



Full wwPDB EM Validation Report ⓘ

Jan 15, 2022 – 08:18 am GMT

PDB ID : 7PXB
EMDB ID : EMD-13696
Title : Substrate-engaged mycobacterial Proteasome-associated ATPase - focused 3D refinement (state B)
Authors : Jomaa, A.; Kavalchuk, M.; Weber-Ban, E.
Deposited on : 2021-10-08
Resolution : 4.00 Å (reported)
Based on initial model : 5KWA

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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

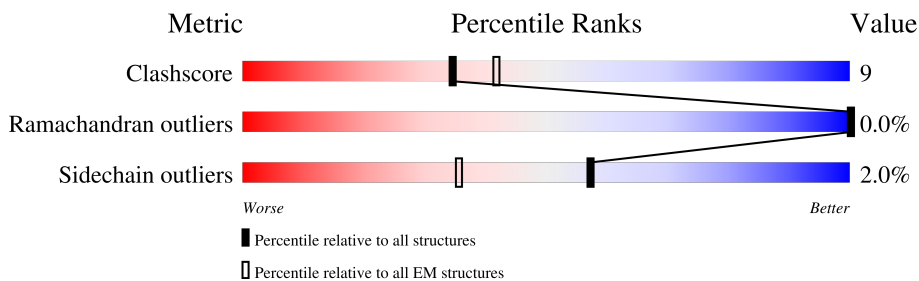
EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

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 4.00 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 $\leq 5\%$. 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	609	
1	B	609	
1	C	609	
1	D	609	
1	E	609	
1	F	609	
2	G	66	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	C	701	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22286 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 AAA ATPase forming ring-shaped complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	466	Total 3650	C 2306	N 630	O 703	S 11	0	0
1	B	476	Total 3719	C 2343	N 642	O 723	S 11	0	0
1	C	464	Total 3629	C 2291	N 625	O 702	S 11	0	0
1	D	452	Total 3542	C 2242	N 607	O 682	S 11	0	0
1	E	476	Total 3719	C 2343	N 642	O 723	S 11	0	0
1	F	477	Total 3723	C 2345	N 643	O 724	S 11	0	0

- Molecule 2 is a protein called Prokaryotic ubiquitin-like protein Pup.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	17	Total 112	C 62	N 23	O 26	S 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP A0A045GWT8
G	0	SER	-	expression tag	UNP A0A045GWT8

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

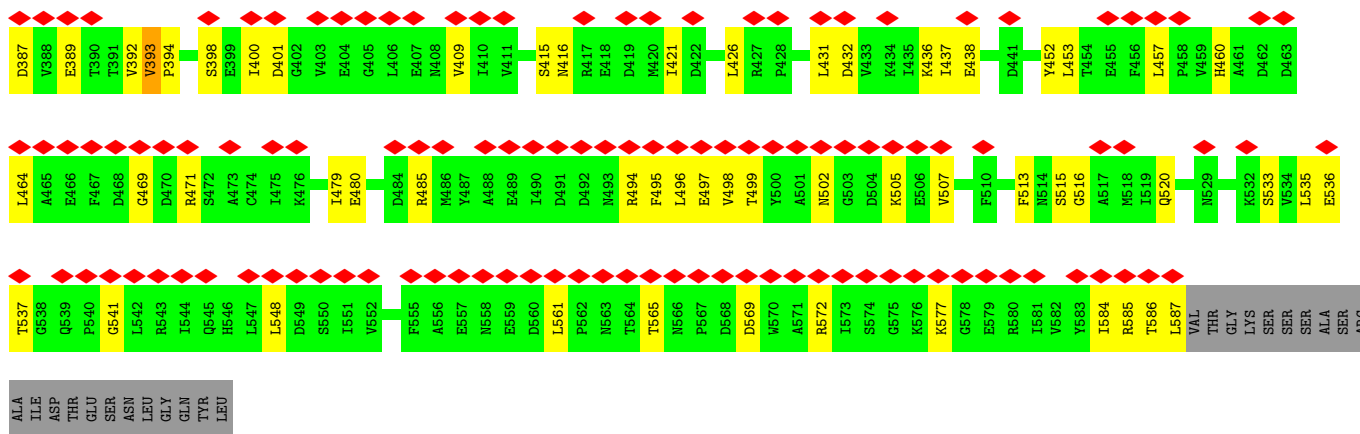
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

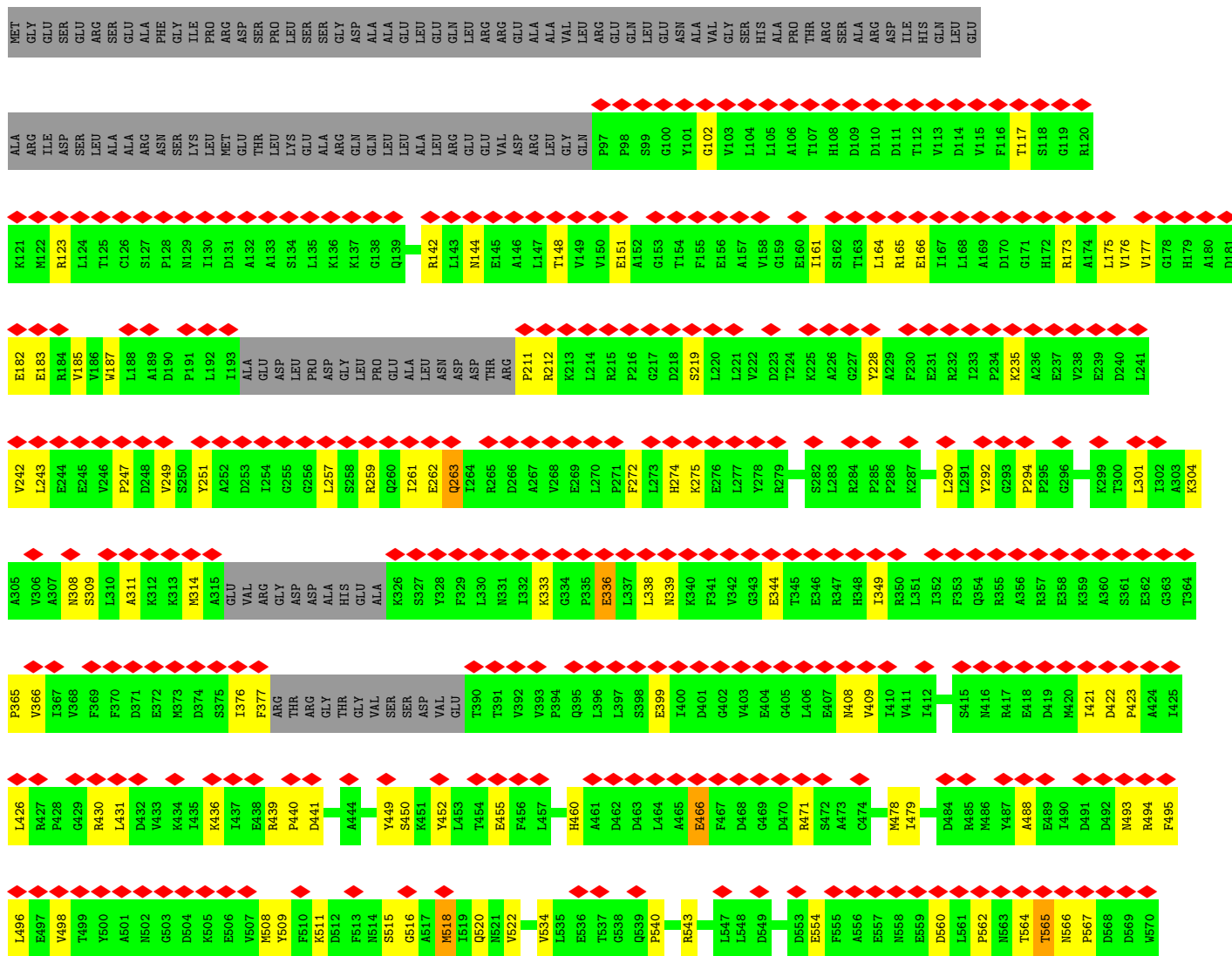
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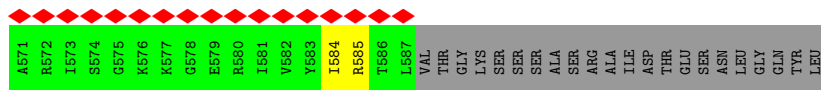
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	F	1	1	1	0

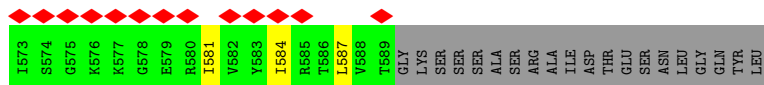
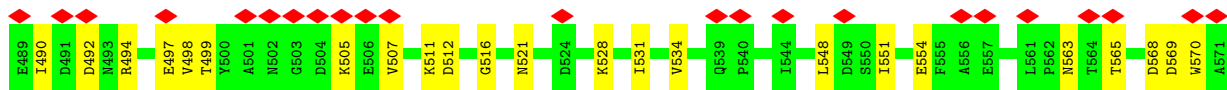
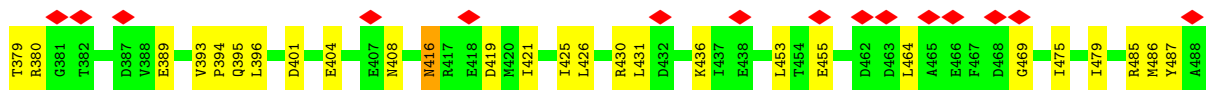
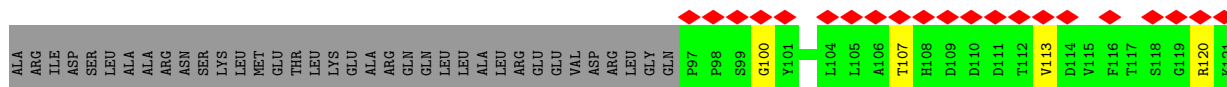


• Molecule 1: AAA ATPase forming ring-shaped complexes

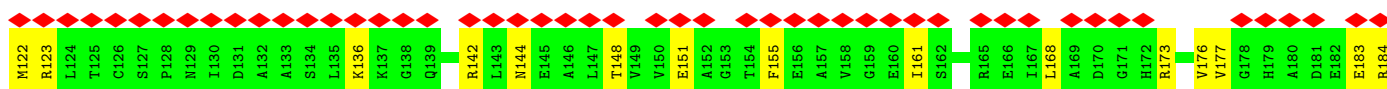
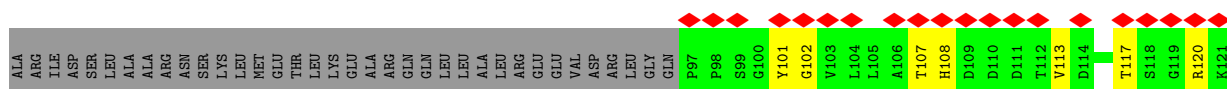


