



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:22 AM UTC

PDB ID : 8XRW / pdb_00008xrw
Title : crystal structure of HpPPAT in complex with ATP
Authors : Yin, H.S.
Deposited on : 2024-01-08
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

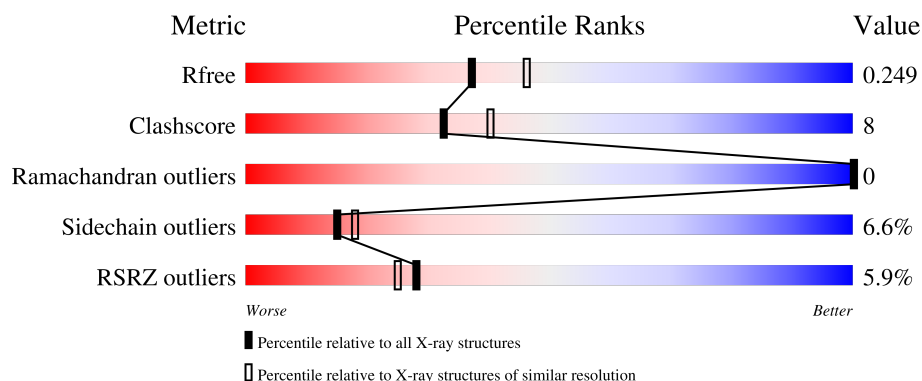
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

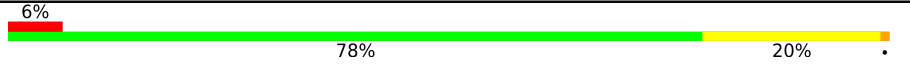
The reported resolution of this entry is 2.20 Å.

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.



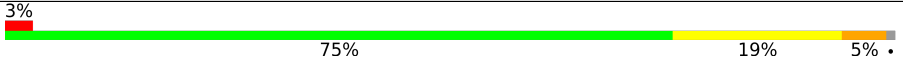
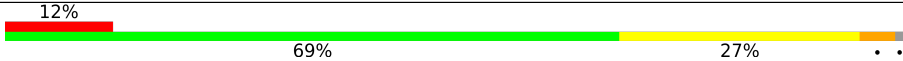
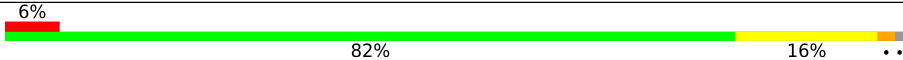
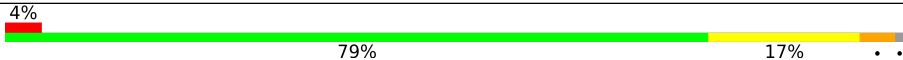
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	

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Mol	Chain	Length	Quality of chain
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	J	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	L	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	A	157	Total	C	N	O	S	0	0	0
			1242	801	209	225	7			
1	B	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	C	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	D	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	E	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	F	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	G	157	Total	C	N	O	S	0	0	0
			1242	801	209	225	7			
1	H	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			
1	K	156	Total	C	N	O	S	0	0	0
			1237	798	208	224	7			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	31	Total	O	0	0
			31	31		
3	J	10	Total	O	0	0
			10	10		
3	L	15	Total	O	0	0
			15	15		
3	A	20	Total	O	0	0
			20	20		
3	B	20	Total	O	0	0
			20	20		
3	C	10	Total	O	0	0
			10	10		
3	D	36	Total	O	0	0
			36	36		
3	E	20	Total	O	0	0
			20	20		
3	F	32	Total	O	0	0
			32	32		

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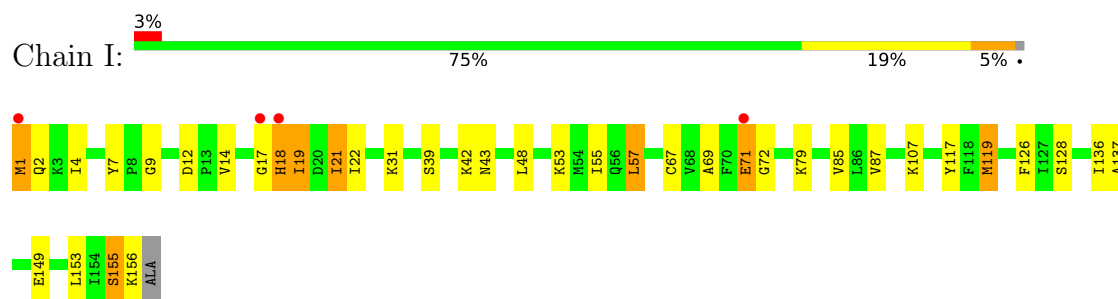
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	18	Total	O	0	0
			18	18		
3	H	20	Total	O	0	0
			20	20		
3	K	17	Total	O	0	0
			17	17		

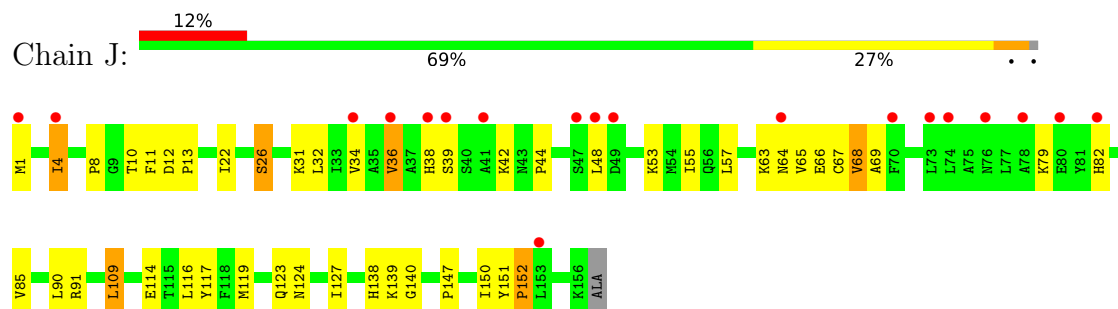
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

