



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 09:35 PM UTC

PDB ID : 6W22 / pdb_00006w22
EMDB ID : EMD-21522
Title : ClpA Engaged1 State bound to RepA-GFP (ClpA Focused Refinement)
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 : 3.00 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:

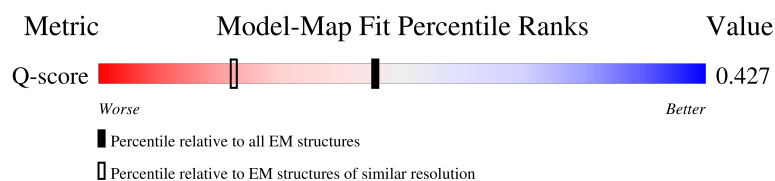
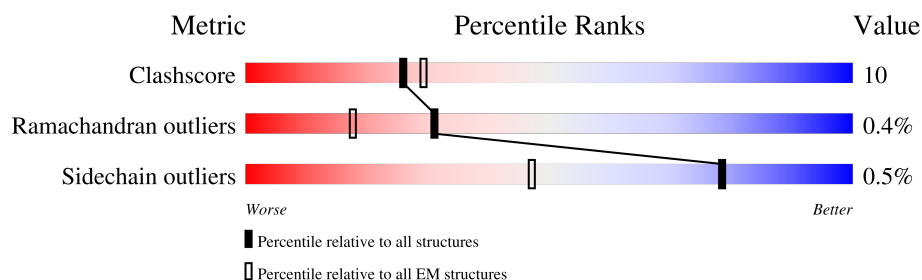
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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.



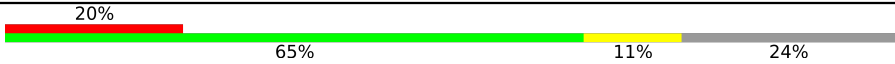
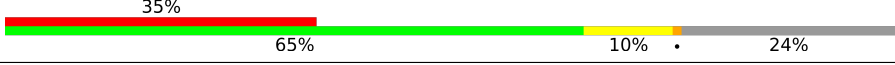
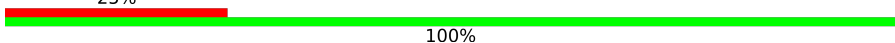
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	 7% 65% 10% 24%
1	B	758	 1% 64% 11% 24%
1	C	758	 1% 63% 12% 24%
1	D	758	 1% 66% 9% 24%

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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	ATP	A	801	-	-	X	-
3	ATP	B	801	-	-	X	-
3	ATP	C	801	-	-	X	-
3	ATP	C	802	-	-	X	-
4	ADP	F	801	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27536 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.

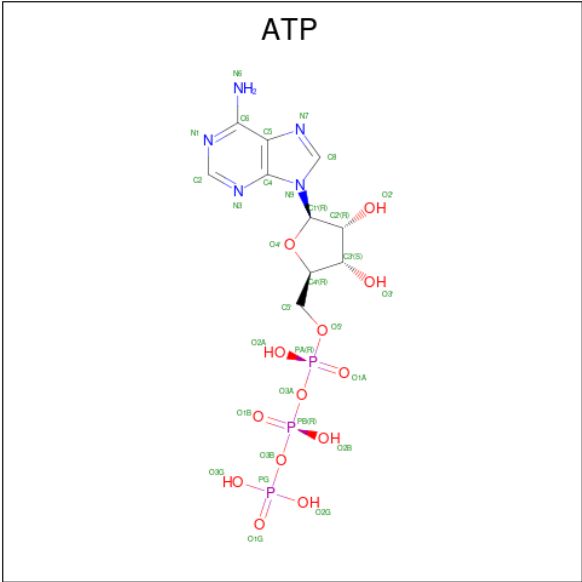
- Molecule 1 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	578	Total	C	N	O	S	0	0
			4510	2841	805	850	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	578	Total	C	N	O	S	0	0
			4510	2841	805	850	14		
1	F	578	Total	C	N	O	S	0	0
			4510	2841	805	850	14		

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

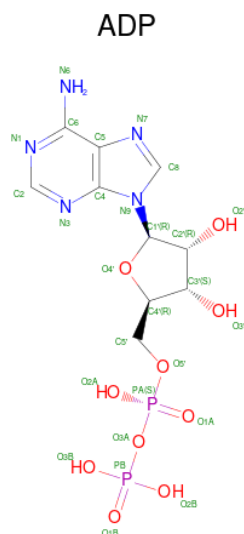
Mol	Chain	Residues	Atoms				AltConf	Trace
2	X	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
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	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	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	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	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

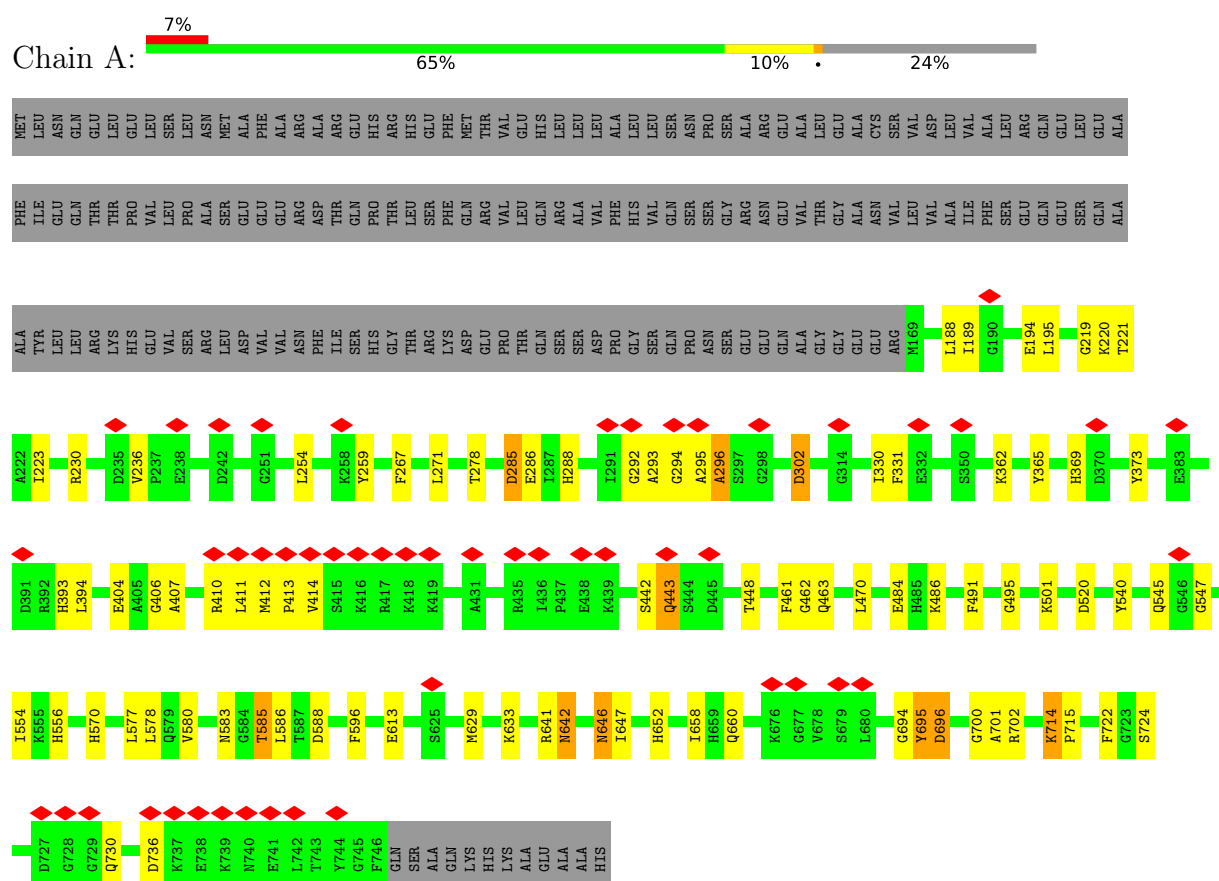


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0

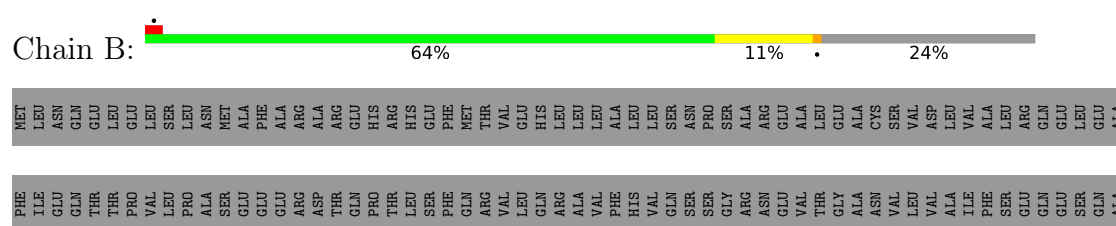
3 Residue-property plots

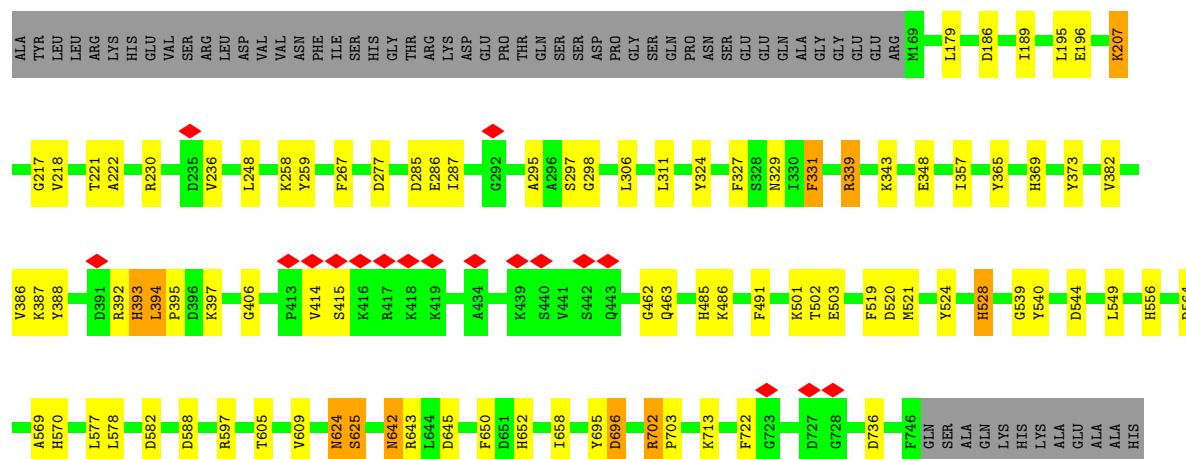
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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



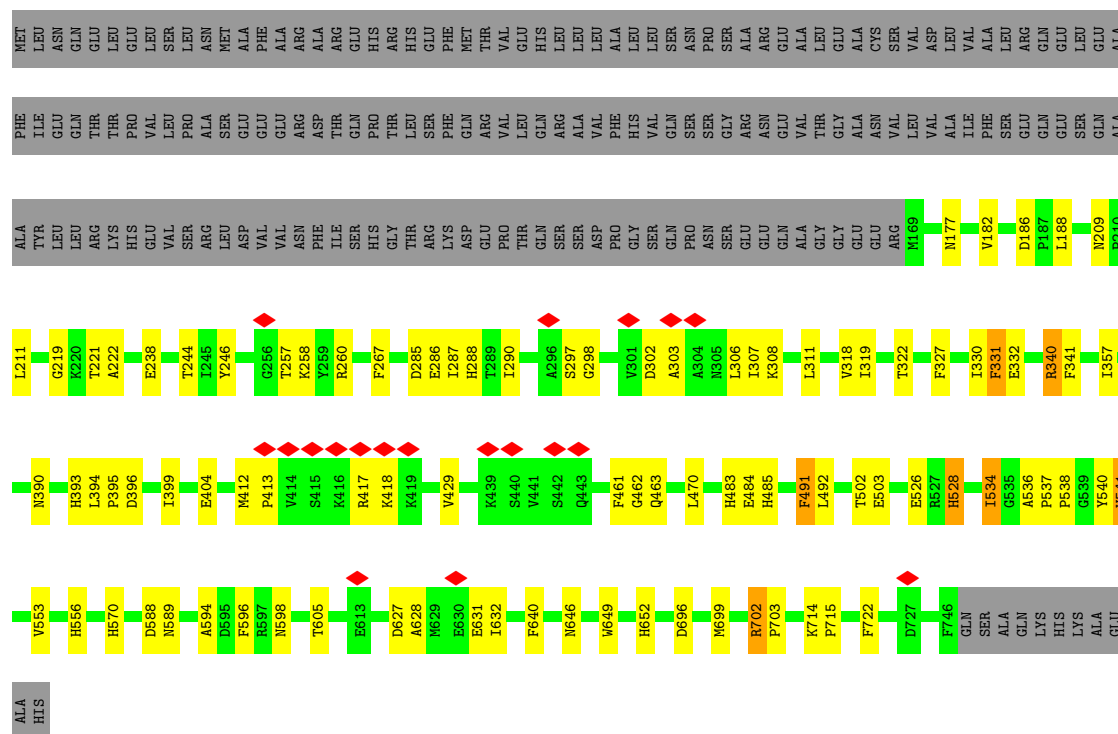
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA





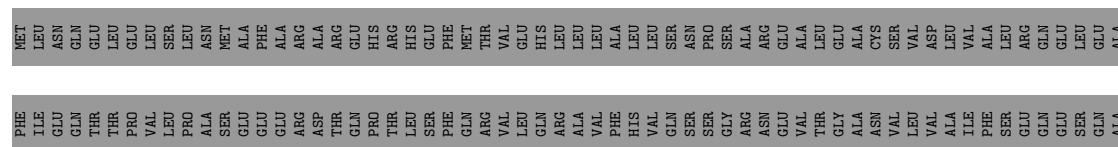
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

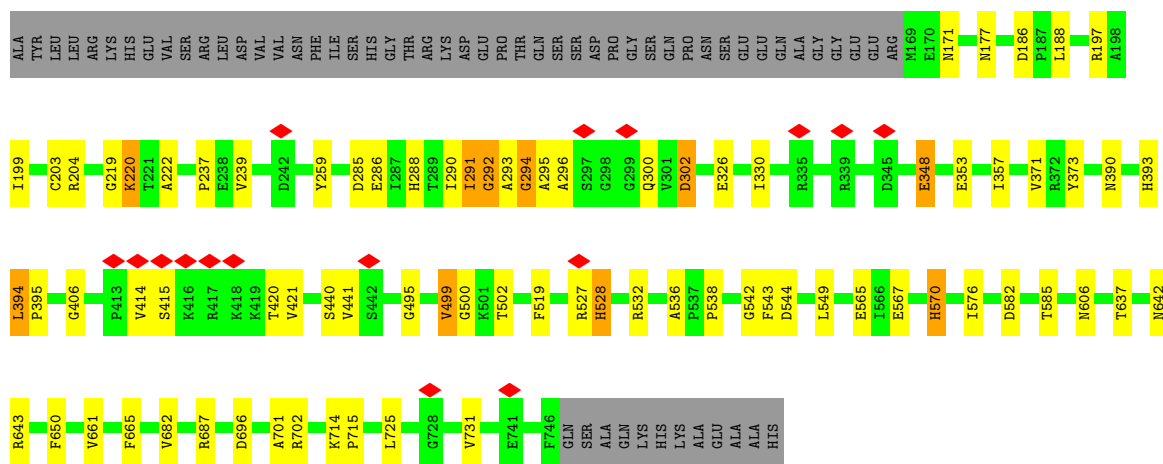
Chain C: 63% 12% 24%



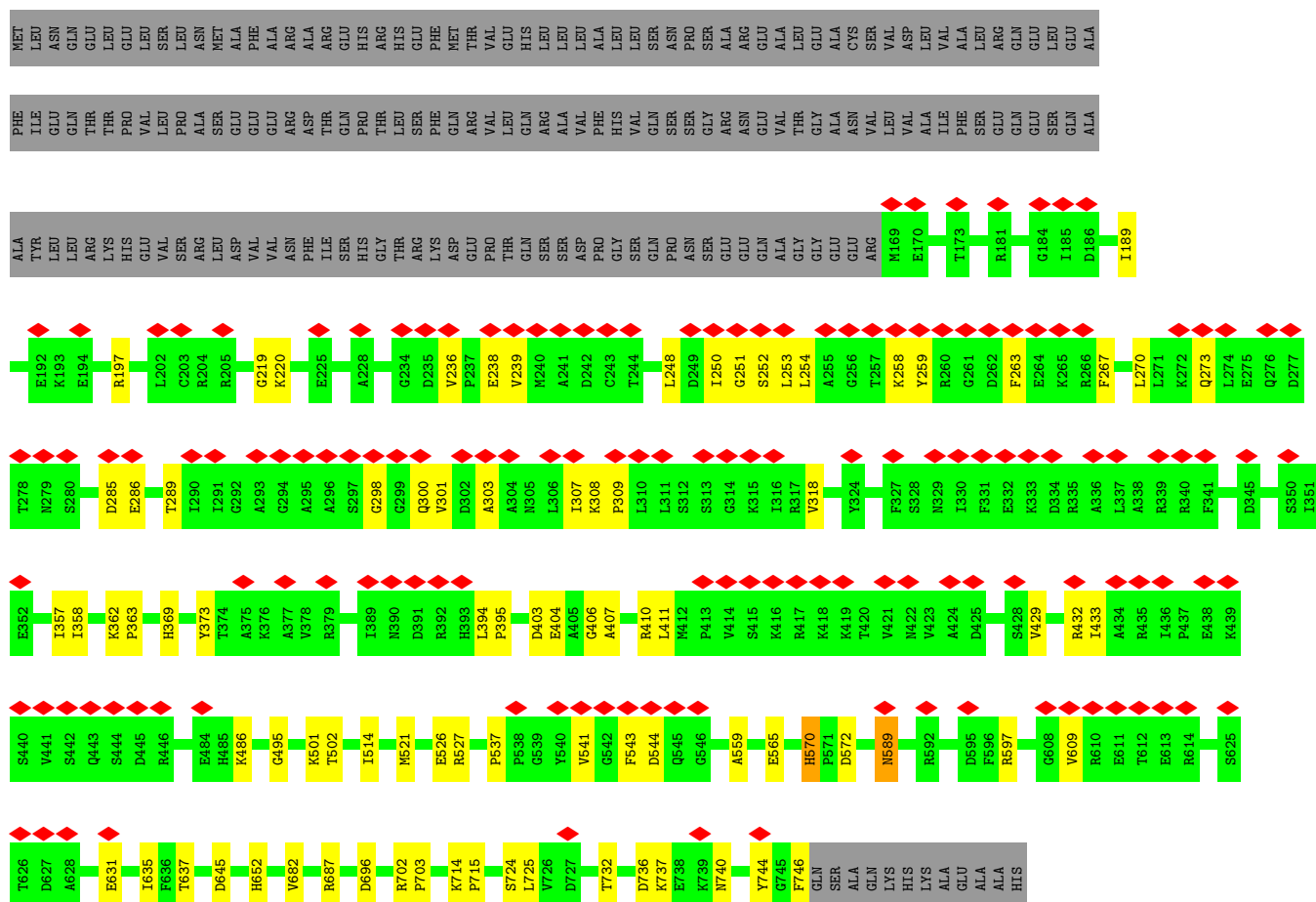
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain D: 66% 9% 24%