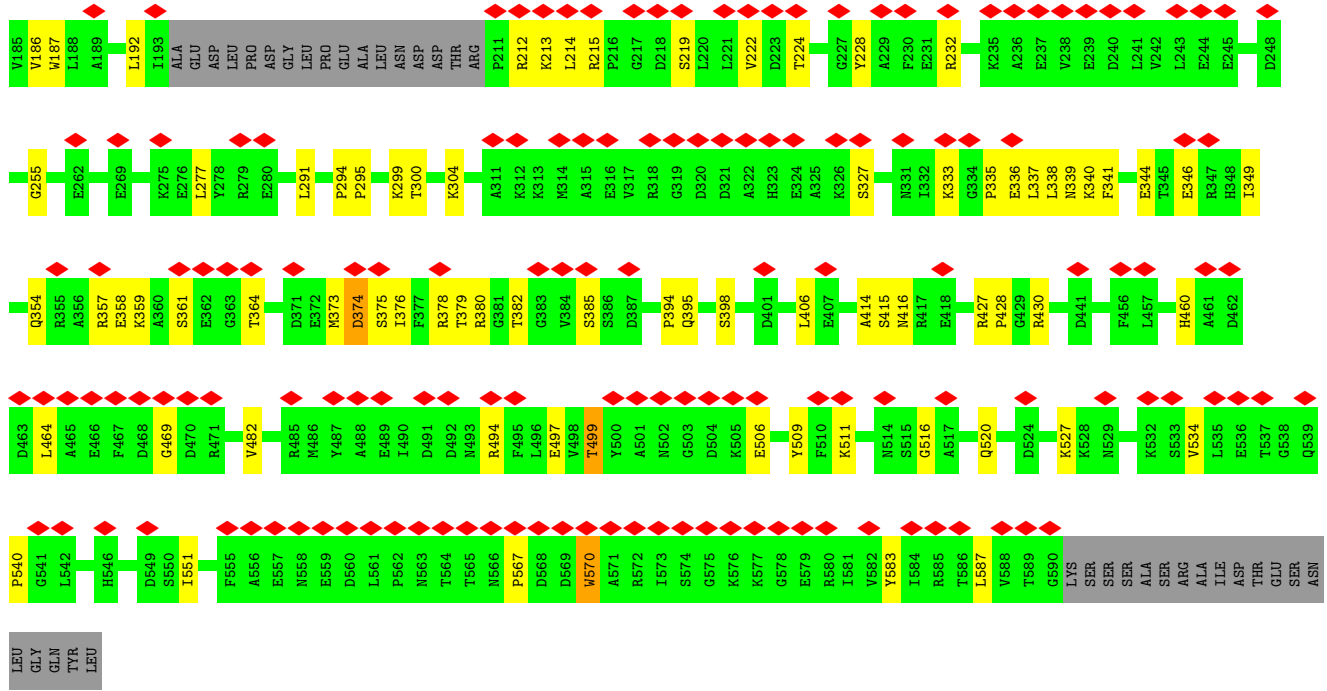


- Molecule 1: AAA ATPase forming ring-shaped complexes

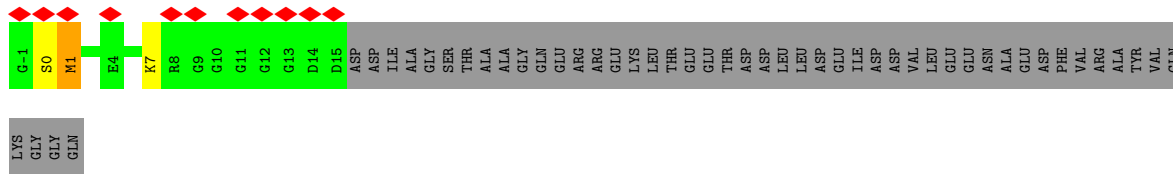


- Molecule 1: AAA ATPase forming ring-shaped complexes





• Molecule 2: Prokaryotic ubiquitin-like protein Pup



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50814	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0247	Depositor
Map size (\AA)	430.144, 430.144, 430.144	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.222, 1.222, 1.222	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.24	0/3709	0.40	0/5015
1	B	0.26	0/3781	0.42	0/5116
1	C	0.26	0/3689	0.41	0/4989
1	D	0.24	0/3601	0.41	0/4869
1	E	0.30	0/3781	0.44	1/5116 (0.0%)
1	F	0.25	0/3785	0.40	0/5121
2	G	0.23	0/111	0.42	0/143
All	All	0.26	0/22457	0.41	1/30369 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	234	PRO	N-CA-CB	-5.27	96.80	102.60

There are no chirality outliers.

There are no planarity outliers.

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	A	3650	0	3677	62	0
1	B	3719	0	3728	77	0
1	C	3629	0	3649	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3542	0	3563	69	0
1	E	3719	0	3727	72	0
1	F	3723	0	3731	66	0
2	G	112	0	102	3	0
3	A	31	0	12	2	0
3	B	31	0	12	2	0
3	C	31	0	12	9	0
3	D	31	0	12	1	0
3	E	31	0	12	4	0
3	F	31	0	12	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	22286	0	22249	391	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 9.