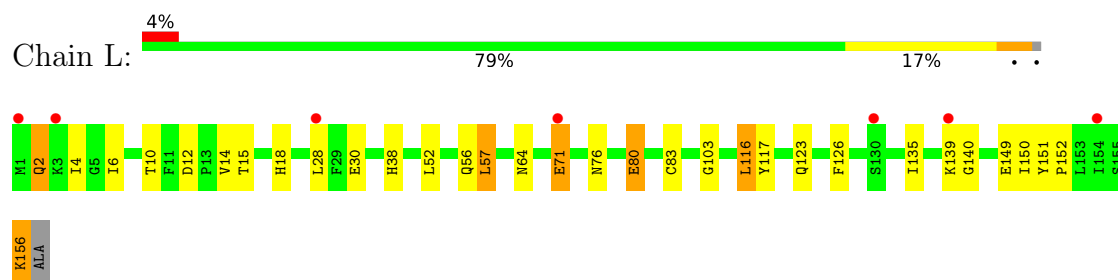
- Molecule 1: Phosphopantetheine adenylyltransferase



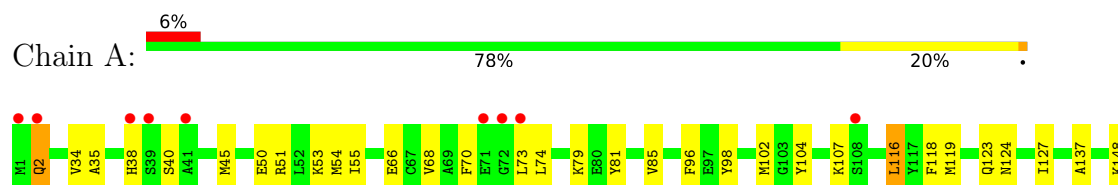
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase

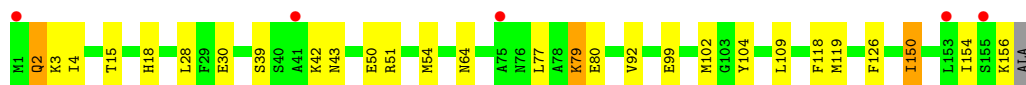
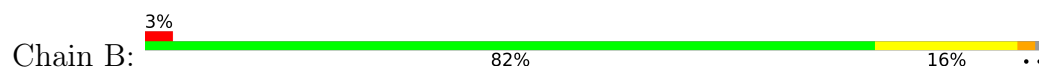


- Molecule 1: Phosphopantetheine adenylyltransferase

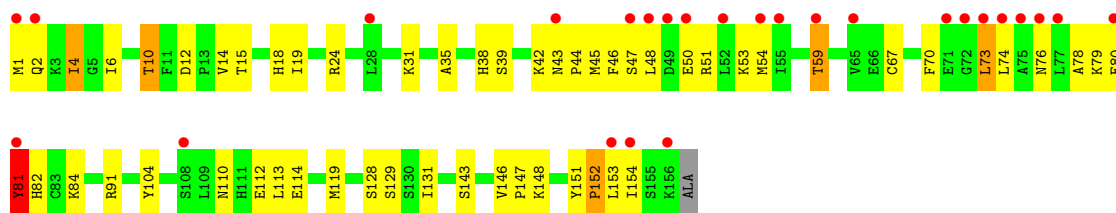




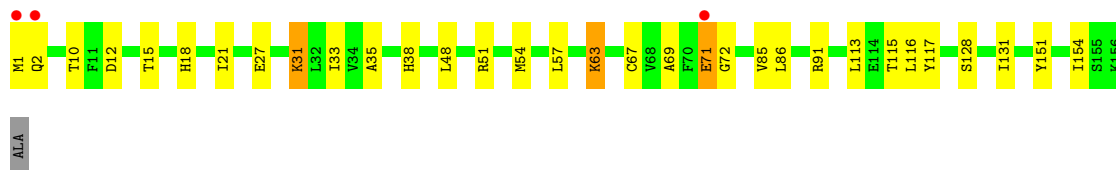
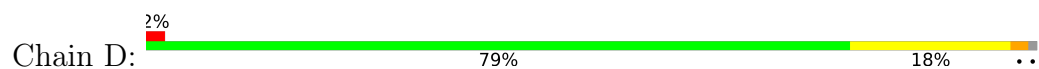
- Molecule 1: Phosphopantetheine adenylyltransferase



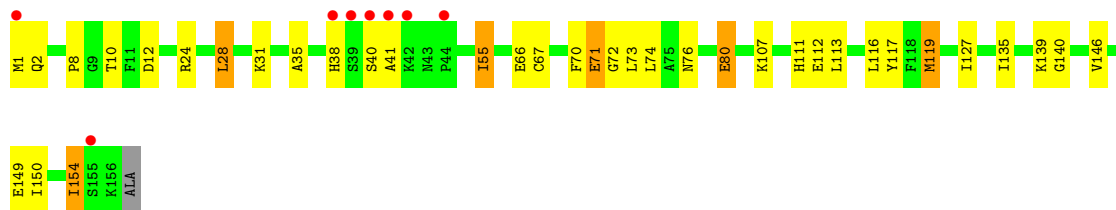
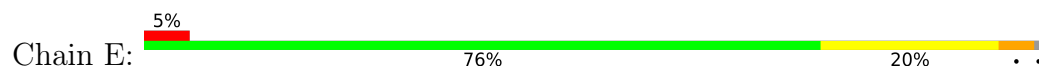
- Molecule 1: Phosphopantetheine adenylyltransferase



