



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:12 AM UTC

PDB ID : 6W23 / pdb_00006w23
EMDB ID : EMD-21523
Title : ClpA Disengaged State bound to RepA-GFP (Focused Classification)
Authors : Lopez, K.L.; Rizo, A.N.; Tse, E.; Lin, J.; Scull, N.W.; Thwin, A.C.; Lucius, A.L.; Shorter, J.; Southworth, D.R.
Deposited on : 2020-03-04
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:

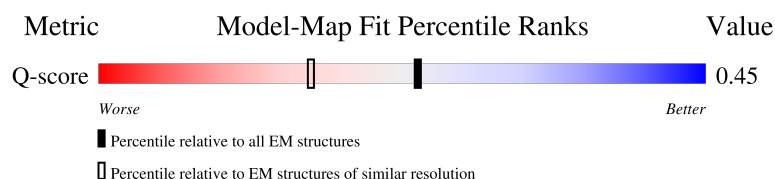
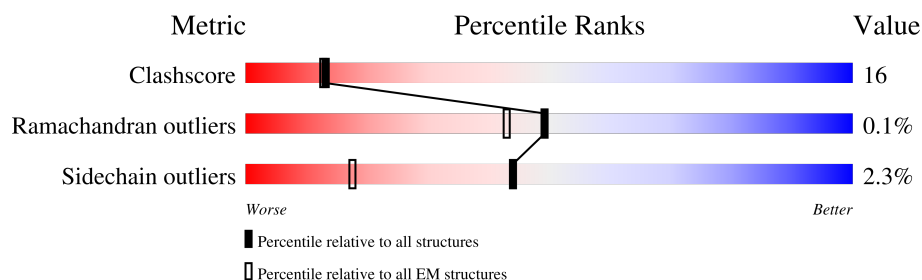
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	758	
1	B	758	
1	C	758	
1	D	758	

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Mol	Chain	Length	Quality of chain
1	E	758	
1	F	758	
2	X	24	

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	ADP	F	801	-	-	X	-
4	ATP	B	801	-	-	X	-
4	ATP	C	801	-	-	X	-
4	ATP	C	802	-	-	X	-
4	ATP	D	802	-	-	X	-
4	ATP	E	801	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27206 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-dependent Clp protease ATP-binding subunit ClpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	552	Total	C	N	O	S	0	0
			4321	2730	767	810	14		
1	B	578	Total	C	N	O	S	0	0
			4510	2841	805	850	14		
1	C	578	Total	C	N	O	S	0	0
			4510	2841	805	850	14		
1	D	578	Total	C	N	O	S	0	0
			4510	2841	805	850	14		
1	E	568	Total	C	N	O	S	0	0
			4453	2809	794	836	14		
1	F	568	Total	C	N	O	S	0	0
			4453	2809	794	836	14		

- Molecule 2 is a protein called RepA, green fluorescent protein fusion.

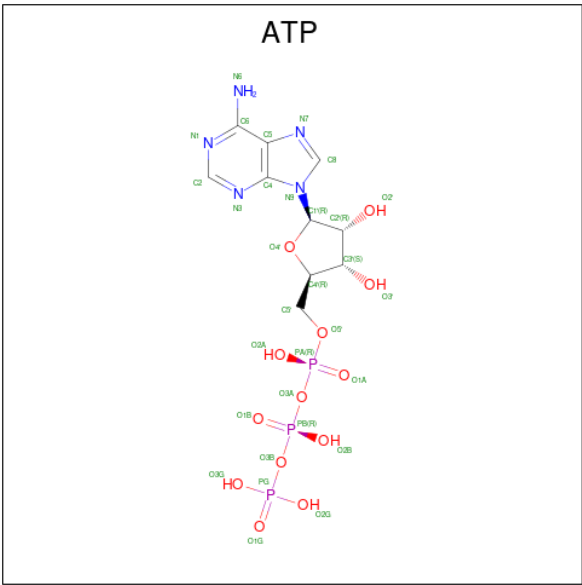
Mol	Chain	Residues	Atoms				AltConf	Trace
2	X	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



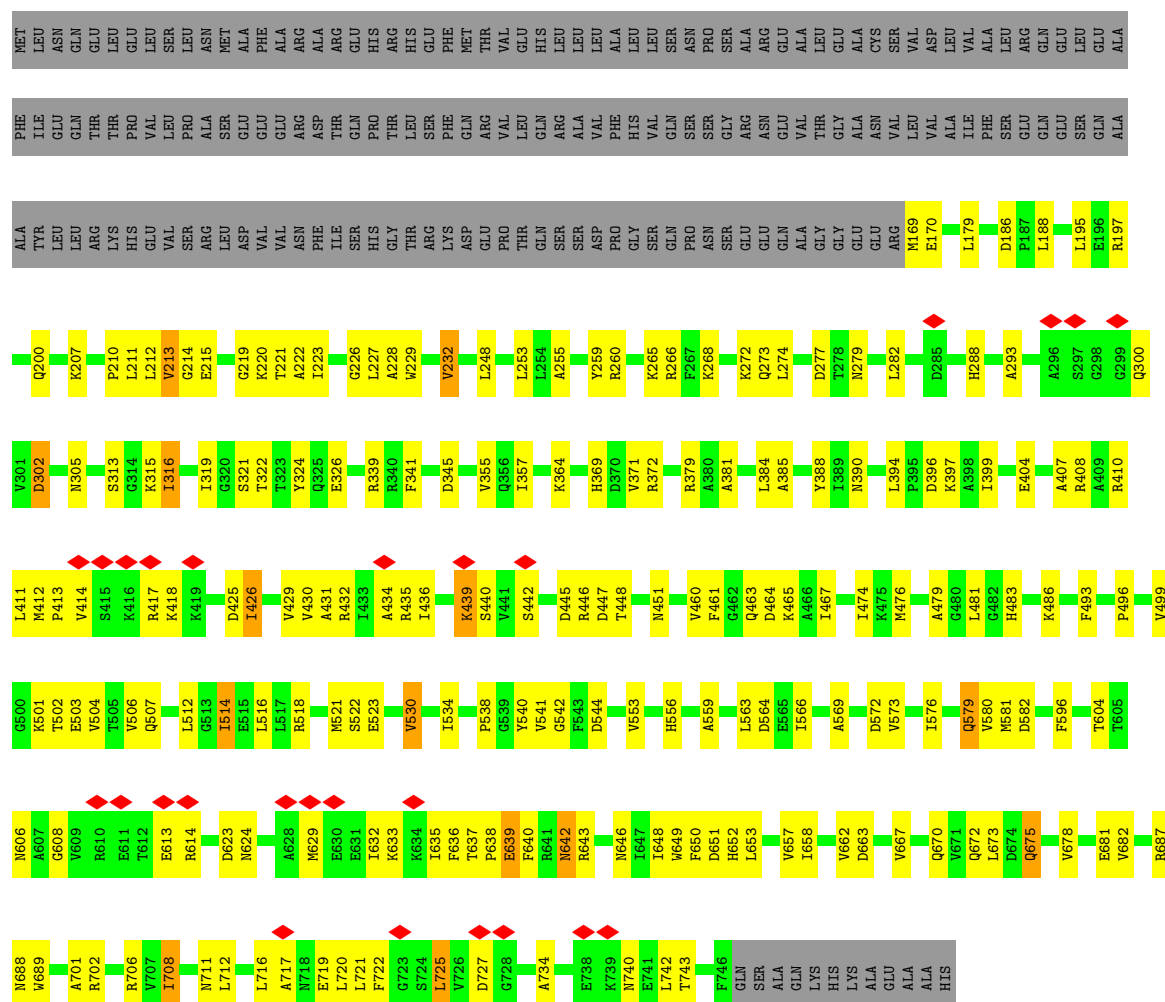
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

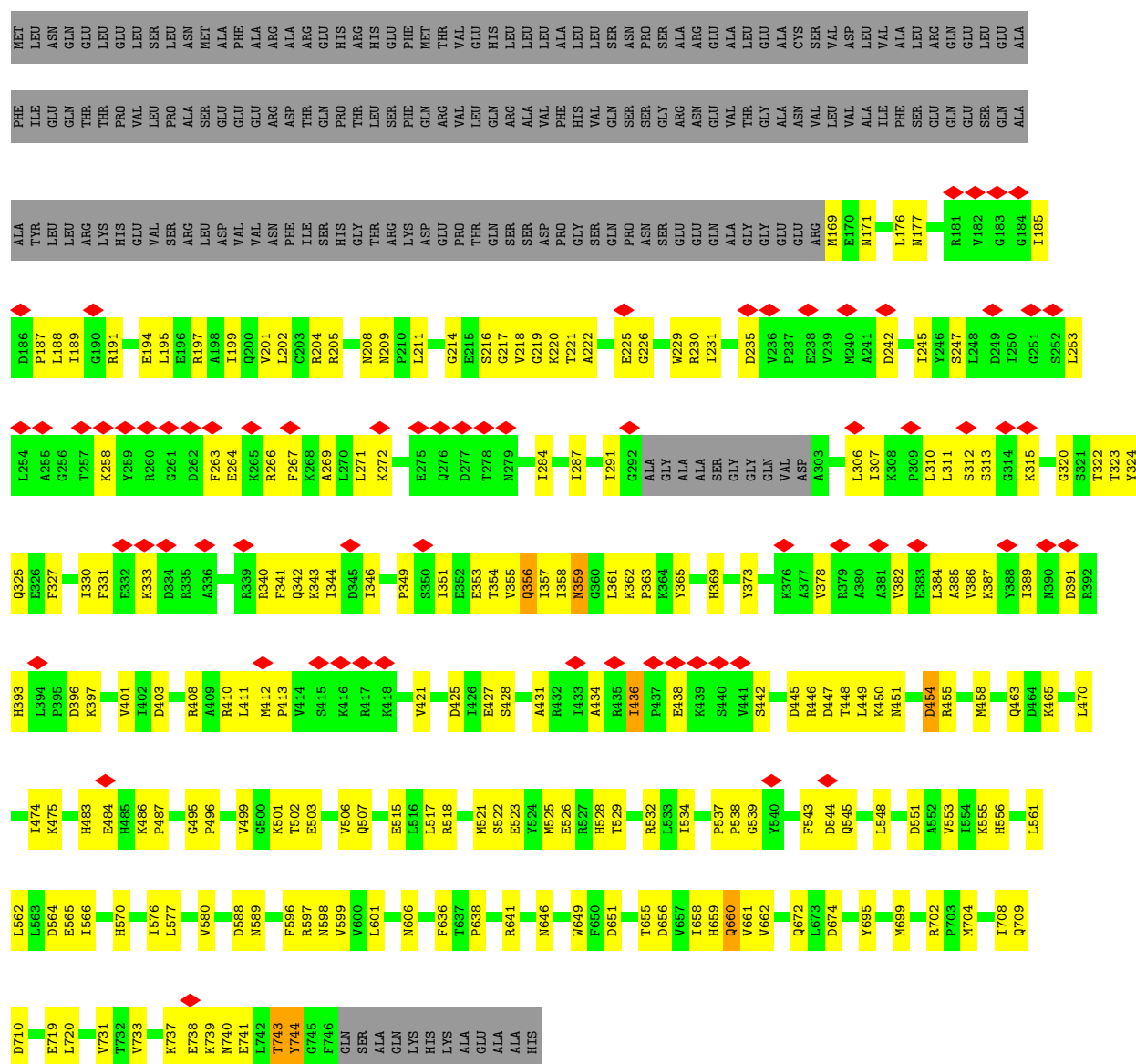
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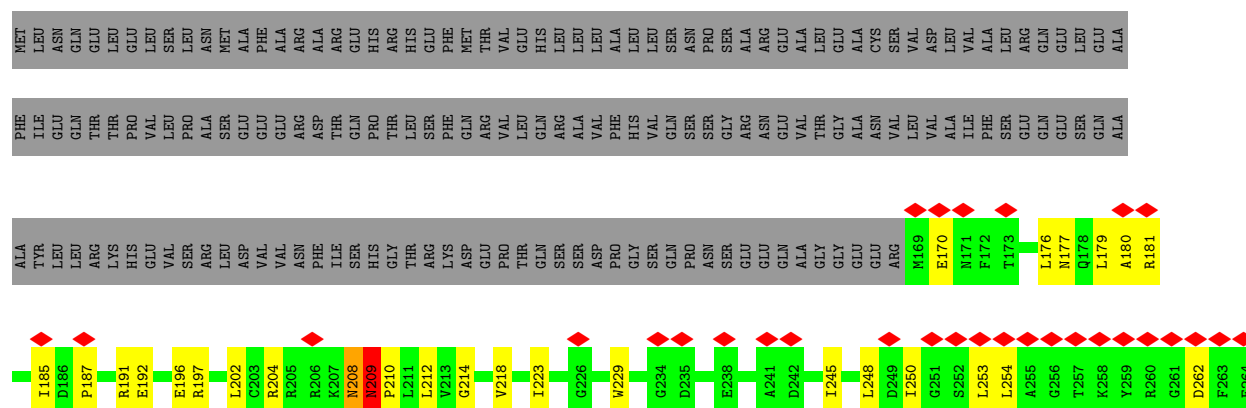
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10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

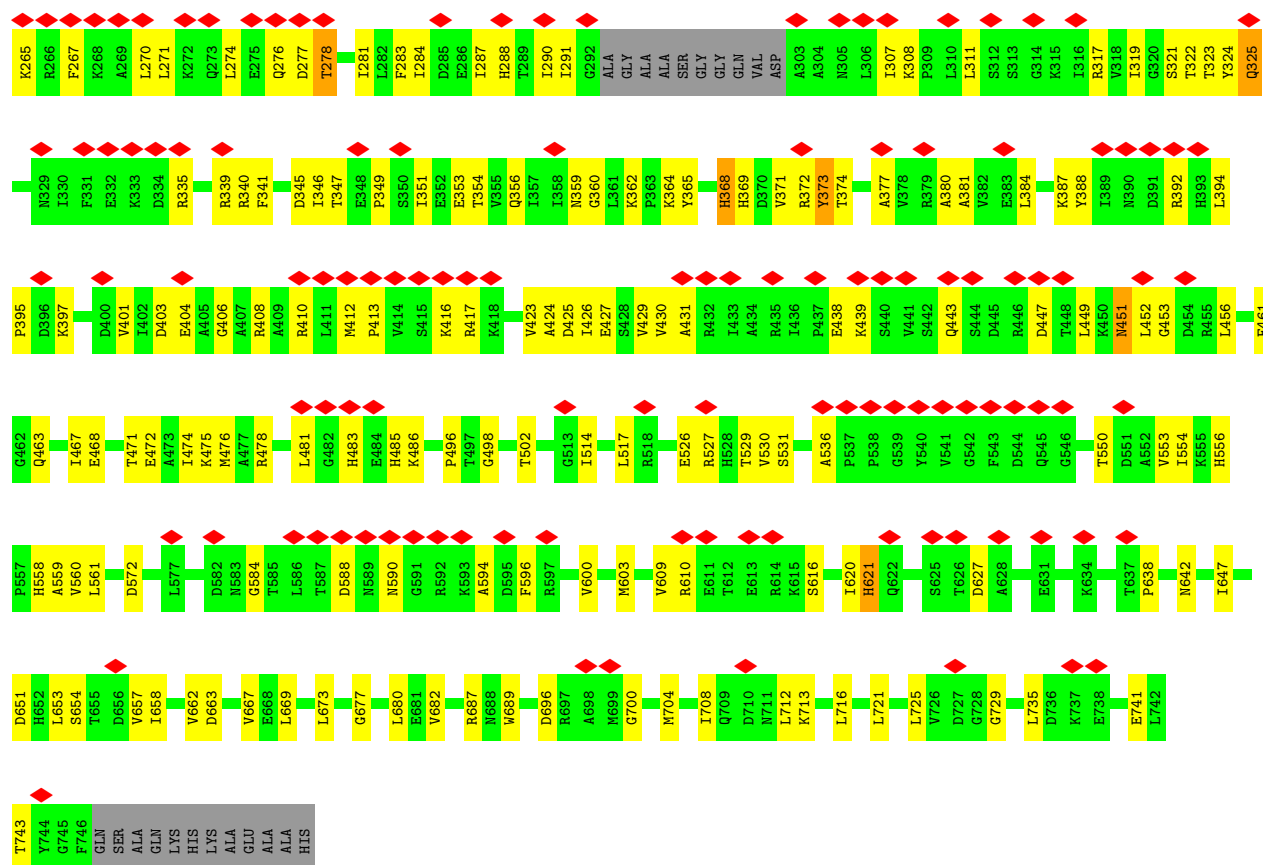
Chain B: 



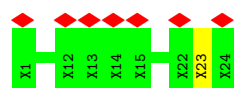


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA





- Molecule 2: RepA, green fluorescent protein fusion



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57848	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 ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	58616	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.725	Depositor
Minimum map value	-0.898	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	7/4384 (0.2%)	0.44	0/5914
1	B	0.35	9/4576 (0.2%)	0.45	2/6175 (0.0%)
1	C	0.46	14/4576 (0.3%)	0.50	8/6175 (0.1%)
1	D	0.39	11/4576 (0.2%)	0.46	6/6175 (0.1%)
1	E	0.36	8/4518 (0.2%)	0.44	2/6095 (0.0%)
1	F	0.36	8/4518 (0.2%)	0.45	4/6095 (0.1%)
All	All	0.38	57/27148 (0.2%)	0.46	22/36629 (0.1%)

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	659	HIS	ND1-CE1	5.34	1.37	1.32
1	E	570	HIS	ND1-CE1	5.33	1.37	1.32
1	C	288	HIS	ND1-CE1	5.28	1.37	1.32
1	F	368	HIS	ND1-CE1	5.28	1.37	1.32
1	D	300	GLN	CD-OE1	5.27	1.33	1.23
1	B	556	HIS	ND1-CE1	5.26	1.37	1.32
1	F	556	HIS	ND1-CE1	5.26	1.37	1.32
1	D	485	HIS	ND1-CE1	5.25	1.37	1.32
1	D	556	HIS	ND1-CE1	5.21	1.37	1.32
1	C	528	HIS	ND1-CE1	5.19	1.37	1.32
1	C	556	HIS	ND1-CE1	5.17	1.37	1.32
1	D	730	GLN	CD-OE1	5.17	1.33	1.23
1	A	672	GLN	CD-OE1	5.15	1.33	1.23
1	E	177	ASN	CG-OD1	5.14	1.33	1.23
1	A	606	ASN	CG-OD1	5.13	1.33	1.23
1	B	675	GLN	CD-OE1	5.13	1.33	1.23
1	E	740	ASN	CG-OD1	5.12	1.33	1.23
1	D	684	GLN	CD-OE1	5.12	1.33	1.23
1	A	200	GLN	CD-OE1	5.12	1.33	1.23
1	C	368	HIS	ND1-CE1	5.12	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	675	GLN	CD-OE1	5.12	1.33	1.23
1	A	279	ASN	CG-OD1	5.12	1.33	1.23
1	B	200	GLN	CD-OE1	5.11	1.33	1.23
1	C	709	GLN	CD-OE1	5.11	1.33	1.23
1	C	325	GLN	CD-OE1	5.11	1.33	1.23
1	F	276	GLN	CD-OE1	5.11	1.33	1.23
1	E	359	ASN	CG-OD1	5.10	1.33	1.23
1	D	305	ASN	CG-OD1	5.10	1.33	1.23
1	C	273	GLN	CD-OE1	5.09	1.33	1.23
1	E	672	GLN	CD-OE1	5.09	1.33	1.23
1	A	507	GLN	CD-OE1	5.09	1.33	1.23
1	D	273	GLN	CD-OE1	5.08	1.33	1.23
1	E	356	GLN	CD-OE1	5.08	1.33	1.23
1	F	208	ASN	CG-OD1	5.08	1.33	1.23
1	B	688	ASN	CG-OD1	5.08	1.33	1.23
1	B	711	ASN	CG-OD1	5.08	1.33	1.23
1	E	598	ASN	CG-OD1	5.07	1.33	1.23
1	F	325	GLN	CD-OE1	5.07	1.33	1.23
1	A	329	ASN	CG-OD1	5.07	1.33	1.23
1	C	276	GLN	CD-OE1	5.07	1.33	1.23
1	C	624	ASN	CG-OD1	5.06	1.33	1.23
1	C	342	GLN	CD-OE1	5.05	1.33	1.23
1	B	305	ASN	CG-OD1	5.05	1.33	1.23
1	B	670	GLN	CD-OE1	5.05	1.33	1.23
1	B	740	ASN	CG-OD1	5.05	1.33	1.23
1	F	356	GLN	CD-OE1	5.05	1.33	1.23
1	C	575	ASN	CG-OD1	5.05	1.33	1.23
1	D	688	ASN	CG-OD1	5.04	1.33	1.23
1	C	740	ASN	CG-OD1	5.04	1.33	1.23
1	C	200	GLN	CD-OE1	5.04	1.33	1.23
1	A	579	GLN	CD-OE1	5.04	1.33	1.23
1	F	451	ASN	CG-OD1	5.02	1.33	1.23
1	F	209	ASN	CG-OD1	5.02	1.33	1.23
1	E	660	GLN	CD-OE1	5.02	1.33	1.23
1	B	642	ASN	CG-OD1	5.01	1.33	1.23
1	D	579	GLN	CD-OE1	5.00	1.33	1.23
1	D	451	ASN	CG-OD1	5.00	1.33	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	485	HIS	CB-CG-CD2	-6.70	122.49	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	570	HIS	CB-CG-CD2	-6.61	122.60	131.20
1	B	556	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	C	288	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	C	528	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	F	368	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	C	556	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	F	556	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	C	368	HIS	CB-CG-CD2	-6.53	122.72	131.20
1	D	556	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	D	659	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	D	485	HIS	CB-CG-ND1	5.75	131.32	122.70
1	C	528	HIS	CB-CG-ND1	5.71	131.26	122.70
1	C	288	HIS	CB-CG-ND1	5.70	131.24	122.70
1	E	570	HIS	CB-CG-ND1	5.69	131.24	122.70
1	F	368	HIS	CB-CG-ND1	5.67	131.21	122.70
1	D	659	HIS	CB-CG-ND1	5.67	131.20	122.70
1	D	556	HIS	CB-CG-ND1	5.65	131.18	122.70
1	B	556	HIS	CB-CG-ND1	5.65	131.17	122.70
1	C	556	HIS	CB-CG-ND1	5.63	131.15	122.70
1	F	556	HIS	CB-CG-ND1	5.63	131.14	122.70
1	C	368	HIS	CB-CG-ND1	5.57	131.06	122.70

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	4321	0	4424	149	0
1	B	4510	0	4609	184	0
1	C	4510	0	4609	163	0
1	D	4510	0	4609	153	0
1	E	4453	0	4558	190	0
1	F	4453	0	4558	152	0
2	X	120	0	27	1	0
3	A	54	0	24	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	27	0	12	15	0
4	B	62	0	24	22	0
4	C	62	0	24	30	0
4	D	62	0	24	18	0
4	E	62	0	24	25	0
All	All	27206	0	27526	892	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 16.