All (391) 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)
1:E:163:THR:HA	1:E:219:SER:HA	1.40	0.99
1:B:429:GLY:H	1:B:432:ASP:HB3	1.49	0.77
1:F:482:VAL:HG23	1:F:551:ILE:HD11	1.67	0.76
1:D:366:VAL:O	1:D:409:VAL:HA	1.85	0.75
1:B:103:VAL:HG13	1:B:116:PHE:HB3	1.71	0.72
1:B:142:ARG:HH21	1:B:151:GLU:HG2	1.55	0.71
1:E:220:LEU:HA	1:E:231:GLU:O	1.90	0.71
1:C:494:ARG:HG2	1:C:507:VAL:HG11	1.74	0.70
1:A:249:VAL:HG11	1:A:304:LYS:HG3	1.74	0.69
1:A:290:LEU:HD22	1:A:426:LEU:HD11	1.75	0.69
1:A:521:ASN:ND2	1:A:554:GLU:OE2	2.26	0.69
1:E:218:ASP:HB3	1:E:232:ARG:HD2	1.74	0.69
1:E:568:ASP:O	1:E:572:ARG:NH2	2.26	0.69
1:F:464:LEU:HB3	1:F:469:GLY:HA2	1.75	0.68
1:D:488:ALA:O	1:D:493:ASN:ND2	2.27	0.67
1:C:569:ASP:O	1:C:572:ARG:HG2	1.94	0.67
1:C:373:MET:HB2	1:C:415:SER:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:LEU:HB3	1:F:214:LEU:HD11	1.76	0.67
1:F:346:GLU:HB3	1:F:395:GLN:HE21	1.60	0.67
1:A:424:ALA:O	1:A:430:ARG:NH2	2.28	0.67
1:C:379:THR:HG22	1:C:381:GLY:H	1.59	0.67
1:A:426:LEU:HD12	1:A:434:LYS:HE3	1.75	0.66
1:A:112:THR:HG22	1:A:125:THR:HG22	1.78	0.66
1:E:531:ILE:HD11	1:F:277:LEU:HB3	1.77	0.66
1:B:255:GLY:O	3:B:701:ATP:N6	2.28	0.66
1:D:534:VAL:HG22	1:D:540:PRO:HA	1.77	0.66
1:D:365:PRO:HA	1:D:408:ASN:HB2	1.78	0.66
1:E:255:GLY:O	3:E:701:ATP:N6	2.29	0.65
1:A:393:VAL:HG13	1:A:394:PRO:HD3	1.78	0.65
1:A:237:GLU:HB2	1:B:165:ARG:HH12	1.60	0.65
1:B:485:ARG:HD3	1:B:548:LEU:HD22	1.78	0.64
1:A:554:GLU:OE1	1:A:558:ASN:ND2	2.29	0.64
1:F:375:SER:O	1:F:378:ARG:NH1	2.30	0.64
1:C:350:ARG:NH2	1:F:335:PRO:O	2.31	0.64
1:A:299:LYS:HG2	1:A:437:ILE:HD13	1.79	0.64
1:D:262:GLU:OE1	1:D:263:GLN:NE2	2.31	0.64
1:F:534:VAL:HG22	1:F:540:PRO:HA	1.80	0.64
1:D:175:LEU:HD11	1:D:183:GLU:HB2	1.80	0.64
1:C:294:PRO:HD2	1:C:438:GLU:HA	1.80	0.63
1:A:139:GLN:NE2	1:A:153:GLY:O	2.29	0.63
1:B:139:GLN:NE2	1:B:153:GLY:O	2.31	0.63
1:F:499:THR:HG23	1:F:583:TYR:HB3	1.81	0.63
1:A:101:TYR:H	1:B:120:ARG:HH12	1.44	0.63
1:B:373:MET:HB3	1:B:415:SER:HB3	1.81	0.62
1:C:287:LYS:NZ	1:C:401:ASP:OD1	2.31	0.62
1:A:585:ARG:HD2	1:B:575:GLY:HA2	1.80	0.62
1:C:193:ILE:O	1:C:213:LYS:NZ	2.33	0.62
1:A:333:LYS:HB2	1:A:336:GLU:HG3	1.81	0.62
1:F:192:LEU:HD22	1:F:214:LEU:HD21	1.81	0.62
1:A:255:GLY:H	3:A:701:ATP:HN61	1.47	0.62
1:A:558:ASN:OD1	1:B:434:LYS:NZ	2.31	0.61
1:B:105:LEU:HD12	1:B:114:ASP:HB3	1.81	0.61
1:F:327:SER:OG	1:F:359:LYS:NZ	2.33	0.61
1:E:464:LEU:HB3	1:E:469:GLY:HA2	1.81	0.61
1:D:439:ARG:HG3	1:D:440:PRO:HD3	1.82	0.61
1:E:521:ASN:ND2	1:E:554:GLU:OE2	2.33	0.61
1:F:509:TYR:HB2	1:F:511:LYS:HG2	1.82	0.61
1:D:249:VAL:O	1:D:308:ASN:ND2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:VAL:HB	1:D:409:VAL:HG22	1.83	0.60
1:F:177:VAL:HG12	1:F:183:GLU:HG3	1.83	0.60
1:B:177:VAL:HG12	1:B:183:GLU:HG3	1.83	0.60
2:G:1:MET:SD	2:G:1:MET:N	2.70	0.60
1:D:294:PRO:HG2	1:D:439:ARG:HG2	1.83	0.60
1:C:291:LEU:HB3	1:C:437:ILE:HD11	1.84	0.60
1:B:266:ASP:HA	1:B:270:LEU:HD13	1.82	0.60
1:D:333:LYS:HE2	1:D:336:GLU:HG2	1.84	0.60
1:D:496:LEU:HB2	1:D:508:MET:HB2	1.84	0.60
1:B:374:ASP:OD2	1:E:380:ARG:NH2	2.34	0.59
1:D:522:VAL:HG22	1:D:554:GLU:HG2	1.85	0.59
1:B:372:GLU:HB3	1:E:394:PRO:HB3	1.85	0.59
1:C:393:VAL:HG13	1:C:394:PRO:HD3	1.84	0.59
1:E:318:ARG:NH2	1:E:364:THR:OG1	2.36	0.59
1:E:233:ILE:HD13	1:E:234:PRO:HD3	1.85	0.58
1:B:164:LEU:HA	1:B:176:VAL:HG12	1.84	0.58
1:C:341:PHE:HB3	1:F:340:LYS:HG3	1.86	0.58
1:E:485:ARG:HG3	1:E:548:LEU:HD22	1.84	0.58
1:A:310:LEU:HD23	1:A:329:PHE:HB2	1.86	0.58
1:B:107:THR:HA	1:B:113:VAL:HG12	1.84	0.58
1:C:123:ARG:NH2	1:F:101:TYR:OH	2.37	0.58
1:A:274:HIS:HB3	1:A:277:LEU:HD23	1.85	0.58
1:A:183:GLU:HG3	1:D:161:ILE:HB	1.86	0.57
1:F:144:ASN:ND2	1:F:148:THR:O	2.37	0.57
1:F:213:LYS:O	1:F:215:ARG:NH1	2.37	0.57
1:B:342:VAL:HA	2:G:7:LYS:HE3	1.85	0.57
1:E:175:LEU:HD11	1:E:183:GLU:HB2	1.87	0.57
1:D:509:TYR:HB2	1:D:511:LYS:HG2	1.86	0.57
1:D:339:ASN:HB3	1:D:344:GLU:HB3	1.84	0.57
1:E:372:GLU:HG2	1:F:394:PRO:HB3	1.86	0.57
1:A:211:PRO:N	1:A:212:ARG:HA	2.20	0.56
1:E:333:LYS:NZ	1:F:398:SER:O	2.36	0.56
1:A:478:MET:HG3	1:A:544:ILE:HD13	1.87	0.56
1:B:144:ASN:HD21	1:B:148:THR:HB	1.68	0.56
1:A:346:GLU:OE2	1:A:350:ARG:NH2	2.38	0.56
1:C:232:ARG:NH1	1:C:233:ILE:O	2.38	0.56
1:F:255:GLY:O	3:F:701:ATP:N6	2.39	0.56
1:E:455:GLU:HA	1:E:475:ILE:HD12	1.88	0.56
1:D:251:TYR:HE2	1:D:309:SER:HB2	1.71	0.56
1:D:562:PRO:O	1:D:565:THR:OG1	2.23	0.56
1:F:107:THR:HA	1:F:113:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ARG:NH2	1:F:224:THR:O	2.39	0.56
1:C:254:ILE:HD11	1:C:301:LEU:HB3	1.88	0.56
1:D:164:LEU:HA	1:D:176:VAL:HG12	1.87	0.56
1:A:425:ILE:HG23	1:A:426:LEU:HD22	1.87	0.55
1:F:335:PRO:HA	1:F:338:LEU:HD13	1.88	0.55
1:C:175:LEU:HD11	1:C:183:GLU:HB3	1.89	0.55
1:C:398:SER:HB2	1:F:333:LYS:HG3	1.86	0.55
1:D:494:ARG:HH21	1:D:509:TYR:HE1	1.53	0.55
1:A:255:GLY:O	3:A:701:ATP:N6	2.39	0.55
1:F:460:HIS:ND1	1:F:540:PRO:O	2.39	0.55
1:A:249:VAL:O	1:A:308:ASN:ND2	2.31	0.55
1:B:563:ASN:OD1	1:B:564:THR:N	2.38	0.55
1:C:212:ARG:HH22	1:C:232:ARG:HE	1.54	0.55
1:F:361:SER:H	1:F:364:THR:HB	1.72	0.55
1:B:255:GLY:H	3:B:701:ATP:HN61	1.55	0.55
1:A:164:LEU:HA	1:A:176:VAL:HG12	1.89	0.55
1:B:288:GLY:HA3	1:B:431:LEU:HA	1.89	0.55
1:D:498:VAL:HG22	1:D:584:ILE:HG23	1.89	0.55
1:E:416:ASN:ND2	3:E:701:ATP:O3G	2.39	0.55
1:B:498:VAL:HG22	1:B:584:ILE:HG22	1.89	0.54
1:E:231:GLU:CD	1:E:232:ARG:H	2.11	0.54
1:F:333:LYS:HB2	1:F:336:GLU:HG3	1.88	0.54
1:C:161:ILE:HD11	1:D:185:VAL:HG23	1.88	0.54
1:B:324:GLU:HA	1:B:327:SER:HB2	1.90	0.54
1:B:554:GLU:OE2	1:B:558:ASN:ND2	2.39	0.54
1:D:450:SER:HA	1:D:479:ILE:HD13	1.90	0.54
1:B:381:GLY:N	1:B:389:GLU:OE2	2.41	0.54
1:C:105:LEU:HD11	1:C:116:PHE:HB2	1.88	0.54
1:E:486:MET:HB3	1:E:551:ILE:HD13	1.90	0.53
1:C:301:LEU:HD11	3:C:701:ATP:H2'	1.90	0.53
1:B:104:LEU:HD22	1:B:135:LEU:HD12	1.90	0.53
1:B:436:LYS:HE2	1:B:438:GLU:HG2	1.90	0.53
1:C:161:ILE:HB	1:D:183:GLU:HG3	1.91	0.53
1:F:295:PRO:HG3	1:F:416:ASN:ND2	2.23	0.53
1:C:384:VAL:HB	1:C:387:ASP:HB2	1.91	0.53
1:F:516:GLY:HA3	3:F:701:ATP:N3	2.24	0.53
1:D:242:VAL:HG13	1:D:243:LEU:H	1.74	0.53
1:A:563:ASN:HD22	1:B:426:LEU:HB3	1.74	0.52
1:B:323:HIS:O	1:B:324:GLU:HB3	2.09	0.52
1:F:494:ARG:HB3	1:F:587:LEU:HD13	1.91	0.52
1:F:108:HIS:CD2	1:F:123:ARG:HH12	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLU:HB2	1:A:587:LEU:HD11	1.91	0.52
1:F:212:ARG:NH2	1:F:358:GLU:O	2.42	0.52
1:D:102:GLY:HA3	1:D:117:THR:HG22	1.91	0.52
1:D:187:TRP:HB2	1:D:228:TYR:CE1	2.45	0.52
1:C:255:GLY:H	3:C:701:ATP:N6	2.08	0.52
1:D:290:LEU:HD12	1:D:431:LEU:HD23	1.91	0.52
1:E:339:ASN:OD1	1:E:340:LYS:N	2.41	0.52
1:C:502:ASN:HD21	1:C:577:LYS:HE3	1.76	0.51
1:E:372:GLU:OE2	1:F:380:ARG:NH1	2.43	0.51
1:C:168:LEU:HD22	1:C:173:ARG:HB2	1.91	0.51
1:F:339:ASN:ND2	1:F:344:GLU:OE2	2.30	0.51
1:C:437:ILE:H	1:C:437:ILE:HD12	1.74	0.51
1:A:487:TYR:OH	1:A:514:ASN:ND2	2.37	0.51
1:C:301:LEU:N	3:C:701:ATP:O1A	2.42	0.51
1:C:457:LEU:O	1:C:471:ARG:NH2	2.44	0.51
1:E:164:LEU:HA	1:E:176:VAL:HG12	1.91	0.51
1:C:292:TYR:O	1:C:436:LYS:HA	2.10	0.51
1:E:497:GLU:HB2	1:E:587:LEU:HD11	1.93	0.51
1:A:380:ARG:HH22	1:A:394:PRO:HG3	1.76	0.50
1:B:335:PRO:HG2	1:E:395:GLN:HB2	1.93	0.50
1:E:100:GLY:HA3	1:F:120:ARG:HH22	1.77	0.50
1:E:290:LEU:HB2	1:E:431:LEU:HD23	1.93	0.50
1:C:187:TRP:HB2	1:C:228:TYR:CE1	2.47	0.50
1:F:255:GLY:H	3:F:701:ATP:HN61	1.59	0.50
1:B:487:TYR:HD2	1:B:511:LYS:HE2	1.75	0.50
1:D:292:TYR:CZ	1:D:436:LYS:HB2	2.47	0.50
1:A:213:LYS:O	1:A:215:ARG:NH1	2.45	0.50
1:B:184:ARG:NH2	1:B:224:THR:O	2.45	0.50
1:C:161:ILE:HD12	1:D:175:LEU:HD13	1.93	0.50
1:F:337:LEU:HD13	1:F:349:ILE:HD11	1.94	0.50
1:B:344:GLU:OE2	1:B:347:ARG:NH2	2.44	0.49
1:E:192:LEU:HD22	1:E:214:LEU:HD11	1.94	0.49
1:D:455:GLU:O	1:D:471:ARG:NH2	2.45	0.49
1:B:117:THR:HG21	1:B:143:LEU:HD22	1.95	0.49
1:A:177:VAL:HG13	1:A:181:ASP:HA	1.94	0.49
1:C:513:PHE:HB3	1:C:561:LEU:HD13	1.95	0.49
1:C:485:ARG:NH1	1:C:548:LEU:HB3	2.28	0.49
1:D:377:PHE:HB2	1:D:422:ASP:HB2	1.93	0.49
1:E:569:ASP:HA	1:E:572:ARG:HH21	1.76	0.49
1:C:215:ARG:NH2	1:C:216:PRO:O	2.41	0.49
1:C:498:VAL:HG22	1:C:584:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:THR:HG22	1:C:505:LYS:HD3	1.95	0.49
1:D:211:PRO:N	1:D:212:ARG:HA	2.27	0.49
1:F:120:ARG:NH1	1:F:122:MET:SD	2.85	0.48
1:F:144:ASN:HD21	1:F:148:THR:HB	1.78	0.48
1:A:142:ARG:HH11	1:B:123:ARG:HD3	1.79	0.48
1:C:460:HIS:HA	1:C:541:GLY:HA3	1.95	0.48
1:E:272:PHE:HE2	1:E:408:ASN:HD21	1.61	0.48
1:B:187:TRP:HB2	1:B:228:TYR:CE1	2.49	0.48
1:A:168:LEU:HD23	1:A:173:ARG:HD2	1.94	0.48
1:A:376:ILE:HD11	1:A:392:VAL:HG11	1.95	0.48
1:D:349:ILE:HG22	1:D:399:GLU:HG3	1.95	0.48
1:E:218:ASP:HB3	1:E:232:ARG:CD	2.43	0.48
1:B:243:LEU:HD11	1:B:327:SER:HA	1.96	0.48
1:C:485:ARG:HD3	1:C:548:LEU:HD22	1.96	0.48
1:D:249:VAL:HG21	1:D:301:LEU:HD22	1.94	0.48
1:A:161:ILE:HB	1:B:183:GLU:HB2	1.96	0.48
1:C:389:GLU:HA	1:C:392:VAL:HG12	1.96	0.48
1:D:495:PHE:CD2	1:D:496:LEU:HG	2.48	0.48
1:A:178:GLY:HA3	1:A:182:GLU:HG2	1.96	0.48
1:A:374:ASP:OD1	1:A:415:SER:OG	2.19	0.48
1:A:430:ARG:H	1:A:430:ARG:HD3	1.80	0.47
1:C:137:LYS:HE3	1:C:172:HIS:HE1	1.78	0.47
1:E:165:ARG:HB2	1:E:177:VAL:HG23	1.95	0.47
1:F:338:LEU:HD11	1:F:376:ILE:HD13	1.96	0.47
1:B:168:LEU:HD12	1:B:173:ARG:HB2	1.96	0.47
1:A:563:ASN:HD22	1:B:426:LEU:HD23	1.80	0.47
1:D:173:ARG:HG2	1:D:187:TRP:CD1	2.49	0.47
1:F:215:ARG:HD3	1:F:354:GLN:HE21	1.79	0.47
1:B:427:ARG:HD2	1:B:428:PRO:O	2.14	0.47
1:C:177:VAL:HG22	1:C:183:GLU:HG3	1.97	0.47
1:C:296:GLY:O	1:C:515:SER:HB2	2.15	0.47
1:F:168:LEU:HD12	1:F:173:ARG:HB2	1.96	0.47
1:A:246:VAL:HG21	1:A:304:LYS:HB2	1.97	0.47
1:C:283:LEU:HD13	1:F:527:LYS:HB2	1.96	0.47
1:F:520:GLN:NE2	3:F:701:ATP:O2'	2.47	0.47
1:D:516:GLY:HA3	3:D:701:ATP:N3	2.30	0.47
1:E:354:GLN:HA	1:E:357:ARG:HG2	1.97	0.47
1:F:497:GLU:HB3	1:F:587:LEU:HD21	1.96	0.47
1:C:251:TYR:HD2	1:C:265:ARG:HH21	1.64	0.46
1:E:570:TRP:HB3	1:E:581:ILE:HD12	1.97	0.46
1:C:296:GLY:N	3:C:701:ATP:O3G	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ILE:HB	1:C:426:LEU:HD11	1.98	0.46
1:A:239:GLU:HB3	1:A:355:ARG:HG2	1.98	0.46
1:E:220:LEU:HD23	1:E:232:ARG:HB3	1.96	0.46
1:E:168:LEU:HD12	1:E:173:ARG:HB2	1.97	0.46
1:E:255:GLY:H	3:E:701:ATP:HN61	1.63	0.46
1:A:333:LYS:HE2	1:B:398:SER:HB2	1.97	0.46
1:E:568:ASP:HB3	1:E:570:TRP:HZ3	1.81	0.46
1:A:116:PHE:HE2	1:A:225:LYS:HZ3	1.64	0.46
1:A:105:LEU:HD12	1:A:114:ASP:HB3	1.98	0.46
1:B:500:TYR:HB2	1:B:503:GLY:HA3	1.98	0.46
1:C:516:GLY:HA3	3:C:701:ATP:N3	2.31	0.46
1:D:249:VAL:HB	1:D:304:LYS:HB2	1.98	0.46
1:C:99:SER:OG	1:D:123:ARG:HB3	2.16	0.46
1:C:299:LYS:HE3	1:C:437:ILE:HD13	1.97	0.46
1:A:158:VAL:HA	1:B:185:VAL:HG23	1.99	0.45
1:C:366:VAL:HG23	1:C:409:VAL:HA	1.98	0.45
1:D:565:THR:HB	1:D:567:PRO:HD2	1.98	0.45
1:D:251:TYR:CE2	1:D:309:SER:HB2	2.51	0.45
1:D:423:PRO:HA	1:D:426:LEU:HB2	1.99	0.45
1:A:388:VAL:HG12	1:A:390:THR:H	1.82	0.45
1:C:189:ALA:HB3	1:C:192:LEU:HD13	1.99	0.45
1:C:533:SER:O	1:C:537:THR:HG22	2.17	0.45
1:D:290:LEU:HD11	1:D:421:ILE:HD13	1.98	0.45
1:B:144:ASN:ND2	1:B:148:THR:O	2.49	0.45
1:B:192:LEU:HB3	1:B:214:LEU:HD11	1.99	0.45
1:B:397:LEU:HD22	1:B:430:ARG:HH11	1.82	0.45
1:C:157:ALA:HB1	1:D:173:ARG:HH11	1.82	0.45
1:B:379:THR:HG22	1:B:422:ASP:HA	1.99	0.45
1:C:437:ILE:HG22	1:C:438:GLU:H	1.82	0.45
1:C:288:GLY:HA3	1:C:431:LEU:HA	1.98	0.45
1:D:165:ARG:HG3	1:D:177:VAL:HG13	1.99	0.45
1:E:419:ASP:OD1	1:E:419:ASP:N	2.50	0.45
1:F:374:ASP:HB3	1:F:415:SER:OG	2.17	0.45
1:E:416:ASN:OD1	1:E:416:ASN:N	2.50	0.45
1:C:142:ARG:HH11	1:D:123:ARG:HD3	1.82	0.44
1:D:338:LEU:HD21	1:D:376:ILE:HG12	1.97	0.44
1:E:401:ASP:OD1	1:E:430:ARG:NE	2.47	0.44
1:A:563:ASN:ND2	1:B:426:LEU:HB3	2.32	0.44
1:C:497:GLU:HB2	1:C:587:LEU:HD11	1.99	0.44
1:E:276:GLU:HG2	1:E:277:LEU:HD22	1.99	0.44
1:E:292:TYR:CZ	1:E:436:LYS:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:379:THR:O	1:F:382:THR:OG1	2.28	0.44
1:A:223:ASP:O	1:A:227:GLY:N	2.44	0.44
1:C:173:ARG:HG2	1:C:187:TRP:CD1	2.52	0.44
1:E:249:VAL:HG23	1:E:253:ASP:HB2	1.99	0.44
1:F:427:ARG:HH21	1:F:430:ARG:CZ	2.29	0.44
1:A:212:ARG:HB3	1:A:215:ARG:HH12	1.83	0.44
1:A:340:LYS:NZ	1:E:181:ASP:OD2	2.34	0.44
1:A:408:ASN:OD1	1:A:408:ASN:N	2.39	0.44
1:C:337:LEU:HD22	1:C:348:HIS:HB3	1.99	0.44
1:C:437:ILE:HD12	1:C:437:ILE:N	2.33	0.44
1:C:464:LEU:HG	1:C:469:GLY:HA2	1.99	0.44
1:A:578:GLY:HA2	1:D:585:ARG:HD3	1.99	0.44
1:C:496:LEU:HD23	1:C:586:THR:HA	2.00	0.44
1:B:497:GLU:HB2	1:B:587:LEU:HD11	1.98	0.44
1:E:163:THR:CA	1:E:219:SER:HA	2.29	0.44
1:E:221:LEU:N	1:E:231:GLU:O	2.46	0.44
1:E:335:PRO:HG3	1:E:375:SER:HB2	2.00	0.44
1:D:247:PRO:HB2	1:D:304:LYS:HB3	2.00	0.44
1:C:287:LYS:HD3	1:C:400:ILE:HG23	2.00	0.43
1:D:272:PHE:HA	1:D:275:LYS:HG2	2.00	0.43
1:E:300:THR:HG22	1:E:304:LYS:HE3	2.00	0.43
1:F:186:VAL:HG11	1:F:222:VAL:HG21	1.99	0.43
1:F:294:PRO:O	1:F:299:LYS:NZ	2.41	0.43
1:B:240:ASP:OD1	1:B:241:LEU:N	2.52	0.43
1:E:107:THR:HG22	1:E:113:VAL:HG12	2.00	0.43
1:F:376:ILE:HD12	1:F:376:ILE:HA	1.91	0.43
1:A:144:ASN:HD21	1:A:146:ALA:HB3	1.83	0.43
1:C:453:LEU:HD12	1:C:479:ILE:HG12	2.01	0.43
1:F:136:LYS:HE3	1:F:155:PHE:HZ	1.82	0.43
1:B:175:LEU:HD11	1:B:183:GLU:HB3	2.01	0.43
1:C:520:GLN:OE1	3:C:701:ATP:O2'	2.36	0.43
1:E:337:LEU:HD13	1:E:349:ILE:HG12	2.01	0.43
1:D:219:SER:H	1:D:235:LYS:NZ	2.16	0.43
1:E:393:VAL:HG13	1:E:425:ILE:HD11	2.00	0.43
1:C:105:LEU:O	1:C:137:LYS:NZ	2.32	0.43
1:B:244:GLU:O	1:B:326:LYS:HD2	2.19	0.43
1:C:452:TYR:OH	3:C:701:ATP:O2'	2.33	0.43
1:D:311:ALA:O	1:D:314:MET:HG2	2.18	0.43
1:F:385:SER:O	2:G:0:SER:OG	2.23	0.43
1:B:243:LEU:HD12	1:B:326:LYS:HG3	2.00	0.43
1:B:495:PHE:HE1	1:B:559:GLU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:LEU:O	1:C:565:THR:HG23	2.19	0.43
1:D:219:SER:H	1:D:235:LYS:HZ2	1.67	0.43
1:E:421:ILE:HB	1:E:426:LEU:HD11	2.00	0.43
1:B:115:VAL:HG11	1:B:143:LEU:HD11	2.01	0.42
1:E:247:PRO:HG2	1:E:304:LYS:HB2	2.01	0.42
1:E:321:ASP:HB2	1:E:324:GLU:HG2	1.99	0.42
1:E:490:ILE:HB	1:E:492:ASP:OD1	2.19	0.42
1:A:165:ARG:HG3	1:A:177:VAL:HG23	2.01	0.42
1:E:531:ILE:HA	1:E:534:VAL:HG12	2.00	0.42
1:B:460:HIS:HE1	1:B:539:GLN:HB3	1.84	0.42
1:B:534:VAL:HG22	1:B:540:PRO:HA	2.01	0.42
1:C:259:ARG:HA	1:C:262:GLU:HG2	2.01	0.42
1:C:495:PHE:HZ	1:C:561:LEU:HB2	1.85	0.42
1:D:257:LEU:O	1:D:261:ILE:HG12	2.18	0.42
1:E:499:THR:HG23	1:E:505:LYS:HG2	2.01	0.42
1:E:528:LYS:O	1:E:531:ILE:HG22	2.19	0.42
1:B:377:PHE:CZ	1:B:396:LEU:HD13	2.54	0.42
1:C:295:PRO:HG3	1:C:416:ASN:CB	2.49	0.42
1:D:566:ASN:N	1:D:567:PRO:HD2	2.35	0.42
1:F:295:PRO:HG3	1:F:416:ASN:HD21	1.83	0.42
1:B:499:THR:HB	1:B:583:TYR:HB3	2.02	0.42
1:E:192:LEU:HD21	1:E:230:PHE:O	2.19	0.42
1:E:494:ARG:HE	1:E:507:VAL:HG21	1.85	0.42
1:B:261:ILE:HG13	1:B:262:GLU:N	2.33	0.42
1:B:349:ILE:HD12	1:B:396:LEU:HD21	2.01	0.42
1:B:495:PHE:HZ	1:B:562:PRO:HD3	1.85	0.42
1:E:531:ILE:HA	1:E:531:ILE:HD12	1.85	0.42
1:F:161:ILE:HB	1:F:219:SER:HB3	2.01	0.42
1:B:528:LYS:HE3	1:B:528:LYS:HB3	1.83	0.42
1:C:295:PRO:HG3	1:C:416:ASN:HB2	2.02	0.42
1:E:498:VAL:HA	1:E:584:ILE:HG22	2.02	0.42
1:E:516:GLY:HA3	3:E:701:ATP:N3	2.34	0.42
1:D:466:GLU:N	1:D:466:GLU:OE1	2.53	0.42
1:E:453:LEU:HD12	1:E:479:ILE:HG12	2.00	0.42
1:F:427:ARG:HD2	1:F:428:PRO:O	2.20	0.42
1:C:432:ASP:OD1	1:C:432:ASP:N	2.53	0.42
1:D:515:SER:H	1:D:518:MET:HG2	1.84	0.42
1:D:560:ASP:O	1:D:564:THR:OG1	2.30	0.42
1:E:563:ASN:ND2	1:E:565:THR:O	2.52	0.42
1:F:102:GLY:HA3	1:F:117:THR:HG22	2.00	0.42
1:C:284:ARG:HH22	1:C:287:LYS:NZ	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:TRP:HB2	1:F:228:TYR:CE1	2.56	0.41
1:F:212:ARG:HB3	1:F:232:ARG:HH22	1.84	0.41
1:D:144:ASN:HD21	1:D:148:THR:HB	1.85	0.41
1:E:221:LEU:HG	1:E:230:PHE:HD2	1.85	0.41
1:B:100:GLY:HA3	1:E:120:ARG:HH21	1.85	0.41
1:B:503:GLY:HA2	1:B:577:LYS:NZ	2.34	0.41
1:C:497:GLU:HB3	1:C:585:ARG:HG2	2.03	0.41
1:D:142:ARG:NE	1:D:151:GLU:OE2	2.54	0.41
1:A:99:SER:OG	1:B:123:ARG:HB3	2.20	0.41
1:A:447:ASP:O	1:A:451:LYS:HG2	2.19	0.41
1:B:336:GLU:HA	1:E:350:ARG:NH2	2.35	0.41
1:B:545:GLN:NE2	1:B:549:ASP:OD1	2.53	0.41
1:C:137:LYS:HE3	1:C:172:HIS:CE1	2.55	0.41
1:C:452:TYR:HH	3:C:701:ATP:HO2'	1.64	0.41
1:A:349:ILE:HD12	1:A:395:GLN:HE21	1.85	0.41
1:C:535:LEU:HD22	1:D:274:HIS:CE1	2.56	0.41
1:D:460:HIS:CE1	1:D:543:ARG:HH11	2.38	0.41
1:E:511:LYS:NZ	1:E:512:ASP:OD1	2.52	0.41
1:A:463:ASP:HB3	1:A:474:CYS:SG	2.60	0.41
1:C:179:HIS:CG	1:D:182:GLU:HB3	2.56	0.41
1:F:291:LEU:O	1:F:414:ALA:HA	2.21	0.41
1:F:142:ARG:HE	1:F:151:GLU:HB3	1.85	0.41
1:F:176:VAL:O	1:F:183:GLU:HA	2.20	0.41
1:A:291:LEU:HD23	1:A:435:ILE:HB	2.03	0.41
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.91	0.41
1:B:500:TYR:HB3	1:B:579:GLU:HB2	2.03	0.41
1:C:255:GLY:H	3:C:701:ATP:HN62	1.68	0.41
1:D:518:MET:O	1:D:522:VAL:HG23	2.21	0.41
1:D:560:ASP:CG	1:D:562:PRO:HD2	2.42	0.41
1:E:261:ILE:HA	1:E:264:ILE:HG22	2.03	0.41
1:F:300:THR:HG22	1:F:304:LYS:HE3	2.01	0.41
1:F:373:MET:HB3	1:F:415:SER:HB2	2.02	0.41
1:D:441:ASP:N	1:D:441:ASP:OD1	2.54	0.41
1:B:142:ARG:O	1:B:149:VAL:HA	2.21	0.40
1:B:367:ILE:HD13	1:B:410:ILE:HB	2.02	0.40
1:F:357:ARG:NH2	1:F:406:LEU:HD23	2.36	0.40
1:A:384:VAL:HG13	1:B:386:SER:HA	2.04	0.40
1:A:523:VAL:HG12	1:A:527:LYS:HE2	2.02	0.40
1:B:475:ILE:HD13	1:B:475:ILE:HA	1.97	0.40
1:C:278:TYR:O	1:C:282:SER:N	2.54	0.40
1:C:339:ASN:HD21	1:C:341:PHE:HD2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:TYR:CE2	1:D:520:GLN:HG2	2.56	0.40
1:F:567:PRO:HA	1:F:570:TRP:NE1	2.35	0.40
1:D:166:GLU:HG2	1:D:175:LEU:HB3	2.03	0.40
1:C:328:TYR:HD2	1:C:359:LYS:HB3	1.86	0.40
1:E:486:MET:HG3	1:E:487:TYR:CD1	2.56	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	A	458/609 (75%)	444 (97%)	14 (3%)	0	100	100
1	B	472/609 (78%)	456 (97%)	16 (3%)	0	100	100
1	C	458/609 (75%)	445 (97%)	13 (3%)	0	100	100
1	D	444/609 (73%)	422 (95%)	22 (5%)	0	100	100
1	E	472/609 (78%)	453 (96%)	18 (4%)	1 (0%)	47	79
1	F	473/609 (78%)	456 (96%)	17 (4%)	0	100	100
2	G	15/66 (23%)	15 (100%)	0	0	100	100
All	All	2792/3720 (75%)	2691 (96%)	100 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	234	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	A	396/511 (78%)	389 (98%)	7 (2%)	59	77
1	B	403/511 (79%)	395 (98%)	8 (2%)	55	73
1	C	394/511 (77%)	387 (98%)	7 (2%)	59	77
1	D	384/511 (75%)	375 (98%)	9 (2%)	50	70
1	E	403/511 (79%)	391 (97%)	12 (3%)	41	64
1	F	403/511 (79%)	398 (99%)	5 (1%)	71	84
2	G	10/50 (20%)	9 (90%)	1 (10%)	7	29
All	All	2393/3116 (77%)	2344 (98%)	49 (2%)	57	73