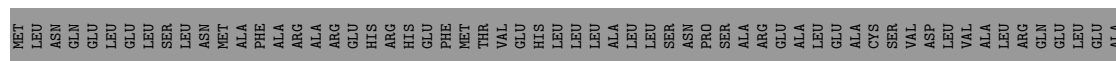


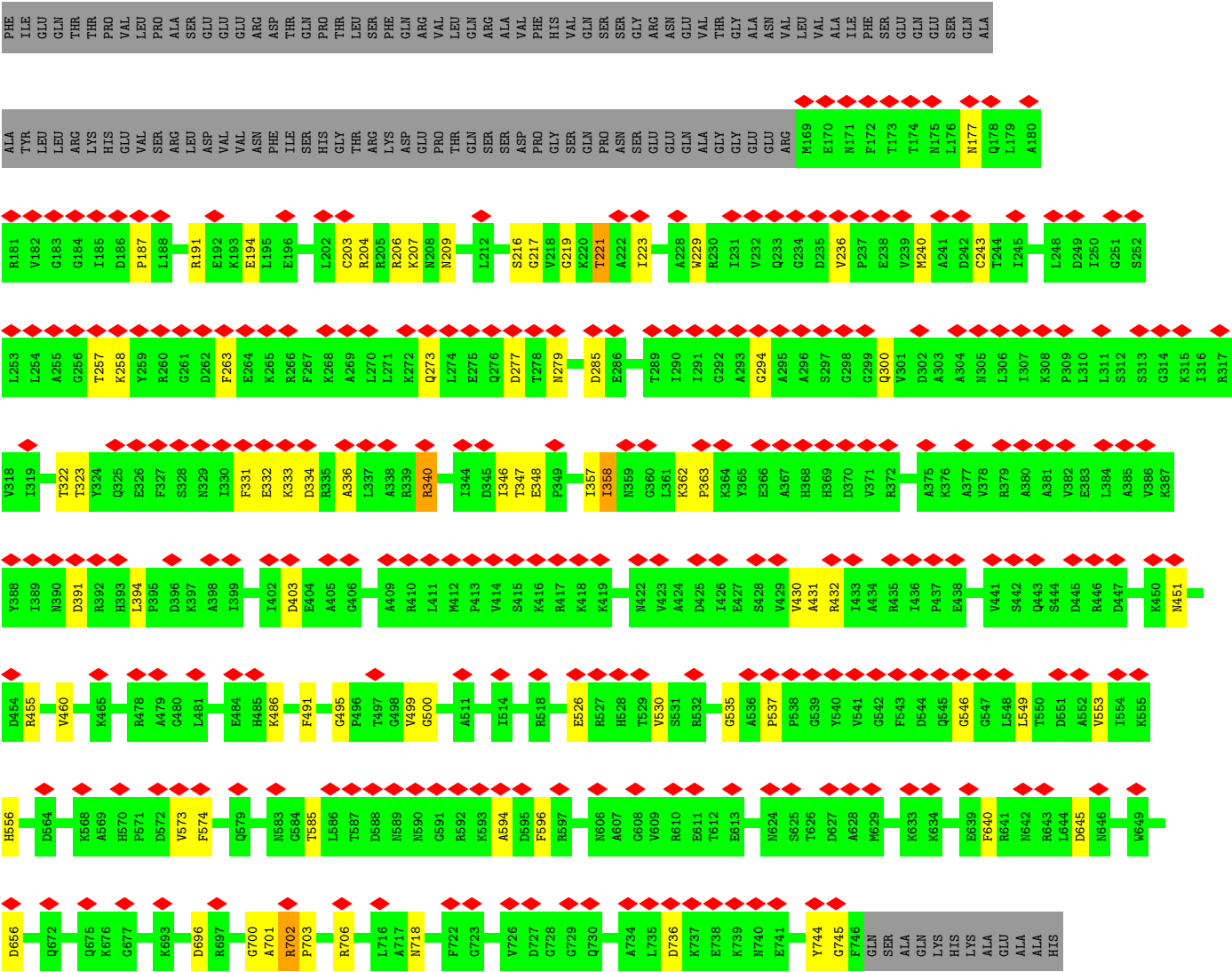


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

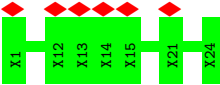


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA





• 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	176232	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	3.753	Depositor
Minimum map value	-1.201	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ADP, 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	1.24	6/4576 (0.1%)	1.26	32/6175 (0.5%)
1	B	1.28	6/4576 (0.1%)	1.25	27/6175 (0.4%)
1	C	1.36	7/4576 (0.2%)	1.24	25/6175 (0.4%)
1	D	1.33	3/4576 (0.1%)	1.25	29/6175 (0.5%)
1	E	1.16	5/4576 (0.1%)	1.27	23/6175 (0.4%)
1	F	1.11	2/4576 (0.0%)	1.28	32/6175 (0.5%)
All	All	1.25	29/27456 (0.1%)	1.26	168/37050 (0.5%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	570	HIS	CB-CG	-6.47	1.41	1.50
1	B	556	HIS	CB-CG	-6.25	1.41	1.50
1	A	570	HIS	CB-CG	-6.13	1.41	1.50
1	B	528	HIS	CB-CG	-6.12	1.41	1.50
1	B	369	HIS	CB-CG	-5.88	1.42	1.50
1	D	570	HIS	CB-CG	-5.81	1.42	1.50
1	E	273	GLN	CD-OE1	5.81	1.34	1.23
1	E	197	ARG	CD-NE	-5.80	1.38	1.46
1	B	485	HIS	CB-CG	-5.70	1.42	1.50
1	B	570	HIS	CB-CG	-5.67	1.42	1.50
1	F	394	LEU	CB-CG	-5.55	1.42	1.53
1	C	485	HIS	CB-CG	-5.50	1.42	1.50
1	C	303	ALA	CA-C	-5.46	1.45	1.52
1	A	652	HIS	CB-CG	-5.43	1.42	1.50
1	D	188	LEU	CB-CG	-5.33	1.42	1.53
1	D	528	HIS	ND1-CE1	5.31	1.37	1.32
1	E	725	LEU	CG-CD2	-5.31	1.35	1.52
1	C	652	HIS	CB-CG	-5.26	1.42	1.50
1	C	528	HIS	ND1-CE1	5.25	1.37	1.32
1	E	597	ARG	CD-NE	-5.24	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	586	LEU	CB-CG	-5.22	1.43	1.53
1	C	288	HIS	ND1-CE1	5.21	1.37	1.32
1	E	369	HIS	CB-CG	-5.20	1.42	1.50
1	A	556	HIS	CB-CG	-5.15	1.43	1.50
1	B	652	HIS	CB-CG	-5.12	1.43	1.50
1	A	642	ASN	CG-OD1	5.10	1.33	1.23
1	C	556	HIS	CB-CG	-5.08	1.43	1.50
1	F	273	GLN	CD-OE1	5.07	1.33	1.23
1	A	288	HIS	CB-CG	-5.05	1.43	1.50

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	VAL	N-CA-C	-12.50	101.28	113.53
1	D	414	VAL	N-CA-C	-11.10	100.44	113.42
1	F	573	VAL	N-CA-C	-8.61	102.47	110.82
1	F	177	ASN	N-CA-C	-8.34	101.44	111.69
1	A	724	SER	N-CA-C	-7.99	102.55	111.82
1	D	495	GLY	CA-C-N	7.72	128.18	119.92
1	D	495	GLY	C-N-CA	7.72	128.18	119.92
1	F	348	GLU	CA-C-N	7.67	128.12	120.52
1	F	348	GLU	C-N-CA	7.67	128.12	120.52
1	B	394	LEU	N-CA-C	7.66	123.88	113.77
1	D	393	HIS	CA-CB-CG	-7.47	106.33	113.80
1	F	495	GLY	CA-C-N	7.41	127.37	120.03
1	F	495	GLY	C-N-CA	7.41	127.37	120.03
1	D	585	THR	N-CA-C	7.12	120.01	108.76
1	B	388	TYR	N-CA-C	7.11	123.07	113.97
1	A	278	THR	N-CA-C	-7.07	105.58	114.56
1	E	307	ILE	N-CA-C	-7.06	104.89	111.45
1	A	393	HIS	CA-CB-CG	-7.02	106.78	113.80
1	C	536	ALA	CA-C-N	6.97	124.75	119.66
1	C	536	ALA	C-N-CA	6.97	124.75	119.66
1	B	486	LYS	CA-C-N	6.88	127.82	120.11
1	B	486	LYS	C-N-CA	6.88	127.82	120.11
1	F	340	ARG	N-CA-C	-6.76	105.98	114.56
1	D	440	SER	N-CA-C	6.71	121.75	113.50
1	A	365	TYR	N-CA-C	-6.65	103.51	111.69
1	D	528	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	D	259	TYR	N-CA-C	6.57	120.00	110.28
1	C	528	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	C	394	LEU	N-CA-C	6.54	122.55	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	F	285	ASP	N-CA-C	-6.45	101.84	110.55
1	D	394	LEU	N-CA-C	6.41	122.36	113.45
1	F	486	LYS	CA-C-N	6.37	126.74	119.92
1	F	486	LYS	C-N-CA	6.37	126.74	119.92
1	C	393	HIS	CA-CB-CG	-6.37	107.43	113.80
1	F	702	ARG	CA-C-N	6.36	126.06	119.82
1	F	702	ARG	C-N-CA	6.36	126.06	119.82
1	E	300	GLN	N-CA-C	6.36	121.11	113.23
1	B	179	LEU	N-CA-C	-6.35	105.18	113.12
1	C	462	GLY	N-CA-C	-6.28	101.28	112.58
1	B	462	GLY	N-CA-C	-6.25	101.33	112.58
1	A	448	THR	N-CA-C	-6.25	106.30	114.04
1	F	535	GLY	N-CA-C	-6.21	104.90	115.08
1	F	556	HIS	CA-C-N	6.17	125.79	119.56
1	F	556	HIS	C-N-CA	6.17	125.79	119.56
1	A	583	ASN	CA-CB-CG	-6.16	106.44	112.60
1	E	236	VAL	CA-C-N	6.13	126.09	119.78
1	E	236	VAL	C-N-CA	6.13	126.09	119.78
1	B	624	ASN	N-CA-C	-6.11	101.15	109.95
1	A	556	HIS	CA-C-N	6.04	125.72	119.56
1	A	556	HIS	C-N-CA	6.04	125.72	119.56
1	E	252	SER	N-CA-C	6.03	118.75	111.40
1	B	311	LEU	N-CA-C	-6.00	105.61	113.12
1	E	301	VAL	CB-CA-C	-5.95	104.23	112.02
1	B	722	PHE	CA-CB-CG	-5.93	107.87	113.80
1	D	576	ILE	N-CA-C	-5.92	104.74	110.72
1	F	537	PRO	CB-CA-C	5.90	118.12	110.92
1	B	393	HIS	CA-CB-CG	-5.89	107.91	113.80
1	F	403	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	177	ASN	N-CA-C	-5.86	104.48	111.69
1	A	443	GLN	N-CA-C	5.84	120.69	113.50
1	C	177	ASN	N-CA-C	-5.82	105.02	111.36
1	A	236	VAL	CA-C-N	5.74	126.06	119.92
1	A	236	VAL	C-N-CA	5.74	126.06	119.92
1	A	554	ILE	N-CA-C	-5.72	106.89	111.81
1	D	186	ASP	CA-C-N	5.72	125.63	119.85
1	D	186	ASP	C-N-CA	5.72	125.63	119.85
1	B	365	TYR	N-CA-C	-5.72	104.66	111.69
1	F	331	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	646	ASN	N-CA-C	5.71	116.09	108.38
1	A	585	THR	N-CA-C	5.69	117.92	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	585	THR	N-CA-C	5.69	117.92	108.99
1	A	495	GLY	CA-C-N	5.68	126.00	119.92
1	A	495	GLY	C-N-CA	5.68	126.00	119.92
1	D	528	HIS	CB-CG-ND1	5.67	131.21	122.70
1	D	292	GLY	N-CA-C	-5.66	101.93	111.73
1	E	570	HIS	CA-C-N	5.65	126.02	119.47
1	E	570	HIS	C-N-CA	5.65	126.02	119.47
1	F	358	ILE	CB-CA-C	-5.65	104.74	111.97
1	C	288	HIS	CB-CG-ND1	5.64	131.16	122.70
1	E	486	LYS	CA-C-N	5.63	125.95	119.92
1	E	486	LYS	C-N-CA	5.63	125.95	119.92
1	C	528	HIS	CB-CG-ND1	5.61	131.12	122.70
1	E	645	ASP	N-CA-C	-5.61	105.25	111.36
1	D	390	ASN	N-CA-C	5.61	119.70	112.41
1	D	702	ARG	CA-C-N	5.61	125.28	119.56
1	D	702	ARG	C-N-CA	5.61	125.28	119.56
1	A	730	GLN	CG-CD-NE2	5.60	124.81	116.40
1	E	637	THR	CA-C-N	5.57	125.93	119.47
1	E	637	THR	C-N-CA	5.57	125.93	119.47
1	D	441	VAL	N-CA-C	5.53	116.26	110.62
1	C	319	ILE	CA-C-N	-5.53	116.72	122.69
1	C	319	ILE	C-N-CA	-5.53	116.72	122.69
1	C	182	VAL	N-CA-C	5.52	116.58	111.45
1	D	291	ILE	N-CA-C	-5.51	97.87	109.34
1	D	237	PRO	N-CA-C	-5.50	102.45	111.15
1	A	714	LYS	CA-C-N	5.48	125.19	119.82
1	A	714	LYS	C-N-CA	5.48	125.19	119.82
1	B	277	ASP	N-CA-C	-5.48	104.71	111.40
1	C	640	PHE	N-CA-C	-5.48	104.72	111.40
1	A	462	GLY	N-CA-C	-5.47	103.53	112.83
1	B	502	THR	N-CA-C	-5.45	106.80	113.50
1	A	302	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	340	ARG	N-CA-C	5.43	119.60	112.92
1	D	570	HIS	CA-C-N	5.42	125.76	119.47
1	D	570	HIS	C-N-CA	5.42	125.76	119.47
1	A	486	LYS	CA-C-N	5.42	126.18	120.11
1	A	486	LYS	C-N-CA	5.42	126.18	120.11
1	E	298	GLY	N-CA-C	-5.42	107.30	115.32
1	A	702	ARG	CA-C-N	5.42	125.50	119.87
1	A	702	ARG	C-N-CA	5.42	125.50	119.87
1	D	499	VAL	N-CA-C	-5.40	100.66	108.87
1	E	652	HIS	N-CA-C	-5.40	102.88	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	589	ASN	CA-CB-CG	-5.40	107.20	112.60
1	B	702	ARG	CA-C-N	5.40	125.01	119.56
1	B	702	ARG	C-N-CA	5.40	125.01	119.56
1	B	248	LEU	N-CA-C	5.39	118.41	109.46
1	C	722	PHE	CA-CB-CG	-5.39	108.41	113.80
1	D	637	THR	CA-C-N	5.38	125.46	119.32
1	D	637	THR	C-N-CA	5.38	125.46	119.32
1	A	189	ILE	N-CA-CB	-5.37	104.70	111.46
1	B	295	ALA	N-CA-C	-5.37	102.45	110.23
1	E	318	VAL	N-CA-C	5.36	116.44	108.46
1	B	186	ASP	CA-C-N	5.35	125.25	119.85
1	B	186	ASP	C-N-CA	5.35	125.25	119.85
1	D	420	THR	N-CA-C	-5.35	102.28	110.14
1	C	322	THR	N-CA-C	5.33	117.17	108.76
1	F	430	VAL	N-CA-C	-5.32	105.19	110.62
1	E	502	THR	N-CA-C	-5.30	106.95	113.41
1	B	221	THR	N-CA-C	-5.29	106.33	112.89
1	C	556	HIS	CA-C-N	5.25	124.91	119.56
1	C	556	HIS	C-N-CA	5.25	124.91	119.56
1	C	462	GLY	CA-C-N	-5.23	114.82	122.40
1	C	462	GLY	C-N-CA	-5.23	114.82	122.40
1	C	534	ILE	N-CA-C	5.23	116.31	111.81
1	E	263	PHE	N-CA-C	5.22	116.66	111.07
1	B	696	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	394	LEU	N-CA-C	5.21	120.69	113.45
1	A	285	ASP	N-CA-C	-5.20	103.17	110.35
1	E	543	PHE	N-CA-C	-5.20	106.20	112.54
1	A	613	GLU	N-CA-C	-5.18	106.73	113.16
1	F	573	VAL	CB-CA-C	-5.15	105.29	112.04
1	A	722	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	700	GLY	CA-C-N	5.15	129.32	120.72
1	A	700	GLY	C-N-CA	5.15	129.32	120.72
1	B	415	SER	CA-C-N	5.15	129.45	122.19
1	B	415	SER	C-N-CA	5.15	129.45	122.19
1	B	609	VAL	N-CA-C	5.14	115.91	110.72
1	F	277	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	713	LYS	N-CA-C	5.13	116.95	111.36
1	F	332	GLU	CA-C-N	5.13	127.15	120.28
1	F	332	GLU	C-N-CA	5.13	127.15	120.28
1	C	598	ASN	CA-CB-CG	-5.11	107.49	112.60
1	C	702	ARG	N-CA-C	5.11	120.41	113.16
1	D	415	SER	N-CA-C	-5.11	106.74	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	537	PRO	CA-C-N	5.10	125.01	119.76
1	E	537	PRO	C-N-CA	5.10	125.01	119.76
1	F	236	VAL	CA-C-N	5.09	125.00	119.85
1	F	236	VAL	C-N-CA	5.09	125.00	119.85
1	F	177	ASN	CA-CB-CG	5.07	117.67	112.60
1	D	544	ASP	CA-CB-CG	-5.06	107.54	112.60
1	B	605	THR	N-CA-C	5.04	116.50	108.79
1	F	391	ASP	N-CA-C	5.04	119.12	112.92
1	E	258	LYS	N-CA-C	-5.03	106.74	112.92
1	F	718	ASN	CA-C-N	-5.02	113.17	120.29
1	F	718	ASN	C-N-CA	-5.02	113.17	120.29
1	C	390	ASN	N-CA-C	5.02	118.93	112.41
1	F	221	THR	N-CA-C	-5.01	105.53	111.69

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	4510	0	4609	96	0
1	B	4510	0	4609	100	0
1	C	4510	0	4609	156	0
1	D	4510	0	4609	97	0
1	E	4510	0	4609	87	0
1	F	4510	0	4609	81	0
2	X	120	0	32	0	0
3	A	31	0	12	11	0
3	B	62	0	24	19	0
3	C	62	0	24	37	0
3	D	62	0	24	15	0
3	E	31	0	12	3	0
4	A	27	0	12	8	0
4	E	27	0	12	5	0
4	F	54	0	24	21	0
All	All	27536	0	27830	563	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 10.