All (892) 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:C:357:ILE:HG23	4:C:801:ATP:C2	1.71	1.23
1:E:361:LEU:CD1	4:E:801:ATP:H1'	1.72	1.19
1:D:502:THR:HG23	4:D:802:ATP:O2B	1.40	1.18
1:C:219:GLY:HA2	4:C:801:ATP:O2A	1.44	1.15
1:E:188:LEU:HD21	1:E:191:ARG:HB2	1.15	1.11
1:E:361:LEU:HD11	4:E:801:ATP:C1'	1.81	1.11
1:D:260:ARG:HA	1:D:300:GLN:HE21	1.15	1.09
1:A:323:THR:CG2	1:F:335:ARG:HH22	1.71	1.03
1:F:502:THR:HG21	3:F:801:ADP:O3B	1.56	1.03
1:E:188:LEU:CD2	1:E:191:ARG:HB2	1.89	1.02
1:C:221:THR:HG22	4:C:801:ATP:O1B	1.56	1.02
1:B:219:GLY:HA2	4:B:801:ATP:PA	2.00	1.00
1:A:323:THR:HG22	1:F:335:ARG:HH22	1.25	0.99
1:D:260:ARG:HA	1:D:300:GLN:NE2	1.80	0.95
1:E:220:LYS:HZ3	1:E:322:THR:C	1.76	0.93
1:C:357:ILE:CG2	4:C:801:ATP:C2	2.51	0.93
1:F:335:ARG:HB3	1:F:339:ARG:NH1	1.86	0.91
1:F:550:THR:O	1:F:554:ILE:HG12	1.71	0.91
1:D:219:GLY:HA2	4:D:801:ATP:O2A	1.72	0.90
1:E:188:LEU:HD21	1:E:191:ARG:CB	2.01	0.88
1:D:399:ILE:CD1	4:D:801:ATP:H1'	2.03	0.88
1:E:408:ARG:HH12	1:E:428:SER:CB	1.86	0.88
1:C:339:ARG:HH11	1:D:396:ASP:CG	1.80	0.88
1:E:205:ARG:HE	1:F:368:HIS:CE1	1.90	0.87
1:E:361:LEU:HD11	4:E:801:ATP:H1'	0.88	0.87
1:C:221:THR:CG2	4:C:801:ATP:O1B	2.22	0.87
1:E:408:ARG:NH1	1:E:428:SER:HB2	1.90	0.85
1:D:550:THR:HG23	1:D:594:ALA:HB2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:OD1	3:A:801:ADP:H4'	1.76	0.84
1:B:274:LEU:CD2	1:B:316:ILE:HB	2.06	0.84
1:A:497:THR:OG1	1:A:702:ARG:CZ	2.27	0.82
1:C:575:ASN:HA	1:C:578:LEU:HG	1.61	0.82
1:B:220:LYS:HE3	1:B:322:THR:O	1.78	0.82
1:E:354:THR:O	1:E:357:ILE:HG12	1.79	0.81
1:B:212:LEU:O	1:B:220:LYS:HD2	1.81	0.80
1:F:502:THR:CG2	3:F:801:ADP:O3B	2.28	0.80
1:C:501:LYS:HG3	4:C:802:ATP:O1B	1.81	0.80
1:D:561:LEU:HD23	1:D:601:LEU:HG	1.62	0.80
1:E:484:GLU:O	1:E:597:ARG:HD3	1.82	0.79
1:F:502:THR:HG21	3:F:801:ADP:PB	2.22	0.79
1:B:222:ALA:HB2	4:B:801:ATP:O2A	1.80	0.79
1:D:502:THR:CG2	4:D:802:ATP:O2B	2.28	0.79
1:A:566:ILE:HG13	1:A:603:MET:HB3	1.65	0.78
1:C:407:ALA:O	1:C:411:LEU:HD13	1.84	0.78
1:D:361:LEU:HD11	4:D:801:ATP:O2'	1.82	0.78
1:F:620:ILE:O	1:F:621:HIS:ND1	2.14	0.78
1:E:176:LEU:HD11	1:E:247:SER:HB2	1.66	0.78
1:E:188:LEU:HD12	1:E:222:ALA:O	1.83	0.78
1:C:357:ILE:HG23	4:C:801:ATP:H2	1.49	0.77
1:A:323:THR:CG2	1:F:335:ARG:NH2	2.46	0.77
1:F:335:ARG:HB3	1:F:339:ARG:HH12	1.48	0.76
1:E:222:ALA:CB	4:E:801:ATP:N7	2.49	0.75
1:E:662:VAL:HG22	1:E:704:MET:HE2	1.68	0.75
1:D:643:ARG:NH2	4:E:802:ATP:O3G	2.21	0.74
1:E:408:ARG:HH12	1:E:428:SER:HB3	1.52	0.74
1:B:222:ALA:CB	4:B:801:ATP:O2A	2.36	0.74
1:A:169:MET:HG3	1:A:173:THR:CG2	2.19	0.73
1:C:219:GLY:CA	4:C:801:ATP:O2A	2.32	0.73
1:C:501:LYS:NZ	4:C:802:ATP:O2G	2.21	0.72
1:C:339:ARG:NH1	1:D:396:ASP:CG	2.48	0.72
1:A:582:ASP:HB2	1:A:643:ARG:NH1	2.05	0.72
1:B:396:ASP:O	1:B:399:ILE:HG12	1.91	0.71
1:E:408:ARG:HH12	1:E:428:SER:HB2	1.48	0.71
1:E:354:THR:O	1:E:357:ILE:CG1	2.39	0.71
1:D:219:GLY:CA	4:D:801:ATP:O2A	2.39	0.71
1:F:311:LEU:O	1:F:340:ARG:NH2	2.24	0.71
1:B:479:ALA:HB1	1:C:720:LEU:HD23	1.72	0.70
1:E:463:GLN:NE2	1:E:651:ASP:O	2.24	0.70
1:B:396:ASP:O	1:B:399:ILE:CG1	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:PHE:CD1	4:C:802:ATP:C2	2.80	0.70
1:C:345:ASP:OD2	1:D:435:ARG:NE	2.25	0.70
1:B:219:GLY:HA2	4:B:801:ATP:O3A	1.91	0.70
1:E:205:ARG:NE	1:F:368:HIS:CE1	2.60	0.70
1:A:432:ARG:NH1	1:A:432:ARG:O	2.25	0.70
1:A:169:MET:HB2	1:A:173:THR:HG22	1.73	0.70
1:F:560:VAL:HG23	1:F:600:VAL:HG13	1.74	0.70
1:B:274:LEU:HD21	1:B:316:ILE:HB	1.74	0.69
1:E:220:LYS:NZ	1:E:322:THR:C	2.49	0.69
1:C:339:ARG:HD2	1:D:396:ASP:OD2	1.92	0.69
1:C:461:PHE:CE1	4:C:802:ATP:H2	2.11	0.69
1:B:461:PHE:O	4:B:802:ATP:N6	2.25	0.69
1:C:461:PHE:CD1	4:C:802:ATP:H2	2.10	0.69
1:C:501:LYS:CE	4:C:802:ATP:O2G	2.41	0.69
1:E:204:ARG:NH1	1:E:342:GLN:OE1	2.24	0.69
1:E:451:ASN:HB3	1:E:455:ARG:HH21	1.56	0.69
1:F:449:LEU:O	1:F:475:LYS:NZ	2.25	0.68
1:E:220:LYS:HZ1	1:E:323:THR:HG22	1.58	0.68
1:E:221:THR:HG22	4:E:801:ATP:O1B	1.93	0.68
1:A:315:LYS:HG3	1:A:316:ILE:HG12	1.75	0.68
1:A:643:ARG:HE	1:B:702:ARG:HD3	1.57	0.68
1:C:661:VAL:HG22	4:C:802:ATP:C2	2.28	0.68
1:C:339:ARG:CZ	1:D:217:GLY:HA2	2.23	0.68
1:E:191:ARG:HH12	1:E:346:ILE:HG23	1.59	0.68
1:F:498:GLY:HA2	3:F:801:ADP:H5'2	1.76	0.68
1:D:204:ARG:NH1	1:D:206:ARG:O	2.26	0.67
1:D:294:GLY:HA3	1:D:302:ASP:HA	1.76	0.67
1:D:722:PHE:O	1:D:722:PHE:CD1	2.47	0.67
1:E:408:ARG:O	1:E:412:MET:N	2.27	0.67
1:F:208:ASN:OD1	1:F:317:ARG:HG2	1.94	0.67
1:A:678:VAL:HG11	1:A:725:LEU:HD21	1.77	0.67
1:B:268:LYS:O	1:B:272:LYS:HG3	1.94	0.67
1:E:191:ARG:NH2	1:E:218:VAL:O	2.27	0.67
1:F:253:LEU:HD22	1:F:270:LEU:HD22	1.77	0.67
1:D:384:LEU:HD11	1:D:427:GLU:HG2	1.75	0.67
1:C:438:GLU:HG3	1:C:439:LYS:HG2	1.77	0.67
1:C:339:ARG:NH1	1:D:396:ASP:OD1	2.28	0.67
1:C:253:LEU:O	1:C:266:ARG:NH1	2.25	0.66
1:E:385:ALA:HB1	1:E:397:LYS:HD2	1.77	0.66
1:A:339:ARG:NH1	4:B:801:ATP:O2B	2.28	0.66
1:C:538:PRO:HB3	1:D:542:GLY:HA3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:ASN:HA	1:C:578:LEU:CD1	2.26	0.66
1:A:271:LEU:HD21	1:A:310:LEU:CD1	2.25	0.66
1:C:575:ASN:HA	1:C:578:LEU:CG	2.25	0.66
1:F:291:ILE:HD13	1:F:307:ILE:HD11	1.76	0.66
1:A:485:HIS:HA	1:A:597:ARG:HH21	1.61	0.66
1:D:212:LEU:HD22	1:D:346:ILE:HD11	1.76	0.66
1:D:209:ASN:ND2	1:D:340:ARG:O	2.29	0.66
1:D:440:SER:OG	1:D:478:ARG:NH2	2.29	0.66
1:D:485:HIS:HA	1:D:597:ARG:HD3	1.77	0.66
1:E:743:THR:HG22	1:E:744:TYR:H	1.61	0.66
1:A:543:PHE:HD2	1:B:541:VAL:HG12	1.61	0.65
1:E:501:LYS:N	4:E:802:ATP:O1B	2.26	0.65
1:A:267:PHE:CE2	1:A:307:ILE:CG2	2.80	0.65
1:E:189:ILE:HB	1:E:357:ILE:HG22	1.77	0.65
1:B:579:GLN:NE2	1:C:523:GLU:OE2	2.29	0.65
1:E:655:THR:O	1:E:659:HIS:ND1	2.28	0.65
1:B:222:ALA:N	4:B:801:ATP:O2A	2.30	0.65
1:B:169:MET:N	1:B:273:GLN:OE1	2.30	0.65
1:C:349:PRO:O	1:C:394:LEU:HD22	1.97	0.65
1:C:446:ARG:NH1	1:D:721:LEU:O	2.30	0.65
1:E:188:LEU:HG	4:E:801:ATP:N6	2.11	0.65
1:A:271:LEU:HD21	1:A:310:LEU:HD11	1.79	0.65
1:E:606:ASN:ND2	4:E:802:ATP:O2G	2.27	0.64
1:E:551:ASP:OD2	1:E:555:LYS:NZ	2.30	0.64
1:E:176:LEU:HD13	1:E:245:ILE:HG22	1.80	0.64
1:A:561:LEU:HD23	1:A:601:LEU:HD13	1.79	0.63
1:A:459:LEU:O	1:A:664:LYS:NZ	2.29	0.63
1:B:339:ARG:NH2	4:C:801:ATP:O2B	2.31	0.63
1:A:199:ILE:HG23	1:A:240:MET:HE3	1.81	0.63
1:C:274:LEU:HD21	1:C:282:LEU:HB2	1.81	0.63
1:A:446:ARG:HH21	1:B:722:PHE:HA	1.64	0.63
1:A:501:LYS:NZ	1:A:605:THR:O	2.31	0.63
1:E:484:GLU:O	1:E:597:ARG:CD	2.47	0.63
1:A:498:GLY:HA3	1:A:700:GLY:HA3	1.79	0.62
1:D:258:LYS:NZ	2:X:23:UNK:O	2.31	0.62
1:E:369:HIS:NE2	1:E:403:ASP:OD1	2.30	0.62
1:B:642:ASN:ND2	1:C:702:ARG:HD2	2.14	0.62
1:E:362:LYS:HG2	1:E:363:PRO:HD3	1.80	0.62
1:C:413:PRO:HG3	1:C:418:LYS:HB2	1.81	0.62
1:B:447:ASP:O	1:B:451:ASN:ND2	2.33	0.62
1:E:235:ASP:OD1	1:E:235:ASP:O	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:521:MET:HG3	1:E:566:ILE:HD12	1.80	0.62
1:A:538:PRO:HB3	1:B:542:GLY:HA3	1.81	0.62
1:A:267:PHE:CZ	1:A:307:ILE:CG2	2.83	0.62
1:E:312:SER:OG	1:E:340:ARG:NH1	2.33	0.62
1:F:253:LEU:HD12	1:F:254:LEU:N	2.15	0.61
1:C:653:LEU:HD22	1:C:657:VAL:HG11	1.83	0.61
1:C:561:LEU:HD23	1:C:601:LEU:HD13	1.83	0.61
1:D:493:PHE:HE1	1:D:648:ILE:HD12	1.65	0.61
1:E:733:VAL:HG13	1:E:741:GLU:HB3	1.81	0.61
1:F:262:ASP:HA	1:F:265:LYS:HG2	1.83	0.61
1:B:682:VAL:O	1:B:687:ARG:NH1	2.32	0.61
1:D:684:GLN:OE1	1:D:688:ASN:ND2	2.32	0.61
1:C:470:LEU:HD13	1:C:508:LEU:HD22	1.81	0.61
1:E:205:ARG:HD3	1:F:365:TYR:CE1	2.36	0.61
1:E:214:GLY:O	1:E:324:TYR:N	2.30	0.61
1:D:173:THR:HG21	1:D:246:TYR:HB3	1.82	0.61
1:A:197:ARG:NH1	1:B:404:GLU:OE2	2.31	0.60
1:A:271:LEU:HG	1:A:275:GLU:OE2	2.01	0.60
1:F:416:LYS:O	1:F:417:ARG:NH1	2.34	0.60
1:C:221:THR:HG22	4:C:801:ATP:PB	2.40	0.60
1:C:527:ARG:NH2	1:D:525:MET:O	2.28	0.60
1:A:714:LYS:N	1:A:715:PRO:HD2	2.16	0.60
1:F:281:ILE:HD11	1:F:317:ARG:HH21	1.67	0.60
1:B:355:VAL:HG21	1:B:379:ARG:HE	1.66	0.60
1:B:502:THR:OG1	4:B:802:ATP:O1A	2.20	0.60
1:C:222:ALA:HB2	4:C:801:ATP:O2A	2.00	0.60
1:B:514:ILE:HG23	1:B:559:ALA:HA	1.84	0.60
1:D:685:GLU:HG3	1:D:735:LEU:HD23	1.82	0.60
1:A:576:ILE:O	1:A:579:GLN:HG2	2.02	0.60
1:C:474:ILE:HD13	1:C:512:LEU:HD11	1.83	0.60
1:E:526:GLU:O	1:E:529:THR:OG1	2.20	0.60
1:E:532:ARG:O	1:E:548:LEU:N	2.33	0.60
1:C:248:LEU:HB2	1:C:282:LEU:HD11	1.84	0.59
1:A:544:ASP:OD1	1:A:544:ASP:O	2.20	0.59
1:C:339:ARG:CZ	1:D:217:GLY:CA	2.80	0.59
1:A:587:THR:OG1	1:A:593:LYS:NZ	2.33	0.59
1:B:188:LEU:HB2	1:B:226:GLY:HA3	1.84	0.59
1:E:222:ALA:HB1	4:E:801:ATP:C5	2.38	0.59
1:B:302:ASP:N	1:B:302:ASP:OD1	2.32	0.59
1:B:483:HIS:HB2	1:B:486:LYS:HB2	1.84	0.59
1:E:205:ARG:NH1	1:F:365:TYR:HE1	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:678:VAL:HA	1:D:729:GLY:HA3	1.84	0.59
1:B:221:THR:HB	4:B:801:ATP:O1B	2.03	0.59
1:B:436:ILE:HD12	1:B:436:ILE:O	2.01	0.59
1:A:656:ASP:OD1	1:A:656:ASP:N	2.35	0.59
1:B:613:GLU:OE2	1:B:614:ARG:HG3	2.02	0.59
1:C:222:ALA:CB	4:C:801:ATP:O2A	2.51	0.59
1:E:222:ALA:HB2	4:E:801:ATP:C8	2.38	0.59
1:B:384:LEU:HB3	1:B:430:VAL:HG11	1.85	0.59
1:D:501:LYS:HE3	4:D:802:ATP:O1B	2.03	0.59
1:E:588:ASP:OD1	1:E:589:ASN:N	2.35	0.59
1:F:439:LYS:HG2	1:F:443:GLN:OE1	2.03	0.59
1:A:579:GLN:OE1	1:A:586:LEU:HD21	2.03	0.59
1:D:361:LEU:CD1	4:D:801:ATP:O2'	2.51	0.59
1:A:682:VAL:HA	1:A:733:VAL:HB	1.85	0.58
1:B:442:SER:HA	1:B:446:ARG:HD2	1.85	0.58
1:D:186:ASP:HA	1:D:364:LYS:HE2	1.85	0.58
1:D:714:LYS:O	1:D:718:ASN:ND2	2.34	0.58
1:E:216:SER:OG	4:E:801:ATP:O2G	2.20	0.58
1:E:222:ALA:HB2	4:E:801:ATP:N7	2.17	0.58
1:A:361:LEU:HD11	3:A:801:ADP:N3	2.18	0.58
1:A:323:THR:HG21	1:F:335:ARG:NH2	2.19	0.58
1:F:364:LYS:O	1:F:368:HIS:ND1	2.37	0.58
1:A:312:SER:HB2	1:A:340:ARG:HE	1.69	0.58
1:B:431:ALA:HA	1:B:434:ALA:HB3	1.85	0.58
1:F:210:PRO:HB2	1:F:319:ILE:HD13	1.86	0.58
1:D:257:THR:OG1	1:D:262:ASP:OD2	2.21	0.58
1:E:191:ARG:HH21	1:E:349:PRO:HD3	1.68	0.58
1:A:446:ARG:O	1:A:446:ARG:NH1	2.37	0.58
1:C:370:ASP:O	1:C:418:LYS:NZ	2.36	0.58
1:E:271:LEU:HD22	1:E:310:LEU:HD12	1.84	0.58
1:F:588:ASP:OD2	1:F:590:ASN:ND2	2.37	0.58
1:C:642:ASN:O	1:D:706:ARG:NH2	2.37	0.57
1:E:327:PHE:HA	1:E:331:PHE:HD2	1.69	0.57
1:A:169:MET:SD	1:A:246:TYR:CE2	2.97	0.57
1:C:652:HIS:HB3	1:C:697:ARG:HG3	1.86	0.57
1:F:387:LYS:O	1:F:387:LYS:HG2	2.04	0.57
1:F:502:THR:OG1	3:F:801:ADP:O2A	2.20	0.57
1:A:641:ARG:HA	1:A:644:LEU:HD12	1.86	0.57
1:B:493:PHE:HE2	1:B:648:ILE:HD12	1.69	0.57
1:D:192:GLU:OE1	1:D:230:ARG:NH1	2.37	0.57
1:E:220:LYS:NZ	1:E:322:THR:O	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:561:LEU:HD23	1:E:601:LEU:HD13	1.86	0.57
1:F:531:SER:HB2	1:F:536:ALA:HB3	1.86	0.57
1:B:658:ILE:O	1:B:662:VAL:HG23	2.04	0.57
1:E:431:ALA:HB2	1:E:438:GLU:HB3	1.87	0.57
1:F:498:GLY:N	3:F:801:ADP:O1A	2.36	0.57
1:F:669:LEU:HD13	1:F:713:LYS:HE3	1.85	0.57
1:B:188:LEU:HD12	4:B:801:ATP:C6	2.40	0.57
1:C:501:LYS:CG	4:C:802:ATP:O1B	2.51	0.57
1:E:361:LEU:CD1	4:E:801:ATP:C1'	2.60	0.57
1:A:403:ASP:OD2	1:F:204:ARG:NE	2.37	0.57
1:B:274:LEU:HD22	1:B:316:ILE:HB	1.87	0.57
1:B:446:ARG:NE	1:C:721:LEU:O	2.38	0.57
1:C:301:VAL:HG11	1:D:254:LEU:HD21	1.87	0.57
1:E:191:ARG:HH12	1:E:346:ILE:CG2	2.16	0.56
1:D:189:ILE:HG12	1:D:360:GLY:HA3	1.87	0.56
1:F:377:ALA:HA	1:F:423:VAL:HG12	1.88	0.56
1:B:663:ASP:O	1:B:667:VAL:HG23	2.05	0.56
1:C:503:GLU:N	4:C:802:ATP:O2A	2.29	0.56
1:E:359:ASN:HA	1:E:362:LYS:HD3	1.87	0.56
1:E:702:ARG:NH2	4:E:802:ATP:O3G	2.38	0.56
1:D:581:MET:HE3	1:D:643:ARG:HG3	1.88	0.56
1:E:220:LYS:HZ1	1:E:323:THR:CG2	2.18	0.56
1:F:368:HIS:O	1:F:410:ARG:NH1	2.39	0.56
1:B:465:LYS:NZ	1:B:649:TRP:O	2.34	0.56
1:B:381:ALA:HB2	1:B:426:ILE:HD13	1.87	0.56
1:A:636:PHE:O	1:A:641:ARG:NH1	2.39	0.56
1:F:408:ARG:HE	1:F:429:VAL:HG22	1.71	0.56
1:F:502:THR:HG23	3:F:801:ADP:O2A	2.06	0.56
1:F:374:THR:OG1	1:F:377:ALA:N	2.39	0.56
1:F:526:GLU:O	1:F:529:THR:OG1	2.22	0.56
1:D:474:ILE:HD13	1:D:512:LEU:HD11	1.88	0.55
1:A:463:GLN:NE2	1:A:651:ASP:O	2.31	0.55
1:E:199:ILE:HA	1:E:202:LEU:HD12	1.86	0.55
1:F:447:ASP:O	1:F:451:ASN:OD1	2.24	0.55
1:B:734:ALA:H	1:B:743:THR:HB	1.70	0.55
1:E:176:LEU:HD12	1:E:176:LEU:H	1.71	0.55
1:B:639:GLU:CA	1:C:497:THR:HG21	2.36	0.55
1:C:221:THR:CG2	4:C:801:ATP:O1A	2.54	0.55
1:C:349:PRO:HD2	1:C:395:PRO:HD3	1.89	0.55
1:A:521:MET:HG3	1:A:566:ILE:HD13	1.89	0.55
1:C:709:GLN:HA	1:C:713:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ILE:HD13	4:D:801:ATP:H1'	1.86	0.55
1:C:188:LEU:HD22	1:C:226:GLY:HA3	1.88	0.55
1:F:180:ALA:HA	1:F:185:ILE:HB	1.89	0.55
1:D:658:ILE:HG13	1:D:695:TYR:HD1	1.71	0.55
1:E:674:ASP:OD1	1:E:674:ASP:O	2.24	0.55
1:B:396:ASP:C	1:B:399:ILE:HG12	2.32	0.55
1:E:205:ARG:NE	1:F:368:HIS:ND1	2.54	0.55
1:A:361:LEU:HD11	3:A:801:ADP:C2	2.42	0.55
1:A:394:LEU:HA	1:A:397:LYS:HE2	1.87	0.55
1:C:451:ASN:OD1	1:C:455:ARG:NH1	2.37	0.55
1:F:277:ASP:O	1:F:278:THR:O	2.25	0.55
1:D:339:ARG:NH2	4:E:801:ATP:O3G	2.40	0.54
1:D:358:ILE:HD11	1:D:378:VAL:HG13	1.89	0.54
1:F:483:HIS:HB2	1:F:486:LYS:HG3	1.89	0.54
1:F:496:PRO:HB3	1:F:609:VAL:HG11	1.89	0.54
1:A:205:ARG:NH2	1:B:186:ASP:OD1	2.40	0.54
1:C:345:ASP:OD1	1:C:345:ASP:O	2.25	0.54
1:E:191:ARG:NH1	1:E:346:ILE:HG23	2.23	0.54
1:F:345:ASP:OD1	1:F:345:ASP:O	2.25	0.54
1:D:214:GLY:O	1:D:220:LYS:NZ	2.40	0.54
1:B:496:PRO:O	1:B:501:LYS:NZ	2.37	0.54
1:D:210:PRO:HG2	1:D:319:ILE:HG23	1.89	0.54
1:E:349:PRO:HG2	1:E:354:THR:OG1	2.07	0.54
1:D:501:LYS:HB2	4:D:802:ATP:O1B	2.07	0.54
1:B:195:LEU:HD21	1:B:227:LEU:HB2	1.89	0.54
1:E:211:LEU:HB3	1:E:343:LYS:HA	1.88	0.54
1:E:408:ARG:HD3	1:E:425:ASP:OD1	2.07	0.54
1:B:396:ASP:O	1:B:399:ILE:HG13	2.06	0.54
1:B:396:ASP:HA	1:B:399:ILE:HG12	1.89	0.54
1:C:350:SER:HB2	1:C:353:GLU:CD	2.33	0.54
1:D:579:GLN:OE1	1:E:522:SER:OG	2.25	0.54
1:E:263:PHE:HA	1:E:266:ARG:HD2	1.88	0.54
1:F:669:LEU:O	1:F:673:LEU:HG	2.07	0.54
1:B:425:ASP:O	1:B:429:VAL:HG23	2.07	0.54
1:D:260:ARG:CA	1:D:300:GLN:HE21	2.03	0.54
1:E:389:ILE:O	1:E:397:LYS:NZ	2.40	0.54
1:F:359:ASN:HA	1:F:362:LYS:HE2	1.89	0.54
1:E:710:ASP:OD1	1:E:710:ASP:O	2.25	0.53
1:F:287:ILE:HD12	1:F:290:ILE:HB	1.90	0.53
1:A:645:ASP:HA	1:B:706:ARG:HE	1.73	0.53
1:C:306:LEU:HD21	1:D:251:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:ASP:OD2	1:C:739:LYS:NZ	2.33	0.53
1:E:534:ILE:HD11	1:E:576:ILE:HD12	1.90	0.53
1:C:682:VAL:O	1:C:687:ARG:NH1	2.41	0.53
1:C:730:GLN:NE2	1:C:731:VAL:O	2.42	0.53
1:C:260:ARG:HD3	1:D:295:ALA:HB3	1.90	0.53
1:F:191:ARG:NH2	1:F:347:THR:O	2.41	0.53
1:F:191:ARG:HH22	1:F:349:PRO:HD3	1.73	0.53
1:F:682:VAL:O	1:F:687:ARG:NH1	2.41	0.53
1:B:371:VAL:HA	1:B:418:LYS:HE2	1.89	0.53
1:B:639:GLU:CB	1:C:497:THR:HG21	2.38	0.53
1:D:350:SER:OG	1:D:351:ILE:N	2.41	0.53
1:E:216:SER:O	1:E:393:HIS:ND1	2.41	0.53
1:E:284:ILE:HG21	1:E:287:ILE:HD13	1.89	0.53
1:E:391:ASP:OD2	1:E:391:ASP:N	2.39	0.53
1:F:253:LEU:HD12	1:F:253:LEU:C	2.34	0.53
1:F:425:ASP:O	1:F:429:VAL:HG23	2.08	0.53
1:D:399:ILE:HD12	4:D:801:ATP:H1'	1.89	0.53
1:D:501:LYS:CB	4:D:802:ATP:O1B	2.56	0.53
1:E:189:ILE:HD12	1:E:357:ILE:HA	1.91	0.53
1:A:497:THR:OG1	1:A:702:ARG:NH2	2.41	0.53
1:B:414:VAL:HG22	1:B:417:ARG:HH12	1.72	0.53
1:B:623:ASP:OD1	1:B:624:ASN:N	2.42	0.53
1:A:446:ARG:NE	1:B:721:LEU:O	2.42	0.53
1:B:464:ASP:HA	1:B:467:ILE:HD12	1.90	0.53
1:B:639:GLU:HA	1:C:497:THR:HG21	1.89	0.53
1:D:310:LEU:HB3	1:D:316:ILE:HG22	1.91	0.53
1:E:658:ILE:O	1:E:662:VAL:HG23	2.09	0.53
1:E:354:THR:HA	1:E:357:ILE:HG12	1.89	0.53
1:B:544:ASP:OD1	1:B:544:ASP:N	2.42	0.53
1:F:369:HIS:NE2	1:F:403:ASP:OD1	2.34	0.53
1:A:497:THR:OG1	1:A:702:ARG:NE	2.41	0.52
1:B:260:ARG:NH1	1:C:257:THR:O	2.43	0.52
1:C:495:GLY:O	1:C:501:LYS:NZ	2.32	0.52
1:B:637:THR:O	1:B:639:GLU:N	2.43	0.52
1:E:636:PHE:O	1:E:641:ARG:NH1	2.39	0.52
1:F:397:LYS:O	1:F:401:VAL:HG23	2.09	0.52
1:F:712:LEU:O	1:F:716:LEU:HG	2.09	0.52
1:A:683:SER:OG	1:A:685:GLU:OE2	2.27	0.52
1:A:575:ASN:HB3	1:B:522:SER:HB2	1.91	0.52
1:A:291:ILE:HG23	1:A:304:ALA:HB2	1.90	0.52
1:A:681:GLU:N	1:A:731:VAL:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ARG:HB2	1:C:208:ASN:HB3	1.92	0.52
1:A:210:PRO:HG2	1:A:319:ILE:HG23	1.91	0.52
1:B:639:GLU:O	1:B:643:ARG:NE	2.42	0.52
1:E:455:ARG:HA	1:E:458:MET:HE2	1.92	0.52
1:A:736:ASP:O	1:A:740:ASN:N	2.33	0.52
1:B:214:GLY:N	1:B:220:LYS:HD3	2.25	0.52
1:B:576:ILE:O	1:B:580:VAL:HG23	2.10	0.52
1:C:339:ARG:NH2	1:D:217:GLY:HA2	2.23	0.52
1:D:352:GLU:HA	1:D:355:VAL:HG12	1.91	0.52
1:B:608:GLY:HA3	1:B:629:MET:HA	1.91	0.52
1:A:543:PHE:CD2	1:B:541:VAL:HG12	2.44	0.52
1:B:521:MET:HB3	1:B:569:ALA:HB2	1.91	0.51
1:C:263:PHE:HZ	1:C:303:ALA:HB2	1.75	0.51
1:C:296:ALA:O	1:C:300:GLN:NE2	2.44	0.51
1:F:191:ARG:HD3	1:F:223:ILE:HD11	1.92	0.51
1:A:312:SER:HB2	1:A:340:ARG:NE	2.24	0.51
1:A:498:GLY:N	3:A:802:ADP:O1B	2.43	0.51
1:D:499:VAL:O	4:D:802:ATP:O3A	2.29	0.51
1:F:456:LEU:HD12	1:F:467:ILE:HG23	1.91	0.51
1:C:277:ASP:OD2	1:C:280:SER:N	2.42	0.51
1:E:496:PRO:HG2	1:E:499:VAL:HG11	1.91	0.51
1:F:653:LEU:HD22	1:F:657:VAL:HG11	1.92	0.51
1:D:526:GLU:HB2	1:D:529:THR:HG23	1.93	0.51
1:A:662:VAL:O	1:A:666:ILE:HG12	2.10	0.51
1:E:354:THR:C	1:E:357:ILE:HG12	2.35	0.51
1:B:572:ASP:O	1:C:525:MET:HE1	2.10	0.51
1:C:437:PRO:HG3	1:C:558:HIS:CE1	2.45	0.51
1:E:737:LYS:O	1:E:739:LYS:NZ	2.37	0.51
1:B:701:ALA:HB3	4:B:802:ATP:C8	2.45	0.51
1:E:351:ILE:O	1:E:355:VAL:HG23	2.10	0.51
1:D:349:PRO:HD2	1:D:395:PRO:HD3	1.93	0.51
1:A:332:GLU:C	1:A:333:LYS:HE2	2.36	0.51
1:A:500:GLY:O	1:A:504:VAL:HG23	2.11	0.51
1:A:539:GLY:HA2	1:B:540:TYR:HB3	1.93	0.51
1:B:413:PRO:HA	1:B:417:ARG:H	1.76	0.51
1:D:606:ASN:OD1	4:D:802:ATP:O2G	2.29	0.51
1:E:486:LYS:HG3	1:E:487:PRO:HD2	1.93	0.51
1:D:282:LEU:HB3	1:D:318:VAL:HG23	1.91	0.50
1:D:567:GLU:OE1	1:D:605:THR:OG1	2.24	0.50
1:E:408:ARG:NH1	1:E:428:SER:CB	2.55	0.50
1:F:502:THR:OG1	3:F:801:ADP:O3B	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLN:HA	1:B:411:LEU:HD11	1.93	0.50
1:A:219:GLY:CA	3:A:801:ADP:O1A	2.60	0.50
1:C:369:HIS:NE2	1:C:403:ASP:OD1	2.35	0.50
1:E:188:LEU:HG	4:E:801:ATP:HN62	1.76	0.50
1:F:218:VAL:HA	1:F:395:PRO:HG2	1.93	0.50
1:A:655:THR:HA	1:A:658:ILE:HD12	1.93	0.50
1:B:431:ALA:O	1:B:435:ARG:N	2.39	0.50
1:B:642:ASN:O	1:C:706:ARG:NH2	2.42	0.50
1:C:199:ILE:HD12	1:C:240:MET:HG3	1.93	0.50
1:D:394:LEU:HA	1:D:397:LYS:HE2	1.94	0.50
1:D:641:ARG:HA	1:D:644:LEU:HD12	1.93	0.50
1:F:283:PHE:HD1	1:F:319:ILE:HG23	1.74	0.50
1:F:308:LYS:HD2	1:F:311:LEU:HD12	1.94	0.50
1:A:206:ARG:HD2	1:A:313:SER:HB3	1.93	0.50
1:C:658:ILE:HG13	1:C:695:TYR:CD1	2.46	0.50
1:D:589:ASN:OD1	1:D:590:ASN:ND2	2.44	0.50
1:A:670:GLN:HG3	1:A:680:LEU:HD23	1.92	0.50
1:B:212:LEU:C	1:B:220:LYS:HD2	2.36	0.50
1:B:673:LEU:HB3	1:B:678:VAL:O	2.11	0.50
1:C:643:ARG:NH2	4:D:802:ATP:O3G	2.42	0.50
1:E:501:LYS:HB2	4:E:802:ATP:O1B	2.12	0.50
1:A:553:VAL:HG21	1:A:596:PHE:CZ	2.47	0.50
1:B:581:MET:HE3	1:B:643:ARG:HG3	1.93	0.50
1:D:466:ALA:HA	1:D:648:ILE:HD13	1.92	0.50
1:E:349:PRO:HB2	1:E:353:GLU:HG3	1.93	0.50
1:A:517:LEU:HB2	1:A:561:LEU:HD12	1.94	0.50
1:C:501:LYS:HE3	4:C:802:ATP:PG	2.52	0.50
1:E:389:ILE:HG12	1:E:434:ALA:HB2	1.93	0.50
1:B:719:GLU:HB3	1:B:725:LEU:HB2	1.93	0.50
1:E:361:LEU:CD1	4:E:801:ATP:O2'	2.60	0.50
1:F:514:ILE:HB	1:F:559:ALA:HA	1.94	0.50
1:D:661:VAL:HG22	4:D:802:ATP:C2	2.47	0.50
1:F:381:ALA:HA	1:F:426:ILE:HG21	1.94	0.50
1:F:502:THR:CB	3:F:801:ADP:O3B	2.60	0.50
1:B:653:LEU:HD12	1:B:657:VAL:HG11	1.94	0.49
1:D:254:LEU:C	1:D:254:LEU:HD12	2.37	0.49
1:F:360:GLY:O	1:F:364:LYS:NZ	2.45	0.49
1:F:517:LEU:HB2	1:F:561:LEU:HD23	1.94	0.49
1:C:357:ILE:CG2	4:C:801:ATP:N3	2.72	0.49
1:E:205:ARG:HB2	1:F:369:HIS:HE1	1.76	0.49
1:B:188:LEU:HD12	4:B:801:ATP:N1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:VAL:O	1:E:382:VAL:HG23	2.11	0.49
1:C:658:ILE:HG13	1:C:695:TYR:HD1	1.77	0.49
1:C:350:SER:HB2	1:C:353:GLU:OE2	2.13	0.49
1:D:264:GLU:HG3	1:D:306:LEU:HD11	1.94	0.49
1:E:171:ASN:OD1	1:E:171:ASN:N	2.44	0.49
1:A:173:THR:HA	1:A:248:LEU:HA	1.94	0.49
1:B:639:GLU:HB3	1:C:497:THR:CG2	2.42	0.49
1:C:563:LEU:HD12	1:C:603:MET:HG2	1.94	0.49
1:E:189:ILE:HG21	1:E:356:GLN:HB3	1.95	0.49
1:A:191:ARG:NH1	1:A:194:GLU:OE2	2.45	0.49
1:A:221:THR:HB	3:A:801:ADP:O2A	2.13	0.49
1:B:313:SER:OG	1:B:315:LYS:HG3	2.12	0.49
1:B:633:LYS:C	1:B:635:ILE:H	2.21	0.49
1:C:662:VAL:HG23	1:C:708:ILE:HD11	1.95	0.49
1:D:324:TYR:OH	1:D:345:ASP:OD1	2.29	0.49
1:F:527:ARG:HD2	1:F:530:VAL:HB	1.94	0.49