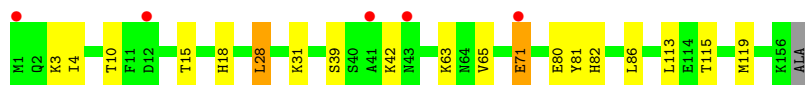
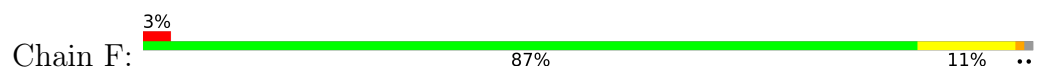
- Molecule 1: Phosphopantetheine adenylyltransferase



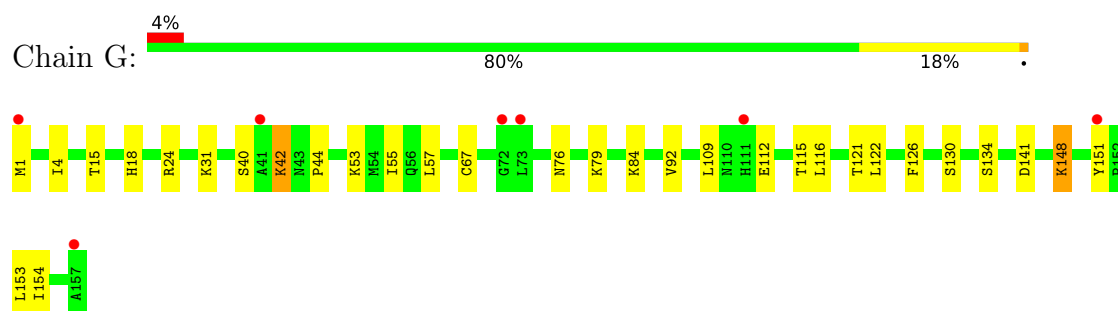
- Molecule 1: Phosphopantetheine adenylyltransferase



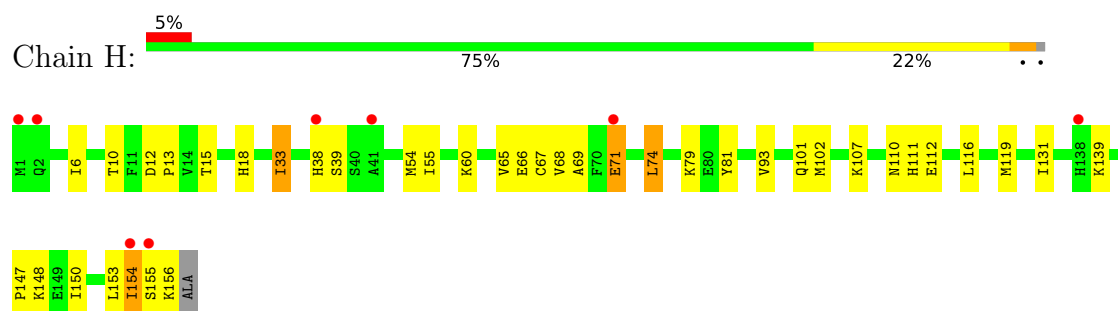
- Molecule 1: Phosphopantetheine adenylyltransferase



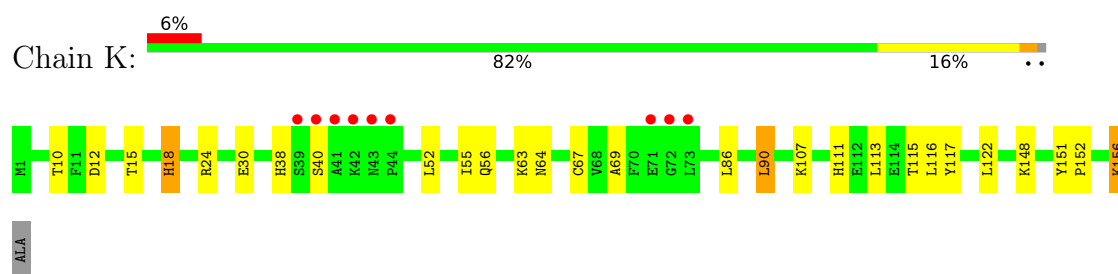
● Molecule 1: Phosphopantetheine adenylyltransferase