All (563) 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:724:SER:HB2	1:E:746:PHE:CD2	1.68	1.28
1:A:220:LYS:HB3	3:A:801:ATP:O1B	1.34	1.28
1:F:206:ARG:NH1	1:F:207:LYS:HE3	1.49	1.26
1:C:221:THR:HB	3:C:801:ATP:O2A	1.39	1.23
1:A:411:LEU:C	1:A:413:PRO:HD2	1.65	1.21
1:C:311:LEU:HD13	1:C:341:PHE:CE1	1.76	1.20
1:A:293:ALA:HA	1:A:302:ASP:CB	1.73	1.19
1:D:239:VAL:HG21	1:E:411:LEU:HG	1.27	1.15
1:F:191:ARG:NH2	1:F:346:ILE:HG23	1.62	1.13
1:A:293:ALA:HA	1:A:302:ASP:HB2	1.29	1.11
1:B:222:ALA:HB2	3:B:801:ATP:H5'2	1.33	1.08
1:D:291:ILE:HD12	1:D:330:ILE:HG22	1.37	1.07
1:C:395:PRO:HB2	3:C:801:ATP:H8	1.03	1.07
1:C:395:PRO:HB2	3:C:801:ATP:C8	1.88	1.07
1:A:220:LYS:HE3	3:A:801:ATP:O1B	1.56	1.06
1:F:206:ARG:HH12	1:F:207:LYS:HE3	1.06	1.04
1:C:470:LEU:HD23	1:C:491:PHE:CZ	1.93	1.03
1:C:395:PRO:CB	3:C:801:ATP:H8	1.71	1.03
1:C:222:ALA:HB1	3:C:801:ATP:C2	1.94	1.02
1:C:540:TYR:OH	1:D:528:HIS:HB2	1.59	1.02
1:A:701:ALA:HB1	4:A:802:ADP:O4'	1.58	1.02
1:B:642:ASN:OD1	1:C:702:ARG:HB3	1.59	1.02
1:C:540:TYR:CZ	1:D:528:HIS:HB2	1.93	1.01
1:F:460:VAL:HG13	4:F:802:ADP:HN62	1.28	0.99
1:C:470:LEU:HD23	1:C:491:PHE:HZ	1.26	0.98
1:C:287:ILE:HG23	1:C:331:PHE:CD1	2.00	0.96
1:E:724:SER:HB2	1:E:746:PHE:HD2	1.19	0.96
1:C:209:ASN:HB3	1:C:341:PHE:CD2	2.00	0.96
1:F:206:ARG:HH12	1:F:207:LYS:CE	1.79	0.95
1:A:411:LEU:C	1:A:413:PRO:CD	2.39	0.94
1:E:702:ARG:HB2	1:E:703:PRO:HD3	1.50	0.91
1:D:538:PRO:HA	1:D:543:PHE:CD1	2.05	0.91
1:A:694:GLY:O	1:A:695:TYR:O	1.87	0.91
1:E:501:LYS:HG2	3:E:802:ATP:O1B	1.69	0.91
1:C:541:VAL:HG13	1:C:542:GLY:H	1.35	0.90
1:C:311:LEU:HD13	1:C:341:PHE:HE1	1.24	0.90
1:A:293:ALA:HB1	1:A:296:ALA:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASN:HB3	1:B:702:ARG:HD2	1.55	0.89
1:F:191:ARG:HH22	1:F:346:ILE:HA	1.37	0.87
1:C:221:THR:CB	3:C:801:ATP:O2A	2.22	0.87
1:B:642:ASN:OD1	1:C:702:ARG:CB	2.22	0.86
1:D:222:ALA:HB2	3:D:801:ATP:H5'1	1.55	0.86
1:D:288:HIS:CE1	1:D:326:GLU:CD	2.53	0.86
1:D:199:ILE:CG2	1:E:411:LEU:HD11	2.07	0.85
1:C:222:ALA:HB2	3:C:801:ATP:H5'2	1.56	0.85
1:C:311:LEU:CD1	1:C:341:PHE:CE1	2.60	0.85
1:B:395:PRO:CB	3:B:801:ATP:H8	1.90	0.85
1:F:191:ARG:CZ	1:F:346:ILE:HG23	2.07	0.84
1:A:188:LEU:HD22	3:A:801:ATP:C6	2.13	0.84
1:F:243:CYS:HB2	1:F:279:ASN:O	1.78	0.84
1:B:285:ASP:HB3	1:B:286:GLU:OE1	1.76	0.84
1:D:291:ILE:HD12	1:D:330:ILE:CG2	2.06	0.84
1:A:220:LYS:CB	3:A:801:ATP:O1B	2.23	0.84
1:A:412:MET:N	1:A:413:PRO:CD	2.41	0.84
1:D:642:ASN:ND2	1:E:702:ARG:HG3	1.91	0.84
1:F:191:ARG:CZ	1:F:194:GLU:HG3	2.08	0.83
1:F:574:PHE:CZ	1:F:640:PHE:HB2	2.13	0.83
1:E:250:ILE:HB	1:E:254:LEU:HD22	1.59	0.83
1:E:404:GLU:HG2	1:E:429:VAL:HB	1.60	0.83
1:C:327:PHE:HA	1:C:331:PHE:HB3	1.59	0.82
1:C:219:GLY:HA2	3:C:801:ATP:O1A	1.80	0.82
1:C:211:LEU:CD2	1:C:331:PHE:CE2	2.62	0.82
1:B:189:ILE:H	3:B:801:ATP:HN62	1.24	0.81
1:F:460:VAL:HG13	4:F:802:ADP:N6	1.95	0.81
1:C:209:ASN:CB	1:C:341:PHE:CD2	2.63	0.81
1:C:327:PHE:CD1	1:C:331:PHE:CD2	2.68	0.81
1:C:211:LEU:HD22	1:C:331:PHE:CE2	2.16	0.81
1:C:327:PHE:CD1	1:C:331:PHE:HD2	2.00	0.80
1:B:222:ALA:HB2	3:B:801:ATP:C5'	2.11	0.80
1:B:395:PRO:HB3	3:B:801:ATP:H8	1.46	0.80
1:A:701:ALA:CB	4:A:802:ADP:C8	2.65	0.80
1:A:295:ALA:O	1:A:296:ALA:O	2.00	0.79
1:F:191:ARG:HE	1:F:223:ILE:HD11	1.45	0.79
1:C:503:GLU:HB2	3:C:802:ATP:H5'1	1.64	0.79
1:C:399:ILE:HG13	3:C:801:ATP:O2'	1.82	0.79
1:C:540:TYR:OH	1:D:528:HIS:CB	2.30	0.79
1:F:221:THR:HG22	4:F:801:ADP:O1A	1.84	0.78
1:F:191:ARG:HH21	1:F:346:ILE:HD12	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ASN:OD1	1:C:702:ARG:CG	2.32	0.77
1:D:239:VAL:CG2	1:E:411:LEU:HG	2.12	0.77
1:F:336:ALA:O	1:F:340:ARG:HG3	1.85	0.77
1:C:222:ALA:CB	3:C:801:ATP:C2	2.68	0.77
1:A:470:LEU:HD23	1:A:491:PHE:CZ	2.20	0.76
1:B:373:TYR:OH	1:B:406:GLY:HA3	1.84	0.76
1:B:544:ASP:OD1	1:B:544:ASP:O	2.03	0.76
1:C:209:ASN:HB3	1:C:341:PHE:CE2	2.20	0.76
1:C:287:ILE:CG2	1:C:331:PHE:CE1	2.68	0.75
1:E:724:SER:HB2	1:E:746:PHE:CE2	2.21	0.75
1:C:287:ILE:CG2	1:C:331:PHE:CD1	2.69	0.75
1:E:248:LEU:HD11	1:E:253:LEU:HD11	1.67	0.75
1:C:628:ALA:HB2	1:C:649:TRP:HE1	1.52	0.75
1:C:222:ALA:HB2	3:C:801:ATP:C5'	2.17	0.74
1:F:191:ARG:NH2	1:F:194:GLU:HG3	2.01	0.74
1:B:395:PRO:HB2	3:B:801:ATP:H1'	1.67	0.74
1:C:541:VAL:HG13	1:C:542:GLY:N	2.03	0.74
1:F:206:ARG:NH1	1:F:207:LYS:CE	2.39	0.73
1:D:293:ALA:O	1:D:302:ASP:HB3	1.88	0.73
1:A:411:LEU:CA	1:A:413:PRO:HD2	2.18	0.73
1:D:293:ALA:O	1:D:295:ALA:N	2.20	0.73
1:E:267:PHE:CE1	1:E:303:ALA:HB1	2.22	0.73
1:A:470:LEU:CD2	1:A:491:PHE:CZ	2.72	0.73
1:A:695:TYR:O	1:A:696:ASP:HB2	1.89	0.72
1:B:327:PHE:CZ	1:B:343:LYS:HD3	2.24	0.72
1:B:540:TYR:CZ	1:C:528:HIS:HB2	2.24	0.72
1:C:244:THR:HG21	1:C:246:TYR:CZ	2.25	0.72
1:D:219:GLY:C	3:D:801:ATP:O2A	2.33	0.72
1:D:219:GLY:CA	3:D:801:ATP:O2A	2.38	0.72
1:A:701:ALA:CB	4:A:802:ADP:O4'	2.36	0.72
1:C:311:LEU:CD1	1:C:341:PHE:HE1	1.98	0.72
1:E:267:PHE:CE2	1:E:303:ALA:HA	2.25	0.71
1:D:239:VAL:HG21	1:E:411:LEU:CG	2.16	0.71
1:F:216:SER:HA	4:F:801:ADP:O2B	1.90	0.71
1:D:296:ALA:H	1:D:300:GLN:HB2	1.54	0.71
1:A:221:THR:HG23	3:A:801:ATP:O2B	1.90	0.70
1:A:501:LYS:NZ	4:A:802:ADP:O1B	2.25	0.70
1:F:240:MET:O	1:F:243:CYS:HB3	1.90	0.70
1:F:553:VAL:HG21	1:F:596:PHE:CE2	2.26	0.70
1:A:293:ALA:CA	1:A:302:ASP:HB2	2.17	0.70
1:E:220:LYS:NZ	4:E:801:ADP:O1B	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:500:GLY:N	4:F:802:ADP:N7	2.39	0.70
1:F:357:ILE:HD13	4:F:801:ADP:C2	2.27	0.70
1:C:188:LEU:HD12	3:C:801:ATP:N6	2.07	0.69
1:F:191:ARG:NH2	1:F:346:ILE:CG2	2.48	0.69
1:D:222:ALA:HB2	3:D:801:ATP:C5'	2.21	0.69
1:E:267:PHE:CZ	1:E:303:ALA:HB1	2.27	0.69
1:E:724:SER:CB	1:E:746:PHE:CD2	2.63	0.69
1:D:203:CYS:SG	1:E:407:ALA:HB1	2.33	0.69
1:D:291:ILE:CD1	1:D:330:ILE:HG22	2.20	0.69
1:E:404:GLU:HG2	1:E:429:VAL:CB	2.22	0.69
1:E:248:LEU:CD1	1:E:253:LEU:HD11	2.23	0.68
1:C:311:LEU:HD13	1:C:341:PHE:CZ	2.28	0.68
1:C:588:ASP:OD1	1:C:589:ASN:OD1	2.11	0.68
1:A:373:TYR:OH	1:A:406:GLY:HA3	1.93	0.68
1:C:211:LEU:HD22	1:C:331:PHE:CZ	2.28	0.68
1:C:287:ILE:HG21	1:C:331:PHE:CE1	2.27	0.68
1:B:503:GLU:N	3:B:802:ATP:O2A	2.27	0.68
1:D:219:GLY:N	3:D:801:ATP:O2A	2.26	0.68
1:F:553:VAL:HG21	1:F:596:PHE:CZ	2.27	0.68
1:B:217:GLY:O	1:B:395:PRO:HG2	1.94	0.68
1:E:250:ILE:HA	1:E:254:LEU:HD13	1.74	0.67
1:F:263:PHE:CD2	1:F:300:GLN:HB3	2.29	0.67
1:A:470:LEU:HD21	1:A:491:PHE:CE1	2.29	0.67
1:F:574:PHE:HZ	1:F:640:PHE:HB2	1.58	0.67
1:D:292:GLY:O	1:D:302:ASP:CB	2.43	0.67
1:C:503:GLU:HB2	3:C:802:ATP:C5'	2.24	0.67
1:D:527:ARG:HG2	1:D:570:HIS:CE1	2.29	0.67
1:C:188:LEU:HD12	3:C:801:ATP:HN62	1.59	0.66
1:F:187:PRO:HB3	1:F:229:TRP:NE1	2.10	0.66
1:C:327:PHE:HD1	1:C:331:PHE:CD2	2.13	0.66
1:F:217:GLY:N	4:F:801:ADP:O1B	2.28	0.66
1:D:500:GLY:HA2	3:D:802:ATP:O1A	1.96	0.66
1:D:204:ARG:HB3	1:E:403:ASP:OD2	1.96	0.66
1:B:189:ILE:N	3:B:801:ATP:HN62	1.94	0.66
1:E:527:ARG:HG3	1:E:572:ASP:OD2	1.96	0.66
1:B:230:ARG:HB3	1:B:236:VAL:HG13	1.79	0.65
1:C:287:ILE:HG23	1:C:331:PHE:CE1	2.30	0.65
1:F:219:GLY:CA	4:F:801:ADP:N7	2.60	0.65
1:B:539:GLY:HA2	1:C:541:VAL:HG12	1.79	0.65
1:D:665:PHE:CZ	3:D:802:ATP:O2'	2.49	0.65
1:A:293:ALA:HA	1:A:302:ASP:HB3	1.74	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:GLU:HG2	1:E:429:VAL:CG1	2.26	0.64
1:A:219:GLY:HA2	3:A:801:ATP:C8	2.32	0.64
1:C:327:PHE:CE1	1:C:331:PHE:CD2	2.85	0.64
1:F:191:ARG:NH2	1:F:346:ILE:HD12	2.12	0.64
1:A:658:ILE:HD11	1:A:695:TYR:CE1	2.33	0.64
1:A:293:ALA:HA	1:A:302:ASP:CG	2.22	0.63
1:C:470:LEU:CD2	1:C:491:PHE:CE1	2.82	0.63
1:C:553:VAL:HG11	1:C:596:PHE:CE2	2.33	0.63
1:A:580:VAL:HB	1:A:596:PHE:CE1	2.34	0.63
1:B:392:ARG:HB2	1:B:397:LYS:CG	2.28	0.63
1:B:395:PRO:HB2	3:B:801:ATP:C8	2.34	0.63
1:F:553:VAL:HB	1:F:594:ALA:HB1	1.82	0.62
1:C:219:GLY:CA	3:C:801:ATP:O1A	2.47	0.62
1:A:220:LYS:CE	3:A:801:ATP:O1B	2.41	0.62
1:E:404:GLU:CG	1:E:429:VAL:HB	2.27	0.62
1:A:470:LEU:CD2	1:A:491:PHE:CE1	2.82	0.62
1:B:287:ILE:HG23	1:B:331:PHE:CE1	2.34	0.62
1:C:412:MET:HB3	1:C:417:ARG:HB2	1.81	0.62
1:B:393:HIS:C	1:B:395:PRO:HD2	2.25	0.62
1:B:540:TYR:CE1	1:C:528:HIS:HB2	2.35	0.62
1:B:395:PRO:HB2	3:B:801:ATP:H8	1.63	0.62
1:F:217:GLY:H	4:F:801:ADP:PB	2.23	0.62
1:F:187:PRO:HA	1:F:229:TRP:CD1	2.34	0.61
1:B:642:ASN:ND2	1:C:699:MET:SD	2.73	0.61
1:D:538:PRO:HA	1:D:543:PHE:CE1	2.34	0.61
1:B:207:LYS:HE2	1:B:339:ARG:HH21	1.65	0.61
1:C:327:PHE:CE1	1:C:331:PHE:HD2	2.18	0.61
1:C:470:LEU:HD23	1:C:491:PHE:CE1	2.35	0.61
1:D:292:GLY:O	1:D:302:ASP:HB2	2.00	0.61
1:D:536:ALA:HB3	1:D:542:GLY:O	2.00	0.61
1:D:543:PHE:CE2	1:E:541:VAL:HG11	2.36	0.61
1:A:461:PHE:CE1	1:A:660:GLN:HB3	2.36	0.61
1:C:244:THR:CG2	1:C:246:TYR:CE1	2.84	0.61
1:A:410:ARG:O	1:A:413:PRO:HG2	2.00	0.61
1:B:501:LYS:HB2	3:B:802:ATP:O1B	2.01	0.61
1:D:725:LEU:HD21	1:D:731:VAL:HG22	1.81	0.61
1:F:191:ARG:NH2	1:F:346:ILE:HA	2.13	0.61
1:F:191:ARG:HH12	1:F:347:THR:H	1.47	0.60
1:D:290:ILE:C	1:D:291:ILE:O	2.33	0.60
1:D:302:ASP:OD1	1:D:302:ASP:N	2.28	0.60
1:B:218:VAL:HA	1:B:395:PRO:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:GLU:HG3	1:D:348:GLU:O	2.02	0.60
1:C:470:LEU:CD2	1:C:491:PHE:CZ	2.78	0.60
1:B:643:ARG:NH2	3:C:802:ATP:O1G	2.34	0.59
1:A:407:ALA:HB2	1:F:204:ARG:HG2	1.84	0.59
1:C:311:LEU:HD22	1:C:341:PHE:CZ	2.37	0.59
1:A:646:ASN:CG	1:A:647:ILE:N	2.61	0.59
1:C:588:ASP:CG	1:C:589:ASN:N	2.61	0.59
1:B:382:VAL:O	1:B:386:VAL:HG23	2.02	0.59
1:D:373:TYR:OH	1:D:406:GLY:HA3	2.02	0.59
1:B:357:ILE:HD13	3:B:801:ATP:C8	2.39	0.58
1:B:642:ASN:OD1	1:C:702:ARG:HG2	2.02	0.58
1:E:404:GLU:OE1	1:E:433:ILE:CG1	2.52	0.58
1:C:260:ARG:HD3	1:D:294:GLY:O	2.03	0.58
1:A:701:ALA:HB3	4:A:802:ADP:H8	1.69	0.58
1:C:188:LEU:HD12	3:C:801:ATP:C6	2.39	0.58
1:E:404:GLU:OE2	1:E:429:VAL:HB	2.04	0.57
1:F:219:GLY:HA2	4:F:801:ADP:N7	2.19	0.57
1:A:642:ASN:O	1:B:702:ARG:HD3	2.05	0.57
1:A:646:ASN:CG	1:A:647:ILE:H	2.12	0.57
1:A:293:ALA:N	1:A:302:ASP:OD2	2.37	0.57
1:C:285:ASP:O	1:C:286:GLU:C	2.46	0.57
1:C:492:LEU:HD21	1:C:605:THR:HG21	1.87	0.57
1:D:288:HIS:CD2	1:D:326:GLU:HB3	2.40	0.57
1:D:295:ALA:HA	1:D:300:GLN:O	2.03	0.57
1:A:701:ALA:HB3	4:A:802:ADP:C8	2.40	0.57
1:B:395:PRO:CB	3:B:801:ATP:C8	2.82	0.57
1:C:311:LEU:CD1	1:C:341:PHE:CZ	2.86	0.57
1:D:288:HIS:CE1	1:D:326:GLU:HB3	2.38	0.57
1:C:470:LEU:HD21	1:C:491:PHE:HE1	1.69	0.57
1:F:206:ARG:CZ	1:F:207:LYS:HE3	2.31	0.57
1:B:373:TYR:OH	1:B:406:GLY:CA	2.51	0.57
1:B:387:LYS:O	1:B:597:ARG:NH1	2.38	0.57
1:A:292:GLY:O	1:A:293:ALA:HB3	2.05	0.57
1:C:483:HIS:ND1	1:C:484:GLU:N	2.52	0.57
1:D:725:LEU:HD11	1:D:731:VAL:HG21	1.85	0.57
1:C:260:ARG:CD	1:D:294:GLY:O	2.53	0.57
1:C:628:ALA:HB2	1:C:649:TRP:NE1	2.19	0.57
1:D:288:HIS:NE2	1:D:326:GLU:CG	2.68	0.57
1:D:661:VAL:HG22	3:D:802:ATP:C2	2.40	0.57
1:B:524:TYR:O	1:B:569:ALA:HA	2.05	0.57
1:C:553:VAL:HG21	1:C:594:ALA:HB1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:ASP:CB	1:B:643:ARG:HH11	2.17	0.56
1:D:642:ASN:CG	1:E:702:ARG:HG3	2.29	0.56
1:A:254:LEU:CD2	1:A:295:ALA:HB2	2.35	0.56
1:D:219:GLY:O	1:D:220:LYS:C	2.46	0.56
1:A:295:ALA:O	1:A:296:ALA:C	2.47	0.56
1:C:330:ILE:C	1:C:332:GLU:H	2.12	0.56
1:C:412:MET:N	1:C:413:PRO:CD	2.68	0.56
1:D:199:ILE:CG2	1:E:411:LEU:CD1	2.83	0.56
1:C:211:LEU:HD21	1:C:331:PHE:CE2	2.40	0.56
1:D:288:HIS:CE1	1:D:326:GLU:OE1	2.58	0.56
1:F:219:GLY:HA3	4:F:801:ADP:N7	2.21	0.56
1:F:491:PHE:CE2	1:F:645:ASP:HB2	2.40	0.56
1:F:187:PRO:HB3	1:F:229:TRP:HE1	1.71	0.56
1:D:292:GLY:O	1:D:293:ALA:HB3	2.05	0.56
1:F:460:VAL:CG1	4:F:802:ADP:HN62	2.10	0.56
1:A:694:GLY:C	1:A:695:TYR:O	2.49	0.56
1:C:209:ASN:HB2	1:C:341:PHE:CD2	2.40	0.56
1:C:491:PHE:CB	1:C:646:ASN:O	2.54	0.56
1:B:357:ILE:HD13	3:B:801:ATP:N7	2.22	0.55
1:D:357:ILE:HG23	3:D:801:ATP:C2	2.41	0.55
1:E:357:ILE:HG12	4:E:801:ADP:C2	2.41	0.55
1:A:412:MET:N	1:A:413:PRO:HD3	2.21	0.55
1:A:540:TYR:CZ	1:B:528:HIS:HB2	2.41	0.55
1:B:394:LEU:N	1:B:395:PRO:HD2	2.20	0.55
1:B:491:PHE:CE2	1:B:645:ASP:HB2	2.40	0.55
1:B:582:ASP:HB2	1:B:643:ARG:HH11	1.71	0.55
1:D:199:ILE:HG22	1:E:411:LEU:CD1	2.37	0.55
1:F:191:ARG:HH21	1:F:346:ILE:HG23	1.61	0.55
1:B:463:GLN:HG2	1:B:650:PHE:CD2	2.42	0.55
1:C:540:TYR:CZ	1:D:528:HIS:CB	2.80	0.55
1:D:204:ARG:CB	1:E:403:ASP:OD2	2.55	0.54
1:F:696:ASP:O	1:F:700:GLY:N	2.40	0.54
1:E:404:GLU:CD	1:E:433:ILE:HG13	2.33	0.54
1:B:392:ARG:CB	1:B:397:LYS:HG3	2.37	0.54
1:C:257:THR:O	1:C:258:LYS:HG3	2.07	0.54
1:C:461:PHE:H	3:C:802:ATP:HN62	1.54	0.54
1:E:714:LYS:HB2	1:E:715:PRO:HD3	1.89	0.54
1:B:539:GLY:H	1:C:541:VAL:HG13	1.72	0.54
1:F:263:PHE:CD2	1:F:300:GLN:CB	2.90	0.54
1:C:188:LEU:HD12	3:C:801:ATP:N1	2.21	0.54
1:C:627:ASP:OD1	1:C:627:ASP:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:VAL:CG1	1:C:542:GLY:H	2.14	0.54
1:F:362:LYS:HB3	1:F:363:PRO:HD3	1.90	0.54
1:F:191:ARG:NH2	1:F:346:ILE:CD1	2.71	0.53
1:B:357:ILE:CD1	3:B:801:ATP:C8	2.91	0.53
1:A:404:GLU:OE1	1:F:204:ARG:HD2	2.08	0.53
1:D:536:ALA:HB3	1:D:542:GLY:C	2.34	0.53
1:B:539:GLY:HA2	1:C:541:VAL:CG1	2.39	0.53
1:D:536:ALA:CB	1:D:542:GLY:O	2.57	0.53
1:E:238:GLU:O	1:E:239:VAL:C	2.49	0.53
1:A:373:TYR:OH	1:A:406:GLY:CA	2.55	0.53
1:A:701:ALA:HB1	4:A:802:ADP:C1'	2.39	0.53
1:B:539:GLY:CA	1:C:541:VAL:HG12	2.38	0.53
1:D:538:PRO:HB3	1:D:543:PHE:CE1	2.44	0.53
1:B:539:GLY:CA	1:C:541:VAL:CG1	2.87	0.53
1:C:470:LEU:HD21	1:C:491:PHE:CE1	2.44	0.53
1:D:353:GLU:O	1:D:357:ILE:HG13	2.08	0.53
1:E:248:LEU:CD1	1:E:253:LEU:CD1	2.87	0.53
1:B:702:ARG:HB3	1:B:703:PRO:HD3	1.90	0.52
1:D:219:GLY:O	3:D:801:ATP:O2A	2.27	0.52
1:D:288:HIS:HE1	1:D:326:GLU:CD	2.15	0.52
1:B:267:PHE:CE2	1:B:306:LEU:HB2	2.44	0.52
1:A:254:LEU:HG	1:A:295:ALA:HB2	1.91	0.52
1:D:219:GLY:O	1:D:222:ALA:N	2.43	0.52
1:F:191:ARG:NH1	1:F:347:THR:H	2.06	0.52
1:C:302:ASP:C	1:C:302:ASP:OD1	2.52	0.52
1:C:553:VAL:CG2	1:C:594:ALA:HB1	2.39	0.52
1:D:725:LEU:HD11	1:D:731:VAL:CG2	2.40	0.52
1:E:527:ARG:HB2	1:E:570:HIS:NE2	2.23	0.52
1:D:499:VAL:HG11	1:D:650:PHE:HB3	1.91	0.52
1:E:219:GLY:HA2	4:E:801:ADP:O5'	2.10	0.52
3:C:801:ATP:C5'	3:C:801:ATP:N3	2.73	0.52
1:E:373:TYR:OH	1:E:406:GLY:HA3	2.10	0.52
1:F:357:ILE:HD13	4:F:801:ADP:N1	2.25	0.52
1:A:219:GLY:HA2	3:A:801:ATP:N7	2.25	0.51
1:D:373:TYR:OH	1:D:406:GLY:CA	2.59	0.51
1:E:267:PHE:HZ	1:E:303:ALA:O	1.92	0.51
1:A:694:GLY:O	1:A:695:TYR:C	2.50	0.51
1:A:658:ILE:CD1	1:A:695:TYR:CD1	2.93	0.51
1:C:538:PRO:HA	1:C:543:PHE:CD1	2.46	0.51
1:D:285:ASP:O	1:D:286:GLU:C	2.53	0.51
1:E:631:GLU:O	1:E:635:ILE:HG12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:PHE:CZ	1:E:303:ALA:CA	2.92	0.51
1:E:189:ILE:O	4:E:801:ADP:N6	2.44	0.51
1:C:395:PRO:O	3:C:801:ATP:H1'	2.10	0.51
1:A:369:HIS:ND1	1:A:410:ARG:HD2	2.25	0.51
1:B:329:ASN:ND2	1:C:544:ASP:OD1	2.44	0.51
1:C:588:ASP:CG	1:C:589:ASN:H	2.18	0.51
1:A:545:GLN:HG3	1:A:547:GLY:H	1.76	0.51
1:D:538:PRO:CA	1:D:543:PHE:CD1	2.90	0.51
1:E:250:ILE:HB	1:E:254:LEU:CD2	2.36	0.50
1:F:194:GLU:OE1	1:F:346:ILE:HD13	2.10	0.50
1:F:358:ILE:O	1:F:362:LYS:N	2.42	0.50
1:D:565:GLU:OE1	1:D:606:ASN:ND2	2.45	0.50
1:E:248:LEU:HD13	1:E:253:LEU:CD1	2.41	0.50
1:A:259:TYR:CE2	1:B:258:LYS:HE3	2.47	0.50
1:A:411:LEU:N	1:A:413:PRO:HD2	2.26	0.50
1:B:519:PHE:HB3	1:B:521:MET:CE	2.41	0.50
1:E:394:LEU:HB2	1:E:395:PRO:HD3	1.93	0.50
1:C:244:THR:HG22	1:C:246:TYR:CE1	2.47	0.50
1:E:724:SER:CB	1:E:746:PHE:CE2	2.89	0.50
1:C:412:MET:H	1:C:413:PRO:CD	2.25	0.50
1:F:333:LYS:O	1:F:334:ASP:OD1	2.29	0.50
1:C:399:ILE:HG13	3:C:801:ATP:HO2'	1.74	0.50
1:B:520:ASP:C	1:B:520:ASP:OD1	2.52	0.50
1:C:502:THR:HG23	3:C:802:ATP:O1B	2.11	0.50
1:D:292:GLY:O	1:D:302:ASP:OD2	2.29	0.50
1:E:248:LEU:HD11	1:E:270:LEU:HD21	1.94	0.50
1:D:643:ARG:HG2	1:E:702:ARG:HH12	1.77	0.50
1:F:553:VAL:HG12	1:F:553:VAL:O	2.11	0.50
1:B:392:ARG:HB3	1:B:397:LYS:HG3	1.93	0.49
1:D:288:HIS:NE2	1:D:326:GLU:CD	2.70	0.49
1:B:642:ASN:O	1:C:702:ARG:CG	2.61	0.49
3:C:801:ATP:N3	3:C:801:ATP:H2'	2.26	0.49
1:A:267:PHE:CE2	1:A:271:LEU:HD11	2.47	0.49
1:B:392:ARG:CB	1:B:397:LYS:CG	2.91	0.49
1:C:307:ILE:O	1:C:308:LYS:C	2.54	0.49
1:B:287:ILE:HG23	1:B:331:PHE:HE1	1.75	0.49
3:C:801:ATP:N3	3:C:801:ATP:H5'1	2.27	0.49
1:A:695:TYR:CG	1:A:696:ASP:N	2.81	0.49
1:E:267:PHE:CZ	1:E:303:ALA:CB	2.95	0.49
1:C:209:ASN:CB	1:C:341:PHE:CE2	2.94	0.48
1:E:404:GLU:HG2	1:E:429:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:ARG:N	1:B:703:PRO:CD	2.76	0.48
1:D:291:ILE:O	1:D:292:GLY:C	2.53	0.48
1:F:219:GLY:HA2	4:F:801:ADP:C8	2.48	0.48
1:C:244:THR:CG2	1:C:246:TYR:CZ	2.95	0.48
1:E:589:ASN:N	1:E:589:ASN:OD1	2.40	0.48
1:B:642:ASN:CG	1:C:702:ARG:HG2	2.39	0.48
1:E:267:PHE:CZ	1:E:303:ALA:HA	2.48	0.48
1:F:526:GLU:O	1:F:530:VAL:HG23	2.13	0.48
1:C:311:LEU:CD2	1:C:341:PHE:CZ	2.97	0.48
1:D:288:HIS:NE2	1:D:326:GLU:HB3	2.27	0.48
1:E:404:GLU:OE2	1:E:433:ILE:HG13	2.12	0.48
1:F:263:PHE:CZ	1:F:294:GLY:HA3	2.49	0.47
1:F:499:VAL:C	4:F:802:ADP:N7	2.72	0.47
1:C:297:SER:OG	1:C:298:GLY:N	2.46	0.47
1:C:534:ILE:O	1:C:588:ASP:OD2	2.31	0.47
1:E:248:LEU:HD11	1:E:270:LEU:CD2	2.45	0.47
1:E:404:GLU:CD	1:E:429:VAL:HB	2.38	0.47
1:A:285:ASP:O	1:A:286:GLU:C	2.57	0.47
1:A:411:LEU:O	1:A:413:PRO:HD2	2.09	0.47
1:E:702:ARG:N	1:E:703:PRO:CD	2.77	0.47
1:B:218:VAL:HA	1:B:395:PRO:CG	2.45	0.47
1:B:222:ALA:HB1	3:B:801:ATP:C2	2.49	0.47
1:C:503:GLU:CB	3:C:802:ATP:H5'1	2.41	0.47
1:A:410:ARG:C	1:A:413:PRO:CD	2.88	0.47
1:A:410:ARG:HD3	1:F:203:CYS:O	2.15	0.47
1:B:285:ASP:CB	1:B:286:GLU:OE1	2.58	0.47
1:B:624:ASN:O	1:B:625:SER:HB2	2.15	0.47
1:E:362:LYS:HB3	1:E:363:PRO:HD3	1.97	0.47
1:B:588:ASP:OD1	1:B:588:ASP:C	2.57	0.47
1:C:330:ILE:C	1:C:332:GLU:N	2.73	0.47
1:C:538:PRO:HB2	1:D:542:GLY:HA3	1.95	0.47
1:D:197:ARG:NH1	1:E:432:ARG:O	2.48	0.47
3:D:802:ATP:N3	3:D:802:ATP:H2'	2.30	0.47
1:E:732:THR:H	1:E:744:TYR:HB3	1.80	0.47
1:E:736:ASP:OD1	1:E:737:LYS:N	2.46	0.47
1:A:219:GLY:CA	3:A:801:ATP:N7	2.77	0.47
1:C:357:ILE:HD13	3:C:801:ATP:N7	2.30	0.47
1:E:501:LYS:CG	3:E:802:ATP:O1B	2.53	0.47
1:E:285:ASP:O	1:E:286:GLU:C	2.58	0.47
1:C:526:GLU:HB3	1:C:528:HIS:CD2	2.51	0.46
1:A:442:SER:OG	1:A:443:GLN:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ALA:CB	3:B:801:ATP:H5'2	2.24	0.46
1:B:339:ARG:NH2	1:C:396:ASP:OD1	2.48	0.46
1:E:702:ARG:HB2	1:E:703:PRO:CD	2.35	0.46
1:F:357:ILE:CD1	4:F:801:ADP:C2	2.98	0.46
1:D:538:PRO:CA	1:D:543:PHE:CE1	2.98	0.46
1:A:188:LEU:HD22	3:A:801:ATP:N6	2.31	0.46
1:A:293:ALA:HA	1:A:302:ASP:OD2	2.16	0.46
1:A:362:LYS:HE3	1:A:373:TYR:HB2	1.97	0.46
1:C:219:GLY:C	3:C:801:ATP:O1A	2.58	0.46
1:D:296:ALA:H	1:D:300:GLN:CB	2.25	0.46
1:E:358:ILE:O	1:E:362:LYS:N	2.45	0.46
1:F:191:ARG:NE	1:F:194:GLU:HG3	2.30	0.46
1:C:340:ARG:C	1:C:341:PHE:CD1	2.94	0.46
1:F:357:ILE:CD1	4:F:801:ADP:N1	2.79	0.46
1:F:216:SER:HA	4:F:801:ADP:PB	2.55	0.46
1:B:230:ARG:HB3	1:B:236:VAL:CG1	2.45	0.46
1:B:386:VAL:CG2	1:B:394:LEU:HD21	2.45	0.46
1:A:194:GLU:CD	1:A:194:GLU:H	2.24	0.45
1:F:191:ARG:NH2	1:F:194:GLU:CG	2.75	0.45
1:B:285:ASP:O	1:B:286:GLU:C	2.59	0.45
1:E:521:MET:HB2	1:E:565:GLU:O	2.17	0.45
1:C:287:ILE:O	1:C:290:ILE:HG12	2.17	0.45
1:F:209:ASN:HB2	1:F:340:ARG:O	2.15	0.45
1:A:461:PHE:CD1	1:A:660:GLN:HB3	2.51	0.45
1:C:395:PRO:CB	3:C:801:ATP:C8	2.67	0.45
1:E:404:GLU:OE1	1:E:433:ILE:HG12	2.16	0.45
1:F:221:THR:CG2	4:F:801:ADP:O1A	2.60	0.45
1:B:207:LYS:HE2	1:C:396:ASP:OD1	2.17	0.45
1:B:521:MET:HB2	1:B:564:ASP:O	2.17	0.45
1:C:287:ILE:CG1	1:C:331:PHE:HE1	2.30	0.45
1:C:483:HIS:CG	1:C:484:GLU:H	2.33	0.45
1:D:567:GLU:OE2	1:D:606:ASN:HB2	2.17	0.45
1:B:642:ASN:O	1:C:702:ARG:HG2	2.17	0.45
1:D:288:HIS:NE2	1:D:326:GLU:HG2	2.32	0.45
1:E:248:LEU:HD13	1:E:253:LEU:HD12	1.99	0.45
1:B:643:ARG:NH2	3:C:802:ATP:PG	2.90	0.44
1:F:357:ILE:HG21	4:F:801:ADP:C2	2.52	0.44
1:B:642:ASN:O	1:C:702:ARG:HD2	2.17	0.44
1:C:627:ASP:OD1	1:C:628:ALA:N	2.50	0.44
1:B:258:LYS:O	1:B:259:TYR:HB2	2.17	0.44
3:B:801:ATP:H3'	3:B:801:ATP:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PHE:CD2	1:C:331:PHE:O	2.71	0.44
1:A:221:THR:CG2	3:A:801:ATP:O2B	2.63	0.44
1:B:642:ASN:CG	1:C:702:ARG:CG	2.91	0.44
1:D:288:HIS:HE1	1:D:326:GLU:OE1	2.01	0.44
1:B:195:LEU:O	1:B:196:GLU:C	2.59	0.44
1:A:293:ALA:CA	1:A:302:ASP:OD2	2.66	0.44
1:B:540:TYR:OH	1:C:528:HIS:HB2	2.16	0.44
1:C:327:PHE:O	1:C:332:GLU:HG3	2.18	0.44
1:C:404:GLU:HG2	1:C:429:VAL:HG13	1.99	0.44
1:C:461:PHE:N	3:C:802:ATP:HN62	2.15	0.44
1:C:714:LYS:HB2	1:C:715:PRO:HD3	2.00	0.44
1:A:714:LYS:N	1:A:715:PRO:CD	2.81	0.43
1:E:250:ILE:CB	1:E:254:LEU:HD22	2.38	0.43
1:E:696:ASP:C	1:E:696:ASP:OD1	2.59	0.43
1:D:567:GLU:CD	1:D:606:ASN:H	2.26	0.43
1:F:357:ILE:CG2	4:F:801:ADP:C2	3.01	0.43
1:A:330:ILE:HG13	1:A:331:PHE:N	2.32	0.43
1:A:642:ASN:HB3	1:B:702:ARG:CD	2.39	0.43
1:C:702:ARG:N	1:C:703:PRO:HD2	2.34	0.43
1:D:519:PHE:CZ	1:D:549:LEU:HA	2.53	0.43
1:E:357:ILE:HG23	4:E:801:ADP:N3	2.34	0.43
1:C:188:LEU:CD1	3:C:801:ATP:HN62	2.28	0.43
1:C:267:PHE:CD2	1:C:306:LEU:HD13	2.53	0.43
1:C:528:HIS:CD2	1:C:528:HIS:H	2.36	0.43
1:A:188:LEU:HD11	1:A:223:ILE:HA	2.01	0.43
3:C:802:ATP:C8	3:C:802:ATP:H5'2	2.53	0.43
1:D:171:ASN:N	1:D:171:ASN:OD1	2.50	0.43
1:D:203:CYS:HB2	1:E:410:ARG:NH2	2.34	0.43
1:E:495:GLY:O	1:E:609:VAL:HG12	2.19	0.43
1:A:412:MET:C	1:A:414:VAL:N	2.77	0.43
1:B:658:ILE:HG13	1:B:695:TYR:CD1	2.54	0.43
1:C:412:MET:HB2	1:C:413:PRO:HD3	2.00	0.43
1:F:702:ARG:N	1:F:703:PRO:HD2	2.33	0.43
1:C:327:PHE:HE1	1:C:331:PHE:CE2	2.37	0.43
1:D:682:VAL:O	1:D:687:ARG:NH1	2.51	0.43
1:F:736:ASP:OD1	1:F:736:ASP:C	2.60	0.43
1:E:501:LYS:N	3:E:802:ATP:O1B	2.51	0.43
1:B:540:TYR:CZ	1:C:528:HIS:CB	2.99	0.42
1:D:199:ILE:HG21	1:E:411:LEU:HD11	1.98	0.42
1:E:736:ASP:HB3	1:E:740:ASN:H	1.83	0.42
1:A:407:ALA:CB	1:F:204:ARG:HG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:LYS:HA	1:A:641:ARG:NE	2.34	0.42
1:A:195:LEU:HD13	1:A:230:ARG:HD2	2.02	0.42
1:A:588:ASP:C	1:A:588:ASP:OD1	2.59	0.42
1:D:696:ASP:OD1	1:D:696:ASP:C	2.58	0.42
1:A:484:GLU:H	1:A:484:GLU:CD	2.25	0.42
1:A:658:ILE:HD11	1:A:695:TYR:CD1	2.54	0.42
1:D:642:ASN:O	1:E:702:ARG:HD2	2.20	0.42
1:A:577:LEU:O	1:A:578:LEU:C	2.60	0.42
1:E:267:PHE:CZ	1:E:303:ALA:O	2.73	0.42
1:A:195:LEU:HD13	1:A:230:ARG:CD	2.49	0.42
1:B:540:TYR:OH	1:C:528:HIS:CB	2.67	0.42
1:B:736:ASP:C	1:B:736:ASP:OD1	2.62	0.42
1:C:287:ILE:HG23	1:C:331:PHE:HD1	1.74	0.42
1:C:318:VAL:HB	1:C:341:PHE:HE2	1.85	0.42
1:C:491:PHE:HB3	1:C:646:ASN:H	1.84	0.42
1:C:696:ASP:C	1:C:696:ASP:OD1	2.60	0.42
1:D:606:ASN:OD1	3:D:802:ATP:O2G	2.37	0.42
1:D:701:ALA:HB3	3:D:802:ATP:H1'	2.00	0.42
1:B:297:SER:OG	1:B:298:GLY:N	2.52	0.42
1:F:744:TYR:CG	1:F:745:GLY:N	2.87	0.42
1:B:519:PHE:CZ	1:B:549:LEU:HA	2.54	0.42
1:B:544:ASP:O	1:B:544:ASP:CG	2.61	0.42
1:C:483:HIS:CG	1:C:484:GLU:N	2.87	0.42
1:D:394:LEU:O	1:D:395:PRO:C	2.61	0.42
1:D:714:LYS:HB2	1:D:715:PRO:HD3	2.02	0.42
1:A:254:LEU:CG	1:A:295:ALA:HB2	2.50	0.42
1:B:577:LEU:O	1:B:578:LEU:C	2.61	0.42
1:F:431:ALA:O	1:F:432:ARG:C	2.63	0.42
1:B:189:ILE:H	3:B:801:ATP:N6	2.04	0.42
1:D:373:TYR:CE2	1:D:421:VAL:HG21	2.55	0.42
1:E:702:ARG:CB	1:E:703:PRO:HD3	2.29	0.42
1:D:288:HIS:CE1	1:D:326:GLU:CG	3.02	0.41
1:F:549:LEU:O	1:F:553:VAL:HG23	2.20	0.41
1:B:582:ASP:CB	1:B:643:ARG:NH1	2.83	0.41
1:C:327:PHE:O	1:C:332:GLU:HB2	2.21	0.41
1:F:322:THR:OG1	1:F:323:THR:N	2.53	0.41
1:B:392:ARG:HB2	1:B:397:LYS:HD3	2.02	0.41
1:C:257:THR:C	1:C:258:LYS:HG3	2.46	0.41
1:E:250:ILE:CG2	1:E:289:THR:HG21	2.50	0.41
1:F:656:ASP:OD1	1:F:656:ASP:N	2.49	0.41
1:A:295:ALA:C	1:A:296:ALA:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ASP:OD2	1:C:418:LYS:NZ	2.54	0.41
1:D:502:THR:HB	3:D:802:ATP:O2A	2.21	0.41
1:E:404:GLU:OE1	1:E:433:ILE:HG13	2.20	0.41
1:A:470:LEU:HD21	1:A:491:PHE:HE1	1.81	0.41
1:A:540:TYR:OH	1:C:526:GLU:HG2	2.21	0.41
1:A:585:THR:HA	1:A:596:PHE:CE2	2.56	0.41
1:D:371:VAL:CG2	1:D:373:TYR:CE1	3.04	0.41
1:D:665:PHE:HZ	3:D:802:ATP:HO2'	1.60	0.41
1:F:451:ASN:O	1:F:455:ARG:HG3	2.21	0.41
1:A:520:ASP:OD1	1:A:520:ASP:C	2.64	0.41
1:B:491:PHE:CE2	1:B:645:ASP:CB	3.03	0.41
1:C:188:LEU:CD1	3:C:801:ATP:N6	2.81	0.41
1:B:702:ARG:CB	1:B:703:PRO:HD3	2.50	0.40
1:C:588:ASP:O	1:D:532:ARG:NH2	2.54	0.40
1:F:257:THR:OG1	1:F:258:LYS:N	2.54	0.40
1:A:701:ALA:HB1	4:A:802:ADP:C8	2.53	0.40
1:B:696:ASP:C	1:B:696:ASP:OD1	2.61	0.40
1:C:257:THR:O	1:C:258:LYS:CG	2.69	0.40
1:C:537:PRO:HG2	1:D:528:HIS:ND1	2.36	0.40
1:E:682:VAL:O	1:E:687:ARG:NH1	2.52	0.40
1:B:339:ARG:NH1	3:C:801:ATP:O2G	2.55	0.40
1:F:701:ALA:O	1:F:702:ARG:C	2.64	0.40
1:F:706:ARG:HD2	1:F:706:ARG:HA	1.84	0.40
1:A:540:TYR:CE1	1:B:528:HIS:HB2	2.57	0.40
1:C:238:GLU:OE1	1:C:238:GLU:N	2.46	0.40
1:C:461:PHE:H	3:C:802:ATP:N6	2.18	0.40
1:C:631:GLU:O	1:C:632:ILE:C	2.61	0.40
1:E:308:LYS:HB2	1:E:309:PRO:HD3	2.02	0.40
1:E:514:ILE:CG2	1:E:559:ALA:HA	2.51	0.40
1:F:491:PHE:CD1	1:F:491:PHE:N	2.89	0.40
1:A:410:ARG:C	1:A:413:PRO:HD2	2.47	0.40
1:A:736:ASP:OD1	1:A:736:ASP:C	2.64	0.40
1:C:267:PHE:CE2	1:C:306:LEU:HB2	2.57	0.40
1:E:248:LEU:HD23	1:E:248:LEU:HA	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/758 (76%)	561 (97%)	10 (2%)	5 (1%)	14	48
1	B	576/758 (76%)	563 (98%)	12 (2%)	1 (0%)	43	76
1	C	576/758 (76%)	550 (96%)	23 (4%)	3 (0%)	24	60
1	D	576/758 (76%)	559 (97%)	15 (3%)	2 (0%)	36	70
1	E	576/758 (76%)	564 (98%)	10 (2%)	2 (0%)	36	70
1	F	576/758 (76%)	563 (98%)	12 (2%)	1 (0%)	43	76
All	All	3456/4548 (76%)	3360 (97%)	82 (2%)	14 (0%)	31	65