1:B:412:MET:O	1:B:414:VAL:N	2.44	0.49
1:C:311:LEU:HB2	1:C:340:ARG:HD3	1.95	0.49
1:D:180:ALA:HB2	1:D:185:ILE:HD12	1.94	0.49
1:E:517:LEU:HB2	1:E:561:LEU:HD12	1.95	0.49
1:F:654:SER:O	1:F:658:ILE:HG13	2.13	0.49
1:A:267:PHE:CE2	1:A:307:ILE:HG23	2.47	0.48
1:A:267:PHE:HZ	1:A:307:ILE:HG21	1.78	0.48
1:B:716:LEU:O	1:B:720:LEU:HG	2.13	0.48
1:C:461:PHE:O	4:C:802:ATP:N6	2.22	0.48
1:E:397:LYS:O	1:E:401:VAL:HG23	2.12	0.48
1:A:267:PHE:HE2	1:A:307:ILE:HG22	1.78	0.48
1:D:191:ARG:NH2	1:D:347:THR:O	2.40	0.48
1:E:355:VAL:HA	1:E:358:ILE:HD12	1.95	0.48
1:E:470:LEU:O	1:E:474:ILE:HG12	2.13	0.48
1:F:248:LEU:HD23	1:F:284:ILE:HG23	1.94	0.48
1:F:527:ARG:NE	1:F:572:ASP:OD2	2.45	0.48
1:A:267:PHE:HE2	1:A:307:ILE:CG2	2.22	0.48
1:D:203:CYS:O	1:E:410:ARG:NH2	2.47	0.48
1:F:177:ASN:HD21	1:F:245:ILE:HD12	1.78	0.48
1:A:248:LEU:HD23	1:A:282:LEU:HD11	1.95	0.48
1:A:716:LEU:HD22	1:F:481:LEU:HD13	1.96	0.48
1:B:339:ARG:NH1	1:C:396:ASP:OD1	2.47	0.48
1:D:493:PHE:CE1	1:D:648:ILE:HD12	2.46	0.48
1:E:291:ILE:HD12	1:E:291:ILE:H	1.79	0.48
1:E:738:GLU:N	1:E:738:GLU:OE1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:GLU:O	1:F:196:GLU:HG3	2.13	0.48
1:E:483:HIS:HB3	1:E:486:LYS:HB3	1.96	0.48
1:E:661:VAL:HG22	4:E:802:ATP:C2	2.48	0.48
1:A:351:ILE:O	1:A:355:VAL:HG23	2.14	0.48
1:B:300:GLN:OE1	1:C:289:THR:HA	2.13	0.48
1:A:432:ARG:HH12	1:A:435:ARG:NH1	2.11	0.48
1:B:460:VAL:HA	4:B:802:ATP:N1	2.29	0.48
1:C:300:GLN:C	1:C:302:ASP:H	2.21	0.48
1:E:446:ARG:HG3	1:E:450:LYS:NZ	2.29	0.48
1:F:176:LEU:HA	1:F:179:LEU:HG	1.96	0.48
1:A:198:ALA:O	1:A:202:LEU:HG	2.14	0.48
1:B:369:HIS:HA	1:B:410:ARG:HH11	1.79	0.48
1:C:517:LEU:HB2	1:C:561:LEU:HD12	1.96	0.48
1:C:666:ILE:O	1:C:670:GLN:HG3	2.13	0.48
1:A:227:LEU:O	1:A:231:ILE:HG13	2.13	0.48
1:B:503:GLU:O	1:B:507:GLN:HG2	2.13	0.48
1:B:662:VAL:HG13	1:B:708:ILE:HD11	1.96	0.48
1:B:506:VAL:HG12	1:B:516:LEU:CD2	2.44	0.47
1:B:639:GLU:CB	1:C:497:THR:CG2	2.92	0.47
1:C:464:ASP:O	1:C:468:GLU:HG2	2.14	0.47
1:C:553:VAL:HG21	1:C:596:PHE:CZ	2.49	0.47
1:D:188:LEU:HD12	4:D:801:ATP:C6	2.49	0.47
1:D:470:LEU:HD13	1:D:508:LEU:HD22	1.95	0.47
1:D:639:GLU:O	1:D:643:ARG:NE	2.47	0.47
1:E:313:SER:O	1:E:315:LYS:NZ	2.36	0.47
1:E:353:GLU:O	1:E:357:ILE:HG23	2.13	0.47
1:F:616:SER:HB2	1:F:621:HIS:HA	1.96	0.47
1:B:248:LEU:HB2	1:B:282:LEU:HD11	1.96	0.47
1:B:259:TYR:HB3	1:C:258:LYS:HG3	1.96	0.47
1:B:396:ASP:HA	1:B:399:ILE:CD1	2.44	0.47
1:B:636:PHE:O	1:B:640:PHE:HB3	2.13	0.47
1:F:449:LEU:HD11	1:F:478:ARG:HG3	1.94	0.47
1:B:530:VAL:HG12	1:B:573:VAL:HG22	1.96	0.47
1:C:264:GLU:HG2	1:D:254:LEU:HD11	1.96	0.47
1:C:358:ILE:HD11	1:C:398:ALA:HB1	1.97	0.47
1:F:267:PHE:O	1:F:270:LEU:HG	2.14	0.47
1:F:453:GLY:HA2	1:F:471:THR:HG21	1.96	0.47
1:A:645:ASP:HA	1:B:706:ARG:NE	2.29	0.47
1:B:255:ALA:O	1:B:266:ARG:NH1	2.47	0.47
1:B:439:LYS:HG3	1:B:440:SER:N	2.30	0.47
1:B:727:ASP:N	1:B:727:ASP:OD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:ALA:O	1:D:589:ASN:ND2	2.42	0.47
1:B:632:ILE:HA	1:B:635:ILE:HD12	1.97	0.47
1:F:663:ASP:O	1:F:667:VAL:HG13	2.15	0.47
1:A:448:THR:O	1:A:455:ARG:NH2	2.48	0.47
1:A:502:THR:OG1	3:A:802:ADP:O2A	2.27	0.47
1:B:646:ASN:N	1:B:646:ASN:OD1	2.46	0.47
1:B:689:TRP:CZ3	1:B:742:LEU:HD21	2.49	0.47
1:E:361:LEU:HD13	4:E:801:ATP:O2'	2.15	0.47
1:F:362:LYS:HG3	1:F:373:TYR:CE1	2.50	0.47
1:A:659:HIS:O	1:A:662:VAL:HG12	2.14	0.47
1:E:544:ASP:OD1	1:E:544:ASP:N	2.45	0.47
1:F:412:MET:HB3	1:F:413:PRO:HD3	1.96	0.47
1:F:502:THR:HG21	3:F:801:ADP:O1B	2.14	0.47
1:C:219:GLY:HA2	4:C:801:ATP:PA	2.51	0.47
1:A:311:LEU:C	1:A:311:LEU:HD12	2.40	0.47
1:A:444:SER:O	1:A:448:THR:HG23	2.14	0.47
1:A:522:SER:HA	1:A:525:MET:HE3	1.96	0.47
1:A:738:GLU:H	1:A:738:GLU:CD	2.23	0.47
1:D:611:GLU:O	1:D:624:ASN:ND2	2.45	0.47
1:F:431:ALA:HB2	1:F:438:GLU:HB3	1.97	0.47
1:A:219:GLY:HA2	3:A:801:ADP:H5'1	1.97	0.46
1:F:362:LYS:HG3	1:F:373:TYR:HE1	1.80	0.46
1:C:443:GLN:CD	1:C:444:SER:H	2.22	0.46
1:F:653:LEU:HD11	3:F:801:ADP:N7	2.30	0.46
1:C:207:LYS:HD2	1:C:340:ARG:HA	1.97	0.46
1:D:499:VAL:O	1:D:501:LYS:N	2.45	0.46
1:D:577:LEU:HA	1:D:580:VAL:HB	1.98	0.46
1:E:226:GLY:O	1:E:230:ARG:HG2	2.15	0.46
1:F:498:GLY:HA2	3:F:801:ADP:C5'	2.43	0.46
1:B:288:HIS:CE1	1:B:326:GLU:HG2	2.51	0.46
1:C:575:ASN:OD1	1:D:568:LYS:HD2	2.16	0.46
1:D:525:MET:HE3	1:D:525:MET:HB2	1.80	0.46
1:A:203:CYS:HB2	1:B:407:ALA:HB1	1.98	0.46
1:B:479:ALA:HB2	1:C:721:LEU:HG	1.98	0.46
1:D:177:ASN:OD1	1:D:244:THR:HA	2.15	0.46
1:D:714:LYS:HB2	1:D:715:PRO:HD3	1.96	0.46
1:A:248:LEU:C	1:A:248:LEU:HD12	2.41	0.46
1:B:228:ALA:O	1:B:232:VAL:HG13	2.15	0.46
1:B:394:LEU:HA	1:B:397:LYS:HE2	1.98	0.46
1:B:412:MET:N	1:B:413:PRO:HD2	2.30	0.46
1:C:481:LEU:HD12	1:C:481:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ASP:O	1:D:418:LYS:HE2	2.16	0.46
1:A:219:GLY:HA2	3:A:801:ADP:O1A	2.15	0.46
1:C:714:LYS:HB2	1:C:715:PRO:HD3	1.98	0.46
1:E:209:ASN:HB3	1:E:341:PHE:CD2	2.51	0.46
1:B:219:GLY:HA2	4:B:801:ATP:O2A	2.16	0.46
1:C:658:ILE:HD12	1:C:704:MET:HG3	1.97	0.46
1:B:502:THR:HG1	4:B:802:ATP:PA	2.39	0.46
1:E:211:LEU:HD13	1:E:341:PHE:CD2	2.50	0.46
1:F:603:MET:HE2	1:F:603:MET:HB2	1.89	0.46
1:B:229:TRP:O	1:B:232:VAL:HG22	2.16	0.46
1:B:734:ALA:O	1:B:743:THR:N	2.48	0.46
1:E:205:ARG:O	1:E:208:ASN:ND2	2.50	0.46
1:E:211:LEU:O	1:E:344:ILE:N	2.47	0.46
1:F:426:ILE:O	1:F:430:VAL:HG23	2.16	0.46
1:C:472:GLU:CD	1:D:714:LYS:HD3	2.41	0.45
1:C:642:ASN:OD1	1:D:497:THR:OG1	2.29	0.45
1:E:737:LYS:HD3	1:E:737:LYS:HA	1.78	0.45
1:A:267:PHE:CZ	1:A:307:ILE:HG23	2.51	0.45
1:B:476:MET:HE1	1:C:709:GLN:HG3	1.98	0.45
1:B:514:ILE:HD13	1:B:514:ILE:HA	1.79	0.45
1:D:192:GLU:O	1:D:196:GLU:HG2	2.17	0.45
1:F:187:PRO:HG3	1:F:229:TRP:CE2	2.51	0.45
1:A:629:MET:HG3	1:A:633:LYS:HE3	1.97	0.45
1:B:371:VAL:HG12	1:B:372:ARG:H	1.82	0.45
1:B:445:ASP:O	1:B:448:THR:OG1	2.29	0.45
1:C:271:LEU:HD13	1:C:310:LEU:HD12	1.98	0.45
1:D:231:ILE:HG12	1:D:236:VAL:HG21	1.97	0.45
1:E:197:ARG:O	1:E:201:VAL:HG23	2.16	0.45
1:E:662:VAL:HG13	1:E:708:ILE:HD11	1.98	0.45
1:F:502:THR:CG2	3:F:801:ADP:O2A	2.64	0.45
1:C:503:GLU:HG2	4:C:802:ATP:H2'	1.97	0.45
1:D:579:GLN:HE22	1:E:523:GLU:CD	2.24	0.45
1:E:384:LEU:HD11	1:E:427:GLU:HG2	1.98	0.45
1:F:250:ILE:O	1:F:254:LEU:HB2	2.16	0.45
1:F:380:ALA:O	1:F:384:LEU:HG	2.17	0.45
1:F:412:MET:HB3	1:F:412:MET:HE3	1.84	0.45
1:F:485:HIS:O	1:F:584:GLY:HA3	2.16	0.45
1:F:284:ILE:HG21	1:F:287:ILE:HD13	1.98	0.45
1:F:584:GLY:O	1:F:596:PHE:HB2	2.17	0.45
1:A:285:ASP:OD1	1:A:285:ASP:O	2.34	0.45
1:A:369:HIS:HB2	1:A:371:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:HD11	1:B:282:LEU:HB2	1.98	0.45
1:C:301:VAL:O	1:C:306:LEU:HG	2.17	0.45
1:C:354:THR:HA	1:C:357:ILE:HD12	1.99	0.45
1:F:214:GLY:HA2	1:F:324:TYR:CE2	2.51	0.45
1:F:408:ARG:HH22	1:F:425:ASP:HB3	1.82	0.45
1:C:205:ARG:HD3	1:D:365:TYR:CD2	2.51	0.45
1:E:211:LEU:HD12	1:E:320:GLY:HA3	1.99	0.45
1:F:177:ASN:HB3	1:F:181:ARG:HH21	1.82	0.45
1:F:351:ILE:O	1:F:354:THR:OG1	2.28	0.45
1:A:714:LYS:HZ3	1:F:476:MET:HB2	1.82	0.45
1:B:211:LEU:HB2	1:B:341:PHE:HB3	1.98	0.45
1:B:460:VAL:HG21	1:B:504:VAL:HA	1.99	0.45
1:E:521:MET:HB2	1:E:564:ASP:O	2.17	0.45
1:A:206:ARG:NH1	1:A:313:SER:O	2.49	0.45
1:A:350:SER:O	1:A:354:THR:OG1	2.34	0.45
1:A:416:LYS:HA	1:A:416:LYS:HD3	1.64	0.45
1:B:518:ARG:NE	1:B:564:ASP:OD2	2.50	0.45
1:C:341:PHE:O	1:D:392:ARG:NH2	2.50	0.45
1:C:633:LYS:HA	1:C:641:ARG:NE	2.32	0.45
1:A:269:ALA:O	1:A:273:GLN:HG2	2.17	0.44
1:C:260:ARG:HH21	1:D:300:GLN:HE22	1.66	0.44
1:C:503:GLU:OE2	1:C:507:GLN:NE2	2.44	0.44
1:D:611:GLU:OE2	1:D:611:GLU:N	2.49	0.44
1:E:330:ILE:HG13	1:E:331:PHE:N	2.32	0.44
1:F:392:ARG:HD2	1:F:397:LYS:HE2	1.98	0.44
1:F:452:LEU:O	1:F:456:LEU:HG	2.18	0.44
1:A:455:ARG:O	1:A:458:MET:HG2	2.18	0.44
1:B:212:LEU:O	1:B:321:SER:HA	2.18	0.44
1:B:219:GLY:O	1:B:223:ILE:HG12	2.17	0.44
1:B:639:GLU:HB3	1:C:497:THR:HG21	2.00	0.44
1:C:693:LYS:NZ	1:C:711:ASN:OD1	2.50	0.44
1:D:417:ARG:HB3	1:D:419:LYS:NZ	2.32	0.44
1:E:188:LEU:CD1	1:E:222:ALA:O	2.61	0.44
1:E:719:GLU:HG3	1:E:744:TYR:CZ	2.52	0.44
1:F:725:LEU:HD23	1:F:729:GLY:HA3	1.98	0.44
1:A:283:PHE:HD1	1:A:319:ILE:HB	1.82	0.44
1:A:286:GLU:HG2	1:F:335:ARG:HD2	1.98	0.44
1:C:412:MET:HB3	1:C:417:ARG:HB3	1.99	0.44
1:A:188:LEU:HD23	1:A:195:LEU:HD11	2.00	0.44
1:E:446:ARG:HH21	1:F:721:LEU:HA	1.83	0.44
1:E:518:ARG:HG2	1:E:562:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLN:NE2	1:B:651:ASP:O	2.45	0.44
1:B:474:ILE:HD13	1:B:512:LEU:HD11	2.00	0.44
1:D:463:GLN:NE2	1:D:651:ASP:O	2.44	0.44
1:E:656:ASP:O	1:E:660:GLN:HG3	2.18	0.44
1:D:656:ASP:OD1	1:D:656:ASP:N	2.49	0.44
1:E:205:ARG:HD3	1:F:365:TYR:CD1	2.53	0.44
1:E:307:ILE:O	1:E:311:LEU:HG	2.18	0.44
1:E:638:PRO:HG3	1:E:641:ARG:HH22	1.82	0.44
1:A:404:GLU:HB3	1:A:429:VAL:HG21	1.99	0.44
1:D:205:ARG:O	1:D:206:ARG:NH1	2.49	0.44
1:D:335:ARG:NH1	1:E:325:GLN:OE1	2.51	0.44
1:E:658:ILE:HG13	1:E:695:TYR:CD1	2.53	0.44
1:A:570:HIS:ND1	1:A:571:PRO:HD2	2.32	0.44
1:B:673:LEU:HD11	1:B:716:LEU:HD23	1.98	0.44
1:C:291:ILE:HA	1:C:304:ALA:HB2	2.00	0.44
1:D:371:VAL:HG11	1:D:421:VAL:HG23	1.99	0.44
1:D:530:VAL:HG21	1:E:525:MET:HE1	1.99	0.44
1:F:209:ASN:O	1:F:341:PHE:HA	2.18	0.44
1:D:272:LYS:HE3	1:D:272:LYS:HB3	1.65	0.44
1:D:308:LYS:HG3	1:D:340:ARG:HH12	1.83	0.44
1:E:191:ARG:NH1	1:E:194:GLU:OE1	2.51	0.44
1:F:202:LEU:HD23	1:F:317:ARG:HD2	2.00	0.44
1:B:253:LEU:O	1:B:266:ARG:NH1	2.49	0.43
1:D:709:GLN:HA	1:D:713:LYS:HG3	2.00	0.43
1:E:447:ASP:OD1	1:E:448:THR:N	2.51	0.43
1:A:267:PHE:HZ	1:A:307:ILE:CG2	2.29	0.43
1:A:717:ALA:HB2	1:F:481:LEU:HD21	1.99	0.43
1:B:188:LEU:HD11	4:B:801:ATP:N6	2.33	0.43
1:B:210:PRO:HG2	1:B:319:ILE:HG12	2.00	0.43
1:B:553:VAL:HG21	1:B:596:PHE:CE2	2.53	0.43
1:D:384:LEU:HB3	1:D:430:VAL:HG11	1.98	0.43
1:E:231:ILE:HD12	1:E:245:ILE:HD11	2.00	0.43
1:E:354:THR:O	1:E:357:ILE:HG13	2.17	0.43
1:B:324:TYR:OH	1:B:345:ASP:OD1	2.36	0.43
1:B:447:ASP:N	1:B:447:ASP:OD1	2.49	0.43
1:B:496:PRO:HG3	1:B:652:HIS:CD2	2.52	0.43
1:C:293:ALA:H	1:C:302:ASP:HB2	1.83	0.43
1:D:288:HIS:HD2	1:D:330:ILE:HD12	1.84	0.43
1:A:725:LEU:HD11	1:A:731:VAL:HG22	2.00	0.43
1:B:672:GLN:HA	1:B:675:GLN:CD	2.43	0.43
1:B:553:VAL:HG21	1:B:596:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:627:ASP:OD2	1:F:627:ASP:N	2.43	0.43
1:C:323:THR:OG1	1:C:326:GLU:OE1	2.36	0.43
1:E:185:ILE:HG23	1:E:225:GLU:HB2	2.00	0.43
1:E:264:GLU:HA	1:E:267:PHE:CD1	2.52	0.43
1:A:315:LYS:HE2	1:A:315:LYS:HB3	1.74	0.43
1:C:413:PRO:HG3	1:C:418:LYS:HE2	2.00	0.43
1:D:409:ALA:O	1:D:413:PRO:HD3	2.18	0.43
1:F:287:ILE:HG22	1:F:321:SER:H	1.84	0.43
1:C:221:THR:CB	4:C:801:ATP:O1B	2.66	0.43
1:C:501:LYS:HE3	4:C:802:ATP:O2G	2.14	0.43
1:C:684:GLN:NE2	1:C:688:ASN:OD1	2.46	0.43
1:D:169:MET:SD	1:D:246:TYR:CE1	3.12	0.43
1:A:446:ARG:NH2	1:B:722:PHE:HA	2.33	0.43
1:B:396:ASP:CA	1:B:399:ILE:HG12	2.48	0.43
1:C:402:ILE:HD13	1:C:402:ILE:HA	1.88	0.43
1:F:288:HIS:CD2	1:F:322:THR:HA	2.54	0.43
1:F:413:PRO:O	1:F:417:ARG:NH1	2.32	0.43
1:F:662:VAL:HG22	1:F:704:MET:SD	2.59	0.43
1:D:220:LYS:HG2	1:D:346:ILE:HG13	2.01	0.43
1:D:537:PRO:HG2	1:E:528:HIS:ND1	2.34	0.43
1:E:217:GLY:HA3	1:E:396:ASP:OD2	2.19	0.43
1:F:461:PHE:N	3:F:801:ADP:HN62	2.17	0.43
1:A:502:THR:HG23	3:A:802:ADP:O2B	2.19	0.42
1:A:582:ASP:CB	1:A:643:ARG:NH1	2.81	0.42
1:B:408:ARG:HG2	1:B:412:MET:HE3	2.01	0.42
1:B:499:VAL:HG23	1:B:650:PHE:HD2	1.83	0.42
1:A:586:LEU:HD23	1:A:586:LEU:HA	1.76	0.42
1:B:357:ILE:HG23	4:B:801:ATP:C2	2.54	0.42
1:B:371:VAL:HG12	1:B:372:ARG:N	2.34	0.42
1:E:436:ILE:H	1:E:436:ILE:HG13	1.78	0.42
1:B:265:LYS:HB3	1:B:265:LYS:HE2	1.82	0.42
1:B:429:VAL:O	1:B:432:ARG:HB3	2.19	0.42
1:D:476:MET:HE1	1:E:709:GLN:HG3	2.00	0.42
1:E:577:LEU:HA	1:E:580:VAL:HG12	2.02	0.42
1:F:461:PHE:H	3:F:801:ADP:HN62	1.67	0.42
1:A:331:PHE:C	1:A:333:LYS:H	2.27	0.42
1:A:476:MET:HA	1:B:717:ALA:HB1	2.00	0.42
1:A:657:VAL:O	1:A:661:VAL:HG13	2.19	0.42
1:E:442:SER:O	1:E:445:ASP:N	2.39	0.42
1:F:696:ASP:O	1:F:700:GLY:N	2.52	0.42
1:B:446:ARG:NH2	1:C:720:LEU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:VAL:HG12	1:B:516:LEU:HD22	2.01	0.42
1:D:501:LYS:HB3	4:D:802:ATP:O1B	2.20	0.42
1:D:642:ASN:ND2	1:E:699:MET:SD	2.91	0.42
1:F:408:ARG:NH2	1:F:425:ASP:HB3	2.34	0.42
1:A:432:ARG:HH21	1:F:197:ARG:CZ	2.32	0.42
1:C:438:GLU:O	1:C:439:LYS:HD2	2.19	0.42
1:C:536:ALA:O	1:C:589:ASN:ND2	2.34	0.42
1:E:195:LEU:HD21	1:E:230:ARG:HG3	2.01	0.42
1:E:387:LYS:HA	1:E:387:LYS:HD3	1.66	0.42
1:E:449:LEU:HD12	1:E:475:LYS:HG2	2.02	0.42
1:F:349:PRO:HB2	1:F:353:GLU:HB2	2.01	0.42
1:A:352:GLU:H	1:A:352:GLU:CD	2.27	0.42
1:A:446:ARG:HA	1:A:446:ARG:HD2	1.89	0.42
1:B:207:LYS:HD3	1:B:339:ARG:NH1	2.34	0.42
1:B:215:GLU:OE2	1:C:555:LYS:NZ	2.42	0.42
1:B:288:HIS:CD2	1:B:326:GLU:HG2	2.54	0.42
1:C:345:ASP:OD2	1:D:435:ARG:CZ	2.67	0.42
1:D:301:VAL:HB	1:D:306:LEU:HD21	2.02	0.42
1:D:577:LEU:HB2	1:D:640:PHE:HE1	1.84	0.42
1:E:442:SER:HB3	1:E:445:ASP:HB2	2.00	0.42
1:F:673:LEU:HD12	1:F:680:LEU:HB2	2.01	0.42
1:A:307:ILE:O	1:A:311:LEU:HG	2.20	0.42
1:B:277:ASP:C	1:B:279:ASN:H	2.26	0.42
1:D:207:LYS:HD2	1:D:339:ARG:O	2.19	0.42
1:D:253:LEU:HG	1:D:263:PHE:HE1	1.85	0.42
1:D:725:LEU:HD13	1:D:728:GLY:O	2.20	0.42
1:E:354:THR:CA	1:E:357:ILE:HG12	2.50	0.42
1:E:553:VAL:HG21	1:E:596:PHE:CZ	2.54	0.42
1:F:394:LEU:HB2	1:F:395:PRO:HD3	2.02	0.42
1:F:553:VAL:HG11	1:F:594:ALA:HB1	2.01	0.42
1:A:410:ARG:O	1:A:413:PRO:HD2	2.20	0.42
1:A:475:LYS:HB3	1:B:721:LEU:HD23	2.01	0.42
1:B:170:GLU:CD	1:B:170:GLU:H	2.28	0.42
1:B:268:LYS:HD3	1:B:268:LYS:HA	1.89	0.42
1:B:288:HIS:NE2	1:B:326:GLU:HG2	2.35	0.42
1:B:712:LEU:O	1:B:716:LEU:HD13	2.19	0.42
1:C:441:VAL:O	1:C:446:ARG:HG3	2.20	0.42
1:D:262:ASP:OD1	1:D:262:ASP:N	2.51	0.42
1:E:411:LEU:HD23	1:E:411:LEU:HA	1.83	0.42
1:E:465:LYS:H	1:E:465:LYS:HG3	1.67	0.42
1:A:579:GLN:HE22	1:B:523:GLU:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:SER:OG	1:A:656:ASP:OD1	2.26	0.42
1:A:719:GLU:HB3	1:A:725:LEU:CB	2.49	0.42
1:B:384:LEU:HD22	1:B:388:TYR:HE1	1.84	0.42
1:C:581:MET:HE2	1:C:643:ARG:HG3	2.01	0.42
1:D:303:ALA:C	1:D:305:ASN:H	2.26	0.42
1:D:323:THR:OG1	1:D:326:GLU:OE1	2.30	0.42
1:D:410:ARG:O	1:D:413:PRO:HD2	2.20	0.42
1:D:495:GLY:O	1:D:501:LYS:NZ	2.53	0.42
1:E:188:LEU:HG	4:E:801:ATP:C6	2.54	0.42
1:E:264:GLU:HG3	1:E:306:LEU:HD21	2.01	0.42
1:E:272:LYS:HA	1:E:272:LYS:HD3	1.84	0.42
1:F:369:HIS:CD2	1:F:406:GLY:HA3	2.55	0.42
1:A:437:PRO:O	1:A:440:SER:OG	2.35	0.41
1:A:654:SER:HB3	1:A:657:VAL:HG23	2.01	0.41
1:B:633:LYS:O	1:B:635:ILE:HG13	2.20	0.41
1:C:501:LYS:CE	4:C:802:ATP:O1B	2.67	0.41
1:C:501:LYS:HE2	4:C:802:ATP:O1B	2.20	0.41
1:C:549:LEU:O	1:C:553:VAL:HG23	2.20	0.41
1:F:307:ILE:H	1:F:307:ILE:HG13	1.73	0.41
1:F:369:HIS:HD2	1:F:406:GLY:HA3	1.85	0.41
1:F:638:PRO:O	1:F:642:ASN:HB2	2.20	0.41
1:C:537:PRO:HG2	1:D:528:HIS:CD2	2.56	0.41
1:C:615:LYS:HE2	1:C:615:LYS:HB2	1.93	0.41
1:D:238:GLU:CD	1:D:238:GLU:H	2.28	0.41
1:E:355:VAL:HG22	1:E:382:VAL:HG21	2.02	0.41
1:E:412:MET:HB3	1:E:413:PRO:HD3	2.02	0.41
1:F:277:ASP:C	1:F:278:THR:O	2.63	0.41
1:F:704:MET:HG3	1:F:708:ILE:HD13	2.02	0.41
1:A:714:LYS:N	1:A:715:PRO:CD	2.83	0.41
1:E:188:LEU:HD21	1:E:191:ARG:CG	2.49	0.41
1:E:221:THR:HG22	4:E:801:ATP:PB	2.61	0.41
1:E:495:GLY:HA2	1:E:649:TRP:CZ3	2.56	0.41
1:F:271:LEU:O	1:F:274:LEU:HG	2.19	0.41
1:F:371:VAL:O	1:F:372:ARG:NH1	2.42	0.41
1:F:463:GLN:NE2	1:F:651:ASP:O	2.36	0.41
1:F:471:THR:HA	1:F:474:ILE:HG22	2.02	0.41
1:B:197:ARG:NH1	1:C:404:GLU:OE2	2.53	0.41
1:B:221:THR:CB	4:B:801:ATP:O1B	2.68	0.41
1:D:195:LEU:O	1:D:199:ILE:HG13	2.20	0.41
1:E:222:ALA:O	1:E:225:GLU:HG2	2.20	0.41
1:E:382:VAL:O	1:E:386:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:ASP:OD1	1:E:454:ASP:N	2.52	0.41
1:E:543:PHE:C	1:E:545:GLN:H	2.28	0.41
1:C:479:ALA:HB2	1:D:721:LEU:HG	2.01	0.41
1:D:204:ARG:HB2	1:D:208:ASN:HB3	2.01	0.41
1:E:564:ASP:OD2	1:E:565:GLU:HG2	2.19	0.41
1:F:468:GLU:O	1:F:472:GLU:HG2	2.20	0.41
1:A:498:GLY:H	3:A:802:ADP:PB	2.43	0.41
1:B:188:LEU:CD1	4:B:801:ATP:C6	3.03	0.41
1:B:521:MET:HG3	1:B:566:ILE:HD12	2.03	0.41
1:D:689:TRP:HB2	1:D:735:LEU:HD22	2.02	0.41
1:E:357:ILE:HG13	1:E:358:ILE:N	2.36	0.41
1:E:373:TYR:HD2	1:E:421:VAL:HG11	1.85	0.41
1:E:503:GLU:O	1:E:507:GLN:HG2	2.20	0.41
1:E:537:PRO:O	1:E:539:GLY:N	2.54	0.41
1:A:439:LYS:HG3	1:A:444:SER:HB3	2.03	0.41
1:C:205:ARG:HD3	1:D:365:TYR:CE2	2.55	0.41
1:D:438:GLU:OE2	1:D:438:GLU:N	2.48	0.41
1:A:381:ALA:HB2	1:A:426:ILE:HG12	2.02	0.41
1:B:219:GLY:CA	4:B:801:ATP:O3A	2.66	0.41
1:C:587:THR:HA	1:C:592:ARG:O	2.20	0.41
1:C:681:GLU:N	1:C:730:GLN:HE22	2.18	0.41
1:D:578:LEU:HD23	1:D:578:LEU:HA	1.87	0.41
1:E:502:THR:O	1:E:506:VAL:HG23	2.21	0.41
1:F:673:LEU:O	1:F:677:GLY:N	2.48	0.41
1:A:173:THR:OG1	1:A:246:TYR:HB3	2.21	0.41
1:A:371:VAL:HA	1:A:419:LYS:HB3	2.03	0.41
1:A:630:GLU:HA	1:A:633:LYS:HD2	2.02	0.41
1:A:658:ILE:HG22	1:A:691:ALA:HB1	2.03	0.41
1:A:696:ASP:HB2	1:A:699:MET:HB2	2.02	0.41
1:B:464:ASP:OD1	1:B:464:ASP:N	2.54	0.41
1:B:481:LEU:HB3	1:C:713:LYS:HE2	2.02	0.41
1:C:353:GLU:OE2	1:C:353:GLU:N	2.53	0.41
1:C:527:ARG:HB2	1:C:570:HIS:CD2	2.56	0.41
1:D:205:ARG:HD3	1:E:365:TYR:CD1	2.56	0.41
1:D:658:ILE:HG13	1:D:695:TYR:CD1	2.55	0.41
1:E:222:ALA:CB	4:E:801:ATP:C5	3.00	0.41
1:F:322:THR:HG22	1:F:323:THR:N	2.36	0.41
1:F:610:ARG:HD2	1:F:610:ARG:HA	1.87	0.41
1:D:582:ASP:HB2	1:D:643:ARG:HD3	2.02	0.41
1:F:212:LEU:HB3	1:F:346:ILE:HD12	2.01	0.41
1:A:317:ARG:H	1:A:317:ARG:HG2	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:THR:HG23	1:C:327:PHE:HB2	2.03	0.40
1:C:702:ARG:N	1:C:703:PRO:HD2	2.36	0.40
1:D:218:VAL:HG13	1:D:348:GLU:HA	2.01	0.40
1:E:187:PRO:HA	1:E:229:TRP:CD1	2.56	0.40
1:E:258:LYS:HE2	1:E:258:LYS:HB3	1.94	0.40
1:B:213:VAL:C	1:B:220:LYS:HD3	2.46	0.40
1:B:385:ALA:HB1	1:B:397:LYS:HG3	2.02	0.40
1:B:399:ILE:CD1	4:B:801:ATP:H4'	2.52	0.40
1:B:481:LEU:O	1:C:713:LYS:NZ	2.44	0.40
1:B:538:PRO:HB3	1:C:542:GLY:HA3	2.04	0.40
1:D:214:GLY:HA2	1:D:324:TYR:CE1	2.56	0.40
1:D:307:ILE:HD12	1:D:310:LEU:HB2	2.02	0.40
1:E:253:LEU:HD12	1:E:267:PHE:CE2	2.56	0.40
1:F:424:ALA:O	1:F:427:GLU:HG2	2.22	0.40
1:F:741:GLU:OE2	1:F:743:THR:OG1	2.35	0.40
1:A:305:ASN:HA	1:A:308:LYS:HD3	2.02	0.40
1:B:582:ASP:OD1	1:C:702:ARG:NH2	2.51	0.40
1:B:720:LEU:HD23	1:B:725:LEU:HB3	2.04	0.40
1:C:440:SER:HB2	1:C:445:ASP:OD2	2.22	0.40
1:C:447:ASP:O	1:C:451:ASN:ND2	2.54	0.40
1:C:667:VAL:O	1:C:671:VAL:HG23	2.22	0.40
1:C:721:LEU:HD23	1:C:721:LEU:HA	1.93	0.40
1:D:191:ARG:HB3	1:D:223:ILE:HD11	2.02	0.40
1:D:230:ARG:O	1:D:234:GLY:N	2.54	0.40
1:E:169:MET:HE2	1:E:269:ALA:HB1	2.03	0.40
1:E:204:ARG:HD2	1:F:404:GLU:HG3	2.03	0.40
1:A:205:ARG:NH2	1:B:364:LYS:HD3	2.37	0.40
1:A:211:LEU:HD12	1:A:320:GLY:HA3	2.02	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.76	0.40
1:B:521:MET:HE3	1:B:563:LEU:HD22	2.03	0.40
1:C:607:ALA:HB1	1:C:635:ILE:HD12	2.03	0.40
1:C:725:LEU:HD23	1:C:725:LEU:HA	1.85	0.40
1:D:191:ARG:NH1	1:D:194:GLU:OE2	2.54	0.40
1:E:219:GLY:HA2	4:E:801:ATP:O2A	2.22	0.40
1:F:202:LEU:HD22	1:F:281:ILE:HD13	2.02	0.40
1:F:387:LYS:HG3	1:F:558:HIS:CD2	2.56	0.40
1:B:188:LEU:CD1	4:B:801:ATP:N6	2.85	0.40
1:B:293:ALA:H	1:B:302:ASP:CB	2.35	0.40
1:C:671:VAL:O	1:C:675:GLN:HG3	2.22	0.40
1:D:335:ARG:HH22	1:E:216:SER:HB3	1.86	0.40
1:D:716:LEU:O	1:D:720:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LYS:HE3	1:E:333:LYS:HB3	1.90	0.40
1:E:515:GLU:OE2	1:E:556:HIS:ND1	2.54	0.40
1:F:689:TRP:HB2	1:F:735:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/758 (72%)	528 (97%)	18 (3%)	0	100	100
1	B	576/758 (76%)	550 (96%)	25 (4%)	1 (0%)	43	73
1	C	576/758 (76%)	542 (94%)	33 (6%)	1 (0%)	43	73
1	D	576/758 (76%)	555 (96%)	21 (4%)	0	100	100
1	E	564/758 (74%)	534 (95%)	29 (5%)	1 (0%)	43	73
1	F	564/758 (74%)	546 (97%)	17 (3%)	1 (0%)	43	73
All	All	3402/4548 (75%)	3255 (96%)	143 (4%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	278	THR
1	C	349	PRO
1	E	538	PRO
1	B	638	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	466/639 (73%)	452 (97%)	14 (3%)	36	65
1	B	485/639 (76%)	467 (96%)	18 (4%)	30	61
1	C	485/639 (76%)	476 (98%)	9 (2%)	50	73
1	D	485/639 (76%)	476 (98%)	9 (2%)	50	73
1	E	481/639 (75%)	472 (98%)	9 (2%)	50	73
1	F	481/639 (75%)	474 (98%)	7 (2%)	57	75
All	All	2883/3834 (75%)	2817 (98%)	66 (2%)	44	70