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLU
1	A	215	ARG
1	A	337	LEU
1	A	393	VAL
1	A	396	LEU
1	A	408	ASN
1	A	430	ARG
1	B	103	VAL
1	B	163	THR
1	B	165	ARG
1	B	212	ARG
1	B	345	THR
1	B	348	HIS
1	B	505	LYS
1	B	559	GLU
1	C	183	GLU
1	C	212	ARG
1	C	232	ARG
1	C	345	THR
1	C	393	VAL
1	C	480	GLU
1	C	536	GLU
1	D	259	ARG
1	D	263	GLN

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Mol	Chain	Res	Type
1	D	336	GLU
1	D	430	ARG
1	D	449	TYR
1	D	466	GLU
1	D	478	MET
1	D	518	MET
1	D	565	THR
1	E	163	THR
1	E	230	PHE
1	E	233	ILE
1	E	234	PRO
1	E	243	LEU
1	E	273	LEU
1	E	345	THR
1	E	379	THR
1	E	389	GLU
1	E	396	LEU
1	E	404	GLU
1	E	416	ASN
1	F	341	PHE
1	F	374	ASP
1	F	499	THR
1	F	506	GLU
1	F	570	TRP
2	G	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	A	539	GLN
1	B	263	GLN
1	B	395	GLN
1	B	460	HIS
1	B	521	ASN
1	B	539	GLN
1	B	546	HIS
1	C	172	HIS
1	C	339	ASN
1	C	514	ASN
1	D	263	GLN
1	D	446	GLN