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ALA
1	A	695	TYR
1	A	696	ASP
1	D	294	GLY
1	F	546	GLY
1	A	294	GLY
1	A	629	MET
1	B	625	SER
1	D	220	LYS
1	C	331	PHE
1	E	259	TYR
1	C	541	VAL
1	C	186	ASP
1	E	251	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/639 (76%)	484 (100%)	1 (0%)	87	92
1	B	485/639 (76%)	479 (99%)	6 (1%)	63	82
1	C	485/639 (76%)	483 (100%)	2 (0%)	84	90
1	D	485/639 (76%)	482 (99%)	3 (1%)	78	88
1	E	485/639 (76%)	483 (100%)	2 (0%)	84	90
1	F	485/639 (76%)	485 (100%)	0	100	100
All	All	2910/3834 (76%)	2896 (100%)	14 (0%)	78	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	GLN
1	B	207	LYS
1	B	324	TYR
1	B	331	PHE
1	B	339	ARG
1	B	348	GLU
1	B	642	ASN
1	C	463	GLN
1	C	491	PHE
1	D	302	ASP
1	D	348	GLU
1	D	582	ASP
1	E	526	GLU
1	E	544	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	368	HIS
1	A	528	HIS
1	A	590	ASN
1	B	273	GLN
1	B	300	GLN
1	B	393	HIS
1	B	558	HIS

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Mol	Chain	Res	Type
1	B	583	ASN
1	B	590	ASN
1	B	652	HIS
1	C	356	GLN
1	C	583	ASN
1	C	684	GLN
1	D	684	GLN
1	E	652	HIS
1	F	177	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 ⓘ

12 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	ATP	E	802	-	32,33,33	4.22	15 (46%)	48,52,52	3.89	15 (31%)
4	ADP	F	801	-	28,29,29	3.00	10 (35%)	43,45,45	1.99	9 (20%)
3	ATP	D	801	-	32,33,33	3.63	11 (34%)	48,52,52	1.81	9 (18%)
3	ATP	D	802	-	32,33,33	3.63	11 (34%)	48,52,52	1.81	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	801	-	32,33,33	4.22	15 (46%)	48,52,52	3.85	14 (29%)
4	ADP	F	802	-	28,29,29	3.00	10 (35%)	43,45,45	1.99	9 (20%)
3	ATP	C	801	-	32,33,33	3.64	11 (34%)	48,52,52	1.80	8 (16%)
4	ADP	A	802	-	28,29,29	2.99	10 (35%)	43,45,45	1.99	9 (20%)
4	ADP	E	801	-	28,29,29	2.99	10 (35%)	43,45,45	1.99	9 (20%)
3	ATP	C	802	-	32,33,33	3.63	11 (34%)	48,52,52	1.81	9 (18%)
3	ATP	B	801	-	32,33,33	3.63	11 (34%)	48,52,52	1.81	9 (18%)
3	ATP	B	802	-	32,33,33	4.23	15 (46%)	48,52,52	3.89	15 (31%)

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	802	-	-	1/22/38/38	0/3/3/3
4	ADP	F	801	-	-	1/16/32/32	0/3/3/3
3	ATP	D	801	-	-	5/22/38/38	0/3/3/3
3	ATP	D	802	-	-	4/22/38/38	0/3/3/3
3	ATP	A	801	-	-	6/22/38/38	0/3/3/3
4	ADP	F	802	-	-	3/16/32/32	0/3/3/3
3	ATP	C	801	-	-	5/22/38/38	0/3/3/3
4	ADP	A	802	-	-	2/16/32/32	0/3/3/3
4	ADP	E	801	-	-	3/16/32/32	0/3/3/3
3	ATP	C	802	-	-	9/22/38/38	0/3/3/3
3	ATP	B	801	-	-	5/22/38/38	0/3/3/3
3	ATP	B	802	-	-	3/22/38/38	0/3/3/3