● Molecule 1: Phosphopantetheine adenylyltransferase



● Molecule 1: Phosphopantetheine adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.15Å 82.06Å 105.51Å 88.02° 73.55° 87.14°	Depositor
Resolution (Å)	101.17 – 2.20 101.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (101.17-2.20) 98.1 (101.17-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.203 , 0.248 0.208 , 0.249	Depositor DCC
R_{free} test set	5330 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15196	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5139e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.21	0/1268	1.15	3/1711 (0.2%)
1	B	1.12	0/1263	1.16	2/1704 (0.1%)
1	C	1.20	2/1263 (0.2%)	1.22	7/1704 (0.4%)
1	D	1.22	2/1263 (0.2%)	1.14	2/1704 (0.1%)
1	E	1.13	1/1263 (0.1%)	1.15	4/1704 (0.2%)
1	F	1.19	2/1263 (0.2%)	1.18	2/1704 (0.1%)
1	G	1.10	0/1268	1.12	1/1711 (0.1%)
1	H	1.19	3/1263 (0.2%)	1.17	1/1704 (0.1%)
1	I	1.26	5/1263 (0.4%)	1.21	9/1704 (0.5%)
1	J	1.08	2/1263 (0.2%)	1.14	4/1704 (0.2%)
1	K	1.13	1/1263 (0.1%)	1.10	1/1704 (0.1%)
1	L	1.17	0/1263	1.14	1/1704 (0.1%)
All	All	1.17	18/15166 (0.1%)	1.16	37/20462 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	10	THR	C-O	-6.71	1.15	1.24
1	D	35	ALA	C-O	-6.59	1.16	1.24
1	I	12	ASP	CA-C	6.55	1.60	1.52
1	D	67	CYS	C-O	-6.35	1.16	1.23
1	C	73	LEU	N-CA	6.27	1.54	1.46
1	I	72	GLY	N-CA	6.26	1.54	1.45
1	E	146	VAL	CA-CB	-6.07	1.49	1.55
1	J	8	PRO	N-CA	-5.42	1.41	1.46
1	J	140	GLY	N-CA	5.37	1.51	1.45
1	H	93	VAL	C-O	-5.27	1.18	1.24
1	K	69	ALA	CA-C	-5.27	1.46	1.52
1	I	79	LYS	C-O	-5.20	1.18	1.24
1	I	18	HIS	CA-C	5.19	1.59	1.52
1	I	87	VAL	CA-CB	-5.16	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	71	GLU	CA-C	5.09	1.58	1.52
1	C	81	TYR	CA-C	5.05	1.59	1.52
1	F	65	VAL	C-O	-5.01	1.18	1.24
1	H	65	VAL	C-O	-5.00	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	LEU	N-CA-C	8.19	121.36	108.67
1	C	10	THR	CA-C-N	-7.96	110.98	123.23
1	C	10	THR	C-N-CA	-7.96	110.98	123.23
1	I	19	ILE	N-CA-C	7.89	118.79	111.45
1	I	71	GLU	CA-C-N	-7.52	106.68	121.41
1	I	71	GLU	C-N-CA	-7.52	106.68	121.41
1	J	4	ILE	N-CA-C	7.34	118.38	106.72
1	J	85	VAL	N-CA-C	7.17	118.67	107.28
1	A	74	LEU	N-CA-C	7.07	118.78	111.14
1	I	71	GLU	O-C-N	-6.99	114.47	122.09
1	C	50	GLU	N-CA-C	-6.96	103.12	111.69
1	C	10	THR	N-CA-C	-6.75	100.98	110.50
1	G	42	LYS	N-CA-C	-6.65	100.67	110.52
1	B	77	LEU	N-CA-C	-5.95	104.80	111.28
1	C	74	LEU	N-CA-C	5.90	118.19	111.11
1	H	33	ILE	CB-CA-C	-5.81	103.93	110.96
1	D	85	VAL	N-CA-C	5.77	116.31	107.77
1	E	71	GLU	N-CA-C	-5.75	99.14	108.52
1	I	71	GLU	CB-CG-CD	5.75	122.37	112.60
1	F	42	LYS	CA-C-N	-5.71	116.42	123.21
1	F	42	LYS	C-N-CA	-5.71	116.42	123.21
1	J	38	HIS	N-CA-C	-5.60	106.12	113.12
1	A	96	PHE	N-CA-C	5.60	117.39	111.28
1	D	21	ILE	CB-CA-C	-5.54	104.67	112.14
1	E	127	ILE	CB-CA-C	-5.49	104.11	110.91
1	I	119	MET	CG-SD-CE	-5.41	88.99	100.90
1	C	6	ILE	N-CA-C	5.38	115.70	108.17
1	I	71	GLU	N-CA-C	5.36	122.40	114.09
1	L	71	GLU	N-CA-C	5.36	119.58	112.72
1	K	18	HIS	N-CA-C	-5.34	105.46	111.28
1	I	21	ILE	CB-CA-C	-5.31	104.89	112.22
1	B	102	MET	N-CA-C	-5.29	105.68	111.82
1	J	82	HIS	N-CA-C	-5.21	104.05	111.24
1	A	85	VAL	N-CA-C	5.14	115.39	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	107	LYS	N-CA-C	-5.07	105.75	111.28
1	E	119	MET	CG-SD-CE	-5.02	89.85	100.90
1	E	72	GLY	N-CA-C	5.00	116.78	110.38

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	1242	0	1270	18	0
1	B	1237	0	1265	15	0
1	C	1237	0	1265	38	0
1	D	1237	0	1265	24	1
1	E	1237	0	1265	20	5
1	F	1237	0	1265	10	1
1	G	1242	0	1270	17	2
1	H	1237	0	1265	21	3
1	I	1237	0	1265	27	0
1	J	1237	0	1265	30	4
1	K	1237	0	1265	22	0
1	L	1237	0	1265	24	0
2	I	31	0	12	3	0
2	J	31	0	12	2	0
2	L	31	0	12	0	0
3	A	20	0	0	2	0
3	B	20	0	0	0	0
3	C	10	0	0	0	0
3	D	36	0	0	0	0
3	E	20	0	0	0	0
3	F	32	0	0	1	0
3	G	18	0	0	2	0
3	H	20	0	0	1	0
3	I	31	0	0	0	0
3	J	10	0	0	0	0
3	K	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	15	0	0	0	0
All	All	15196	0	15226	238	8

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 8.