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Mol	Chain	Res	Type
1	D	520	GLN
1	D	546	HIS
1	D	558	ASN
1	E	108	HIS
1	E	354	GLN
1	E	408	ASN
1	E	520	GLN
1	F	108	HIS
1	F	348	HIS
1	F	354	GLN
1	F	395	GLN
1	F	520	GLN
1	F	546	HIS

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
3	ATP	E	701	4	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	D	701	4	26,33,33	0.92	1 (3%)	31,52,52	1.52	5 (16%)
3	ATP	B	701	4	26,33,33	0.92	1 (3%)	31,52,52	1.63	5 (16%)
3	ATP	A	701	4	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
3	ATP	C	701	4	26,33,33	0.94	1 (3%)	31,52,52	1.50	5 (16%)
3	ATP	F	701	4	26,33,33	0.93	1 (3%)	31,52,52	1.64	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	701	4	-	0/18/38/38	0/3/3/3
3	ATP	D	701	4	-	0/18/38/38	0/3/3/3
3	ATP	B	701	4	-	0/18/38/38	0/3/3/3
3	ATP	A	701	4	-	0/18/38/38	0/3/3/3
3	ATP	C	701	4	-	0/18/38/38	0/3/3/3
3	ATP	F	701	4	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	701	ATP	C5-C4	2.51	1.47	1.40
3	C	701	ATP	C5-C4	2.49	1.47	1.40
3	D	701	ATP	C5-C4	2.49	1.47	1.40
3	E	701	ATP	C5-C4	2.49	1.47	1.40
3	A	701	ATP	C5-C4	2.47	1.47	1.40
3	B	701	ATP	C5-C4	2.44	1.47	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	ATP	PB-O3B-PG	-4.52	117.31	132.83
3	A	701	ATP	PB-O3B-PG	-4.42	117.66	132.83
3	F	701	ATP	PB-O3B-PG	-4.36	117.85	132.83
3	E	701	ATP	PB-O3B-PG	-4.34	117.94	132.83
3	F	701	ATP	PA-O3A-PB	-4.23	118.33	132.83
3	B	701	ATP	PA-O3A-PB	-4.10	118.77	132.83
3	A	701	ATP	PA-O3A-PB	-4.08	118.84	132.83
3	E	701	ATP	PA-O3A-PB	-4.01	119.07	132.83
3	D	701	ATP	PB-O3B-PG	-3.91	119.41	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	ATP	PB-O3B-PG	-3.54	120.69	132.83
3	D	701	ATP	PA-O3A-PB	-3.53	120.73	132.83
3	C	701	ATP	PA-O3A-PB	-3.36	121.31	132.83
3	C	701	ATP	N3-C2-N1	-3.17	123.72	128.68
3	A	701	ATP	N3-C2-N1	-3.12	123.81	128.68
3	B	701	ATP	N3-C2-N1	-3.11	123.82	128.68
3	F	701	ATP	N3-C2-N1	-3.11	123.82	128.68
3	D	701	ATP	N3-C2-N1	-3.09	123.84	128.68
3	E	701	ATP	N3-C2-N1	-3.04	123.93	128.68
3	E	701	ATP	C3'-C2'-C1'	2.88	105.31	100.98
3	B	701	ATP	C3'-C2'-C1'	2.81	105.20	100.98
3	A	701	ATP	C3'-C2'-C1'	2.77	105.15	100.98
3	C	701	ATP	C3'-C2'-C1'	2.75	105.12	100.98
3	F	701	ATP	C3'-C2'-C1'	2.67	105.00	100.98
3	C	701	ATP	C4-C5-N7	-2.66	106.63	109.40
3	A	701	ATP	C4-C5-N7	-2.63	106.66	109.40
3	D	701	ATP	C4-C5-N7	-2.62	106.67	109.40
3	F	701	ATP	C4-C5-N7	-2.58	106.71	109.40
3	E	701	ATP	C4-C5-N7	-2.49	106.80	109.40
3	D	701	ATP	C3'-C2'-C1'	2.46	104.69	100.98
3	B	701	ATP	C4-C5-N7	-2.42	106.88	109.40

There are no chirality outliers.

There are no torsion outliers.

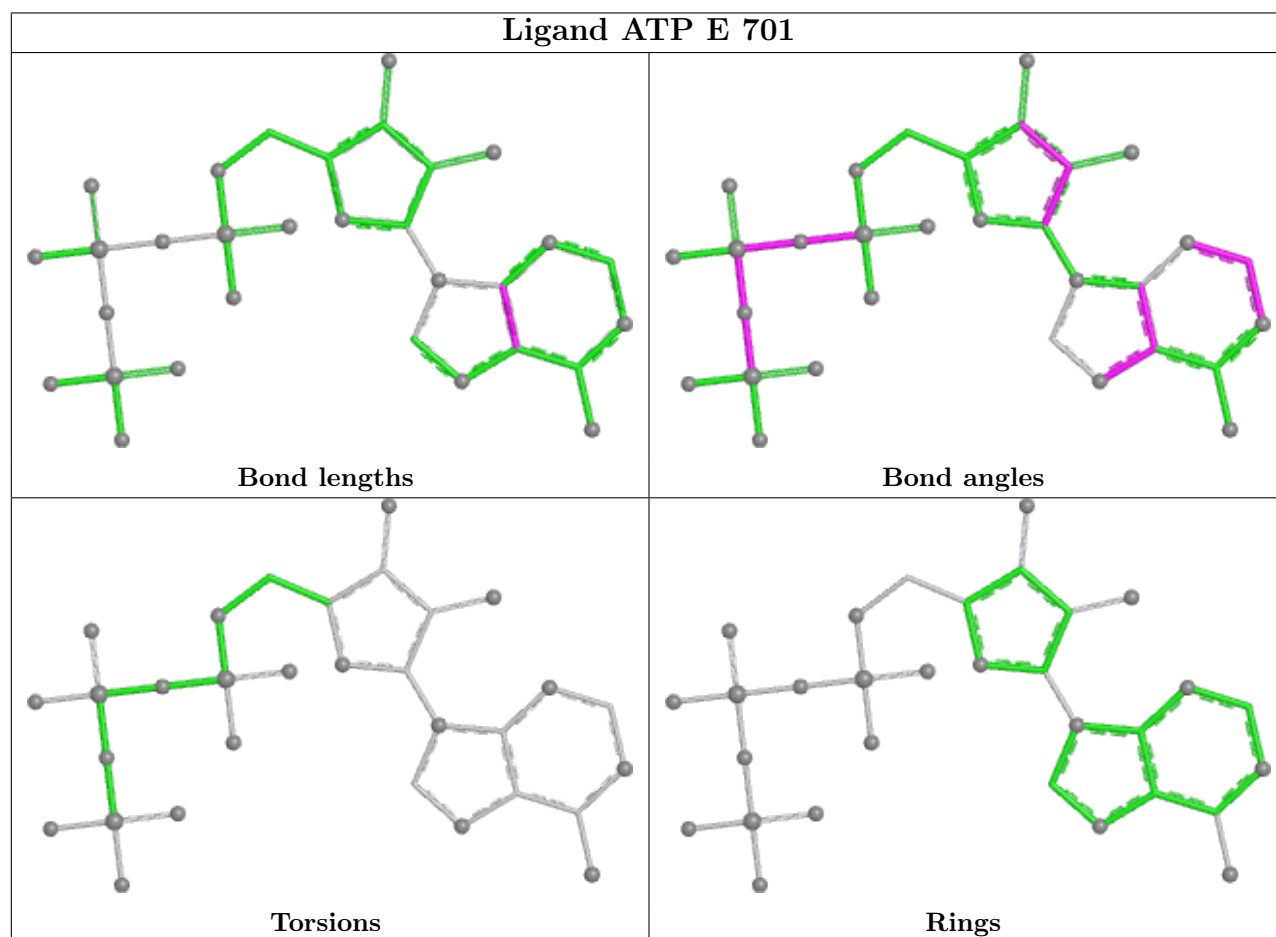
There are no ring outliers.

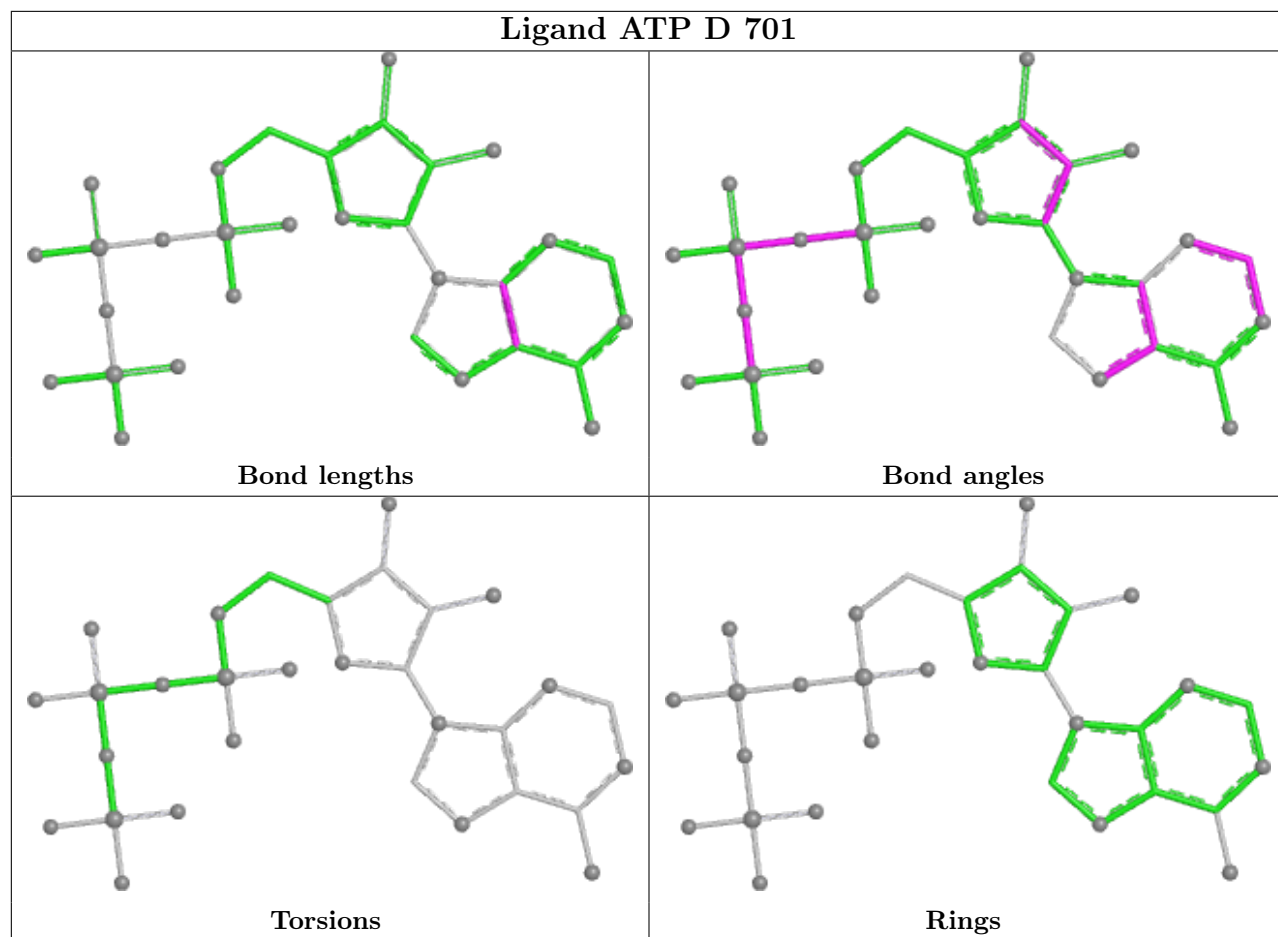
6 monomers are involved in 22 short contacts:

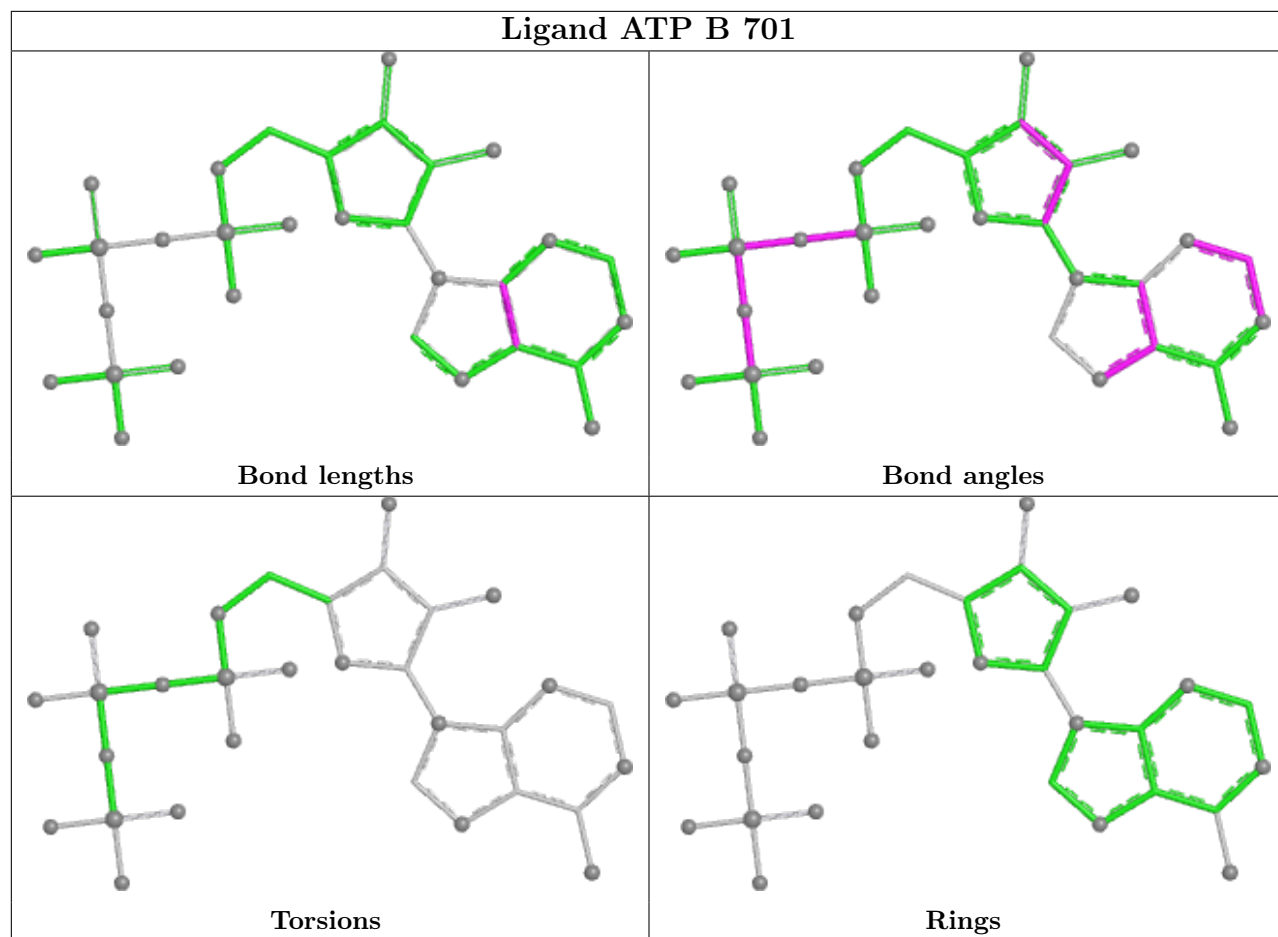
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	701	ATP	4	0
3	D	701	ATP	1	0
3	B	701	ATP	2	0
3	A	701	ATP	2	0
3	C	701	ATP	9	0
3	F	701	ATP	4	0

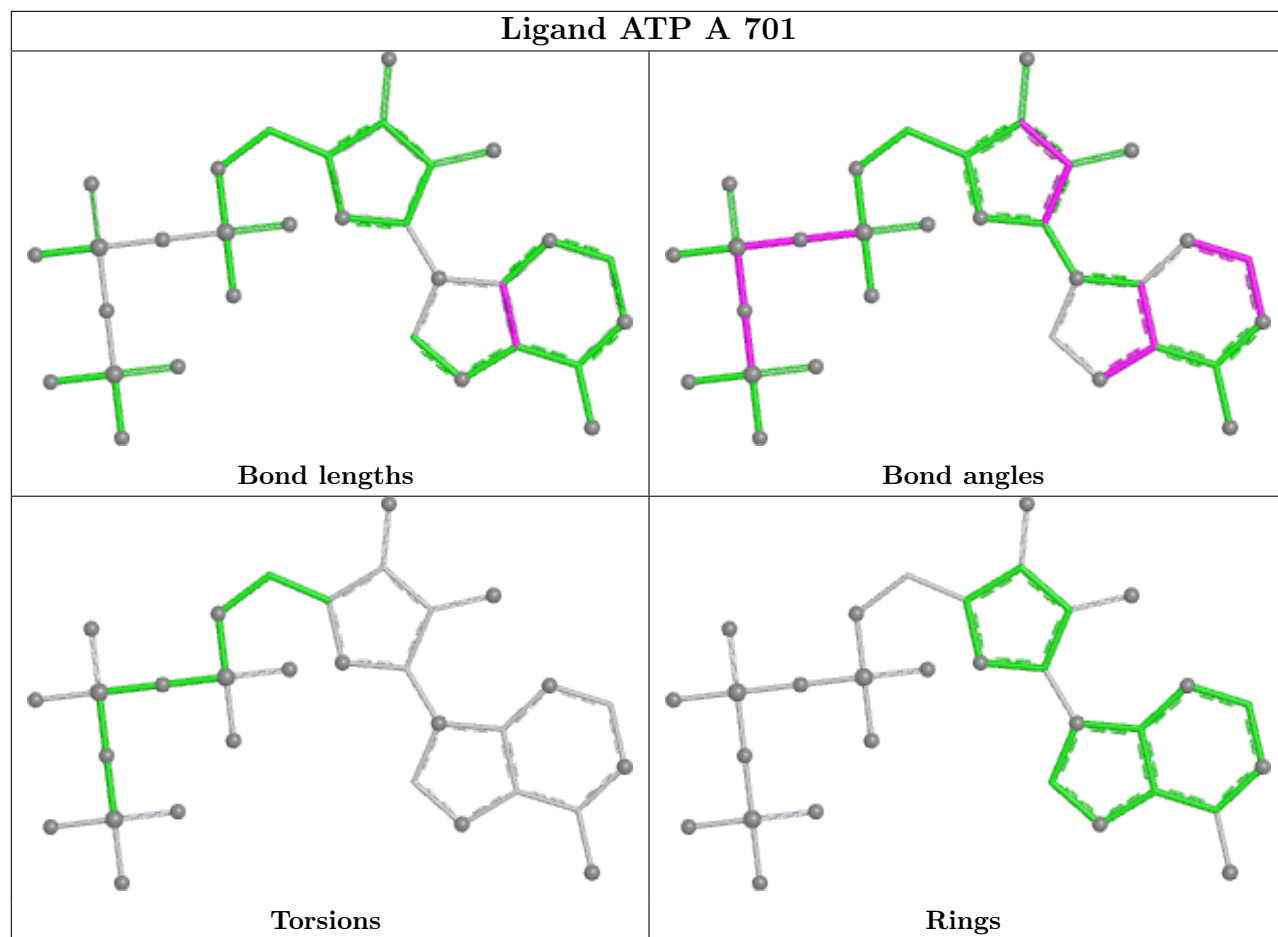
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

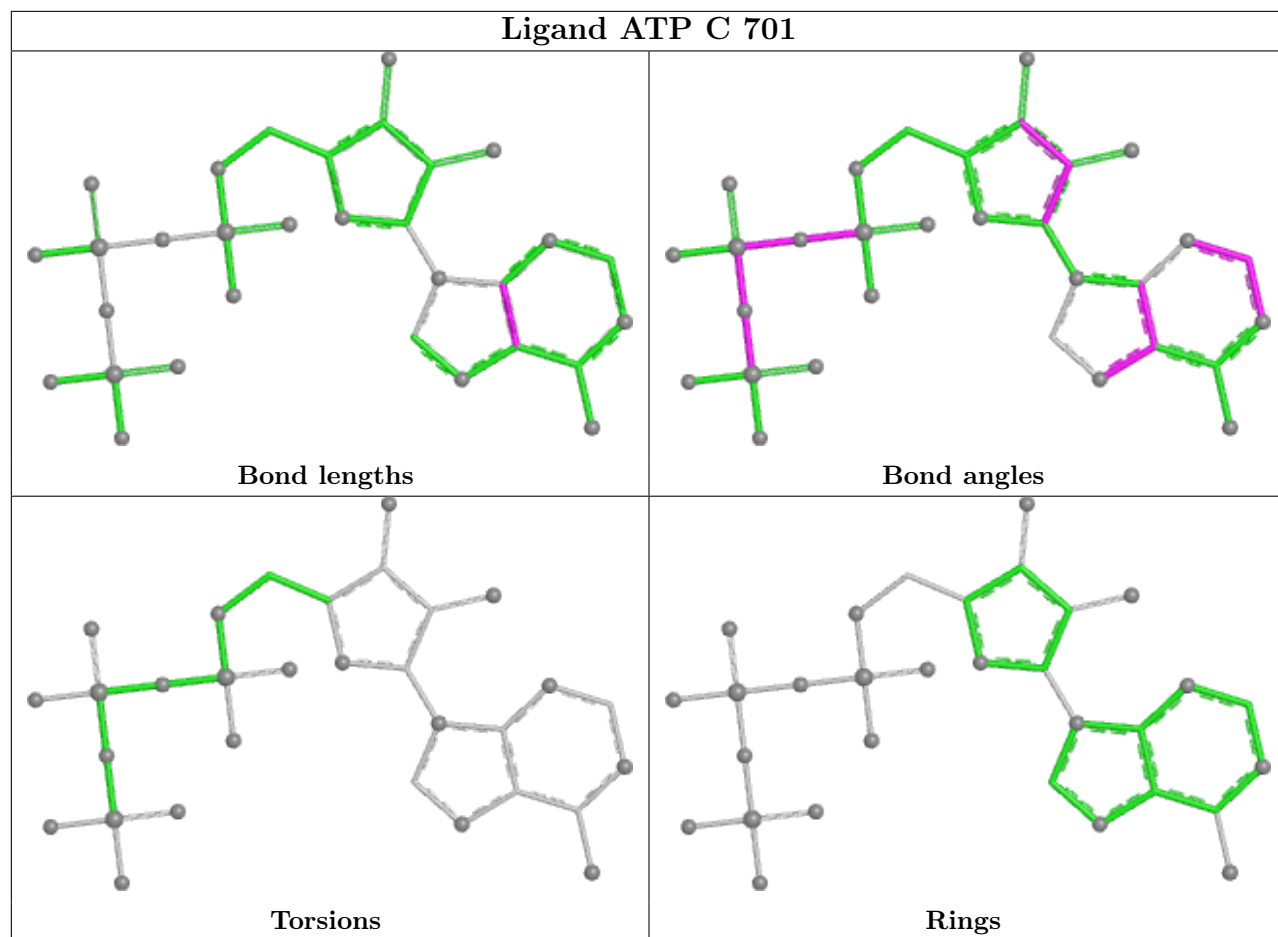
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