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	MET
1	A	189	ILE
1	A	239	VAL
1	A	317	ARG
1	A	323	THR
1	A	403	ASP
1	A	470	LEU
1	A	510	LYS
1	A	529	THR
1	A	534	ILE
1	A	560	VAL
1	A	599	VAL
1	A	604	THR
1	A	656	ASP
1	B	179	LEU
1	B	213	VAL
1	B	232	VAL
1	B	302	ASP
1	B	316	ILE
1	B	390	ASN
1	B	426	ILE
1	B	439	LYS
1	B	514	ILE
1	B	530	VAL
1	B	534	ILE
1	B	579	GLN

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Mol	Chain	Res	Type
1	B	604	THR
1	B	606	ASN
1	B	639	GLU
1	B	681	GLU
1	B	708	ILE
1	B	725	LEU
1	C	374	THR
1	C	399	ILE
1	C	454	ASP
1	C	514	ILE
1	C	579	GLN
1	C	603	MET
1	C	622	GLN
1	C	642	ASN
1	C	707	VAL
1	D	223	ILE
1	D	231	ILE
1	D	262	ASP
1	D	272	LYS
1	D	310	LEU
1	D	374	THR
1	D	567	GLU
1	D	706	ARG
1	D	720	LEU
1	E	242	ASP
1	E	436	ILE
1	E	454	ASP
1	E	599	VAL
1	E	646	ASN
1	E	720	LEU
1	E	731	VAL
1	E	743	THR
1	E	744	TYR
1	F	170	GLU
1	F	209	ASN
1	F	325	GLN
1	F	373	TYR
1	F	388	TYR
1	F	621	HIS
1	F	647	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	HIS
1	A	390	ASN
1	A	579	GLN
1	A	652	HIS
1	A	709	GLN
1	B	273	GLN
1	B	305	ASN
1	B	483	HIS
1	B	590	ASN
1	B	621	HIS
1	B	718	ASN
1	C	288	HIS
1	C	579	GLN
1	C	672	GLN
1	D	359	ASN
1	D	483	HIS
1	D	528	HIS
1	D	570	HIS
1	D	583	ASN
1	D	590	ASN
1	D	606	ASN
1	D	652	HIS
1	D	675	GLN
1	D	709	GLN
1	E	279	ASN
1	E	368	HIS
1	E	390	ASN
1	E	545	GLN
1	E	583	ASN
1	E	711	ASN
1	F	233	GLN
1	F	273	GLN
1	F	528	HIS
1	F	659	HIS
1	F	718	ASN

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 ⓘ

11 ligands are modelled in this entry.