All (238) 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:D:71:GLU:OE2	1:D:72:GLY:N	1.99	0.94
1:A:2:GLN:HB3	3:A:202:HOH:O	1.70	0.90
1:C:59:THR:HG21	1:C:67:CYS:SG	2.12	0.89
1:K:156:LYS:HA	1:K:156:LYS:NZ	1.89	0.88
1:E:38:HIS:CE1	1:E:40:SER:HB3	2.10	0.86
1:A:73:LEU:HA	3:A:201:HOH:O	1.81	0.80
1:D:71:GLU:H	1:D:71:GLU:CD	1.93	0.77
1:D:71:GLU:CD	1:D:71:GLU:N	2.44	0.75
1:J:119:MET:CE	1:K:115:THR:HB	2.17	0.74
1:I:9:GLY:HA3	2:I:201:ATP:H5'2	1.68	0.74
1:J:36:VAL:HG23	1:J:48:LEU:HD11	1.70	0.73
1:I:71:GLU:HG3	1:I:71:GLU:O	1.88	0.73
3:G:215:HOH:O	1:H:119:MET:HE3	1.90	0.71
1:K:156:LYS:HA	1:K:156:LYS:HZ3	1.55	0.71
1:L:57:LEU:HG	1:L:149:GLU:HB3	1.71	0.70
1:L:38:HIS:CD2	1:L:71:GLU:OE2	2.45	0.69
1:D:116:LEU:HD11	1:E:116:LEU:HG	1.74	0.69
1:C:38:HIS:O	1:C:51:ARG:NH2	2.16	0.69
1:D:31:LYS:HE2	1:D:33:ILE:HD11	1.76	0.68
1:G:42:LYS:O	1:G:44:PRO:HD3	1.94	0.68
1:G:115:THR:HB	1:H:119:MET:HE1	1.75	0.68
1:I:14:VAL:HG23	1:I:18:HIS:HB2	1.77	0.66
1:L:135:ILE:HG23	1:L:140:GLY:HA3	1.78	0.66
1:H:155:SER:O	1:H:156:LYS:C	2.39	0.66
1:H:54:MET:O	1:H:150:ILE:HD11	1.97	0.65
1:L:38:HIS:CG	1:L:71:GLU:OE2	2.50	0.65
1:E:38:HIS:ND1	1:E:40:SER:HB3	2.13	0.64
1:I:14:VAL:HA	1:I:18:HIS:ND1	2.13	0.63
1:A:2:GLN:HE22	1:B:2:GLN:HB2	1.64	0.63
1:E:107:LYS:HD3	1:E:113:LEU:O	1.98	0.63
1:H:68:VAL:HG11	1:H:81:TYR:OH	1.97	0.63
1:G:115:THR:HB	1:H:119:MET:CE	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:HE2	1:B:104:TYR:CZ	2.33	0.62
1:B:3:LYS:O	1:B:30:GLU:HB3	1.99	0.62
1:E:55:ILE:CG2	1:E:67:CYS:SG	2.88	0.61
1:D:116:LEU:HD12	1:E:117:TYR:O	2.00	0.61
1:H:107:LYS:NZ	1:H:111:HIS:O	2.33	0.60
1:L:52:LEU:O	1:L:56:GLN:HG3	2.01	0.60
1:D:71:GLU:N	1:D:71:GLU:OE1	2.35	0.60
1:E:24:ARG:NH1	1:E:119:MET:O	2.35	0.60
1:I:71:GLU:O	1:I:71:GLU:CG	2.50	0.59
1:E:10:THR:HG22	1:E:12:ASP:HB2	1.84	0.59
1:B:15:THR:H	1:B:18:HIS:HD2	1.49	0.59
1:H:55:ILE:HG22	1:H:67:CYS:SG	2.43	0.59
1:E:107:LYS:NZ	1:E:111:HIS:O	2.19	0.59
1:C:1:MET:HE3	1:C:114:GLU:HG3	1.83	0.59
1:C:44:PRO:HB2	1:C:46:PHE:O	2.03	0.58
1:I:17:GLY:O	1:I:18:HIS:C	2.46	0.58
1:A:116:LEU:HD23	1:A:118:PHE:CE1	2.38	0.58
1:F:15:THR:H	1:F:18:HIS:HD2	1.52	0.57
1:J:116:LEU:HG	1:K:116:LEU:HD11	1.86	0.57
1:A:68:VAL:HG11	1:A:81:TYR:OH	2.05	0.56
1:J:119:MET:HE1	1:K:115:THR:HB	1.86	0.56
1:K:156:LYS:HA	1:K:156:LYS:HZ2	1.68	0.56
1:H:147:PRO:HG2	1:H:150:ILE:HG12	1.87	0.56
1:L:57:LEU:HD21	1:L:149:GLU:O	2.06	0.56
1:K:52:LEU:O	1:K:56:GLN:HG3	2.05	0.56
1:C:78:ALA:HB1	1:C:113:LEU:HD13	1.88	0.55
1:K:15:THR:H	1:K:18:HIS:HD2	1.53	0.55
1:L:6:ILE:HG13	1:L:83:CYS:SG	2.46	0.55
1:I:117:TYR:HB2	1:L:117:TYR:HB2	1.88	0.55
1:C:119:MET:HE3	1:F:115:THR:HB	1.88	0.55
1:K:30:GLU:O	1:K:64:ASN:HB2	2.07	0.55
1:J:91:ARG:HD2	2:J:201:ATP:C5	2.42	0.55
1:L:126:PHE:CD1	1:K:122:LEU:HD11	2.42	0.55
1:E:135:ILE:HG23	1:E:140:GLY:HA3	1.88	0.55
1:C:35:ALA:HB1	1:C:70:PHE:CD1	2.42	0.54
1:I:17:GLY:C	1:I:19:ILE:N	2.63	0.54
1:J:42:LYS:O	1:J:44:PRO:HD3	2.07	0.54
1:J:36:VAL:HG23	1:J:36:VAL:O	2.08	0.54
1:J:151:TYR:HB2	1:J:152:PRO:HD3	1.89	0.53
1:E:150:ILE:HD12	1:E:154:ILE:HD13	1.90	0.53
1:D:38:HIS:HA	1:D:48:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:THR:H	1:K:18:HIS:CD2	2.27	0.53
1:B:92:VAL:HG11	1:B:126:PHE:CE1	2.44	0.53
1:D:15:THR:H	1:D:18:HIS:HD2	1.57	0.53
1:C:44:PRO:HG2	1:C:51:ARG:NH2	2.23	0.52
1:C:44:PRO:O	1:C:45:MET:C	2.50	0.52
1:I:17:GLY:O	1:I:19:ILE:N	2.43	0.52
1:A:148:LYS:HA	1:A:151:TYR:CZ	2.45	0.52
1:G:15:THR:H	1:G:18:HIS:HD2	1.59	0.51
1:C:51:ARG:HA	1:C:54:MET:HE3	1.91	0.51