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	ATP	C5-C4	13.38	1.63	1.39
3	E	802	ATP	C5-C4	13.38	1.63	1.39
3	A	801	ATP	C5-C4	13.37	1.62	1.39
3	C	801	ATP	C2'-C3'	-10.72	1.24	1.53
3	D	801	ATP	C2'-C3'	-10.71	1.24	1.53
3	C	802	ATP	C2'-C3'	-10.68	1.24	1.53
3	B	801	ATP	C2'-C3'	-10.67	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	ATP	C2'-C3'	-10.66	1.24	1.53
3	A	801	ATP	C8-N7	-9.60	1.13	1.31
3	B	802	ATP	C8-N7	-9.54	1.13	1.31
3	E	802	ATP	C8-N7	-9.54	1.13	1.31
3	E	802	ATP	C8-N9	-8.36	1.23	1.37
3	B	802	ATP	C8-N9	-8.35	1.23	1.37
3	D	801	ATP	O4'-C4'	-8.19	1.26	1.45
3	A	801	ATP	C8-N9	-8.16	1.23	1.37
3	C	802	ATP	O4'-C4'	-8.16	1.26	1.45
3	B	801	ATP	O4'-C4'	-8.16	1.26	1.45
3	D	802	ATP	O4'-C4'	-8.15	1.26	1.45
3	C	801	ATP	O4'-C4'	-8.13	1.26	1.45
4	E	801	ADP	C3'-C4'	-7.60	1.33	1.53
4	F	801	ADP	C3'-C4'	-7.57	1.33	1.53
4	F	802	ADP	C3'-C4'	-7.57	1.33	1.53
4	A	802	ADP	C3'-C4'	-7.55	1.33	1.53
4	F	802	ADP	O4'-C4'	6.66	1.59	1.45
4	A	802	ADP	O4'-C4'	6.64	1.59	1.45
4	E	801	ADP	O4'-C4'	6.64	1.59	1.45
4	F	801	ADP	O4'-C4'	6.63	1.59	1.45
3	D	802	ATP	PA-O3A	6.31	1.66	1.59
3	B	801	ATP	C6-N6	6.30	1.50	1.34
3	C	801	ATP	C6-N6	6.29	1.50	1.34
3	C	802	ATP	C6-N6	6.28	1.50	1.34
3	D	802	ATP	C6-N6	6.27	1.50	1.34
3	C	802	ATP	PA-O3A	6.27	1.66	1.59
3	C	801	ATP	PA-O3A	6.27	1.66	1.59
3	D	801	ATP	PA-O3A	6.26	1.66	1.59
3	D	801	ATP	C6-N6	6.26	1.50	1.34
3	B	801	ATP	PA-O3A	6.23	1.66	1.59
3	B	801	ATP	PB-O3B	6.18	1.66	1.59
3	D	802	ATP	PB-O3B	6.18	1.66	1.59
3	C	801	ATP	PB-O3B	6.16	1.66	1.59
3	C	802	ATP	PB-O3B	6.16	1.66	1.59
3	D	801	ATP	PB-O3B	6.12	1.66	1.59
3	A	801	ATP	PB-O3B	5.39	1.65	1.59
3	B	802	ATP	PB-O3B	5.38	1.65	1.59
3	B	802	ATP	PB-O3A	5.37	1.65	1.59
3	A	801	ATP	PA-O3A	5.34	1.65	1.59
3	B	802	ATP	PA-O3A	5.33	1.65	1.59
3	E	802	ATP	PB-O3A	5.33	1.65	1.59
3	E	802	ATP	PA-O3A	5.33	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	802	ATP	PB-O3B	5.30	1.65	1.59
3	A	801	ATP	PB-O3A	5.30	1.65	1.59
4	A	802	ADP	O4'-C1'	5.21	1.54	1.42
4	F	801	ADP	C6-N6	5.21	1.47	1.34
3	B	801	ATP	C3'-C4'	5.20	1.66	1.53
3	D	801	ATP	C3'-C4'	5.20	1.66	1.53
3	C	801	ATP	C3'-C4'	5.20	1.66	1.53
4	E	801	ADP	O4'-C1'	5.19	1.54	1.42
3	C	802	ATP	C3'-C4'	5.19	1.66	1.53
4	F	802	ADP	C6-N6	5.19	1.47	1.34
4	E	801	ADP	C6-N6	5.19	1.47	1.34
4	A	802	ADP	C6-N6	5.19	1.47	1.34
3	D	802	ATP	C3'-C4'	5.18	1.66	1.53
4	F	801	ADP	O4'-C1'	5.17	1.54	1.42
4	F	802	ADP	O4'-C1'	5.17	1.54	1.42
4	F	802	ADP	PA-O3A	5.13	1.65	1.59
4	F	801	ADP	PA-O3A	5.08	1.65	1.59
4	F	802	ADP	C2'-C1'	-5.07	1.37	1.53
4	F	801	ADP	C2'-C1'	-5.07	1.37	1.53
4	A	802	ADP	C2'-C1'	-5.06	1.37	1.53
4	E	801	ADP	C2'-C1'	-5.06	1.37	1.53
3	B	802	ATP	C4-N3	-5.02	1.25	1.34
3	E	802	ATP	C4-N3	-5.01	1.25	1.34
4	A	802	ADP	PA-O3A	5.01	1.64	1.59
3	A	801	ATP	C4-N3	-5.01	1.25	1.34
4	E	801	ADP	PA-O3A	4.99	1.64	1.59
3	C	801	ATP	O4'-C1'	4.75	1.53	1.42
3	C	802	ATP	O4'-C1'	4.74	1.53	1.42
3	B	801	ATP	O4'-C1'	4.74	1.53	1.42
3	D	802	ATP	O4'-C1'	4.72	1.52	1.42
3	D	801	ATP	O4'-C1'	4.72	1.52	1.42
3	D	802	ATP	C1'-N9	-4.68	1.33	1.46
3	D	801	ATP	C1'-N9	-4.67	1.33	1.46
3	B	801	ATP	C1'-N9	-4.66	1.33	1.46
3	C	802	ATP	C1'-N9	-4.64	1.33	1.46
3	C	801	ATP	C1'-N9	-4.64	1.33	1.46
3	A	801	ATP	C6-N6	4.45	1.45	1.34
3	E	802	ATP	C6-N6	4.44	1.45	1.34
3	B	802	ATP	C6-N6	4.41	1.45	1.34
3	A	801	ATP	O4'-C1'	4.38	1.52	1.42
3	E	802	ATP	C2-N3	-4.34	1.26	1.33
3	A	801	ATP	C2-N3	-4.31	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	ATP	C2-N3	-4.30	1.26	1.33
3	A	801	ATP	C4-N9	4.26	1.46	1.37
3	E	802	ATP	O4'-C1'	4.21	1.51	1.42
3	B	802	ATP	O4'-C1'	4.20	1.51	1.42
3	B	802	ATP	C4-N9	4.14	1.46	1.37
3	B	801	ATP	PB-O3A	4.13	1.64	1.59
3	E	802	ATP	C4-N9	4.12	1.46	1.37
3	C	801	ATP	PB-O3A	4.12	1.63	1.59
3	C	802	ATP	PB-O3A	4.12	1.63	1.59
3	D	801	ATP	PB-O3A	4.11	1.63	1.59
3	D	802	ATP	PB-O3A	4.06	1.63	1.59
3	C	801	ATP	O2'-C2'	3.56	1.51	1.43
3	C	802	ATP	O2'-C2'	3.56	1.51	1.43
3	B	801	ATP	O2'-C2'	3.55	1.51	1.43
3	D	801	ATP	O2'-C2'	3.54	1.51	1.43
3	D	802	ATP	O2'-C2'	3.54	1.51	1.43
4	A	802	ADP	C5-N7	-3.35	1.33	1.39
4	F	801	ADP	C5-N7	-3.34	1.33	1.39
4	E	801	ADP	C5-N7	-3.28	1.33	1.39
4	F	802	ADP	C5-N7	-3.26	1.33	1.39
4	E	801	ADP	C2'-C3'	3.24	1.62	1.53
4	F	802	ADP	C2'-C3'	3.23	1.62	1.53
4	A	802	ADP	C2'-C3'	3.23	1.62	1.53
4	F	801	ADP	C2'-C3'	3.21	1.62	1.53
3	B	802	ATP	O4'-C4'	2.99	1.51	1.45
3	E	802	ATP	O4'-C4'	2.96	1.51	1.45
3	A	801	ATP	O4'-C4'	2.93	1.51	1.45
3	E	802	ATP	C2'-C3'	-2.90	1.45	1.53
3	B	802	ATP	C2'-C3'	-2.89	1.45	1.53
3	A	801	ATP	C2'-C3'	-2.89	1.45	1.53
4	F	802	ADP	C8-N9	-2.74	1.32	1.37
4	A	802	ADP	C8-N9	-2.73	1.32	1.37
4	F	801	ADP	C8-N9	-2.69	1.33	1.37
4	E	801	ADP	C8-N9	-2.68	1.33	1.37
3	D	802	ATP	O3'-C3'	2.52	1.49	1.43
3	B	801	ATP	O3'-C3'	2.50	1.49	1.43
3	C	801	ATP	O3'-C3'	2.50	1.49	1.43
3	C	802	ATP	O3'-C3'	2.50	1.49	1.43
3	D	801	ATP	O3'-C3'	2.50	1.49	1.43
3	B	802	ATP	C6-N1	2.42	1.42	1.35
3	E	802	ATP	C6-N1	2.40	1.42	1.35
3	A	801	ATP	C6-N1	2.39	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ATP	C5-C6	2.28	1.47	1.41
4	F	802	ADP	C4-N9	-2.27	1.33	1.37
4	F	801	ADP	C4-N9	-2.26	1.33	1.37
3	B	802	ATP	C5-C6	2.26	1.47	1.41
4	E	801	ADP	C4-N9	-2.23	1.33	1.37
3	E	802	ATP	C5-C6	2.23	1.47	1.41
4	A	802	ADP	C4-N9	-2.23	1.33	1.37

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	ATP	C5-C4-N9	-13.53	91.07	105.81
3	E	802	ATP	C5-C4-N9	-13.50	91.09	105.81
3	E	802	ATP	N3-C4-N9	13.35	149.88	127.17
3	B	802	ATP	N3-C4-N9	13.33	149.84	127.17
3	A	801	ATP	C5-C4-N9	-13.27	91.34	105.81
3	A	801	ATP	N3-C4-N9	13.20	149.62	127.17
3	E	802	ATP	C4-N9-C8	9.77	116.00	105.74
3	B	802	ATP	C4-N9-C8	9.75	115.97	105.74
3	A	801	ATP	C4-N9-C8	9.22	115.42	105.74
3	A	801	ATP	C6-C5-N7	6.85	145.29	132.09
3	E	802	ATP	C6-C5-N7	6.80	145.21	132.09
3	B	802	ATP	C6-C5-N7	6.80	145.20	132.09
3	A	801	ATP	C2-N3-C4	6.28	127.17	111.83
3	E	802	ATP	C2-N3-C4	6.28	127.16	111.83
3	B	802	ATP	C2-N3-C4	6.26	127.12	111.83
4	E	801	ADP	C5-C4-N3	-6.25	118.11	126.72
4	F	802	ADP	C5-C4-N3	-6.24	118.13	126.72
4	F	801	ADP	C5-C4-N3	-6.23	118.14	126.72
4	A	802	ADP	C5-C4-N3	-6.18	118.21	126.72
3	C	801	ATP	C5-C4-N3	-6.07	118.36	126.72
3	B	801	ATP	C5-C4-N3	-6.07	118.36	126.72
3	D	801	ATP	C5-C4-N3	-6.04	118.40	126.72
3	D	802	ATP	C5-C4-N3	-6.03	118.41	126.72
3	C	802	ATP	C5-C4-N3	-6.03	118.41	126.72
3	A	801	ATP	C5-N7-C8	5.76	112.50	103.45
3	B	802	ATP	C5-N7-C8	5.72	112.43	103.45
3	E	802	ATP	C5-N7-C8	5.71	112.42	103.45
3	E	802	ATP	C5-C4-N3	-5.58	119.03	126.72
3	A	801	ATP	C5-C4-N3	-5.58	119.04	126.72
3	B	802	ATP	C5-C4-N3	-5.53	119.10	126.72
3	A	801	ATP	C4-C5-N7	-5.42	104.39	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	802	ATP	C4-C5-N7	-5.38	104.42	110.58
3	B	802	ATP	C4-C5-N7	-5.35	104.47	110.58
3	A	801	ATP	C6-C5-C4	-5.02	110.32	117.18
3	B	802	ATP	C6-C5-C4	-5.01	110.33	117.18
3	E	802	ATP	C6-C5-C4	-4.99	110.37	117.18
4	E	801	ADP	N3-C4-N9	4.86	135.44	127.17
4	F	802	ADP	N3-C4-N9	4.86	135.43	127.17
4	F	801	ADP	N3-C4-N9	4.85	135.42	127.17
4	A	802	ADP	N3-C4-N9	4.84	135.40	127.17
4	E	801	ADP	N3-C2-N1	-4.41	121.91	128.58
4	F	801	ADP	N3-C2-N1	-4.41	121.91	128.58
4	A	802	ADP	N3-C2-N1	-4.40	121.92	128.58
4	F	802	ADP	N3-C2-N1	-4.39	121.94	128.58
3	B	801	ATP	N3-C4-N9	4.34	134.54	127.17
3	C	801	ATP	N3-C4-N9	4.34	134.54	127.17
3	C	802	ATP	N3-C4-N9	4.33	134.53	127.17
3	D	802	ATP	N3-C4-N9	4.31	134.50	127.17
3	D	801	ATP	N3-C4-N9	4.31	134.49	127.17
3	D	801	ATP	N3-C2-N1	-4.21	122.20	128.58
3	C	801	ATP	N3-C2-N1	-4.20	122.22	128.58
3	D	802	ATP	N3-C2-N1	-4.18	122.25	128.58
3	C	802	ATP	N3-C2-N1	-4.16	122.28	128.58
3	B	801	ATP	N3-C2-N1	-4.15	122.30	128.58
4	E	801	ADP	C2-N3-C4	3.83	121.17	111.83
4	F	801	ADP	C2-N3-C4	3.82	121.16	111.83
4	F	802	ADP	C2-N3-C4	3.81	121.14	111.83
4	A	802	ADP	C2-N3-C4	3.81	121.13	111.83
3	C	801	ATP	C2-N3-C4	3.67	120.80	111.83
3	B	801	ATP	C2-N3-C4	3.65	120.75	111.83
3	D	801	ATP	C2-N3-C4	3.65	120.73	111.83
3	C	802	ATP	C2-N3-C4	3.64	120.73	111.83
3	D	802	ATP	C2-N3-C4	3.64	120.73	111.83
3	A	801	ATP	C3'-C2'-C1'	3.60	108.28	101.46
3	B	802	ATP	N3-C2-N1	-3.47	123.32	128.58
3	E	802	ATP	N3-C2-N1	-3.47	123.33	128.58
3	A	801	ATP	N3-C2-N1	-3.47	123.34	128.58
4	F	801	ADP	N9-C8-N7	-3.46	109.03	113.94
4	A	802	ADP	N9-C8-N7	-3.46	109.03	113.94
3	D	801	ATP	C4-C5-N7	-3.43	106.66	110.58
4	E	801	ADP	N9-C8-N7	-3.43	109.06	113.94
4	F	802	ADP	N9-C8-N7	-3.43	109.07	113.94
3	D	802	ATP	C4-C5-N7	-3.41	106.69	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	802	ATP	C3'-C2'-C1'	3.40	107.89	101.46
3	B	801	ATP	C4-C5-N7	-3.40	106.70	110.58
3	C	801	ATP	C4-C5-N7	-3.39	106.70	110.58
3	B	802	ATP	C3'-C2'-C1'	3.38	107.86	101.46
3	C	802	ATP	C4-C5-N7	-3.38	106.72	110.58
4	F	801	ADP	C5-N7-C8	3.34	108.69	103.45
4	A	802	ADP	C5-N7-C8	3.33	108.68	103.45
4	E	801	ADP	C5-N7-C8	3.29	108.63	103.45
4	F	802	ADP	C5-N7-C8	3.26	108.57	103.45
3	D	801	ATP	C5-N7-C8	3.25	108.55	103.45
3	D	802	ATP	C5-N7-C8	3.22	108.52	103.45
3	C	802	ATP	C5-N7-C8	3.22	108.51	103.45
3	B	801	ATP	C5-N7-C8	3.21	108.50	103.45
4	F	801	ADP	C4-C5-N7	-3.19	106.93	110.58
3	C	801	ATP	C5-N7-C8	3.19	108.46	103.45
4	F	802	ADP	C4-C5-N7	-3.16	106.97	110.58
4	E	801	ADP	C4-C5-N7	-3.16	106.97	110.58
4	A	802	ADP	C4-C5-N7	-3.16	106.97	110.58
3	C	802	ATP	N9-C8-N7	-3.14	109.48	113.94
3	D	801	ATP	N9-C8-N7	-3.13	109.50	113.94
3	B	801	ATP	N9-C8-N7	-3.12	109.51	113.94
3	D	802	ATP	N9-C8-N7	-3.11	109.53	113.94
3	C	801	ATP	N9-C8-N7	-3.06	109.59	113.94
4	F	802	ADP	C4-N9-C8	3.05	108.94	105.74
4	A	802	ADP	C4-N9-C8	3.03	108.92	105.74
4	F	801	ADP	C4-N9-C8	3.02	108.90	105.74
4	E	801	ADP	C4-N9-C8	3.00	108.89	105.74
3	B	802	ATP	C2'-C3'-C4'	2.65	107.72	102.61
3	E	802	ATP	C2'-C3'-C4'	2.63	107.68	102.61
3	A	801	ATP	C2'-C3'-C4'	2.54	107.51	102.61
3	C	802	ATP	C4-N9-C8	2.37	108.23	105.74
3	B	801	ATP	C4-N9-C8	2.35	108.21	105.74
3	D	801	ATP	C4-N9-C8	2.33	108.19	105.74
3	D	802	ATP	C4-N9-C8	2.33	108.19	105.74
3	C	801	ATP	C4-N9-C8	2.29	108.14	105.74
4	A	802	ADP	C3'-C2'-C1'	2.28	105.78	101.46
4	F	801	ADP	C3'-C2'-C1'	2.26	105.74	101.46
4	E	801	ADP	C3'-C2'-C1'	2.25	105.71	101.46
4	F	802	ADP	C3'-C2'-C1'	2.24	105.71	101.46
3	E	802	ATP	C1'-N9-C8	-2.22	122.17	127.09
3	B	802	ATP	C1'-N9-C8	-2.21	122.18	127.09
3	A	801	ATP	C4-N9-C1'	-2.20	121.48	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	802	ATP	C4'-O4'-C1'	-2.18	104.66	109.47
3	B	802	ATP	C4'-O4'-C1'	-2.17	104.67	109.47
3	A	801	ATP	C4'-O4'-C1'	-2.15	104.71	109.47
3	D	802	ATP	C3'-C2'-C1'	2.07	105.38	101.46
3	D	801	ATP	C3'-C2'-C1'	2.06	105.36	101.46
3	C	802	ATP	C3'-C2'-C1'	2.06	105.35	101.46
3	B	801	ATP	C3'-C2'-C1'	2.05	105.34	101.46
3	E	802	ATP	C4-N9-C1'	-2.05	121.84	126.63
3	B	802	ATP	C4-N9-C1'	-2.05	121.85	126.63

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	ATP	C4'-C5'-O5'-PA
3	B	801	ATP	C3'-C4'-C5'-O5'
3	B	802	ATP	PB-O3B-PG-O3G
3	C	801	ATP	O4'-C4'-C5'-O5'
3	D	801	ATP	C5'-O5'-PA-O3A
3	D	801	ATP	C3'-C4'-C5'-O5'
3	D	802	ATP	PB-O3B-PG-O2G
3	D	802	ATP	C5'-O5'-PA-O1A
4	E	801	ADP	C5'-O5'-PA-O1A
4	F	802	ADP	C5'-O5'-PA-O3A
3	A	801	ATP	O4'-C4'-C5'-O5'
3	B	801	ATP	O4'-C4'-C5'-O5'
3	C	801	ATP	C3'-C4'-C5'-O5'
3	C	802	ATP	C3'-C4'-C5'-O5'
3	D	801	ATP	O4'-C4'-C5'-O5'
3	A	801	ATP	C3'-C4'-C5'-O5'
3	C	802	ATP	O4'-C4'-C5'-O5'
3	A	801	ATP	C4'-C5'-O5'-PA
3	D	802	ATP	C3'-C4'-C5'-O5'
3	D	802	ATP	O4'-C4'-C5'-O5'
3	E	802	ATP	PG-O3B-PB-O1B
3	C	801	ATP	C4'-C5'-O5'-PA
3	C	802	ATP	PB-O3B-PG-O1G
3	B	801	ATP	PA-O3A-PB-O1B
3	B	802	ATP	PA-O3A-PB-O2B
3	C	802	ATP	PA-O3A-PB-O2B
4	F	801	ADP	PB-O3A-PA-O2A
4	E	801	ADP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	A	801	ATP	C5'-O5'-PA-O1A
3	B	801	ATP	C5'-O5'-PA-O1A
3	C	802	ATP	C5'-O5'-PA-O3A
3	D	801	ATP	C5'-O5'-PA-O1A
4	A	802	ADP	C5'-O5'-PA-O2A
4	A	802	ADP	C5'-O5'-PA-O3A
4	E	801	ADP	C5'-O5'-PA-O3A
4	F	802	ADP	C5'-O5'-PA-O2A
3	A	801	ATP	PB-O3A-PA-O2A
3	D	801	ATP	C4'-C5'-O5'-PA
3	C	802	ATP	PB-O3B-PG-O2G
3	C	802	ATP	PB-O3B-PG-O3G
4	F	802	ADP	PA-O3A-PB-O3B
3	A	801	ATP	PG-O3B-PB-O2B
3	B	802	ATP	PA-O3A-PB-O1B
3	C	801	ATP	PG-O3B-PB-O2B
3	C	801	ATP	O4'-C1'-N9-C8
3	C	802	ATP	C4'-C5'-O5'-PA
3	C	802	ATP	PG-O3B-PB-O2B