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	ADP	F	801	-	28,29,29	3.00	10 (35%)	43,45,45	1.99	9 (20%)
4	ATP	E	802	-	32,33,33	4.23	15 (46%)	48,52,52	3.90	15 (31%)
3	ADP	A	802	-	28,29,29	2.99	10 (35%)	43,45,45	1.98	9 (20%)
4	ATP	B	801	-	32,33,33	4.22	15 (46%)	48,52,52	3.89	15 (31%)
4	ATP	C	802	-	32,33,33	4.23	15 (46%)	48,52,52	3.90	15 (31%)
3	ADP	A	801	-	28,29,29	2.99	10 (35%)	43,45,45	1.99	9 (20%)
4	ATP	D	802	-	32,33,33	4.23	15 (46%)	48,52,52	3.89	15 (31%)
4	ATP	E	801	-	32,33,33	4.23	15 (46%)	48,52,52	3.91	14 (29%)
4	ATP	C	801	-	32,33,33	4.22	15 (46%)	48,52,52	3.90	15 (31%)
4	ATP	B	802	-	32,33,33	4.22	15 (46%)	48,52,52	3.87	14 (29%)
4	ATP	D	801	-	32,33,33	4.21	15 (46%)	48,52,52	3.85	14 (29%)

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	ADP	F	801	-	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	E	802	-	-	2/22/38/38	0/3/3/3
3	ADP	A	802	-	-	2/16/32/32	0/3/3/3
4	ATP	B	801	-	-	1/22/38/38	0/3/3/3
4	ATP	C	802	-	-	2/22/38/38	0/3/3/3
3	ADP	A	801	-	-	4/16/32/32	0/3/3/3
4	ATP	D	802	-	-	2/22/38/38	0/3/3/3
4	ATP	E	801	-	-	4/22/38/38	0/3/3/3
4	ATP	C	801	-	-	7/22/38/38	0/3/3/3
4	ATP	B	802	-	-	4/22/38/38	0/3/3/3
4	ATP	D	801	-	-	2/22/38/38	0/3/3/3

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	801	ATP	C5-C4	13.43	1.63	1.39
4	E	802	ATP	C5-C4	13.41	1.63	1.39
4	C	801	ATP	C5-C4	13.40	1.63	1.39
4	C	802	ATP	C5-C4	13.40	1.63	1.39
4	B	802	ATP	C5-C4	13.40	1.63	1.39
4	D	802	ATP	C5-C4	13.37	1.62	1.39
4	D	801	ATP	C5-C4	13.36	1.62	1.39
4	B	801	ATP	C5-C4	13.34	1.62	1.39
4	C	802	ATP	C8-N7	-9.60	1.13	1.31
4	B	802	ATP	C8-N7	-9.58	1.13	1.31
4	E	802	ATP	C8-N7	-9.58	1.13	1.31
4	D	801	ATP	C8-N7	-9.57	1.13	1.31
4	E	801	ATP	C8-N7	-9.57	1.13	1.31
4	B	801	ATP	C8-N7	-9.56	1.13	1.31
4	C	801	ATP	C8-N7	-9.54	1.13	1.31
4	D	802	ATP	C8-N7	-9.54	1.13	1.31
4	D	802	ATP	C8-N9	-8.38	1.23	1.37
4	B	801	ATP	C8-N9	-8.34	1.23	1.37
4	C	801	ATP	C8-N9	-8.33	1.23	1.37
4	E	802	ATP	C8-N9	-8.32	1.23	1.37
4	E	801	ATP	C8-N9	-8.32	1.23	1.37
4	C	802	ATP	C8-N9	-8.32	1.23	1.37
4	D	801	ATP	C8-N9	-8.17	1.23	1.37
4	B	802	ATP	C8-N9	-8.13	1.23	1.37
3	A	801	ADP	C3'-C4'	-7.61	1.33	1.53
3	F	801	ADP	C3'-C4'	-7.59	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	ADP	C3'-C4'	-7.57	1.33	1.53
3	F	801	ADP	O4'-C4'	6.66	1.59	1.45
3	A	801	ADP	O4'-C4'	6.64	1.59	1.45
3	A	802	ADP	O4'-C4'	6.61	1.59	1.45
4	B	802	ATP	PB-O3A	5.39	1.65	1.59
4	D	802	ATP	PB-O3A	5.37	1.65	1.59
4	C	802	ATP	PA-O3A	5.36	1.65	1.59
4	C	801	ATP	PB-O3A	5.36	1.65	1.59
4	E	801	ATP	PB-O3B	5.36	1.65	1.59
4	D	802	ATP	PB-O3B	5.35	1.65	1.59
4	C	802	ATP	PB-O3B	5.35	1.65	1.59
4	E	802	ATP	PA-O3A	5.35	1.65	1.59
4	B	802	ATP	PB-O3B	5.33	1.65	1.59
4	B	801	ATP	PB-O3A	5.33	1.65	1.59
4	D	801	ATP	PA-O3A	5.33	1.65	1.59
4	E	802	ATP	PB-O3B	5.32	1.65	1.59
4	D	801	ATP	PB-O3A	5.32	1.65	1.59
4	D	801	ATP	PB-O3B	5.32	1.65	1.59
4	C	801	ATP	PB-O3B	5.31	1.65	1.59
4	B	801	ATP	PB-O3B	5.31	1.65	1.59
4	E	802	ATP	PB-O3A	5.30	1.65	1.59
4	E	801	ATP	PB-O3A	5.30	1.65	1.59
4	C	802	ATP	PB-O3A	5.30	1.65	1.59
4	B	801	ATP	PA-O3A	5.29	1.65	1.59
4	D	802	ATP	PA-O3A	5.28	1.65	1.59
4	C	801	ATP	PA-O3A	5.28	1.65	1.59
4	B	802	ATP	PA-O3A	5.27	1.65	1.59
4	E	801	ATP	PA-O3A	5.25	1.65	1.59
3	A	802	ADP	O4'-C1'	5.22	1.54	1.42
3	F	801	ADP	C6-N6	5.20	1.47	1.34
3	F	801	ADP	O4'-C1'	5.20	1.54	1.42
3	A	801	ADP	O4'-C1'	5.19	1.54	1.42
3	A	802	ADP	C6-N6	5.18	1.47	1.34
3	A	801	ADP	C6-N6	5.16	1.47	1.34
3	A	802	ADP	C2'-C1'	-5.08	1.37	1.53
3	A	801	ADP	C2'-C1'	-5.07	1.37	1.53
3	F	801	ADP	C2'-C1'	-5.06	1.37	1.53
4	E	801	ATP	C4-N3	-5.05	1.25	1.34
4	B	802	ATP	C4-N3	-5.04	1.25	1.34
4	E	802	ATP	C4-N3	-5.04	1.25	1.34
4	C	802	ATP	C4-N3	-5.03	1.25	1.34
4	D	802	ATP	C4-N3	-5.03	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	801	ADP	PA-O3A	5.03	1.64	1.59
3	A	802	ADP	PA-O3A	5.01	1.64	1.59
3	A	801	ADP	PA-O3A	5.00	1.64	1.59
4	B	801	ATP	C4-N3	-5.00	1.25	1.34
4	C	801	ATP	C4-N3	-4.99	1.25	1.34
4	D	801	ATP	C4-N3	-4.96	1.25	1.34
4	B	801	ATP	C6-N6	4.45	1.45	1.34
4	D	802	ATP	C6-N6	4.45	1.45	1.34
4	E	801	ATP	C6-N6	4.45	1.45	1.34
4	D	801	ATP	C6-N6	4.44	1.45	1.34
4	B	802	ATP	C6-N6	4.43	1.45	1.34
4	C	801	ATP	C6-N6	4.43	1.45	1.34
4	C	802	ATP	C6-N6	4.43	1.45	1.34
4	E	802	ATP	C6-N6	4.41	1.45	1.34
4	D	801	ATP	C2-N3	-4.36	1.26	1.33
4	D	801	ATP	O4'-C1'	4.36	1.52	1.42
4	E	802	ATP	C2-N3	-4.36	1.26	1.33
4	B	802	ATP	C2-N3	-4.35	1.26	1.33
4	C	802	ATP	C2-N3	-4.35	1.26	1.33
4	E	801	ATP	C2-N3	-4.34	1.26	1.33
4	B	802	ATP	O4'-C1'	4.34	1.52	1.42
4	B	801	ATP	C2-N3	-4.30	1.26	1.33
4	D	802	ATP	C2-N3	-4.30	1.26	1.33
4	C	801	ATP	C2-N3	-4.29	1.26	1.33
4	E	802	ATP	O4'-C1'	4.24	1.51	1.42
4	D	802	ATP	O4'-C1'	4.22	1.51	1.42
4	E	801	ATP	O4'-C1'	4.22	1.51	1.42
4	C	802	ATP	O4'-C1'	4.22	1.51	1.42
4	B	801	ATP	O4'-C1'	4.21	1.51	1.42
4	C	801	ATP	O4'-C1'	4.20	1.51	1.42
4	D	801	ATP	C4-N9	4.18	1.46	1.37
4	B	802	ATP	C4-N9	4.18	1.46	1.37
4	E	802	ATP	C4-N9	4.13	1.46	1.37
4	C	802	ATP	C4-N9	4.13	1.46	1.37
4	D	802	ATP	C4-N9	4.12	1.46	1.37
4	E	801	ATP	C4-N9	4.12	1.46	1.37
4	B	801	ATP	C4-N9	4.12	1.46	1.37
4	C	801	ATP	C4-N9	4.10	1.46	1.37
3	A	802	ADP	C5-N7	-3.31	1.33	1.39
3	A	801	ADP	C5-N7	-3.31	1.33	1.39
3	F	801	ADP	C5-N7	-3.30	1.33	1.39
3	F	801	ADP	C2'-C3'	3.24	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ADP	C2'-C3'	3.24	1.62	1.53
3	A	802	ADP	C2'-C3'	3.23	1.62	1.53
4	D	802	ATP	O4'-C4'	3.00	1.51	1.45
4	C	802	ATP	O4'-C4'	3.00	1.51	1.45
4	E	802	ATP	O4'-C4'	2.99	1.51	1.45
4	B	801	ATP	O4'-C4'	2.97	1.51	1.45
4	C	801	ATP	O4'-C4'	2.95	1.51	1.45
4	E	801	ATP	O4'-C4'	2.91	1.51	1.45
4	D	802	ATP	C2'-C3'	-2.91	1.45	1.53
4	D	801	ATP	O4'-C4'	2.90	1.51	1.45
4	B	802	ATP	O4'-C4'	2.89	1.51	1.45
4	E	802	ATP	C2'-C3'	-2.88	1.45	1.53
4	C	802	ATP	C2'-C3'	-2.87	1.45	1.53
4	D	801	ATP	C2'-C3'	-2.87	1.45	1.53
4	B	801	ATP	C2'-C3'	-2.86	1.45	1.53
4	E	801	ATP	C2'-C3'	-2.85	1.45	1.53
4	C	801	ATP	C2'-C3'	-2.83	1.45	1.53
4	B	802	ATP	C2'-C3'	-2.83	1.45	1.53
3	F	801	ADP	C8-N9	-2.74	1.32	1.37
3	A	802	ADP	C8-N9	-2.72	1.32	1.37
3	A	801	ADP	C8-N9	-2.72	1.32	1.37
4	D	802	ATP	C6-N1	2.42	1.42	1.35
4	B	802	ATP	C6-N1	2.41	1.42	1.35
4	E	802	ATP	C6-N1	2.41	1.42	1.35
4	C	801	ATP	C6-N1	2.40	1.42	1.35
4	E	801	ATP	C6-N1	2.40	1.42	1.35
4	C	802	ATP	C6-N1	2.40	1.42	1.35
4	D	801	ATP	C6-N1	2.40	1.42	1.35
4	B	801	ATP	C6-N1	2.36	1.42	1.35
4	E	802	ATP	C5-C6	2.28	1.47	1.41
4	C	801	ATP	C5-C6	2.27	1.47	1.41
4	B	801	ATP	C5-C6	2.27	1.47	1.41
4	D	801	ATP	C5-C6	2.26	1.47	1.41
4	E	801	ATP	C5-C6	2.26	1.47	1.41
4	B	802	ATP	C5-C6	2.26	1.47	1.41
3	F	801	ADP	C4-N9	-2.25	1.33	1.37
4	C	802	ATP	C5-C6	2.25	1.47	1.41
3	A	801	ADP	C4-N9	-2.24	1.33	1.37
4	D	802	ATP	C5-C6	2.23	1.47	1.41
3	A	802	ADP	C4-N9	-2.20	1.33	1.37

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	801	ATP	C5-C4-N9	-13.59	91.00	105.81
4	C	802	ATP	C5-C4-N9	-13.55	91.04	105.81
4	E	802	ATP	C5-C4-N9	-13.55	91.04	105.81
4	C	801	ATP	C5-C4-N9	-13.53	91.07	105.81
4	D	802	ATP	C5-C4-N9	-13.52	91.08	105.81
4	B	801	ATP	C5-C4-N9	-13.49	91.10	105.81
4	E	801	ATP	N3-C4-N9	13.37	149.91	127.17
4	C	802	ATP	N3-C4-N9	13.36	149.88	127.17
4	E	802	ATP	N3-C4-N9	13.36	149.88	127.17
4	D	802	ATP	N3-C4-N9	13.34	149.86	127.17
4	C	801	ATP	N3-C4-N9	13.33	149.84	127.17
4	B	801	ATP	N3-C4-N9	13.33	149.83	127.17
4	B	802	ATP	C5-C4-N9	-13.29	91.33	105.81
4	B	802	ATP	N3-C4-N9	13.26	149.71	127.17
4	D	801	ATP	C5-C4-N9	-13.25	91.37	105.81
4	D	801	ATP	N3-C4-N9	13.24	149.69	127.17
4	E	801	ATP	C4-N9-C8	9.86	116.09	105.74
4	D	802	ATP	C4-N9-C8	9.81	116.03	105.74
4	C	801	ATP	C4-N9-C8	9.79	116.02	105.74
4	C	802	ATP	C4-N9-C8	9.78	116.00	105.74
4	E	802	ATP	C4-N9-C8	9.77	116.00	105.74
4	B	801	ATP	C4-N9-C8	9.74	115.97	105.74
4	B	802	ATP	C4-N9-C8	9.34	115.54	105.74
4	D	801	ATP	C4-N9-C8	9.26	115.46	105.74
4	E	801	ATP	C6-C5-N7	6.83	145.25	132.09
4	E	802	ATP	C6-C5-N7	6.83	145.25	132.09
4	D	801	ATP	C6-C5-N7	6.83	145.25	132.09
4	C	801	ATP	C6-C5-N7	6.82	145.25	132.09
4	B	802	ATP	C6-C5-N7	6.82	145.24	132.09
4	B	801	ATP	C6-C5-N7	6.81	145.22	132.09
4	D	802	ATP	C6-C5-N7	6.81	145.21	132.09
4	C	802	ATP	C6-C5-N7	6.80	145.20	132.09
4	B	802	ATP	C2-N3-C4	6.33	127.28	111.83
4	D	801	ATP	C2-N3-C4	6.30	127.22	111.83
4	E	802	ATP	C2-N3-C4	6.27	127.14	111.83
4	C	802	ATP	C2-N3-C4	6.27	127.14	111.83
4	E	801	ATP	C2-N3-C4	6.27	127.13	111.83
4	B	801	ATP	C2-N3-C4	6.27	127.13	111.83
4	D	802	ATP	C2-N3-C4	6.25	127.10	111.83
4	C	801	ATP	C2-N3-C4	6.24	127.06	111.83
3	F	801	ADP	C5-C4-N3	-6.22	118.15	126.72
3	A	801	ADP	C5-C4-N3	-6.21	118.17	126.72
3	A	802	ADP	C5-C4-N3	-6.21	118.17	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	801	ATP	C5-N7-C8	5.76	112.50	103.45
4	E	802	ATP	C5-N7-C8	5.74	112.47	103.45
4	D	801	ATP	C5-N7-C8	5.73	112.46	103.45
4	B	802	ATP	C5-N7-C8	5.73	112.46	103.45
4	C	801	ATP	C5-N7-C8	5.73	112.46	103.45
4	D	802	ATP	C5-N7-C8	5.73	112.46	103.45
4	B	801	ATP	C5-N7-C8	5.72	112.44	103.45
4	C	802	ATP	C5-N7-C8	5.71	112.42	103.45
4	D	801	ATP	C5-C4-N3	-5.65	118.94	126.72
4	B	802	ATP	C5-C4-N3	-5.64	118.96	126.72
4	B	801	ATP	C5-C4-N3	-5.56	119.06	126.72
4	D	802	ATP	C5-C4-N3	-5.55	119.07	126.72
4	C	802	ATP	C5-C4-N3	-5.55	119.08	126.72
4	E	802	ATP	C5-C4-N3	-5.55	119.08	126.72
4	C	801	ATP	C5-C4-N3	-5.54	119.09	126.72
4	E	801	ATP	C5-C4-N3	-5.53	119.10	126.72
4	D	801	ATP	C4-C5-N7	-5.43	104.38	110.58
4	B	802	ATP	C4-C5-N7	-5.42	104.38	110.58
4	D	802	ATP	C4-C5-N7	-5.39	104.42	110.58
4	C	801	ATP	C4-C5-N7	-5.37	104.44	110.58
4	B	801	ATP	C4-C5-N7	-5.37	104.44	110.58
4	E	802	ATP	C4-C5-N7	-5.36	104.45	110.58
4	E	801	ATP	C4-C5-N7	-5.36	104.45	110.58
4	C	802	ATP	C4-C5-N7	-5.35	104.46	110.58
4	E	801	ATP	C6-C5-C4	-5.04	110.29	117.18
4	E	802	ATP	C6-C5-C4	-5.04	110.30	117.18
4	C	801	ATP	C6-C5-C4	-5.03	110.31	117.18
4	C	802	ATP	C6-C5-C4	-5.01	110.34	117.18
4	B	801	ATP	C6-C5-C4	-5.01	110.34	117.18
4	D	802	ATP	C6-C5-C4	-4.99	110.37	117.18
4	D	801	ATP	C6-C5-C4	-4.98	110.37	117.18
4	B	802	ATP	C6-C5-C4	-4.98	110.38	117.18
3	F	801	ADP	N3-C4-N9	4.86	135.44	127.17
3	A	802	ADP	N3-C4-N9	4.86	135.43	127.17
3	A	801	ADP	N3-C4-N9	4.84	135.39	127.17
3	F	801	ADP	N3-C2-N1	-4.41	121.90	128.58
3	A	802	ADP	N3-C2-N1	-4.41	121.91	128.58
3	A	801	ADP	N3-C2-N1	-4.39	121.94	128.58
3	F	801	ADP	C2-N3-C4	3.82	121.16	111.83
3	A	802	ADP	C2-N3-C4	3.81	121.13	111.83
3	A	801	ADP	C2-N3-C4	3.81	121.13	111.83
4	B	802	ATP	C3'-C2'-C1'	3.75	108.56	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	801	ATP	C3'-C2'-C1'	3.62	108.31	101.46
4	E	801	ATP	C3'-C2'-C1'	3.52	108.12	101.46
4	C	801	ATP	C3'-C2'-C1'	3.51	108.10	101.46
4	B	802	ATP	N3-C2-N1	-3.50	123.29	128.58
4	B	801	ATP	N3-C2-N1	-3.49	123.30	128.58
4	C	802	ATP	N3-C2-N1	-3.47	123.32	128.58
4	E	801	ATP	N3-C2-N1	-3.47	123.34	128.58
4	E	802	ATP	N3-C2-N1	-3.45	123.36	128.58
4	D	801	ATP	N3-C2-N1	-3.44	123.37	128.58
4	D	802	ATP	N3-C2-N1	-3.44	123.37	128.58
3	A	801	ADP	N9-C8-N7	-3.44	109.06	113.94
3	A	802	ADP	N9-C8-N7	-3.44	109.06	113.94
3	F	801	ADP	N9-C8-N7	-3.43	109.07	113.94
4	C	801	ATP	N3-C2-N1	-3.43	123.39	128.58
4	E	802	ATP	C3'-C2'-C1'	3.41	107.91	101.46
4	B	801	ATP	C3'-C2'-C1'	3.39	107.87	101.46
4	C	802	ATP	C3'-C2'-C1'	3.38	107.85	101.46
4	D	802	ATP	C3'-C2'-C1'	3.37	107.84	101.46
3	A	801	ADP	C5-N7-C8	3.32	108.66	103.45
3	F	801	ADP	C5-N7-C8	3.31	108.65	103.45
3	A	802	ADP	C5-N7-C8	3.28	108.60	103.45
3	F	801	ADP	C4-C5-N7	-3.19	106.93	110.58
3	A	801	ADP	C4-C5-N7	-3.18	106.94	110.58
3	A	802	ADP	C4-C5-N7	-3.11	107.03	110.58
3	F	801	ADP	C4-N9-C8	3.04	108.93	105.74
3	A	802	ADP	C4-N9-C8	3.02	108.91	105.74
3	A	801	ADP	C4-N9-C8	3.01	108.90	105.74
4	B	802	ATP	C2'-C3'-C4'	2.68	107.78	102.61
4	D	802	ATP	C2'-C3'-C4'	2.66	107.74	102.61
4	E	802	ATP	C2'-C3'-C4'	2.65	107.74	102.61
4	B	801	ATP	C2'-C3'-C4'	2.64	107.71	102.61
4	C	802	ATP	C2'-C3'-C4'	2.63	107.69	102.61
4	E	801	ATP	C2'-C3'-C4'	2.60	107.63	102.61
4	C	801	ATP	C2'-C3'-C4'	2.60	107.62	102.61
4	D	801	ATP	C2'-C3'-C4'	2.55	107.53	102.61
4	B	802	ATP	C4'-O4'-C1'	-2.42	104.13	109.47
4	E	801	ATP	C4'-O4'-C1'	-2.37	104.23	109.47
4	C	801	ATP	C4'-O4'-C1'	-2.34	104.29	109.47
4	E	801	ATP	C1'-N9-C8	-2.32	121.95	127.09
3	A	801	ADP	C3'-C2'-C1'	2.30	105.82	101.46
3	F	801	ADP	C3'-C2'-C1'	2.30	105.81	101.46
4	C	801	ATP	C1'-N9-C8	-2.28	122.04	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ADP	C3'-C2'-C1'	2.27	105.75	101.46
4	B	802	ATP	C4-N9-C1'	-2.26	121.35	126.63
4	B	801	ATP	C1'-N9-C8	-2.23	122.14	127.09
4	E	802	ATP	C1'-N9-C8	-2.23	122.14	127.09
4	D	802	ATP	C1'-N9-C8	-2.23	122.14	127.09
4	C	802	ATP	C1'-N9-C8	-2.22	122.17	127.09
4	D	802	ATP	C4'-O4'-C1'	-2.19	104.63	109.47
4	D	801	ATP	C4-N9-C1'	-2.19	121.52	126.63
4	E	802	ATP	C4'-O4'-C1'	-2.18	104.65	109.47
4	C	802	ATP	C4'-O4'-C1'	-2.18	104.65	109.47
4	B	801	ATP	C4'-O4'-C1'	-2.16	104.69	109.47
4	D	801	ATP	C4'-O4'-C1'	-2.16	104.71	109.47
4	D	802	ATP	C4-N9-C1'	-2.06	121.82	126.63
4	C	802	ATP	C4-N9-C1'	-2.05	121.83	126.63
4	E	802	ATP	C4-N9-C1'	-2.04	121.86	126.63
4	B	801	ATP	C4-N9-C1'	-2.02	121.90	126.63
4	C	801	ATP	C4-N9-C1'	-2.00	121.95	126.63