1:C:119:MET:CE	1:F:115:THR:HB	2.40	0.51
1:K:107:LYS:NZ	1:K:111:HIS:O	2.41	0.51
1:F:71:GLU:OE1	1:F:71:GLU:O	2.28	0.51
1:C:104:TYR:CZ	1:F:119:MET:HE2	2.45	0.51
1:L:2:GLN:NE2	1:L:30:GLU:OE1	2.44	0.51
1:I:39:SER:HB3	1:I:42:LYS:HD3	1.93	0.51
1:H:13:PRO:HG3	1:H:154:ILE:HD11	1.93	0.51
1:C:84:LYS:HE3	1:C:112:GLU:HG2	1.93	0.50
1:K:148:LYS:HA	1:K:151:TYR:CZ	2.47	0.50
1:B:150:ILE:HD12	1:B:154:ILE:HG23	1.93	0.50
1:K:10:THR:HG22	1:K:12:ASP:HB2	1.94	0.50
1:J:117:TYR:HB2	1:K:117:TYR:HB2	1.93	0.50
1:L:151:TYR:N	1:L:152:PRO:HD2	2.27	0.50
1:H:68:VAL:HG11	1:H:81:TYR:HH	1.76	0.50
1:C:76:ASN:HA	1:C:79:LYS:HB3	1.94	0.50
1:K:148:LYS:HA	1:K:151:TYR:CE2	2.47	0.50
1:J:55:ILE:HG22	1:J:67:CYS:SG	2.52	0.49
1:J:36:VAL:HG22	1:J:68:VAL:O	2.13	0.49
1:C:1:MET:HB3	1:F:28:LEU:HD12	1.93	0.49
1:C:151:TYR:HB2	1:C:152:PRO:HD3	1.94	0.49
1:D:117:TYR:HB2	1:E:117:TYR:HB2	1.92	0.49
1:I:7:TYR:CE1	2:I:201:ATP:H4'	2.47	0.49
1:C:10:THR:HG22	1:C:12:ASP:HB2	1.94	0.49
1:H:102:MET:HE3	3:H:211:HOH:O	2.11	0.49
1:J:4:ILE:HD12	1:J:31:LYS:HB3	1.94	0.49
1:G:151:TYR:HA	1:G:154:ILE:HG12	1.94	0.49
1:E:35:ALA:HB1	1:E:70:PHE:CD1	2.48	0.49
1:F:15:THR:H	1:F:18:HIS:CD2	2.29	0.49
1:A:116:LEU:CD2	1:A:118:PHE:CE1	2.96	0.48
1:L:15:THR:H	1:L:18:HIS:HD2	1.60	0.48
1:B:15:THR:H	1:B:18:HIS:CD2	2.29	0.48
1:E:76:ASN:O	1:E:80:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:GLY:C	1:I:19:ILE:H	2.22	0.48
1:A:119:MET:HE2	1:B:104:TYR:CE1	2.48	0.48
1:C:151:TYR:HB2	1:C:152:PRO:CD	2.43	0.48
1:I:126:PHE:CD2	1:G:122:LEU:HD11	2.49	0.48
1:C:1:MET:CE	1:C:114:GLU:HG3	2.43	0.48
1:C:2:GLN:NE2	3:F:201:HOH:O	2.42	0.47
1:G:151:TYR:CD1	1:G:154:ILE:HD11	2.50	0.47
1:J:34:VAL:HG23	1:J:65:VAL:HG13	1.96	0.47
1:A:98:TYR:CE2	1:A:102:MET:HE2	2.50	0.47
1:J:10:THR:HG22	1:J:12:ASP:HB2	1.96	0.46
1:A:45:MET:HE1	1:A:137:ALA:HB2	1.98	0.46
1:L:156:LYS:HD2	1:L:156:LYS:C	2.40	0.46
1:I:14:VAL:HG23	1:I:18:HIS:CB	2.45	0.46
1:I:128:SER:HB2	1:H:101:GLN:HE22	1.80	0.46
1:L:15:THR:H	1:L:18:HIS:CD2	2.34	0.46
1:I:1:MET:HG3	1:I:85:VAL:CG2	2.46	0.46
1:A:50:GLU:O	1:A:54:MET:HG3	2.15	0.46
1:B:79:LYS:O	1:B:80:GLU:C	2.59	0.46
1:J:22:ILE:O	1:J:26:SER:HB2	2.16	0.45
1:C:4:ILE:HA	1:C:31:LYS:O	2.17	0.45
1:D:151:TYR:CE1	1:D:154:ILE:HD11	2.50	0.45
1:C:10:THR:HG23	1:C:51:ARG:NH1	2.32	0.45
1:J:11:PHE:CD1	1:J:55:ILE:HD11	2.52	0.45
1:A:104:TYR:CZ	1:B:119:MET:HE3	2.51	0.45
1:B:15:THR:N	1:B:18:HIS:HD2	2.14	0.45
1:D:48:LEU:HD21	1:D:69:ALA:HB1	1.98	0.45
1:G:53:LYS:HA	1:G:53:LYS:HD3	1.88	0.45
1:E:31:LYS:NZ	1:E:66:GLU:OE1	2.37	0.45
1:A:38:HIS:CD2	1:A:40:SER:H	2.35	0.44
1:K:151:TYR:N	1:K:152:PRO:CD	2.80	0.44
1:I:53:LYS:HD2	1:I:57:LEU:HD22	2.00	0.44
1:F:86:LEU:HG	1:F:113:LEU:HD11	1.99	0.44
1:F:81:TYR:O	1:F:82:HIS:C	2.59	0.44
1:C:43:ASN:N	1:C:44:PRO:HD3	2.32	0.44
1:I:42:LYS:O	1:I:43:ASN:C	2.61	0.44
1:J:48:LEU:HD21	1:J:69:ALA:HB1	1.99	0.44
1:D:15:THR:H	1:D:18:HIS:CD2	2.35	0.44
1:H:38:HIS:CG	1:H:39:SER:N	2.86	0.44
1:B:118:PHE:CD1	1:B:118:PHE:N	2.86	0.44
1:J:109:LEU:HD12	1:J:109:LEU:HA	1.82	0.44
1:A:34:VAL:HG11	1:A:55:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HB1	1:A:70:PHE:CD1	2.52	0.44
1:L:116:LEU:HD12	1:L:117:TYR:N	2.33	0.43
1:D:51:ARG:HA	1:D:54:MET:HE2	2.01	0.43
1:I:21:ILE:HD11	2:I:201:ATP:H2	1.83	0.43
1:J:32:LEU:O	1:J:65:VAL:HA	2.18	0.43
1:J:124:ASN:HD22	1:J:127:ILE:CD1	2.32	0.43
1:C:51:ARG:HA	1:C:54:MET:CE	2.49	0.43
1:C:143:SER:O	1:C:151:TYR:OH	2.18	0.43
1:G:15:THR:H	1:G:18:HIS:CD2	2.36	0.43
1:G:55:ILE:HG23	1:G:67:CYS:SG	2.59	0.43