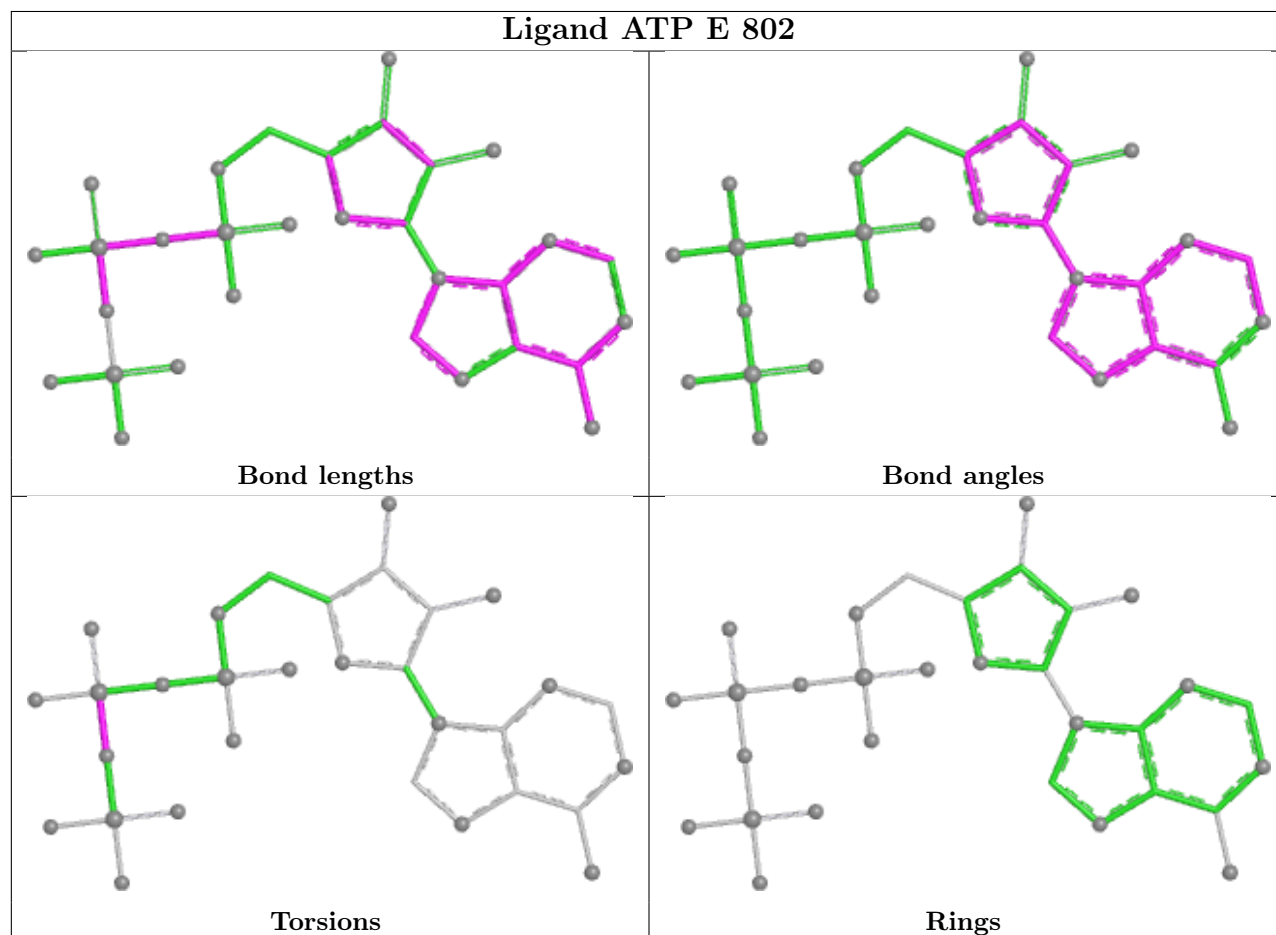
There are no ring outliers.

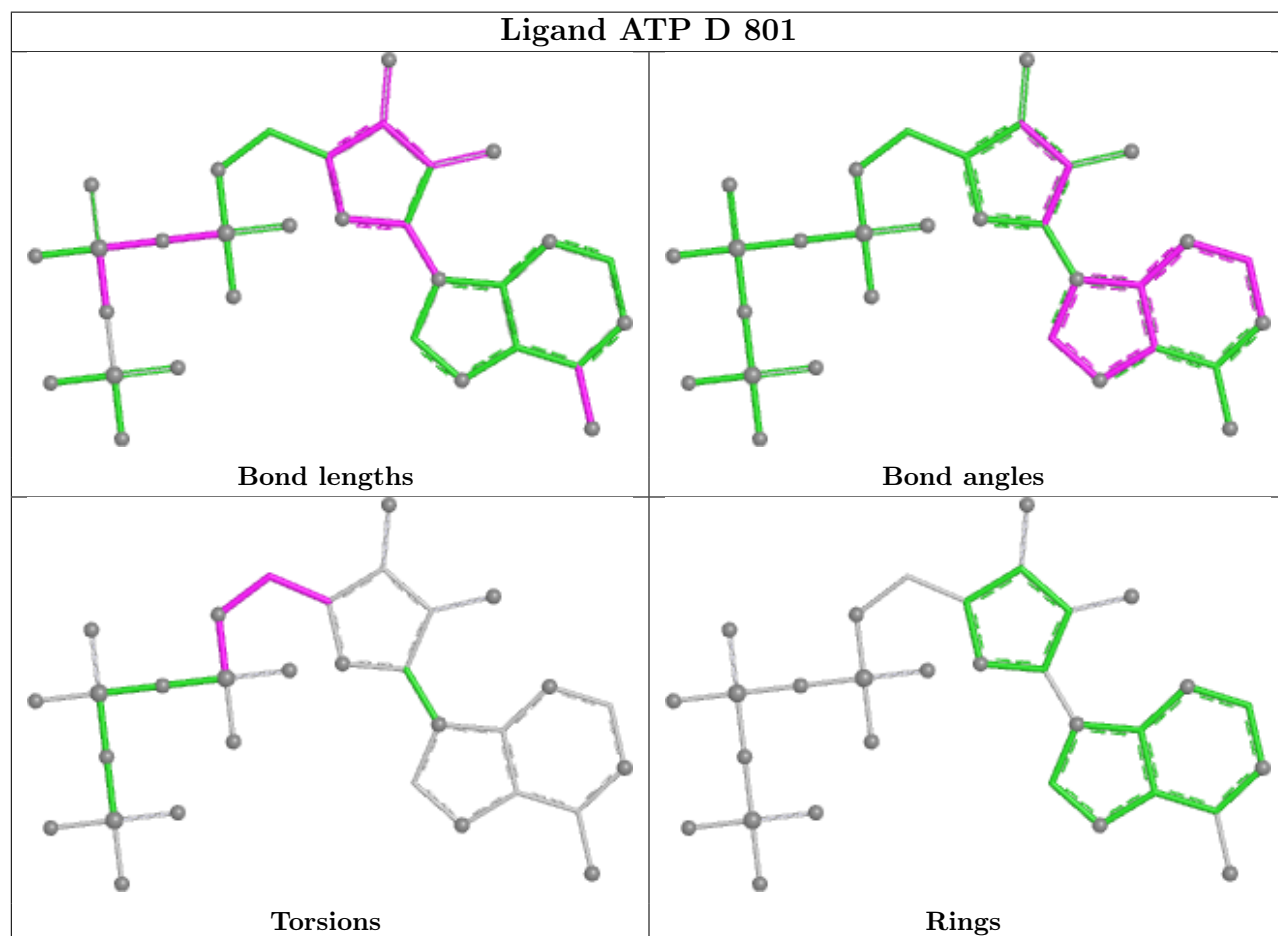
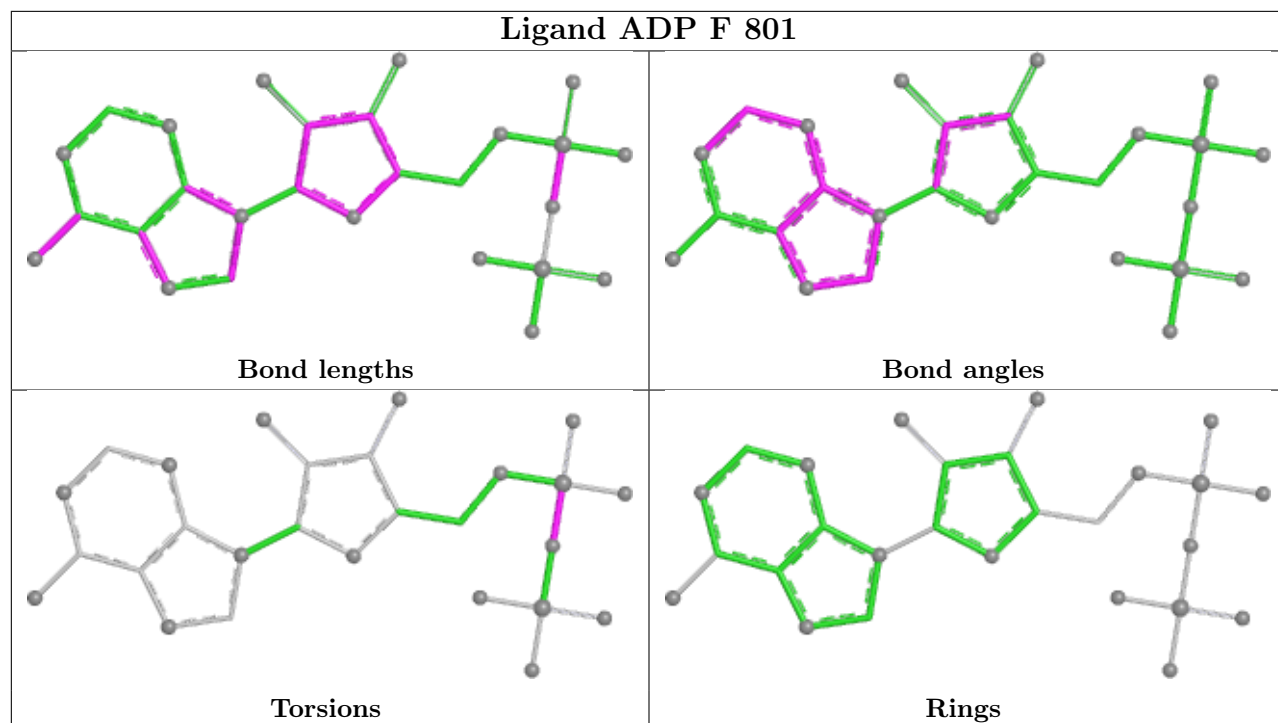
12 monomers are involved in 119 short contacts:

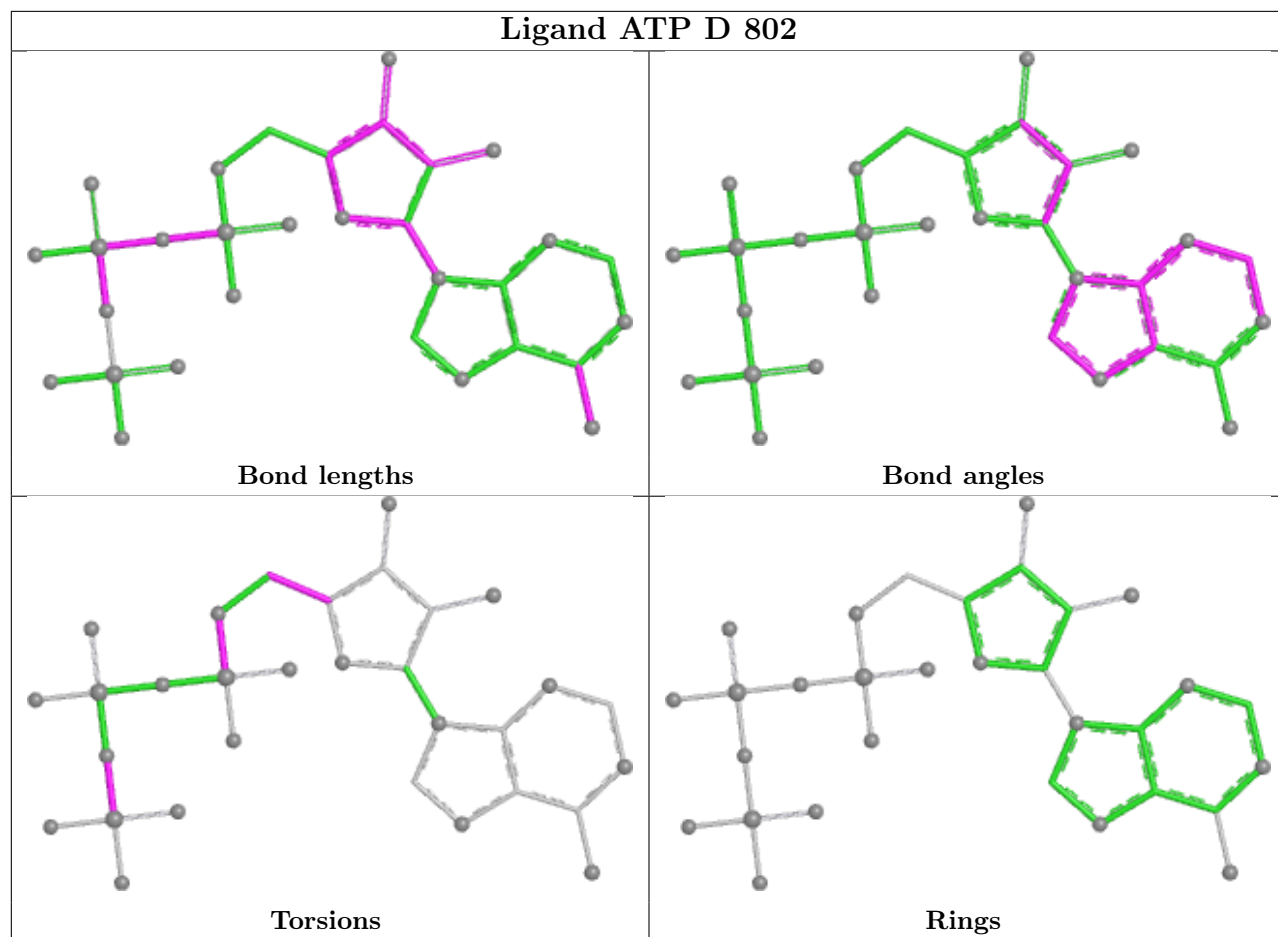
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	802	ATP	3	0
4	F	801	ADP	16	0
3	D	801	ATP	7	0
3	D	802	ATP	8	0
3	A	801	ATP	11	0
4	F	802	ADP	5	0
3	C	801	ATP	27	0
4	A	802	ADP	8	0
4	E	801	ADP	5	0
3	C	802	ATP	10	0
3	B	801	ATP	17	0
3	B	802	ATP	2	0

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

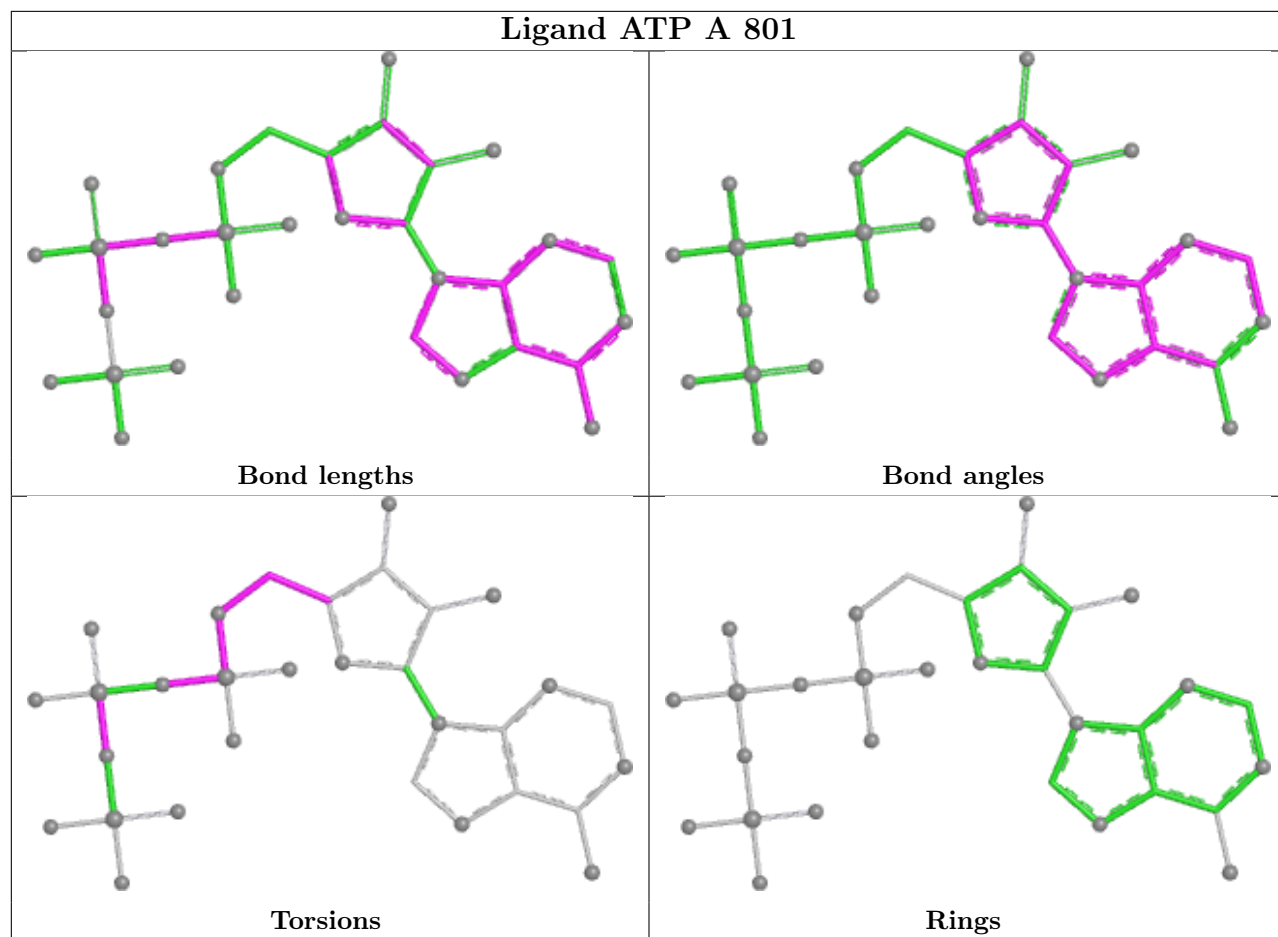
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