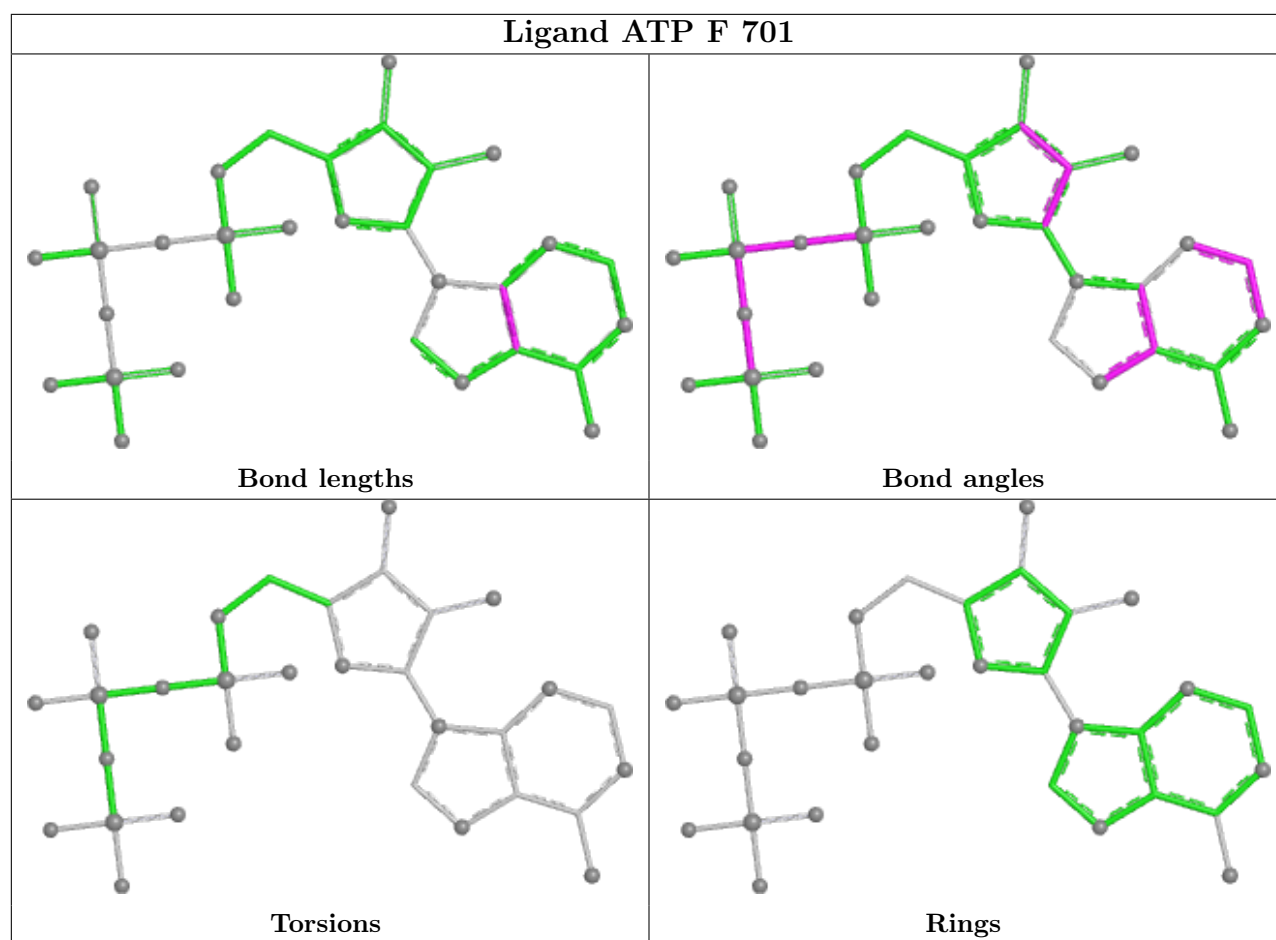












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

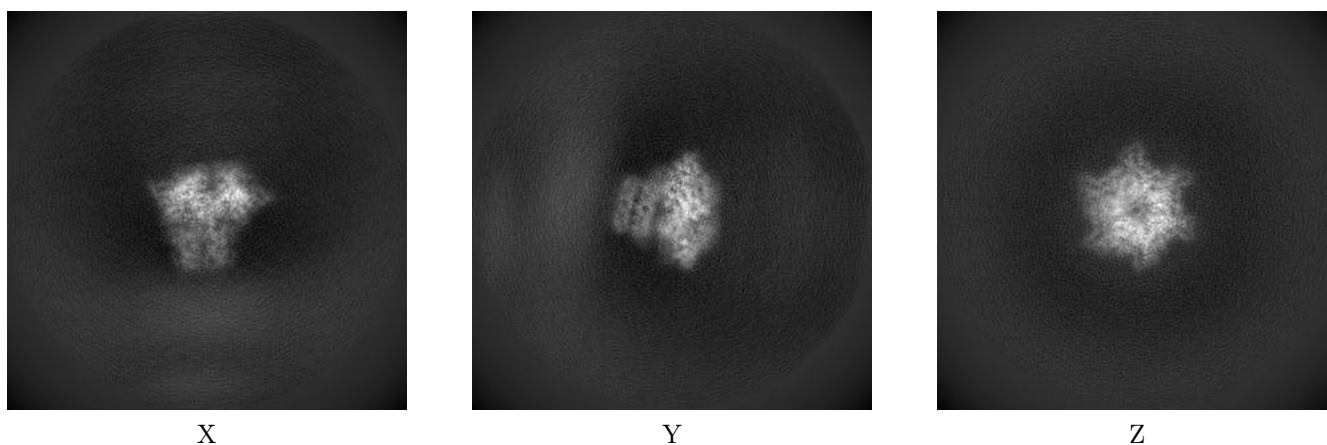
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13696. 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](#)

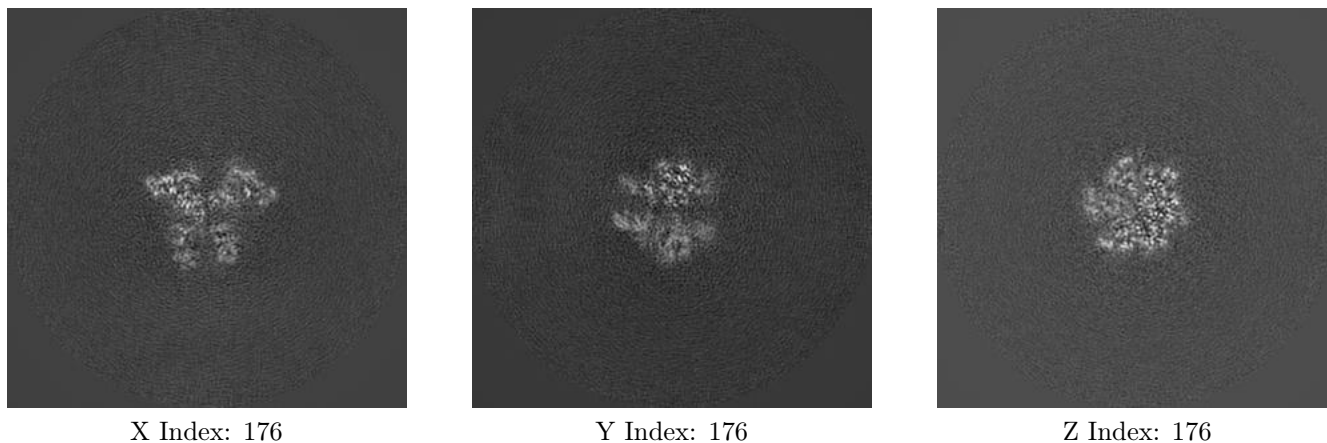
6.1.1 Primary map



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

6.2 Central slices [i](#)

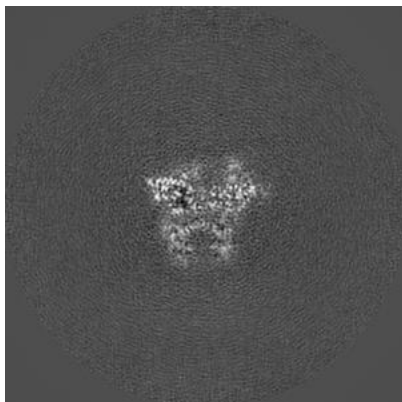
6.2.1 Primary map



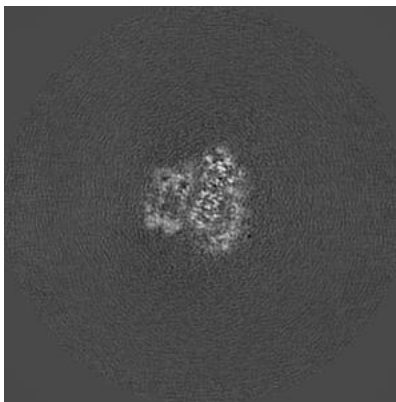
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

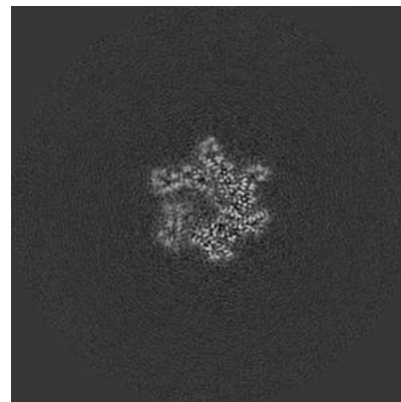
6.3.1 Primary map



X Index: 183



Y Index: 164

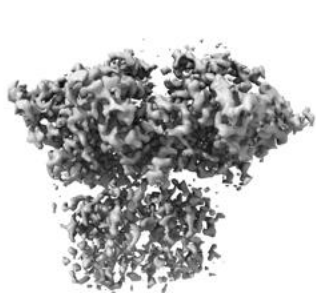


Z Index: 189

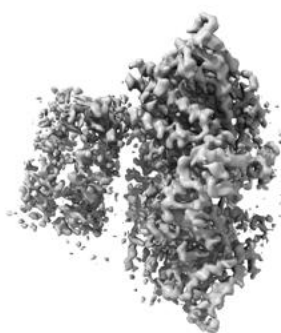
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

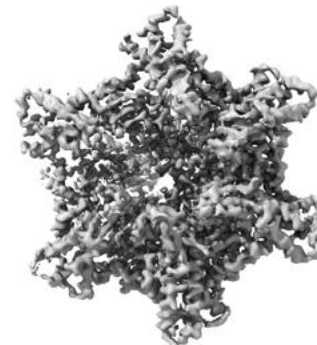
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0247. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