1:G:92:VAL:HG11	1:G:126:PHE:CE1	2.54	0.43
1:K:38:HIS:O	1:K:40:SER:N	2.52	0.43
1:J:67:CYS:C	1:J:68:VAL:CG1	2.91	0.43
1:C:81:TYR:O	1:C:82:HIS:HB2	2.19	0.43
1:D:151:TYR:CD1	1:D:154:ILE:HD11	2.53	0.43
1:K:55:ILE:HG23	1:K:67:CYS:SG	2.59	0.43
1:I:18:HIS:O	1:I:22:ILE:HG13	2.18	0.43
1:I:119:MET:HE1	1:L:103:GLY:HA3	2.00	0.43
1:A:38:HIS:HA	1:A:51:ARG:HH22	1.83	0.43
1:D:2:GLN:O	1:D:2:GLN:HG3	2.19	0.43
1:D:115:THR:HB	1:E:119:MET:HE2	2.00	0.43
1:L:80:GLU:N	1:L:80:GLU:OE1	2.51	0.43
1:A:124:ASN:HD22	1:A:127:ILE:HD12	1.83	0.43
1:G:15:THR:N	1:G:18:HIS:HD2	2.16	0.43
1:D:63:LYS:HA	1:D:63:LYS:HE2	2.01	0.42
1:F:15:THR:N	1:F:18:HIS:HD2	2.16	0.42
1:B:51:ARG:HA	1:B:54:MET:HE2	2.02	0.42
1:C:110:ASN:O	1:C:112:GLU:N	2.52	0.42
1:E:8:PRO:HG3	1:E:74:LEU:HD21	2.01	0.42
1:H:74:LEU:HA	1:H:74:LEU:HD13	1.63	0.42
1:L:57:LEU:CG	1:L:149:GLU:HB3	2.46	0.42
1:G:148:LYS:HE2	3:G:214:HOH:O	2.18	0.42
1:H:15:THR:H	1:H:18:HIS:HD2	1.68	0.42
1:L:80:GLU:OE1	1:L:80:GLU:CA	2.68	0.42
1:D:2:GLN:O	1:D:2:GLN:NE2	2.52	0.42
1:J:36:VAL:O	1:J:36:VAL:CG2	2.67	0.42
1:J:127:ILE:O	2:J:201:ATP:N6	2.47	0.42
1:K:86:LEU:HG	1:K:113:LEU:HD11	2.01	0.42
1:I:55:ILE:HG23	1:I:67:CYS:SG	2.59	0.42
1:J:114:GLU:HG2	1:K:24:ARG:HE	1.83	0.42
1:C:38:HIS:HA	1:C:48:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:HA	1:C:53:LYS:HD3	1.88	0.42
1:D:86:LEU:HG	1:D:113:LEU:HD11	2.02	0.42
1:L:14:VAL:HA	1:L:18:HIS:HD2	1.85	0.42
1:B:39:SER:HB3	1:B:42:LYS:HD2	2.01	0.42
1:I:155:SER:O	1:I:156:LYS:HB2	2.19	0.41
1:J:147:PRO:O	1:J:150:ILE:HG12	2.20	0.41
1:H:6:ILE:HG12	1:H:33:ILE:HB	2.02	0.41
1:J:36:VAL:O	1:J:69:ALA:HA	2.20	0.41
1:L:10:THR:HG22	1:L:12:ASP:HB2	2.01	0.41
1:L:76:ASN:O	1:L:80:GLU:CD	2.64	0.41
1:C:45:MET:HE2	1:C:46:PHE:CE2	2.56	0.41
1:D:31:LYS:HE2	1:D:33:ILE:CD1	2.47	0.41
1:G:79:LYS:HB2	1:G:79:LYS:HE3	1.88	0.41
1:H:10:THR:HG22	1:H:12:ASP:HB2	2.03	0.41
1:L:30:GLU:O	1:L:64:ASN:HB2	2.21	0.41
1:B:42:LYS:O	1:B:43:ASN:C	2.64	0.41
1:J:67:CYS:O	1:J:68:VAL:HG12	2.21	0.41
1:C:14:VAL:HA	1:C:18:HIS:HD2	1.84	0.41
1:C:91:ARG:HH22	1:C:128:SER:CB	2.34	0.41
1:J:90:LEU:HD11	1:K:90:LEU:HD11	2.02	0.41
1:C:44:PRO:C	1:C:46:PHE:N	2.78	0.41
1:C:38:HIS:HD2	1:C:48:LEU:HB2	1.86	0.41
1:G:40:SER:O	1:G:42:LYS:O	2.39	0.41
1:H:110:ASN:OD1	1:H:112:GLU:HG2	2.21	0.41
1:I:48:LEU:HD21	1:I:69:ALA:HB1	2.02	0.40
1:C:15:THR:O	1:C:19:ILE:HG12	2.21	0.40
1:C:146:VAL:HB	1:C:147:PRO:HD2	2.02	0.40
1:D:91:ARG:HH11	1:D:128:SER:HB2	1.86	0.40
1:G:116:LEU:HG	1:H:116:LEU:HD11	2.01	0.40
1:I:4:ILE:HD12	1:I:31:LYS:HD3	2.02	0.40
1:I:128:SER:CB	1:H:101:GLN:HE22	2.34	0.40
1:J:11:PHE:O	1:J:13:PRO:HA	2.19	0.40
1:J:138:HIS:O	1:J:139:LYS:HB2	2.22	0.40
1:L:4:ILE:HG23	1:L:83:CYS:HA	2.02	0.40
1:I:136:ILE:O	1:I:137:ALA:C	2.65	0.40
1:D:10:THR:HG22	1:D:12:ASP:HB2	2.03	0.40
1:G:24:ARG:NH1	1:G:121:THR:HG22	2.37	0.40
1:C:38:HIS:CD2	1:C:48:LEU:HB2	2.56	0.40
1:C:59:THR:CG2	1:C:67:CYS:SG	2.97	0.40
1:D:1:MET:HB3	1:E:28:LEU:CD1	2.51	0.40
1:E:40:SER:O	1:E:41:ALA:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ILE:HG23	1:E:67:CYS:SG	2.61	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:139:LYS:O	1:E:139:LYS:NZ[1_546]	1.04	1.16
1:J:139:LYS:O	1:E:139:LYS:CE[1_546]	1.38	0.82
1:G:141:ASP:OD1	1:H:156:LYS:NZ[1_455]	1.45	0.75
1:J:139:LYS:C	1:E:139:LYS:NZ[1_546]	1.77	0.43
1:J:139:LYS:O	1:E:139:LYS:CD[1_546]	1.89	0.31
1:D:71:GLU:OE1	1:H:69:ALA:O[1_465]	2.02	0.18
1:G:141:ASP:CG	1:H:156:LYS:NZ[1_455]	2.07	0.13
1:E:38:HIS:NE2	1:F:80:GLU:OE1[1_655]	2.10	0.10