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	ADP	C5'-O5'-PA-O1A
3	A	801	ADP	C5'-O5'-PA-O2A
3	A	801	ADP	C5'-O5'-PA-O3A
3	A	802	ADP	O4'-C4'-C5'-O5'
3	F	801	ADP	PA-O3A-PB-O2B
3	F	801	ADP	PA-O3A-PB-O3B
3	F	801	ADP	C5'-O5'-PA-O1A
3	F	801	ADP	C5'-O5'-PA-O2A
3	F	801	ADP	C5'-O5'-PA-O3A
4	B	802	ATP	PB-O3B-PG-O2G
4	C	801	ATP	C5'-O5'-PA-O1A
4	D	801	ATP	C5'-O5'-PA-O2A
4	D	801	ATP	C5'-O5'-PA-O3A
4	E	801	ATP	C5'-O5'-PA-O1A
4	E	801	ATP	C5'-O5'-PA-O3A
3	A	802	ADP	C3'-C4'-C5'-O5'
3	F	801	ADP	PB-O3A-PA-O1A
4	C	801	ATP	PB-O3A-PA-O1A
4	E	802	ATP	PG-O3B-PB-O2B
4	B	802	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	C	801	ATP	C5'-O5'-PA-O2A
4	C	801	ATP	C5'-O5'-PA-O3A
4	E	801	ATP	C5'-O5'-PA-O2A
4	B	802	ATP	PB-O3A-PA-O2A
4	C	802	ATP	PA-O3A-PB-O2B
4	D	802	ATP	PA-O3A-PB-O2B
4	B	801	ATP	C4'-C5'-O5'-PA
4	C	801	ATP	C4'-C5'-O5'-PA
4	B	802	ATP	PB-O3A-PA-O1A
4	E	801	ATP	C4'-C5'-O5'-PA
4	C	802	ATP	PA-O3A-PB-O1B
4	D	802	ATP	PA-O3A-PB-O1B
4	E	802	ATP	PG-O3B-PB-O1B
3	F	801	ADP	PA-O3A-PB-O1B
4	C	801	ATP	O4'-C4'-C5'-O5'
3	A	801	ADP	O4'-C4'-C5'-O5'
4	C	801	ATP	PB-O3A-PA-O2A

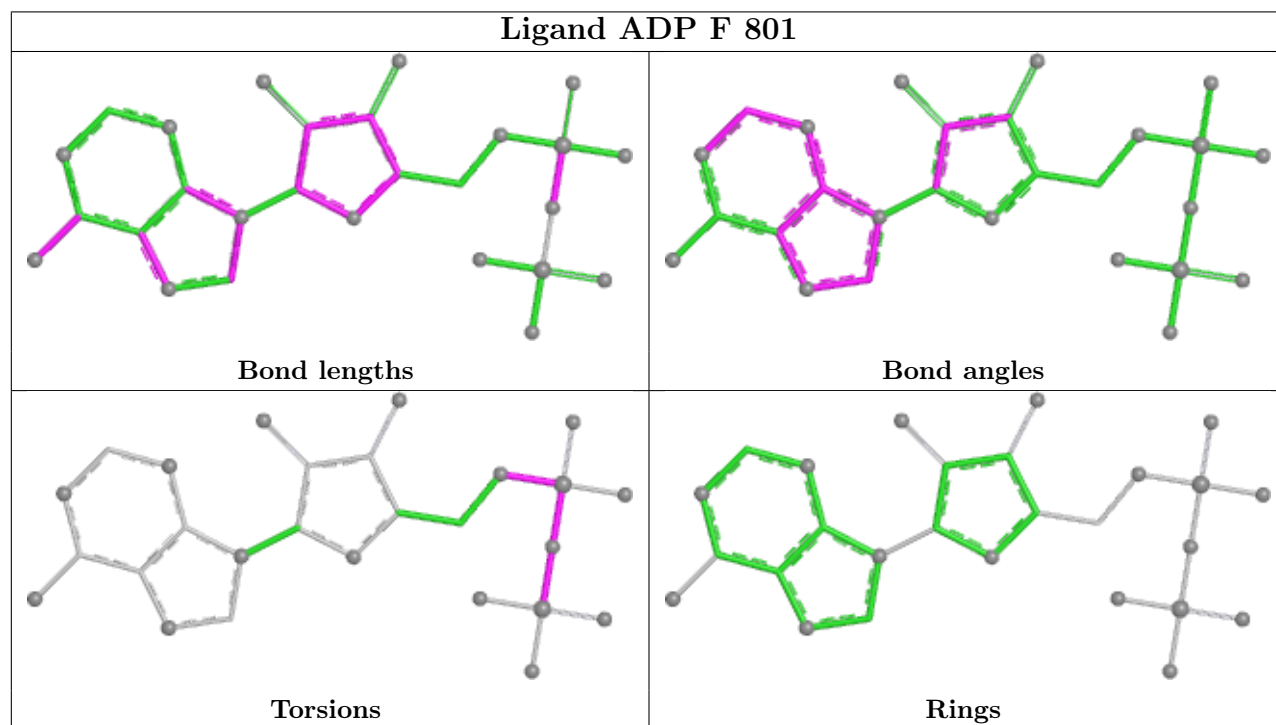
There are no ring outliers.

11 monomers are involved in 121 short contacts:

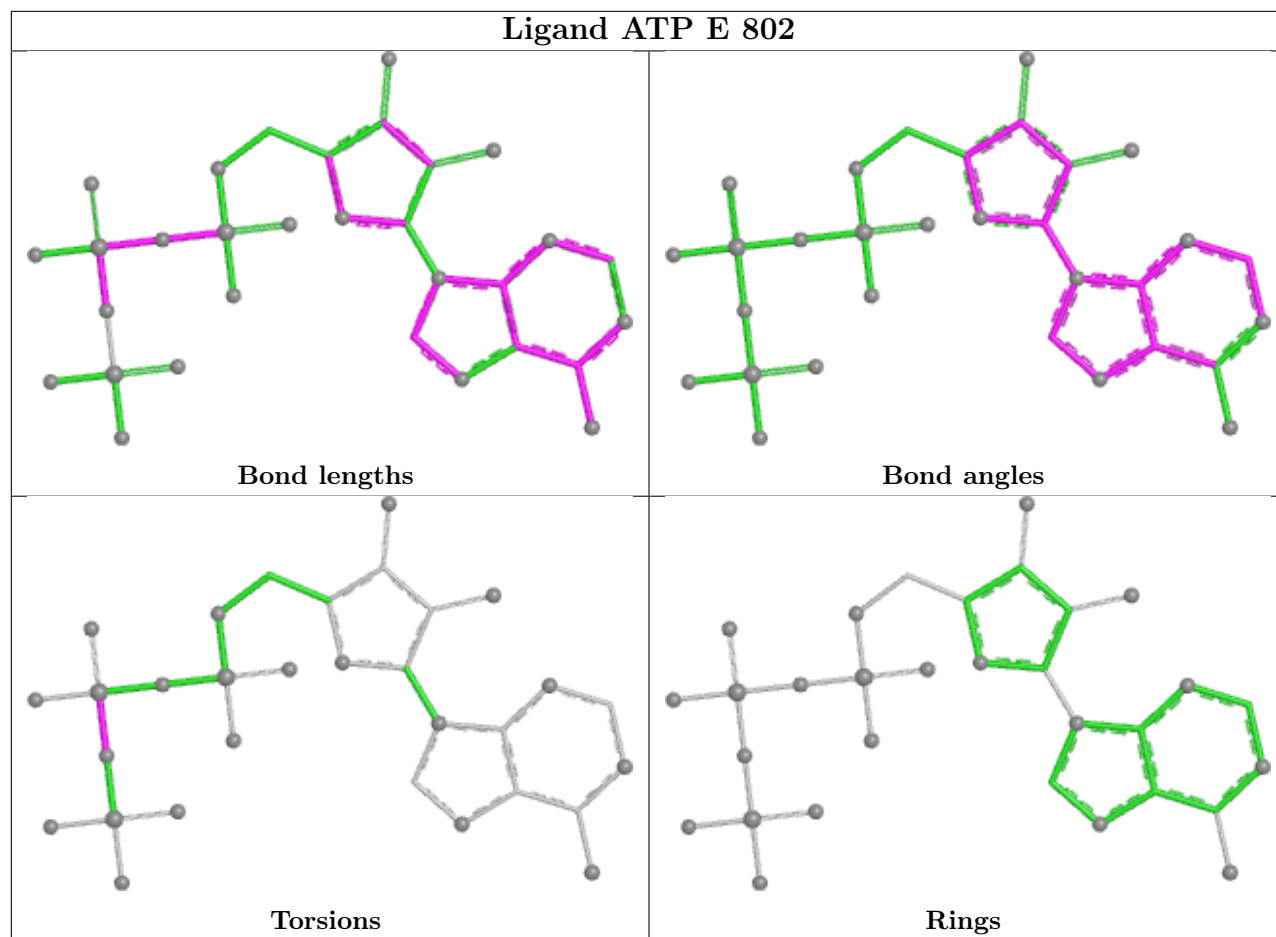
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	ADP	15	0
4	E	802	ATP	6	0
3	A	802	ADP	4	0
4	B	801	ATP	17	0
4	C	802	ATP	15	0
3	A	801	ADP	7	0
4	D	802	ATP	10	0
4	E	801	ATP	19	0
4	C	801	ATP	15	0
4	B	802	ATP	5	0
4	D	801	ATP	8	0

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

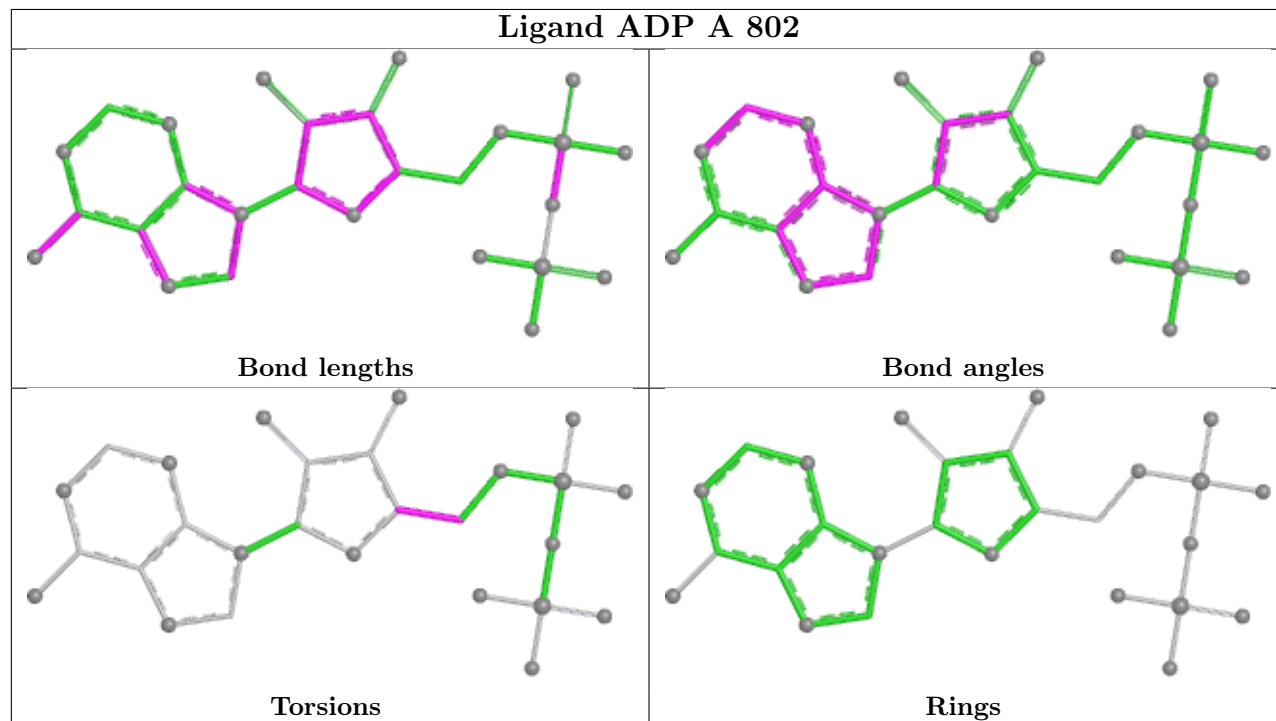
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

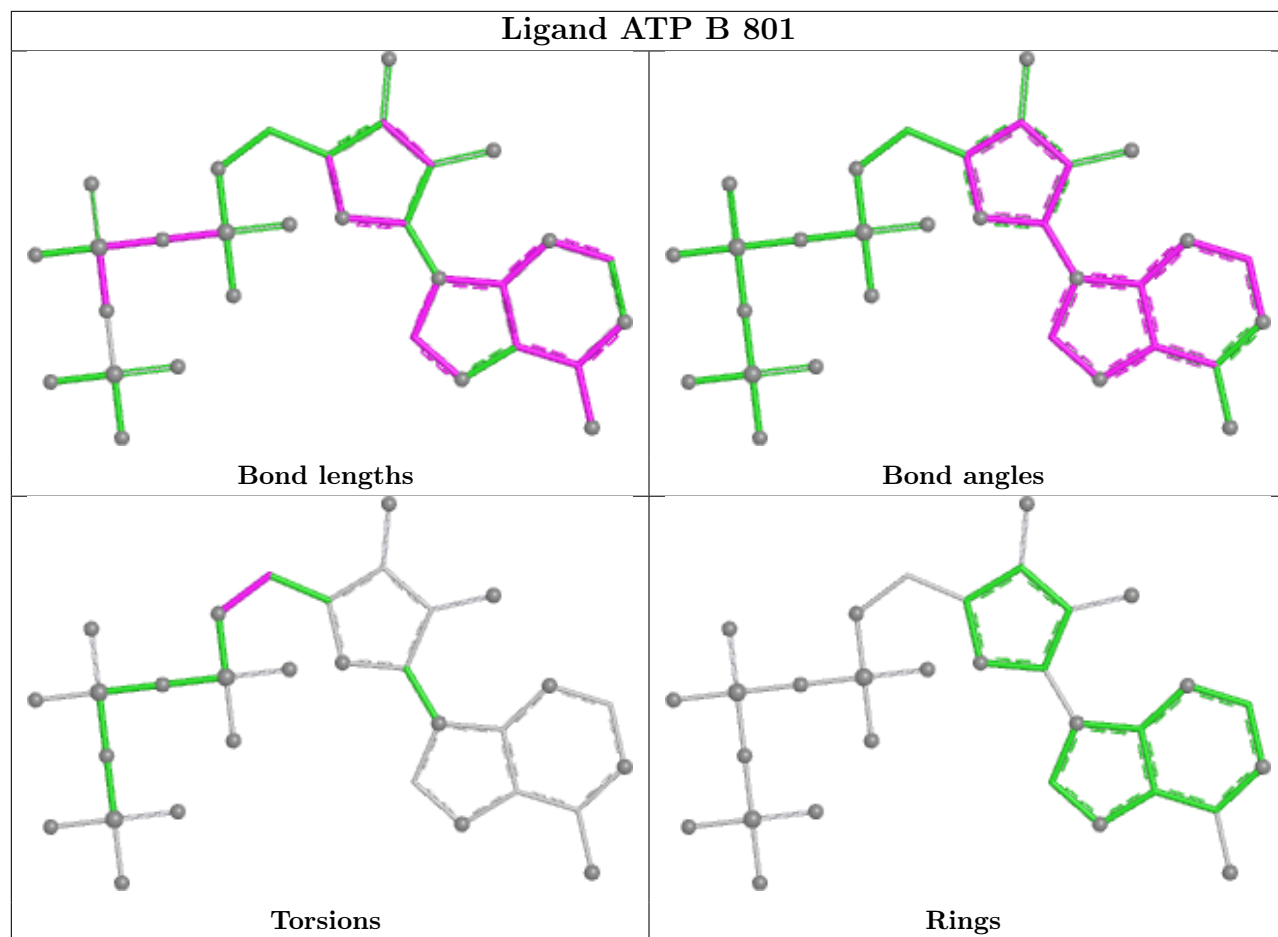


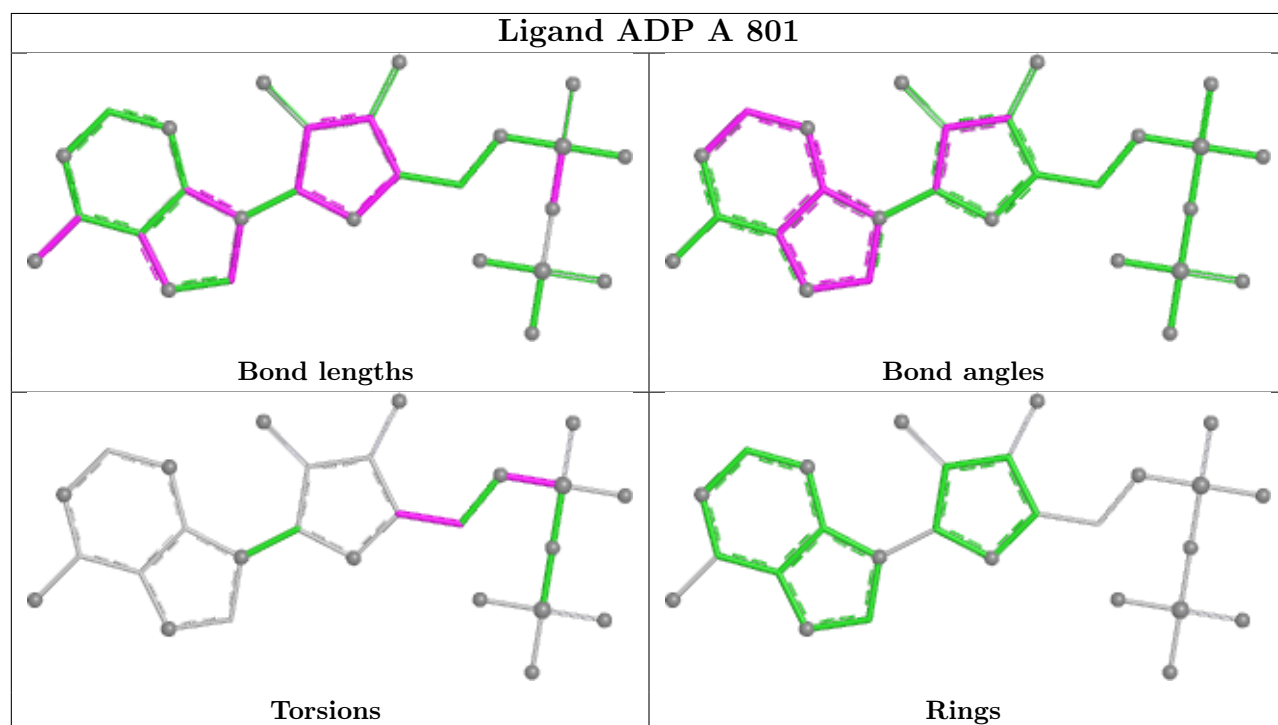
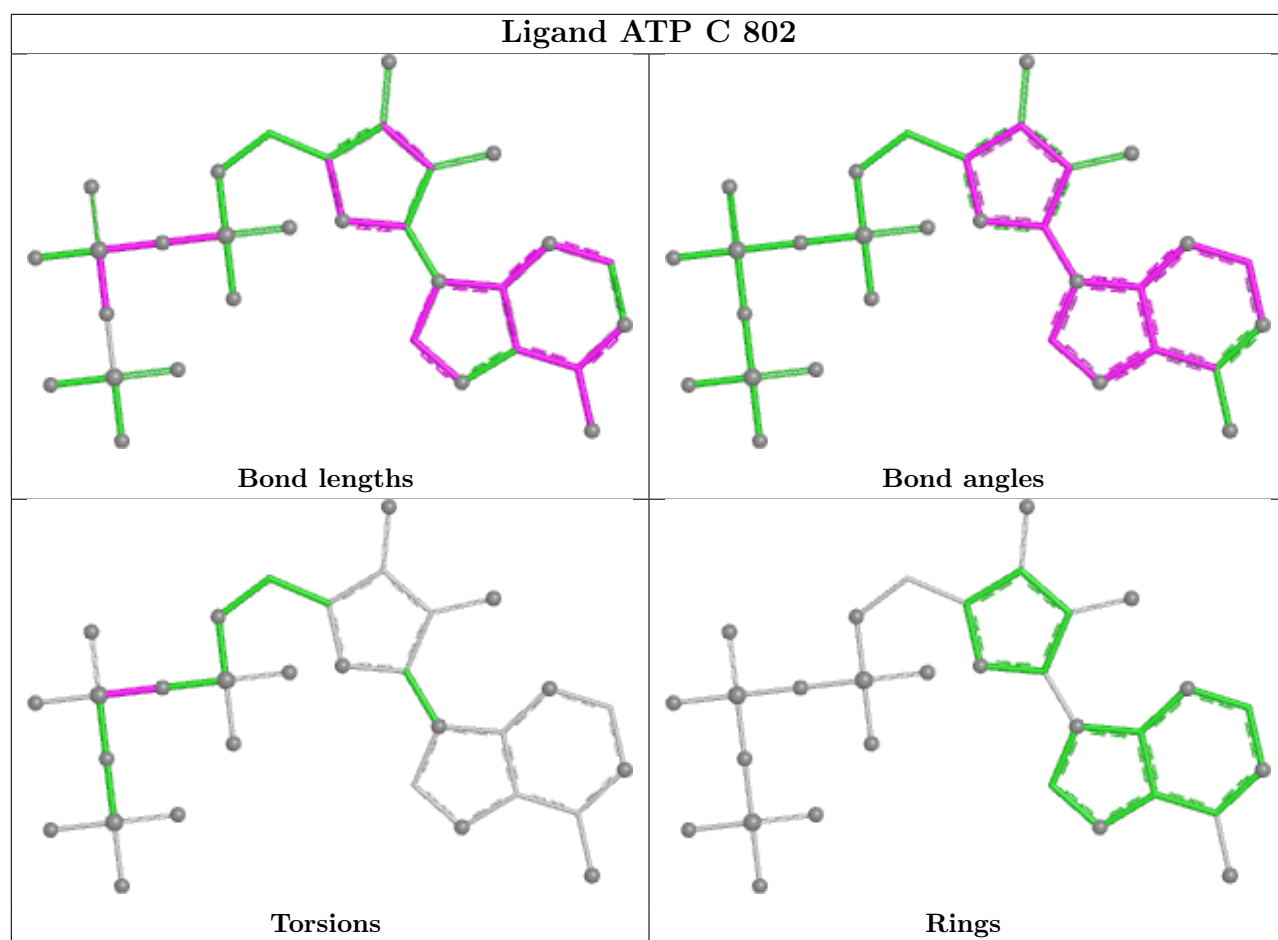
Ligand ATP E 802