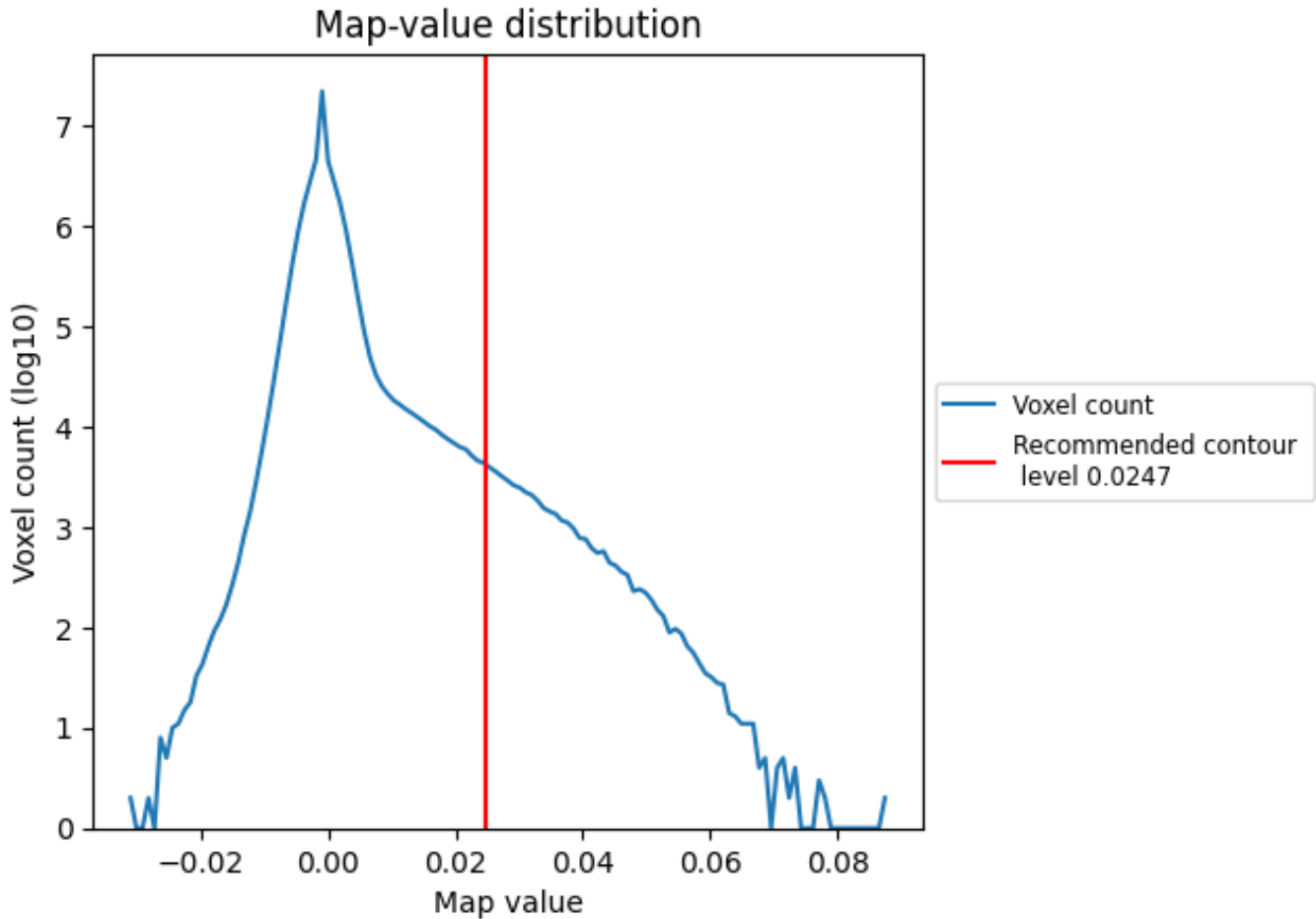
6.5 Mask visualisation

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

7 Map analysis [i](#)

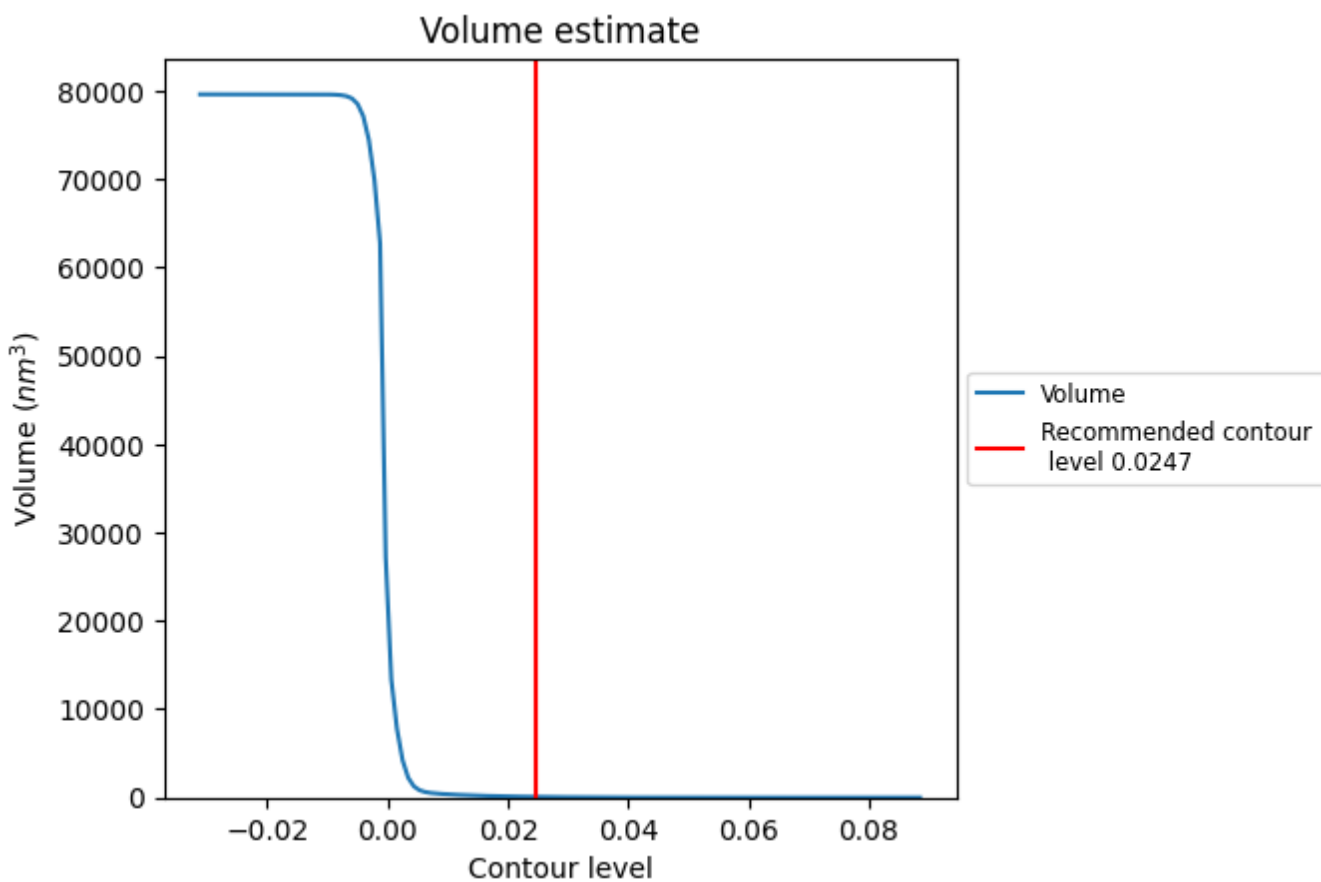
This section contains the results of statistical analysis of the map.

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.

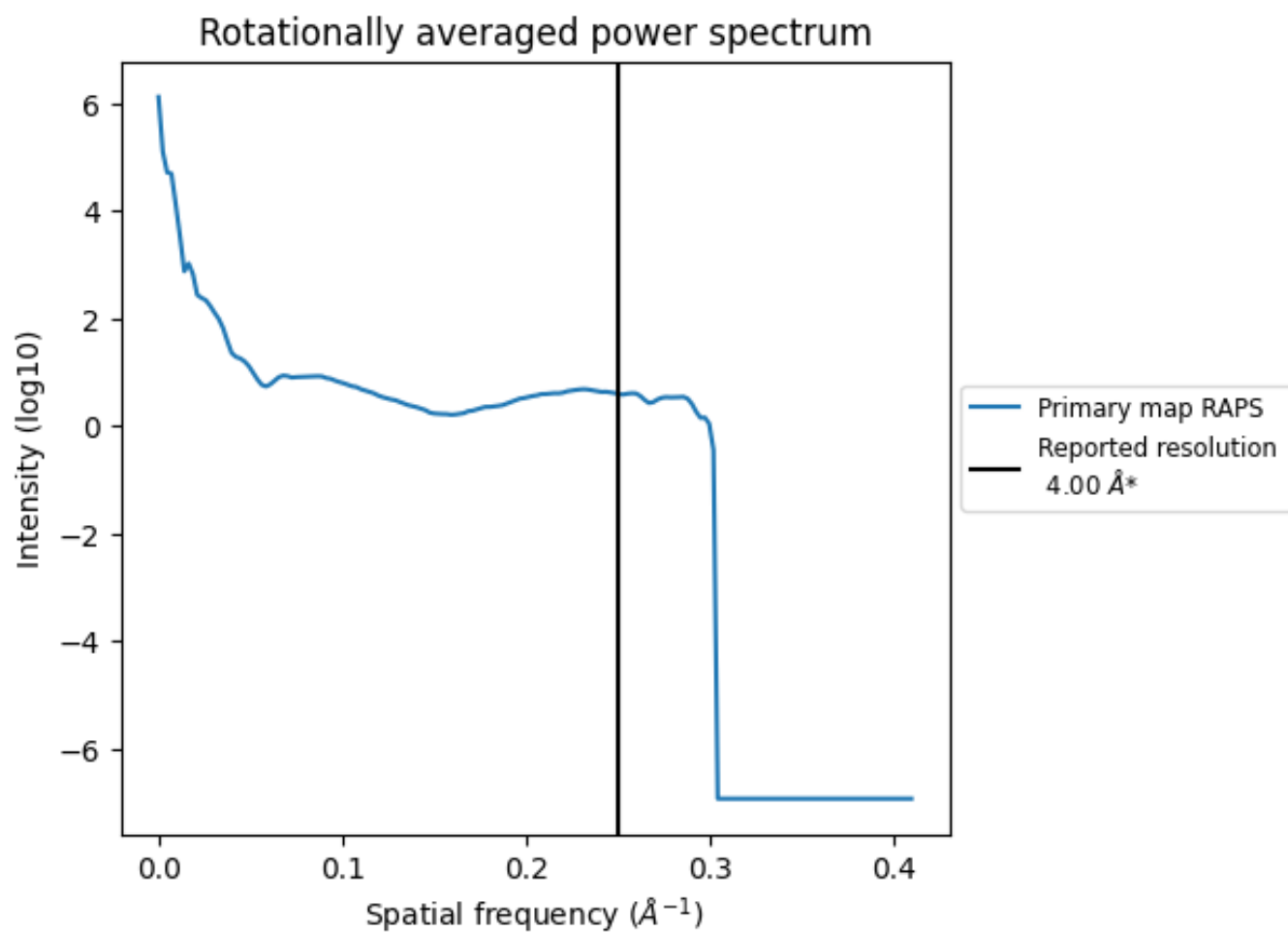
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm³; this corresponds to an approximate mass of 70 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 0.250 Å⁻¹

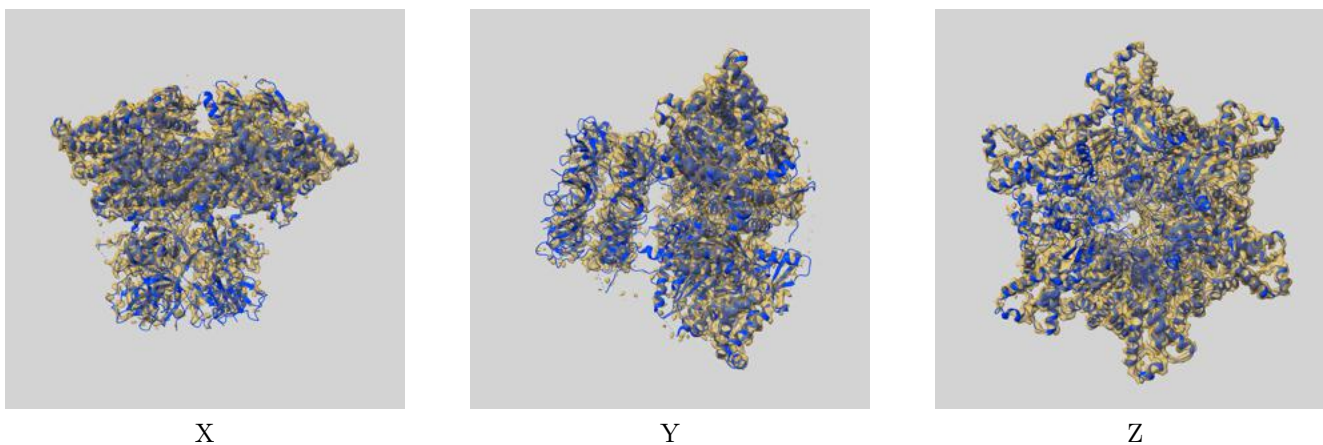
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

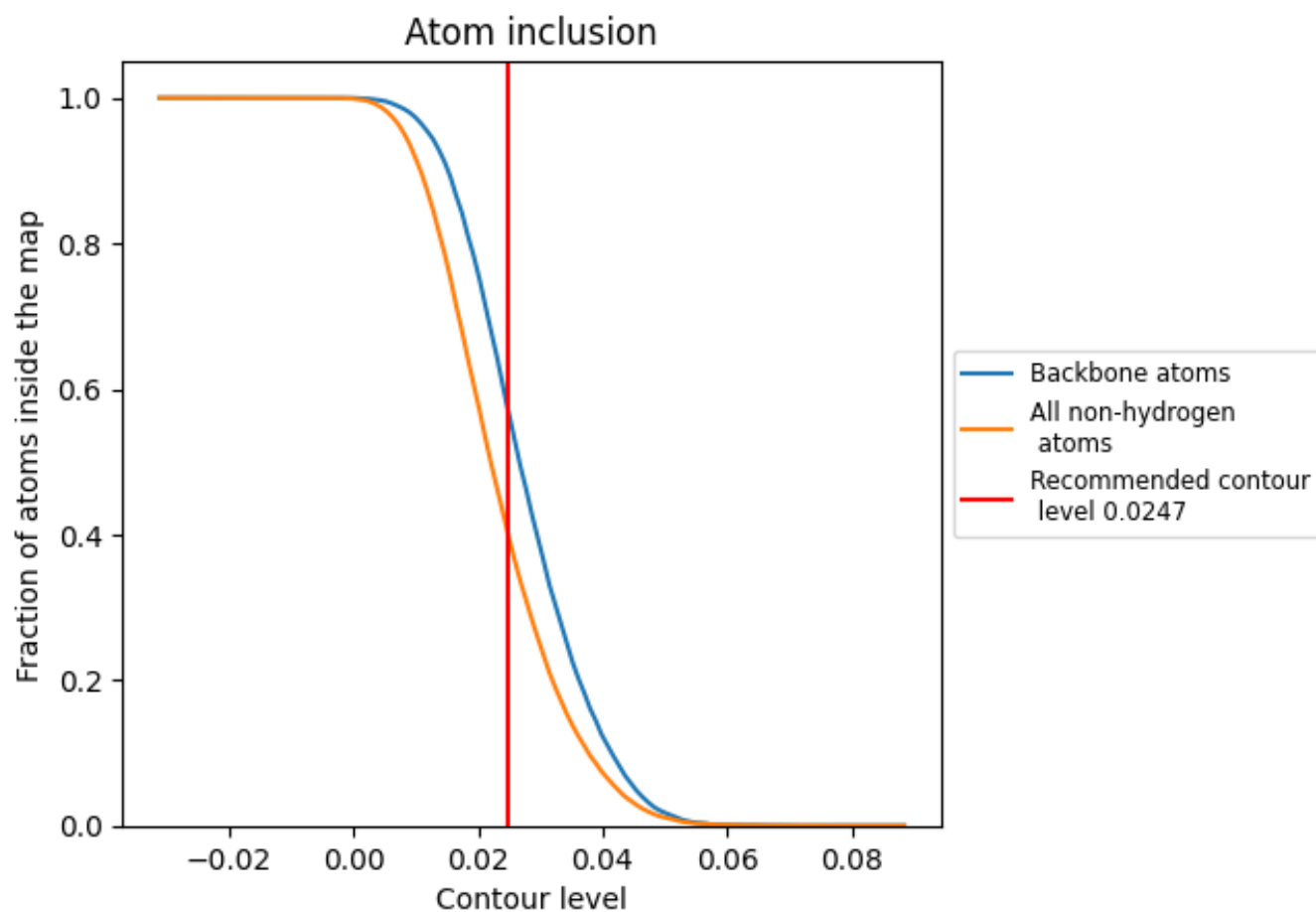
This section contains information regarding the fit between EMDB map EMD-13696 and PDB model 7PXB. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0247 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 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.