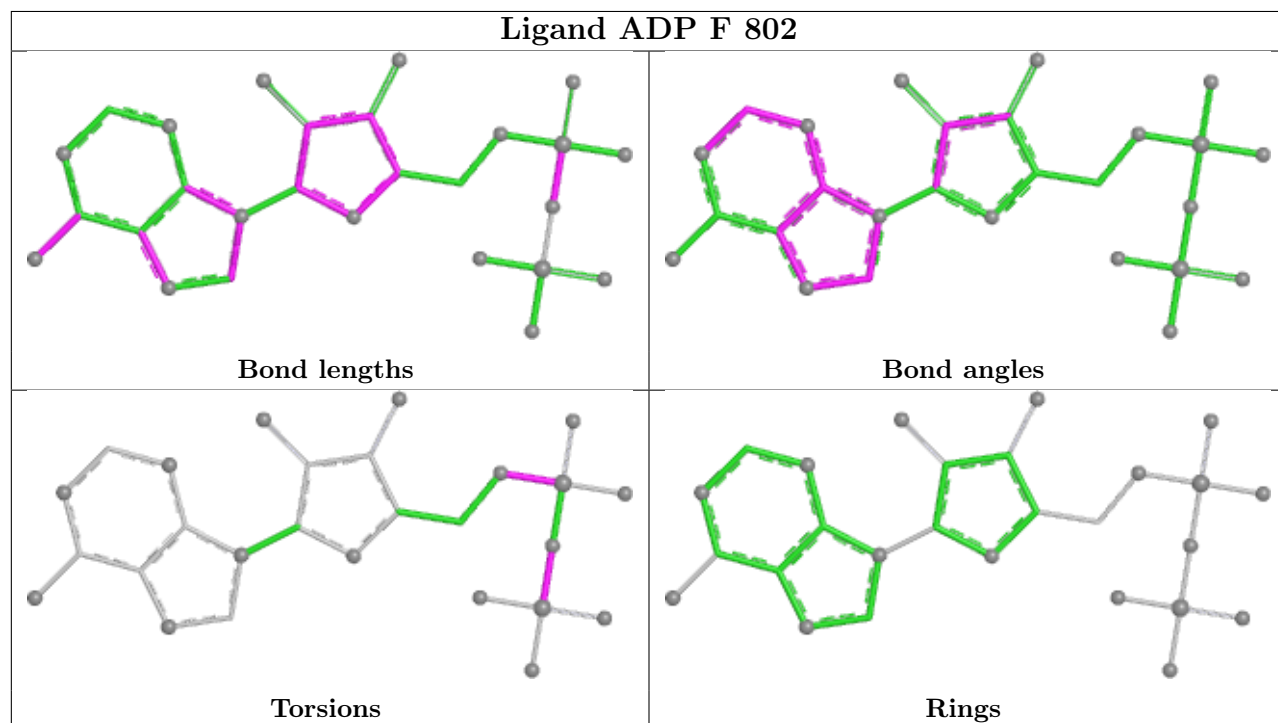




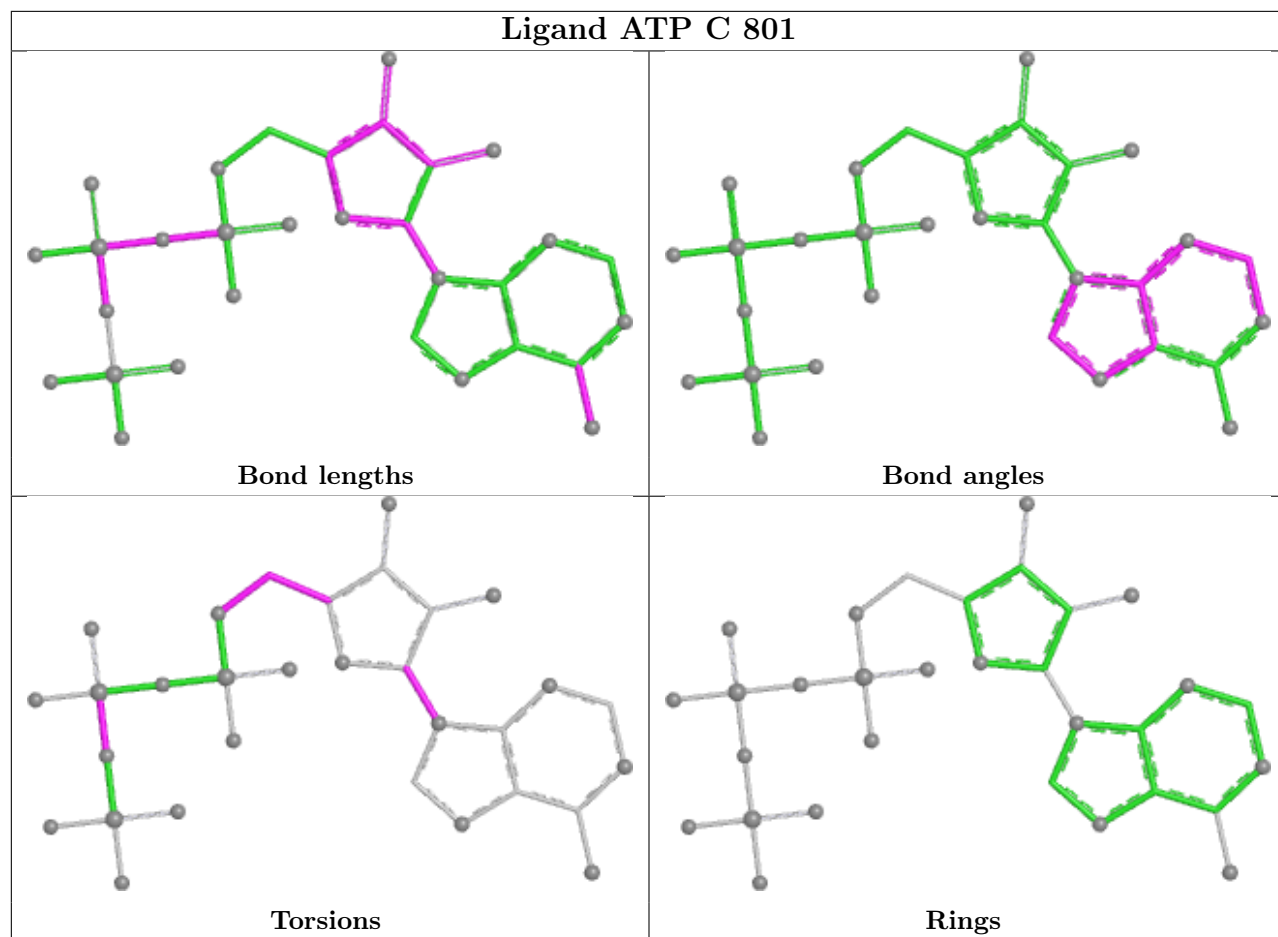
Ligand ATP A 801



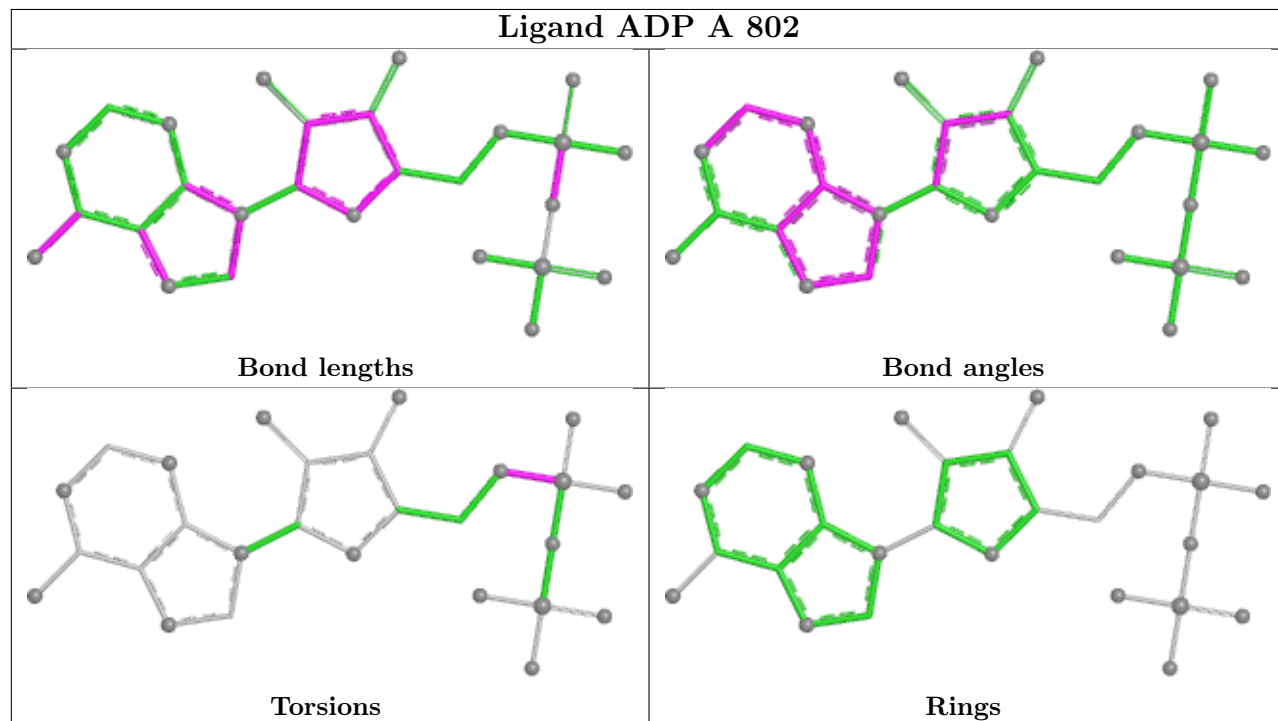
Ligand ADP F 802

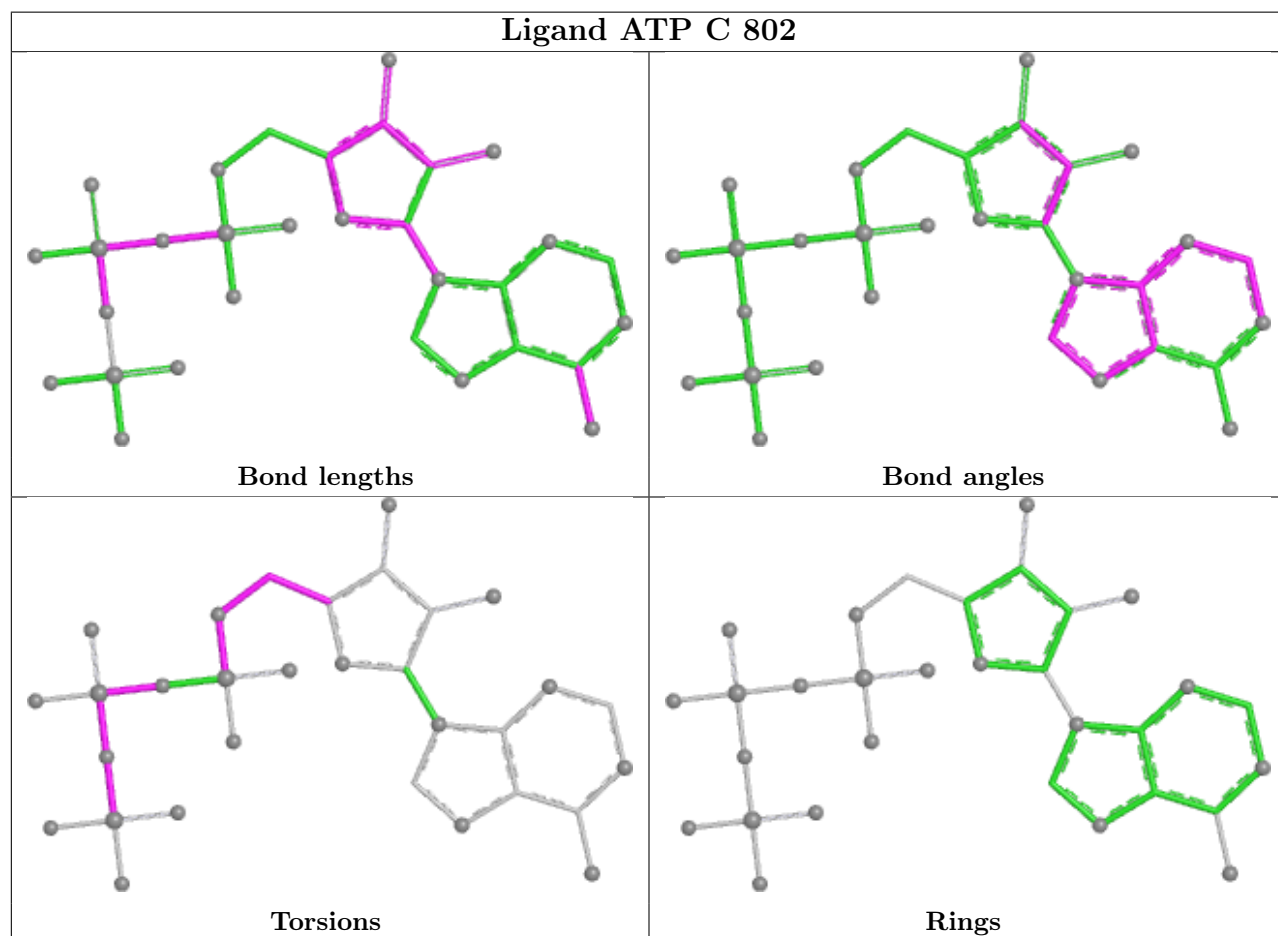
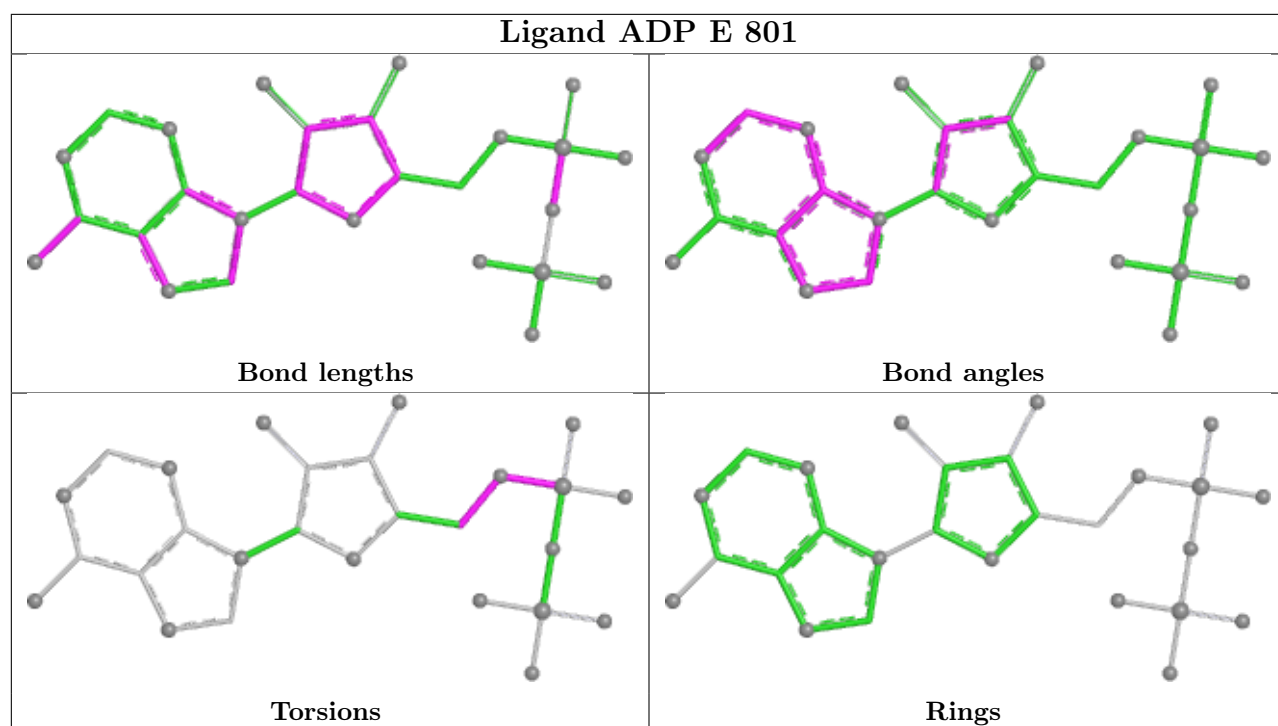


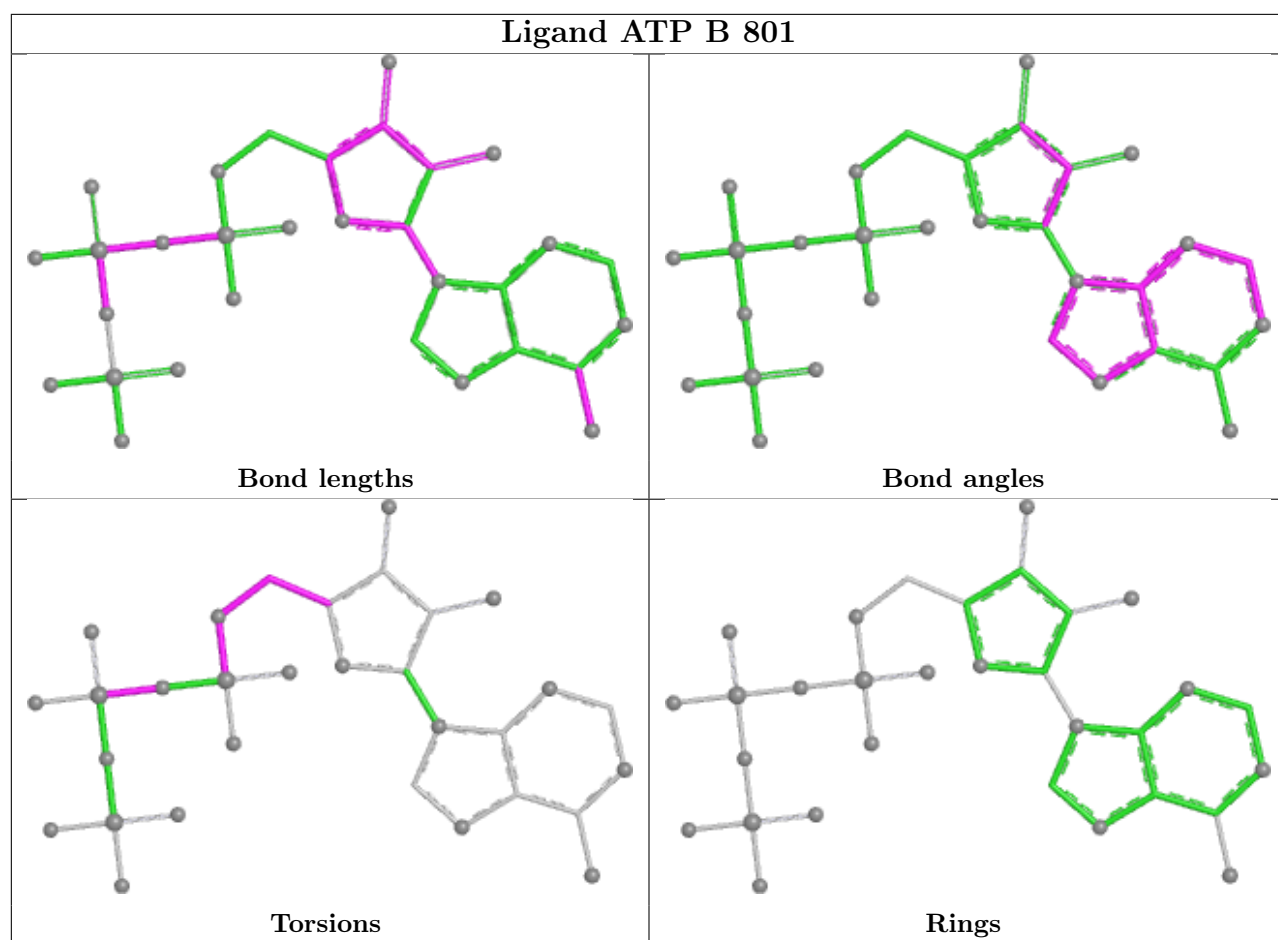
Ligand ATP C 801

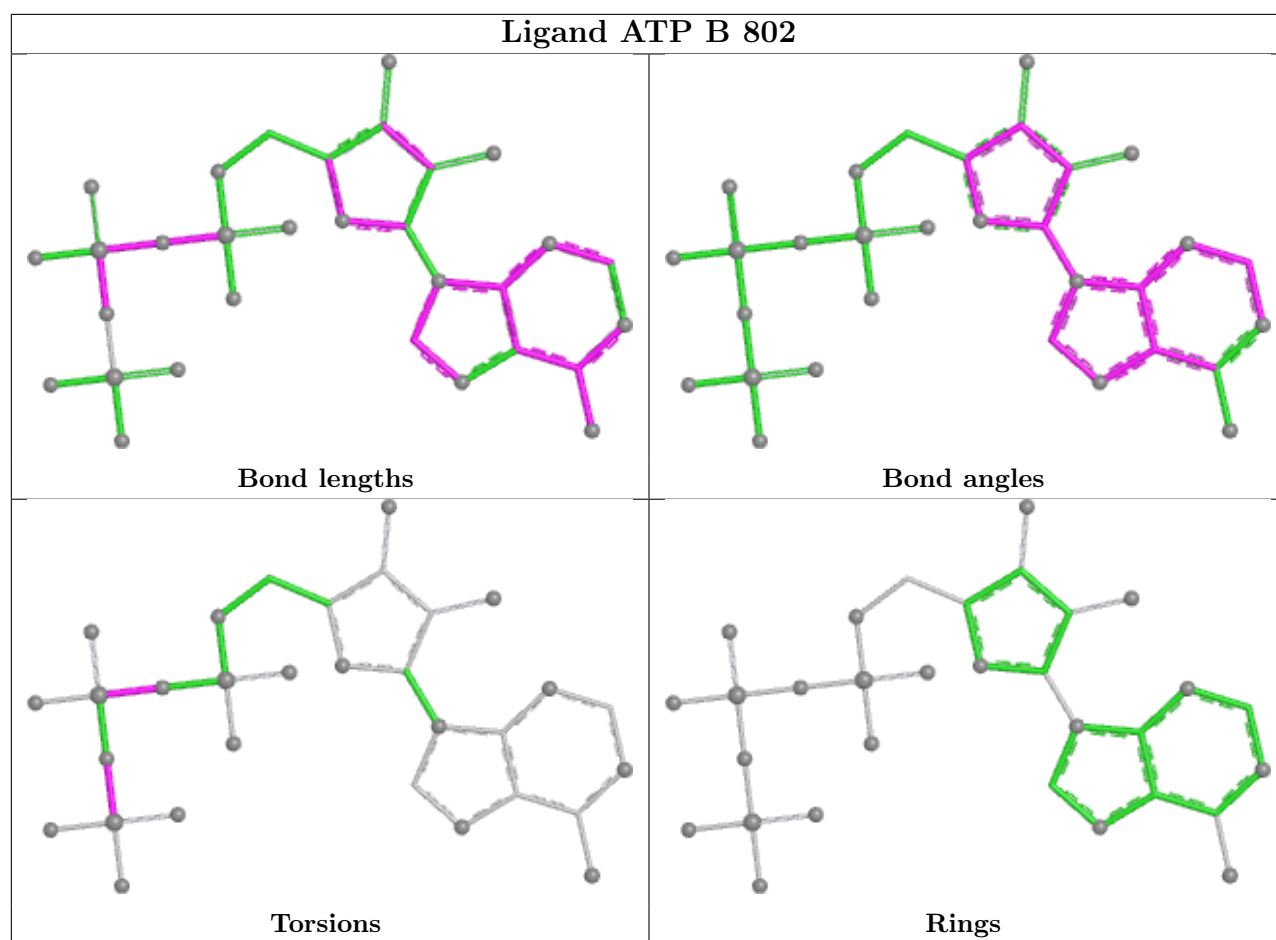


Ligand ADP A 802









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.

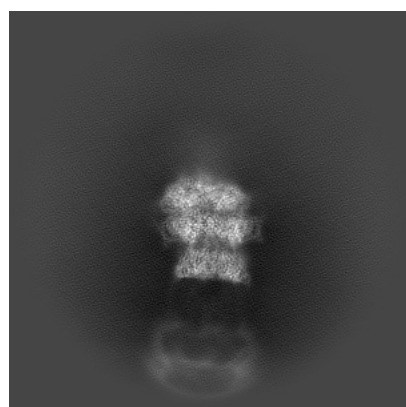
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21522. These allow visual inspection of the internal detail of the map and identification of artifacts.