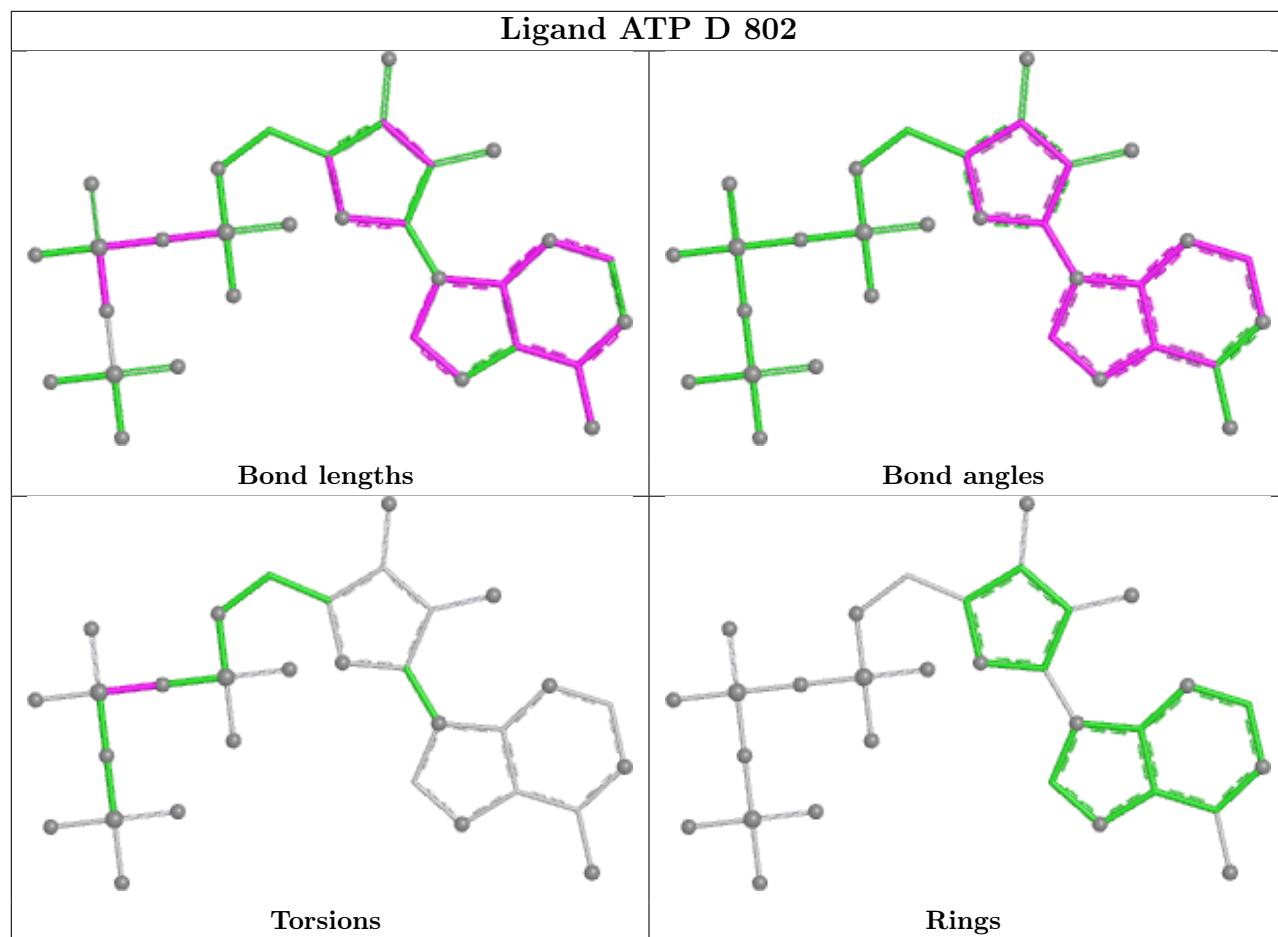


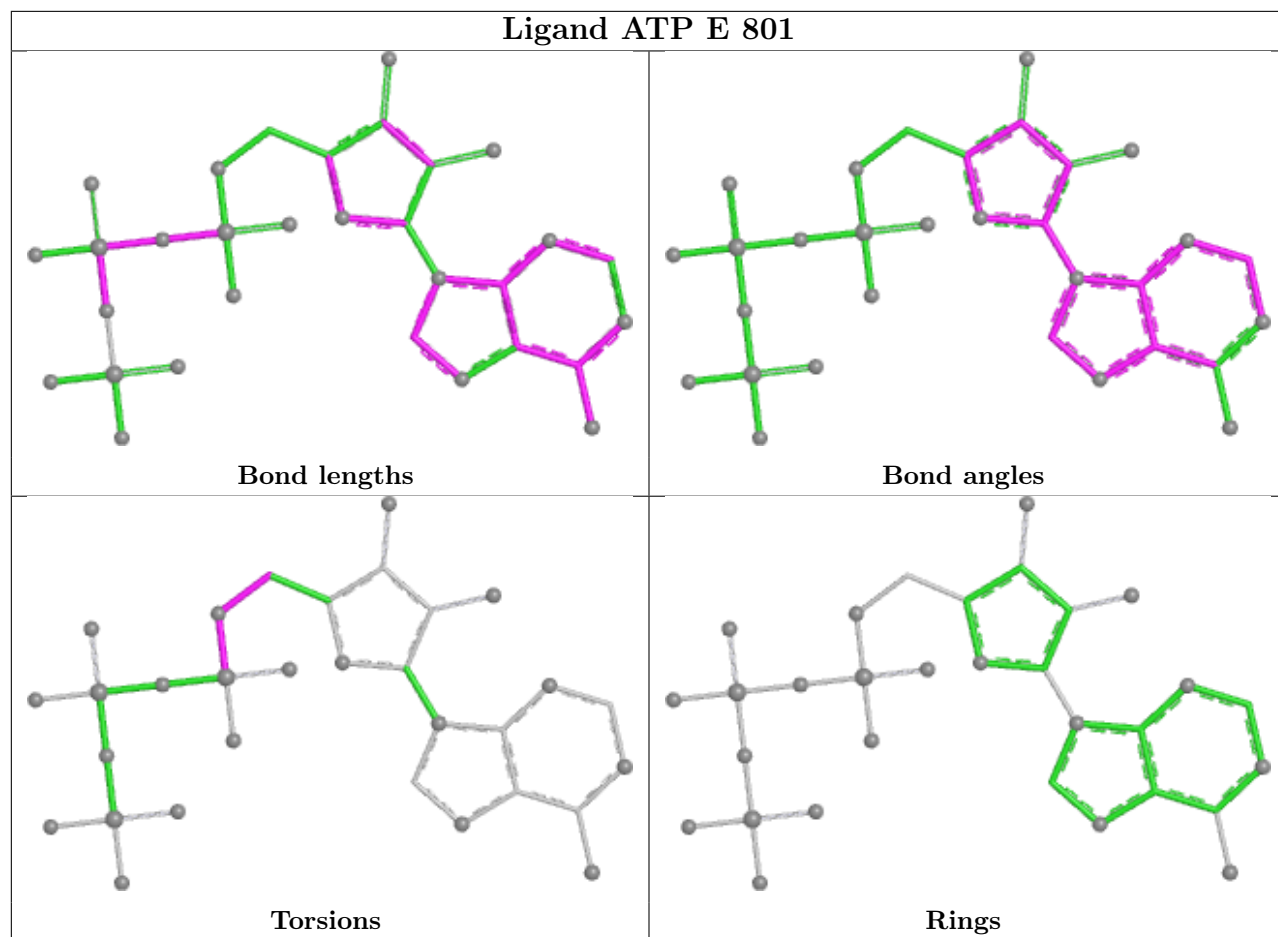
Ligand ADP A 802

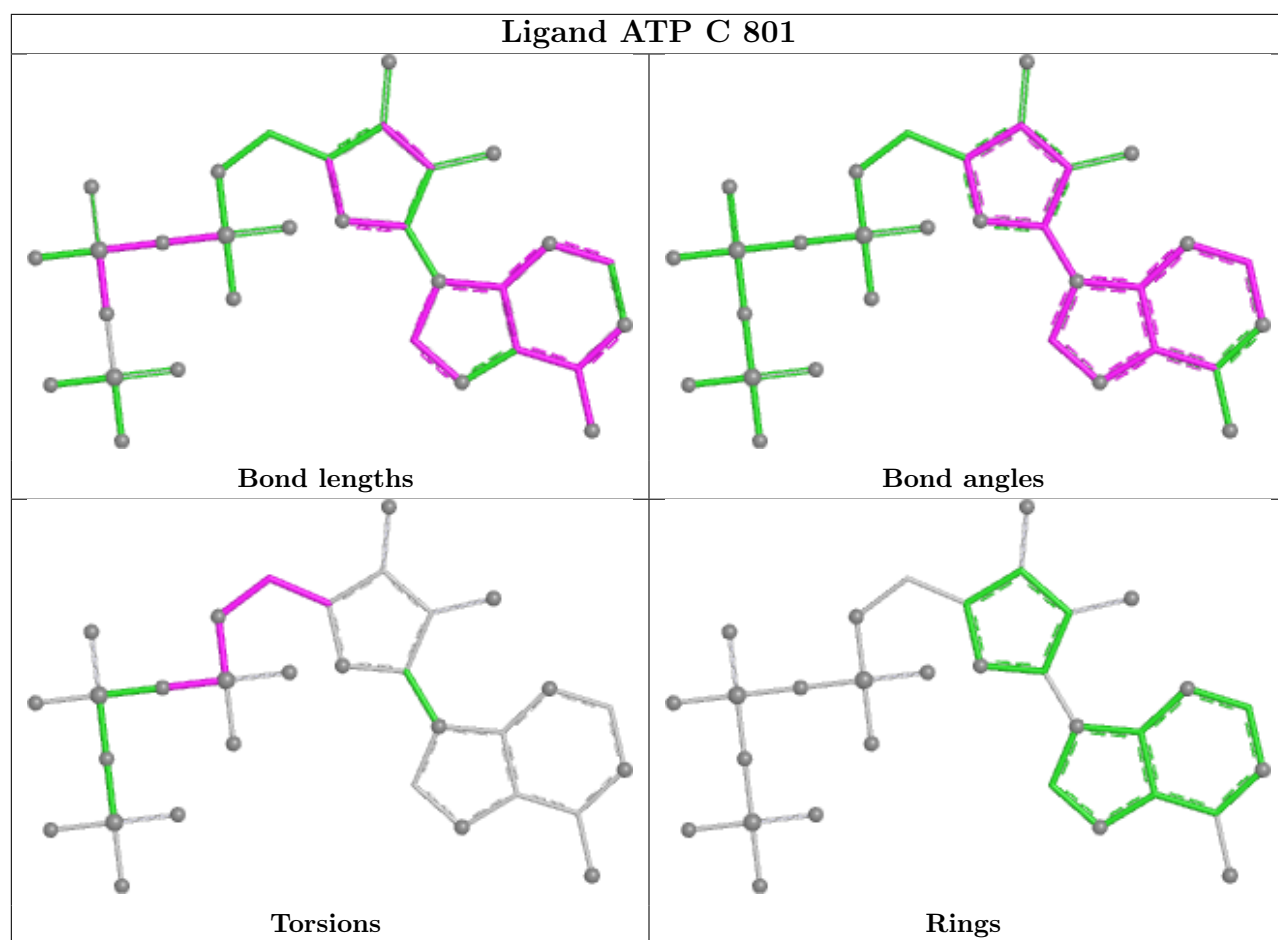


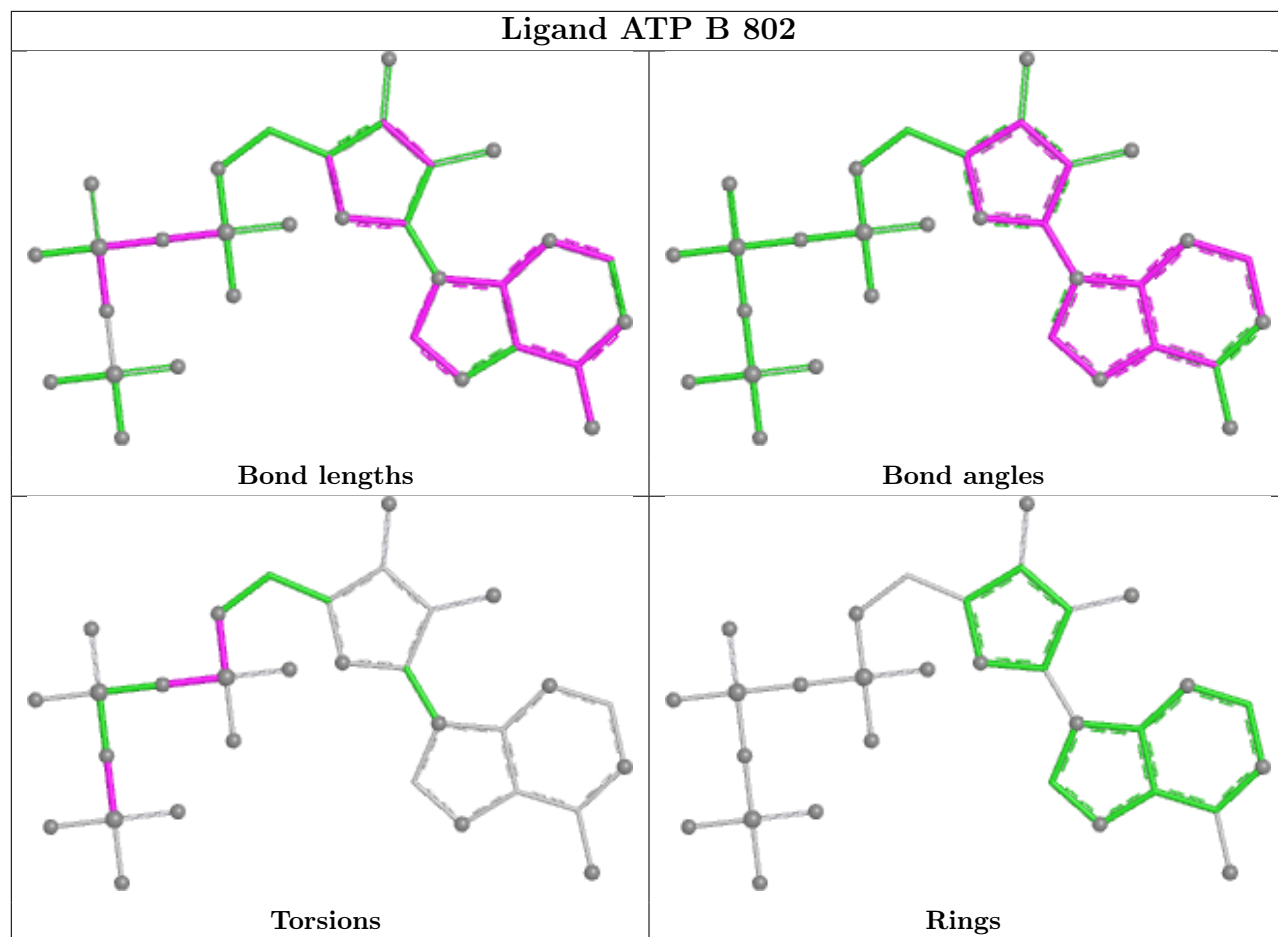


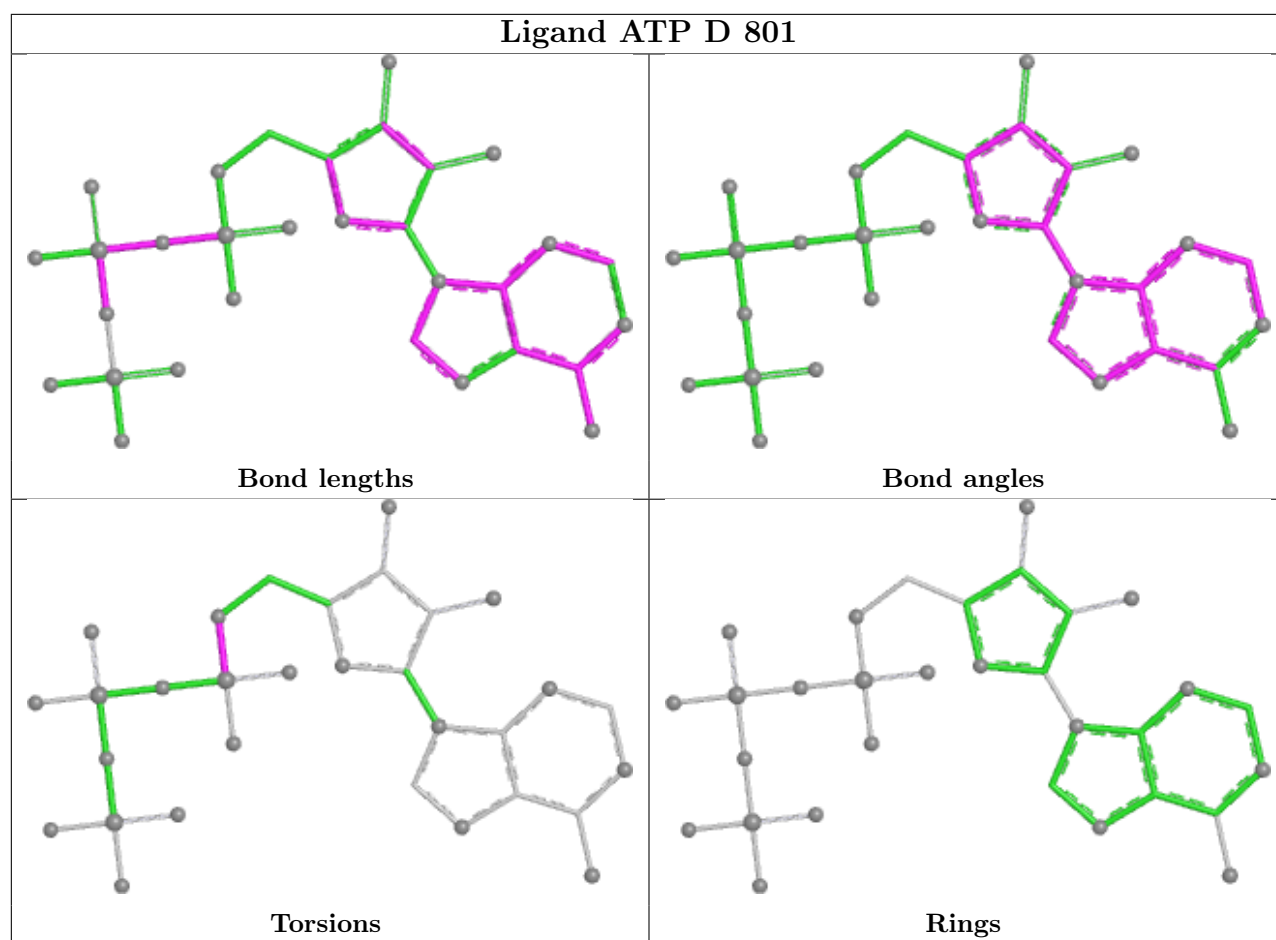












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

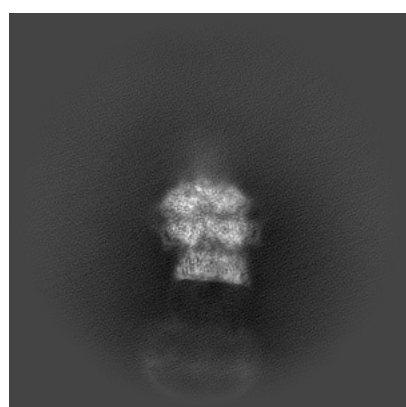
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21523. These allow visual inspection of the internal detail of the map and identification of artifacts.

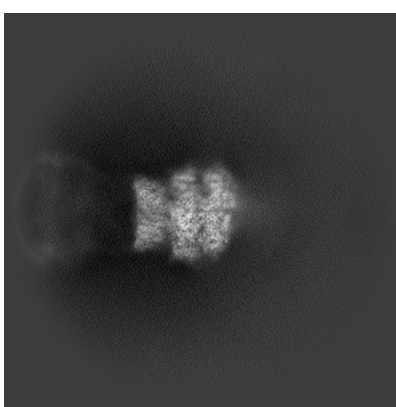
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

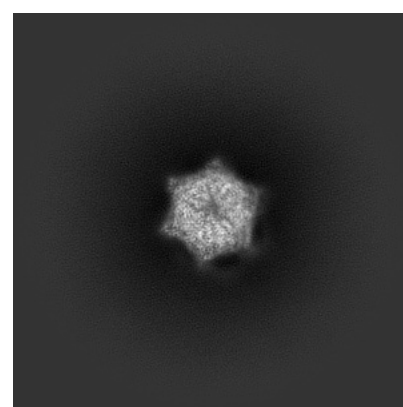
6.1.1 Primary map



X



Y

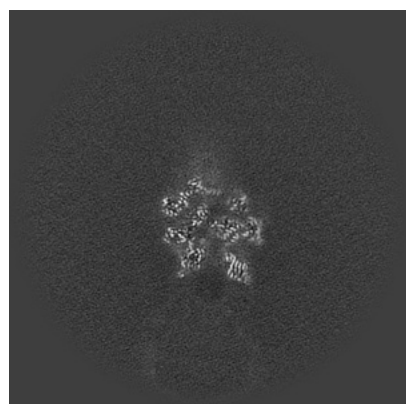


Z

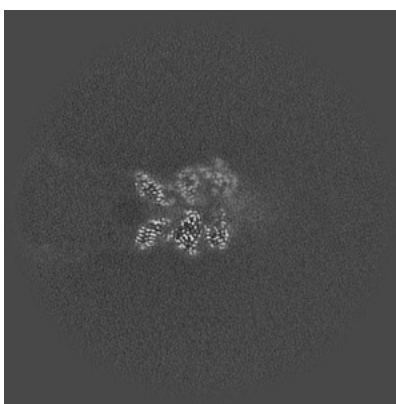
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

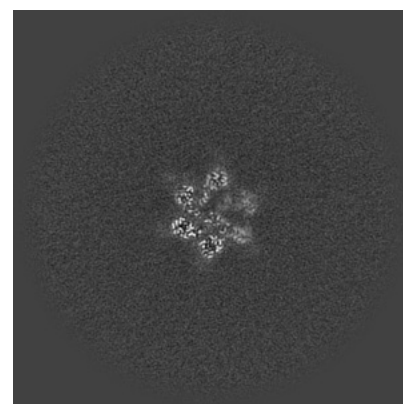
6.2.1 Primary map



X Index: 300



Y Index: 300

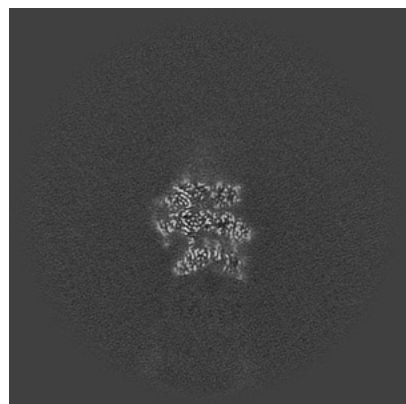


Z Index: 300

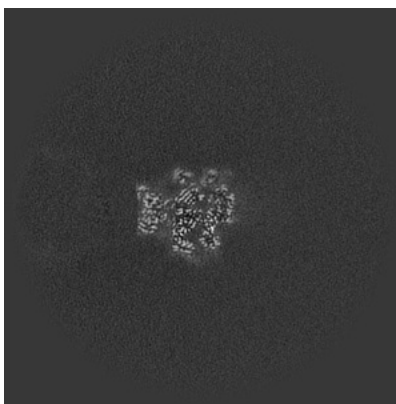
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

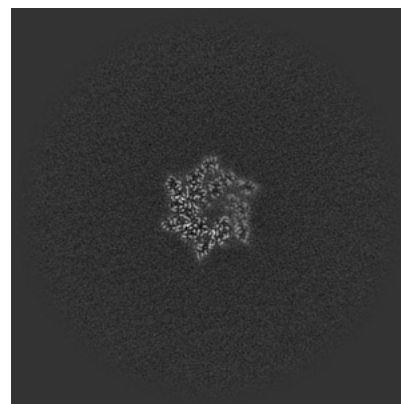
6.3.1 Primary map



X Index: 281



Y Index: 269

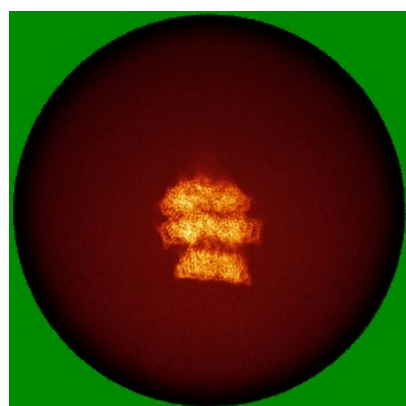


Z Index: 268

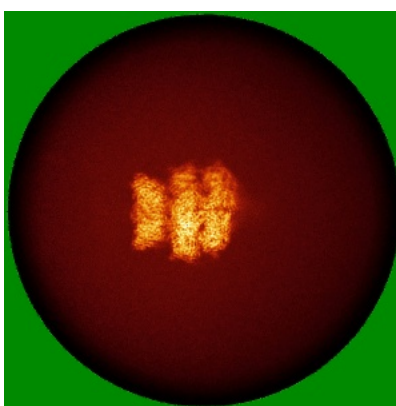
The images above show the largest variance slices of the map in three orthogonal directions.

