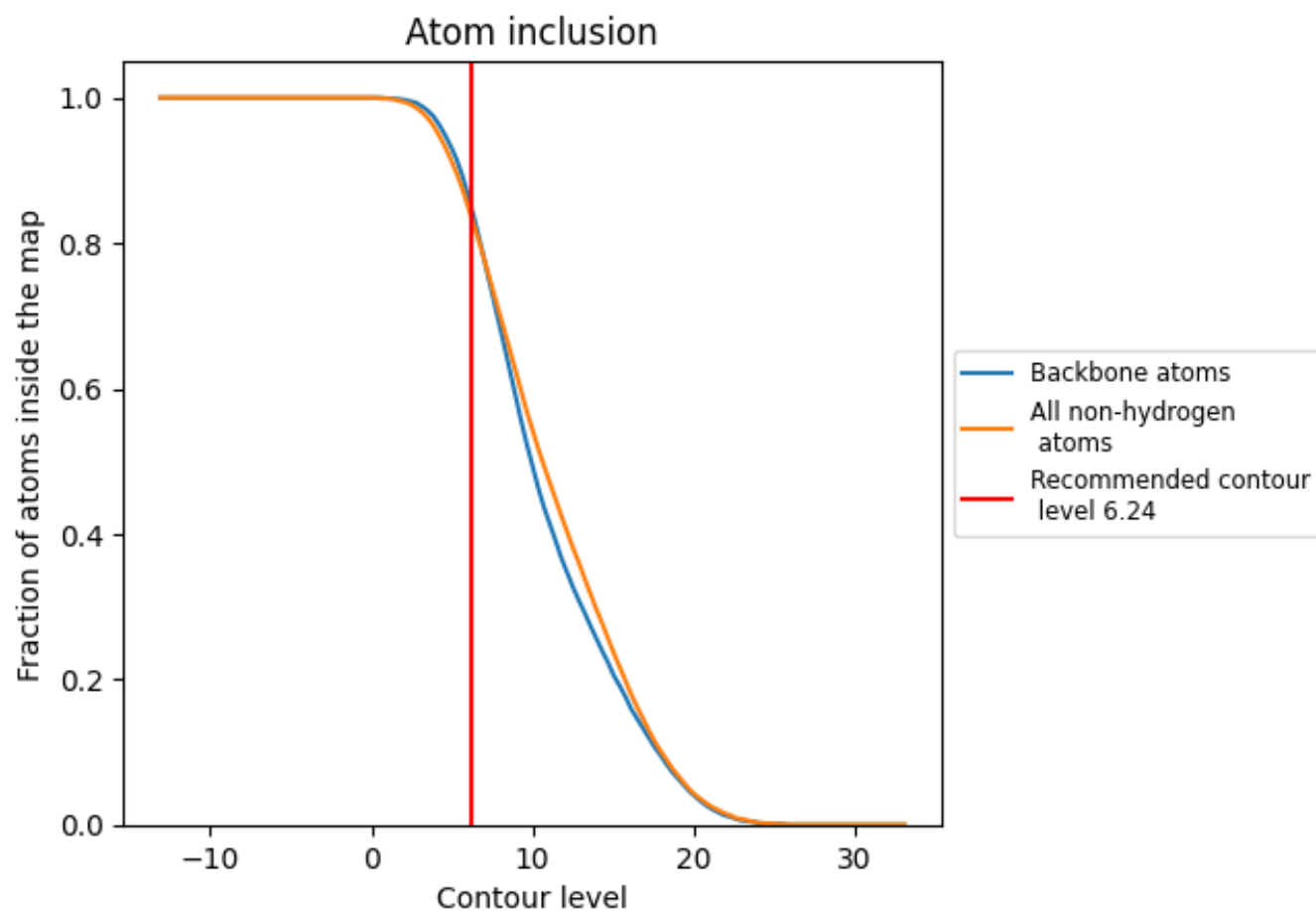
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (6.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.4780
A	 0.8630	 0.5200
B	 0.8850	 0.5350
C	 0.8920	 0.5410
D	 0.9040	 0.5510
E	 0.8160	 0.5120
F	 0.8830	 0.5380
G	 0.8020	 0.3800
H	 0.8230	 0.3570
J	 0.8550	 0.3660
K	 0.8980	 0.3880
L	 0.8960	 0.3940
O	 0.9150	 0.3960
P	 0.8740	 0.3830
Q	 0.8420	 0.3850
R	 0.8070	 0.3880
S	 0.7960	 0.3880
a	 0.7350	 0.3050
b	 0.6180	 0.3010
d	 0.8240	 0.4800
e	 0.7980	 0.5000
g	 0.8020	 0.5020
p	 0.6570	 0.3170