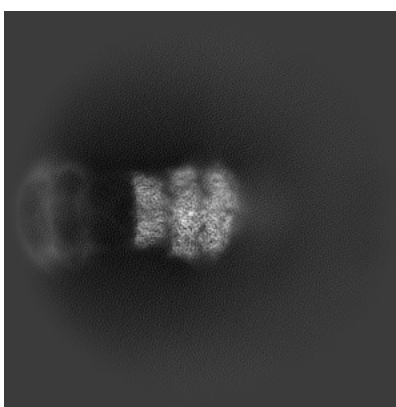
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

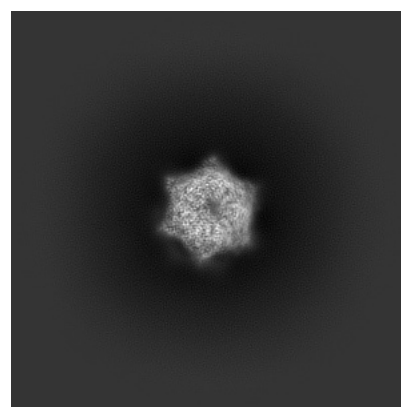
6.1.1 Primary map



X



Y

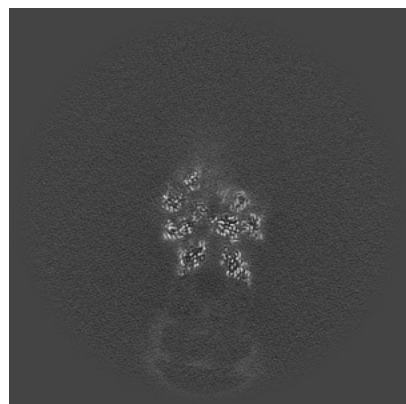


Z

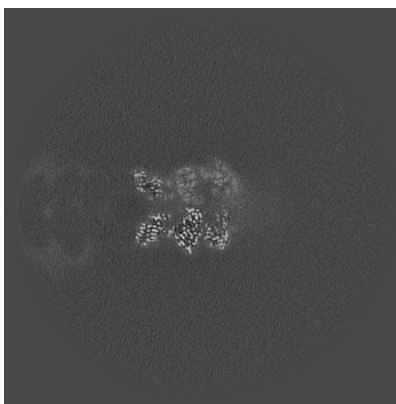
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

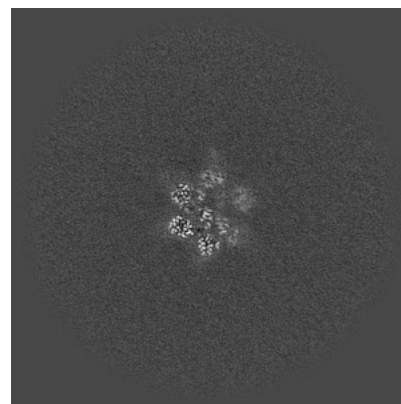
6.2.1 Primary map



X Index: 300



Y Index: 300

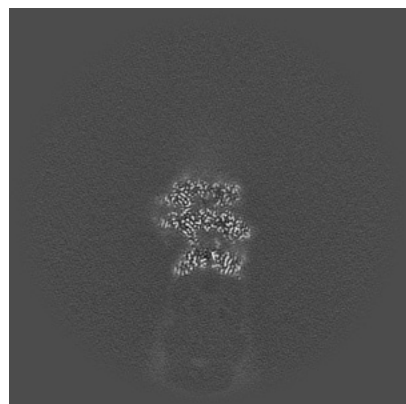


Z Index: 300

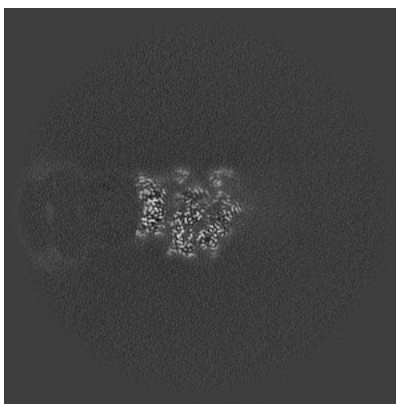
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

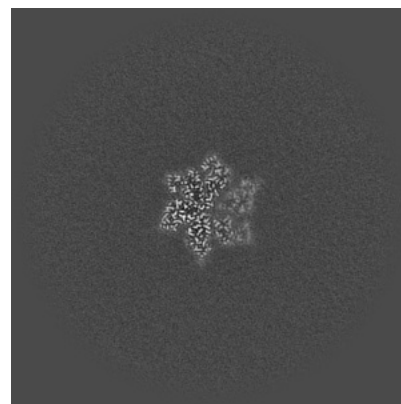
6.3.1 Primary map



X Index: 280



Y Index: 278

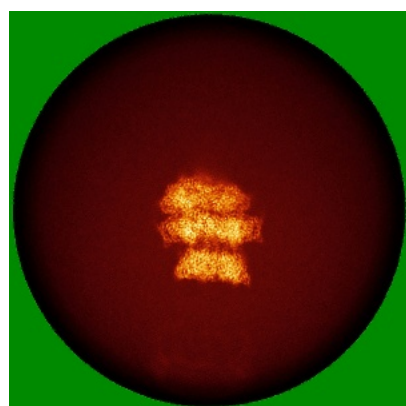


Z Index: 278

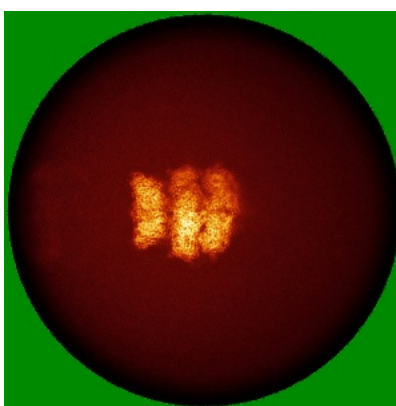
The images above show the largest variance slices of the map in three orthogonal directions.

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

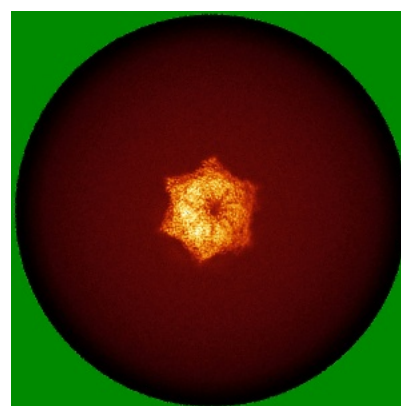
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

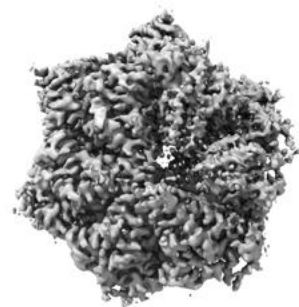
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

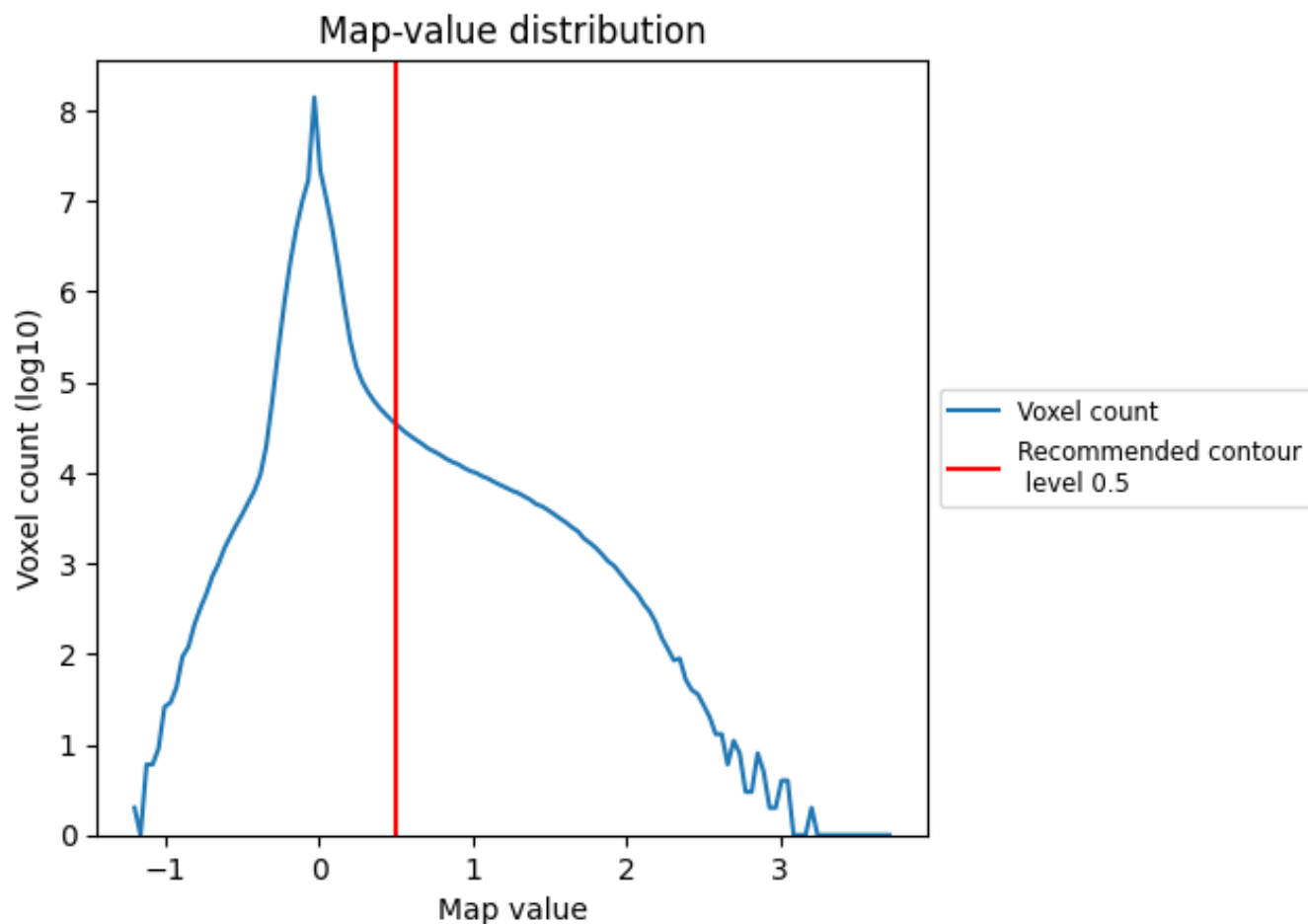
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

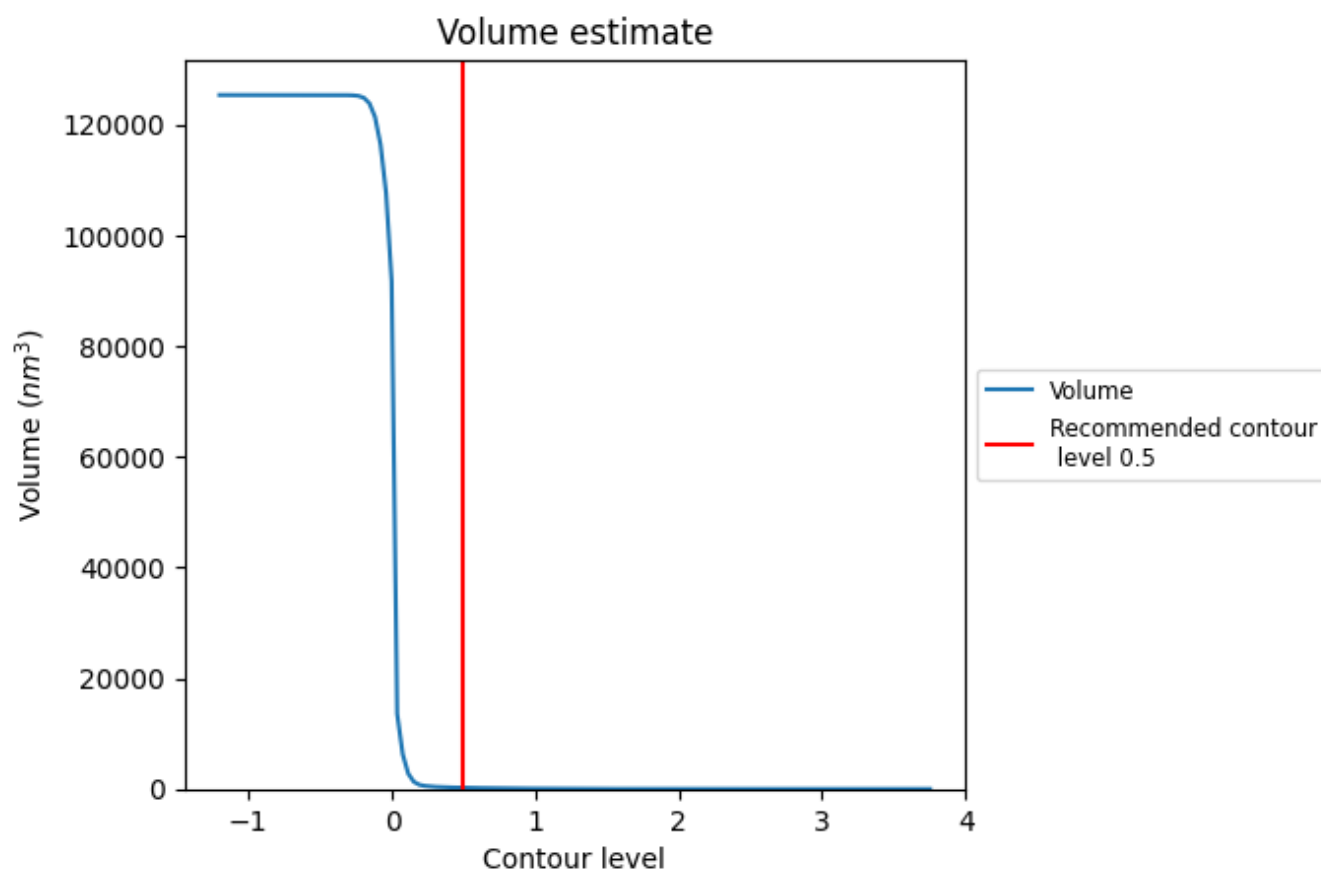
This section contains the results of statistical analysis of the map.

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.

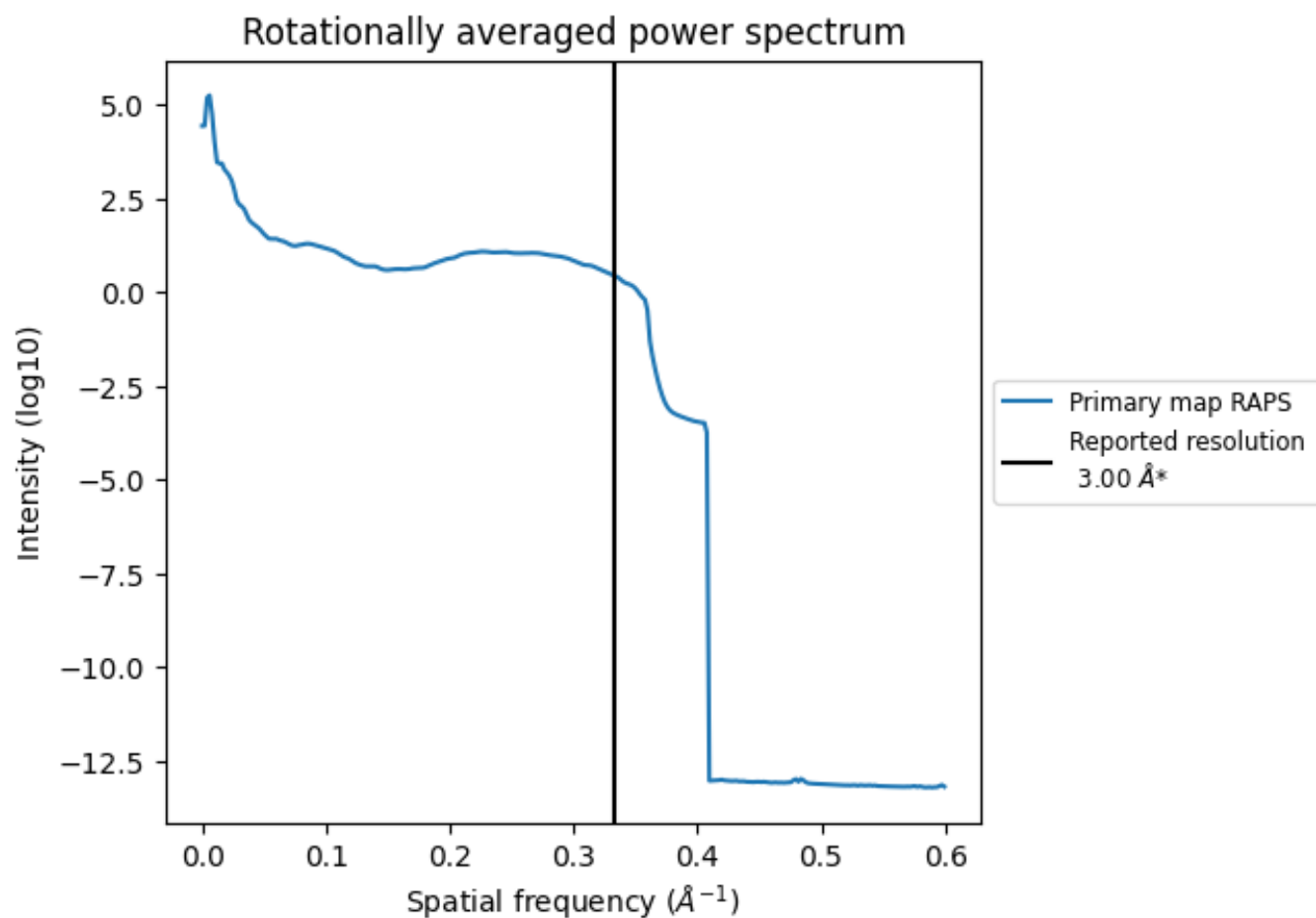
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm³; this corresponds to an approximate mass of 194 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 0.333 Å⁻¹

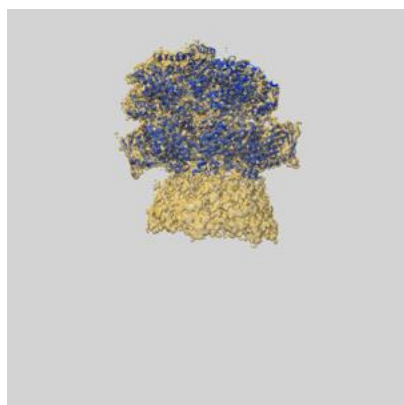
8 Fourier-Shell correlation ⓘ

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

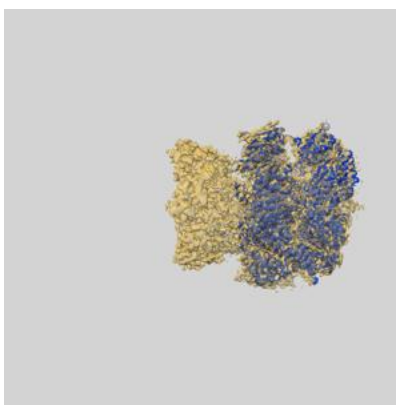
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21522 and PDB model 6W22. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

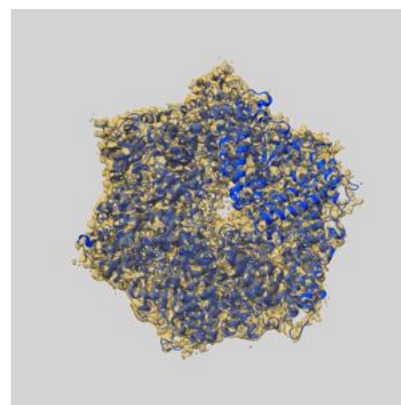
9.1 Map-model overlay [i](#)



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](#)



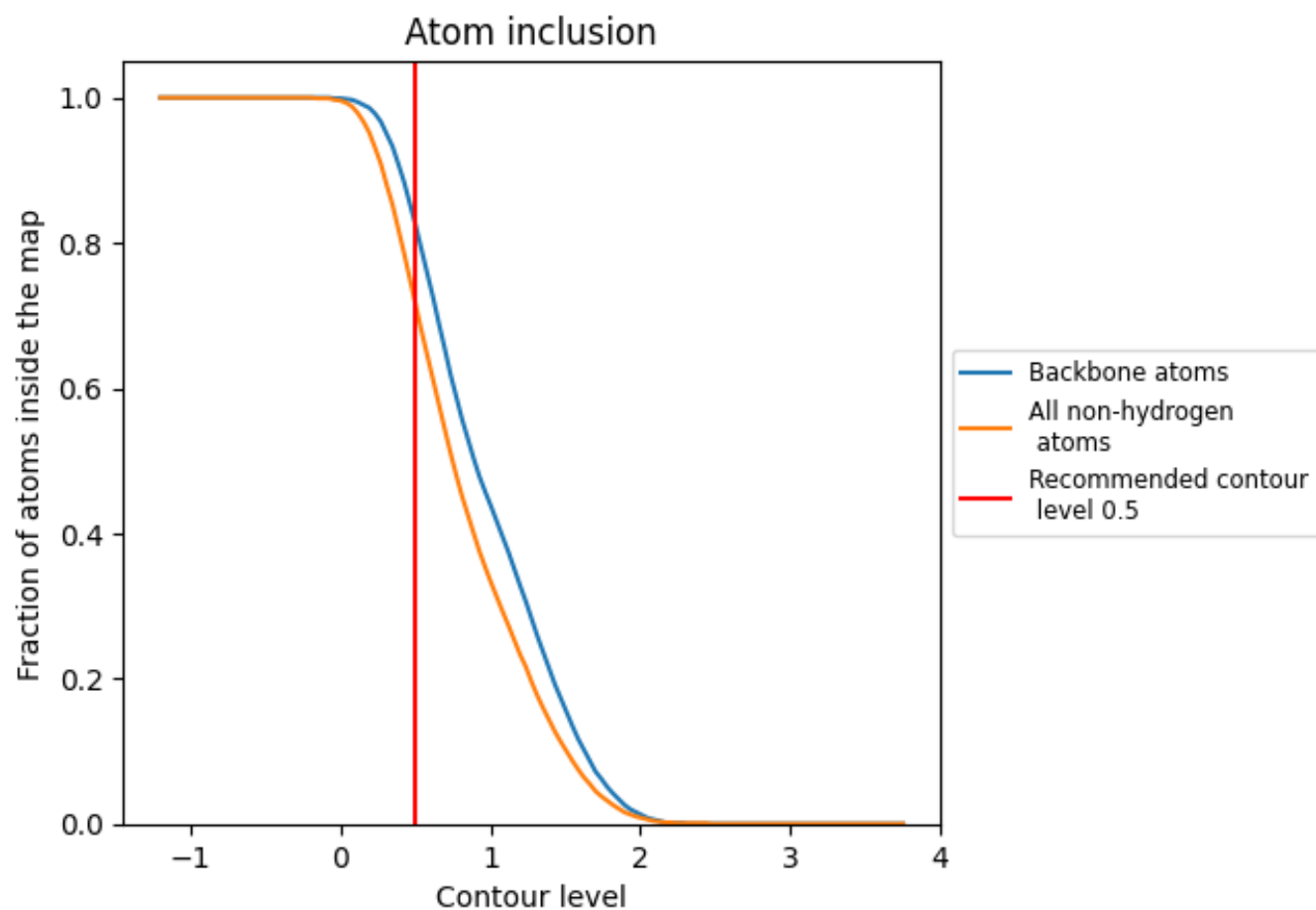
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 83% 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	0.7160	0.4270
A	0.7350	0.4370
B	0.8420	0.5070
C	0.8580	0.5190
D	0.8300	0.5090
E	0.5950	0.3430
F	0.4370	0.2470
X	0.6830	0.3880

1.0

0.0

<0.0