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

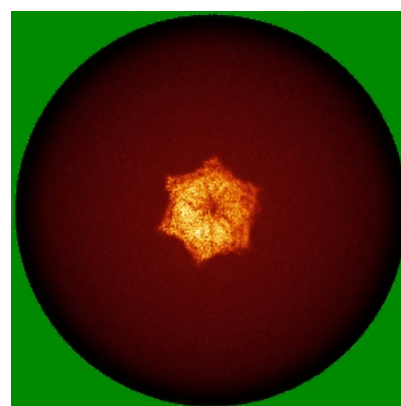
6.4.1 Primary map



X



Y

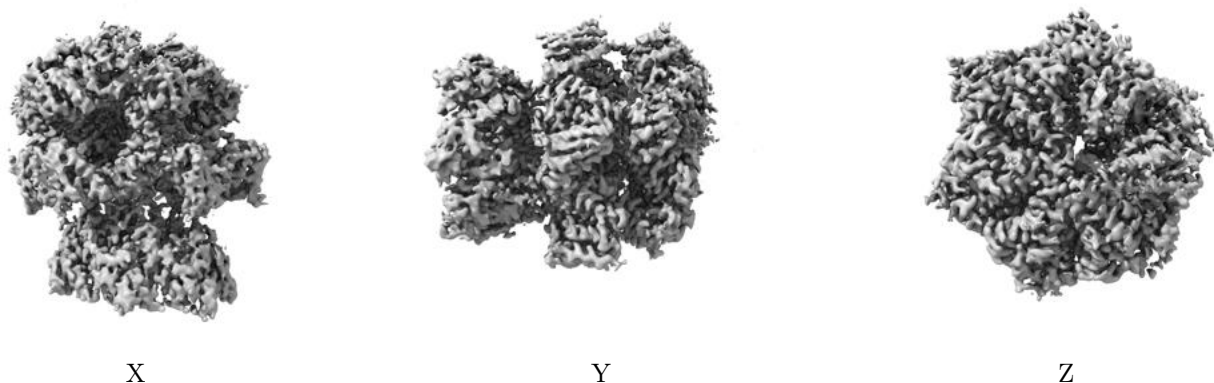


Z

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 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

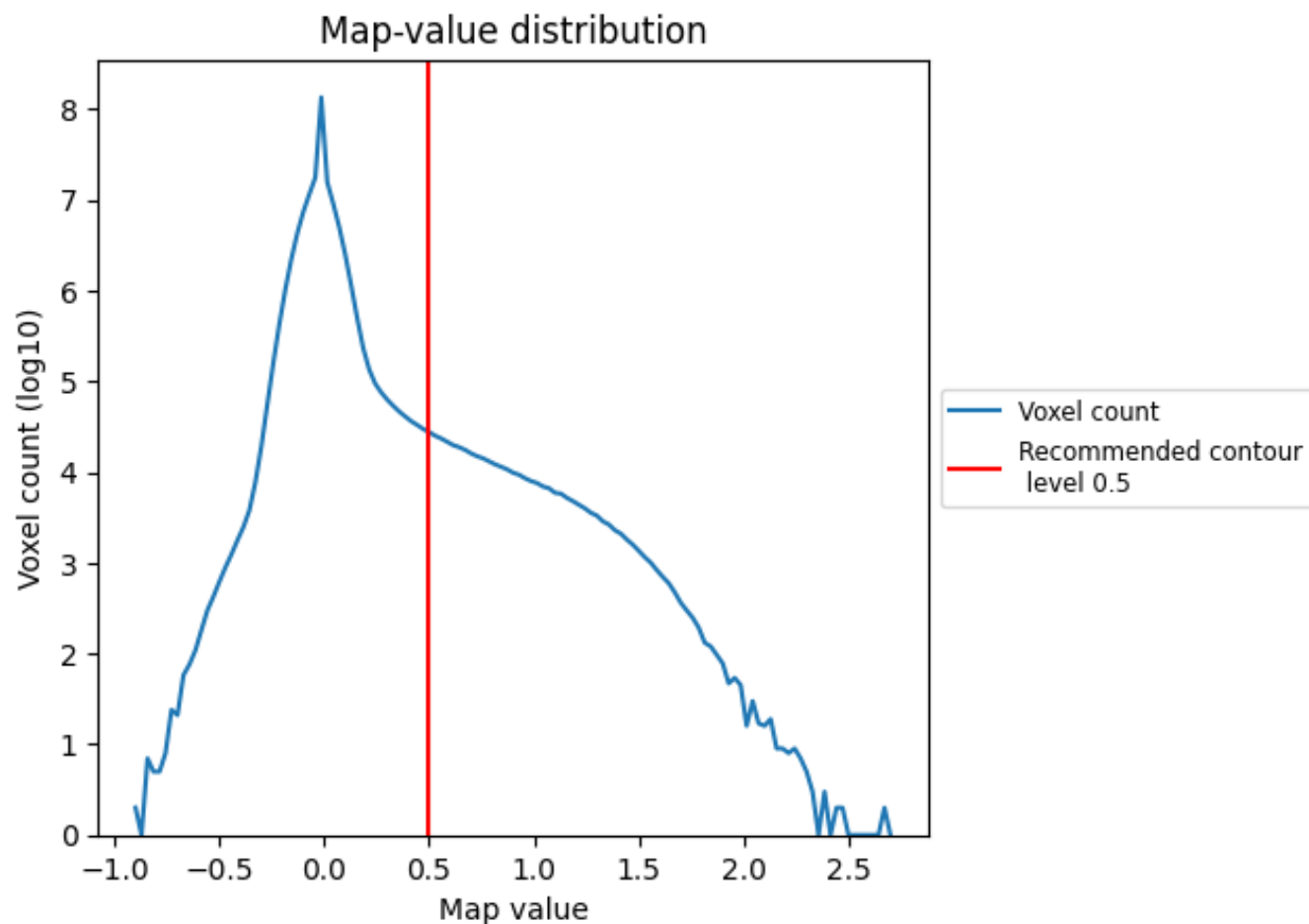
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

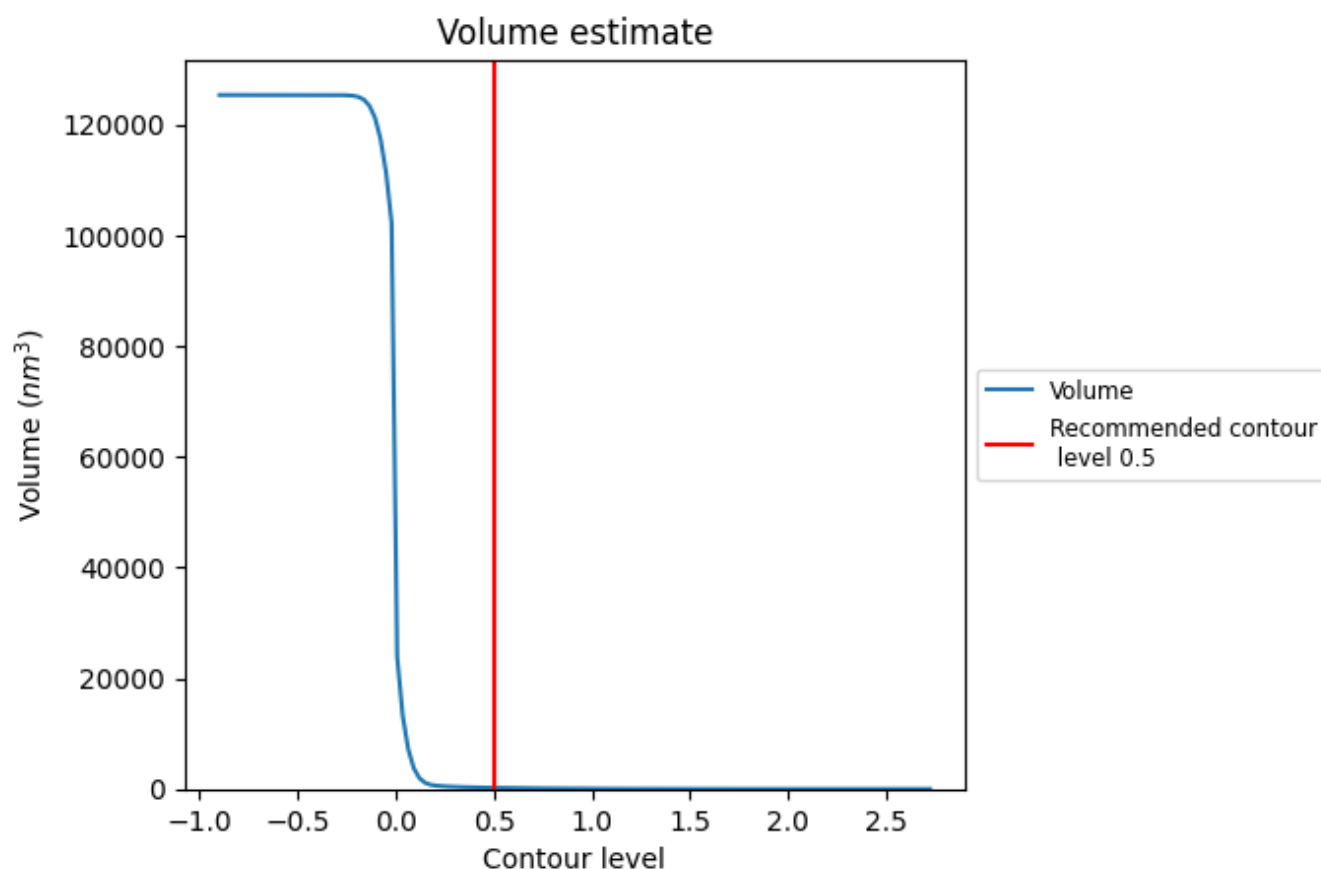
This section contains the results of statistical analysis of the map.

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.

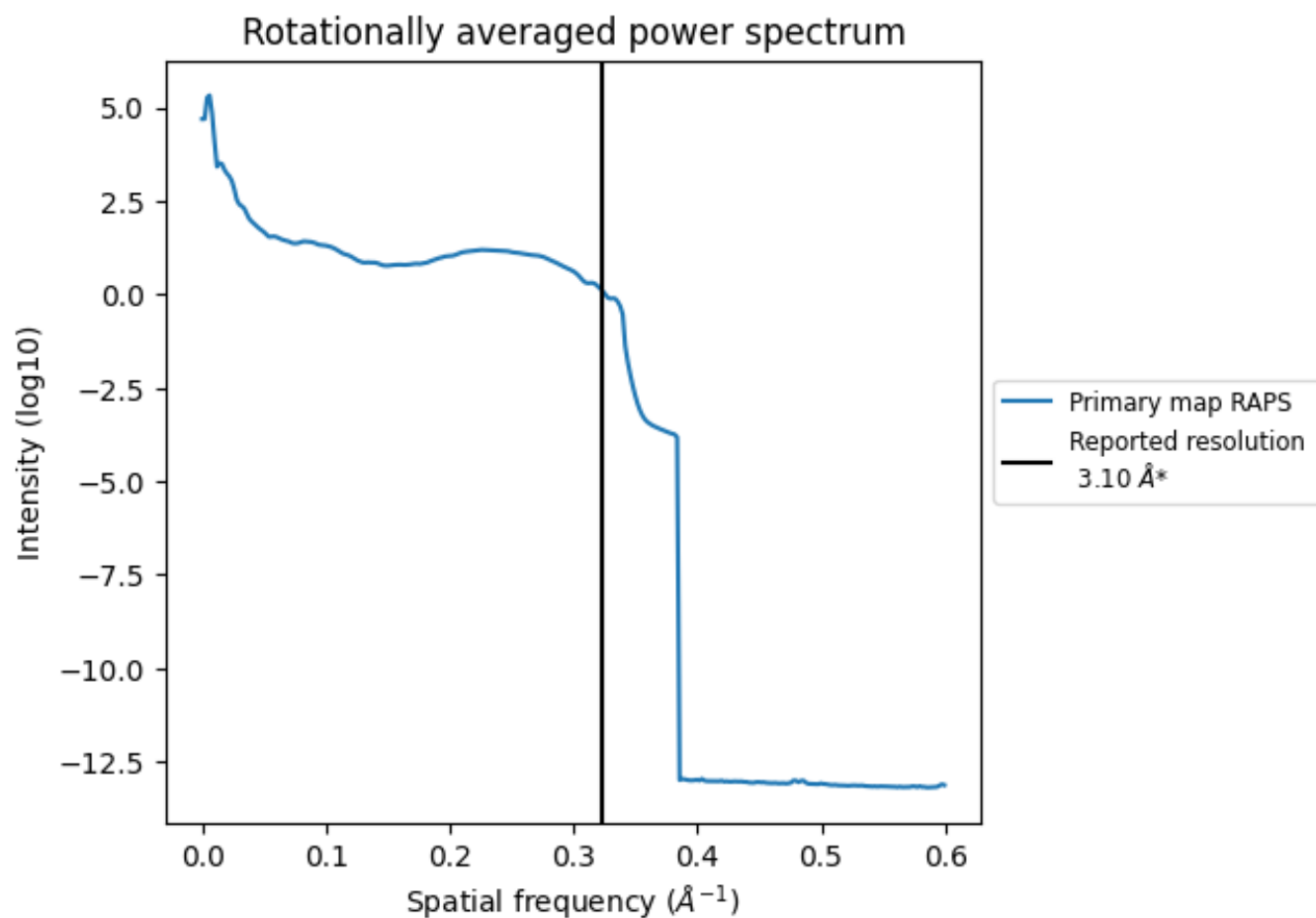
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 $\text{\AA}^{-1}$

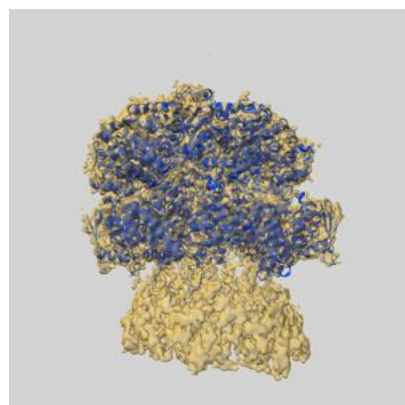
8 Fourier-Shell correlation

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

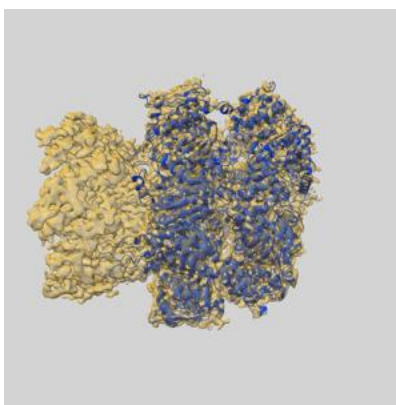
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21523 and PDB model 6W23. Per-residue inclusion information can be found in section [3](#) on page [7](#).

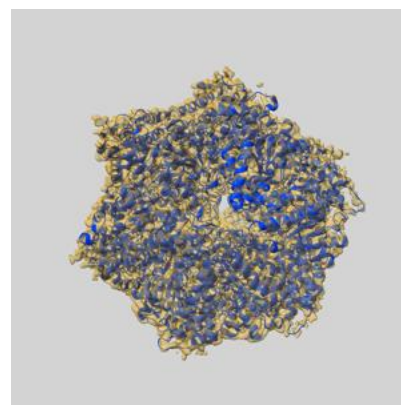
9.1 Map-model overlay [i](#)



X



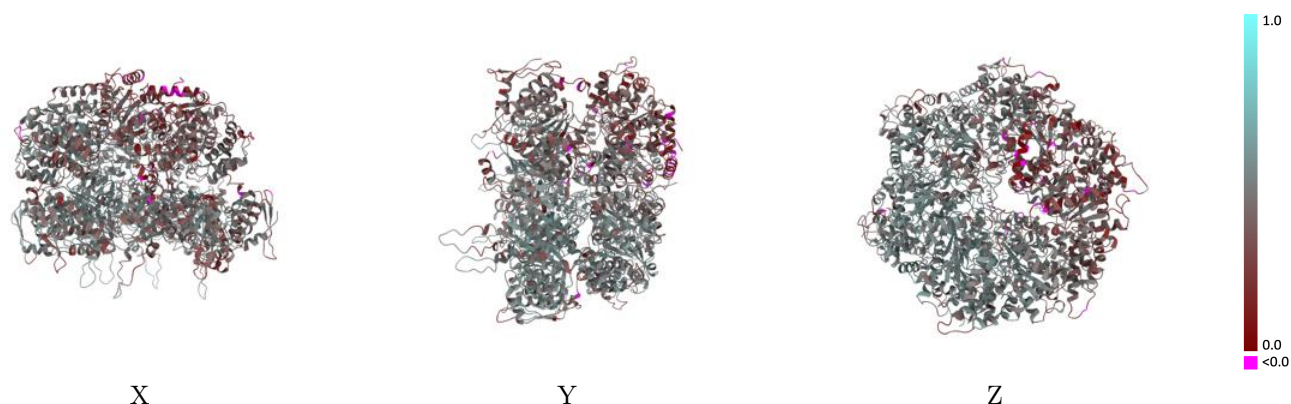
Y



Z

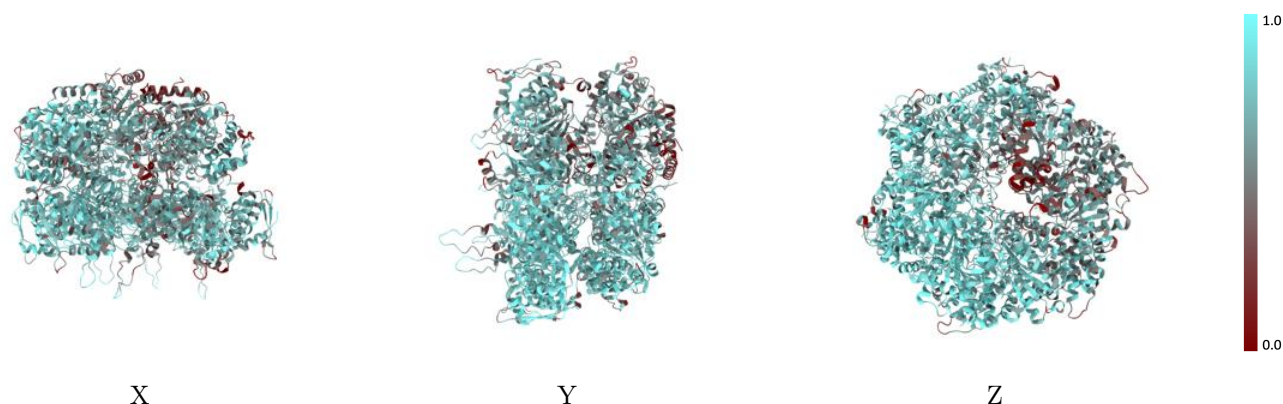
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



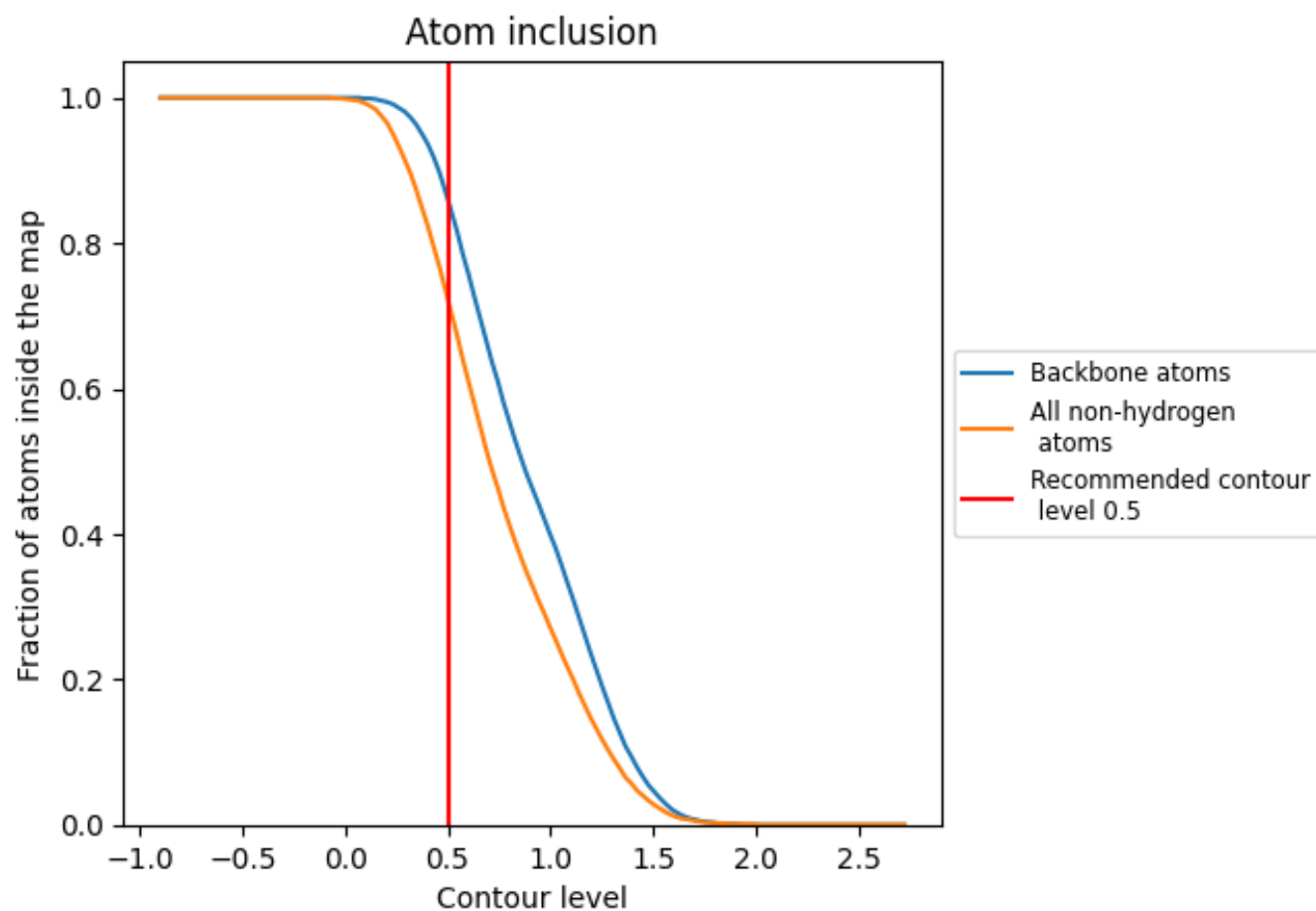
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7240	0.4500
A	0.6800	0.4360
B	0.7890	0.4820
C	0.8330	0.5140
D	0.8090	0.5010
E	0.6860	0.4220
F	0.5410	0.3430
X	0.6500	0.4290

1.0

0.0

<0.0