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 X-ray entries followed by that with respect to entries of similar resolution.

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	155/157 (99%)	152 (98%)	3 (2%)	0	100	100
1	B	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
1	C	154/157 (98%)	142 (92%)	12 (8%)	0	100	100
1	D	154/157 (98%)	152 (99%)	2 (1%)	0	100	100
1	E	154/157 (98%)	151 (98%)	3 (2%)	0	100	100
1	F	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
1	G	155/157 (99%)	151 (97%)	4 (3%)	0	100	100
1	H	154/157 (98%)	151 (98%)	3 (2%)	0	100	100
1	I	154/157 (98%)	152 (99%)	2 (1%)	0	100	100
1	J	154/157 (98%)	145 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	154/157 (98%)	151 (98%)	3 (2%)	0	100	100
1	L	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
All	All	1850/1884 (98%)	1796 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	138/138 (100%)	130 (94%)	8 (6%)	18	22
1	B	138/138 (100%)	128 (93%)	10 (7%)	13	15
1	C	138/138 (100%)	123 (89%)	15 (11%)	6	6
1	D	138/138 (100%)	132 (96%)	6 (4%)	26	35
1	E	138/138 (100%)	128 (93%)	10 (7%)	13	15
1	F	138/138 (100%)	131 (95%)	7 (5%)	21	27
1	G	138/138 (100%)	126 (91%)	12 (9%)	9	10
1	H	138/138 (100%)	128 (93%)	10 (7%)	13	15
1	I	138/138 (100%)	132 (96%)	6 (4%)	26	35
1	J	138/138 (100%)	124 (90%)	14 (10%)	7	7
1	K	138/138 (100%)	135 (98%)	3 (2%)	45	61
1	L	138/138 (100%)	129 (94%)	9 (6%)	15	18
All	All	1656/1656 (100%)	1546 (93%)	110 (7%)	15	18

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	1	MET
1	I	2	GLN
1	I	57	LEU
1	I	149	GLU

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Mol	Chain	Res	Type
1	I	153	LEU
1	I	155	SER
1	J	1	MET
1	J	26	SER
1	J	36	VAL
1	J	39	SER
1	J	53	LYS
1	J	57	LEU
1	J	63	LYS
1	J	64	ASN
1	J	66	GLU
1	J	68	VAL
1	J	79	LYS
1	J	109	LEU
1	J	123	GLN
1	J	152	PRO
1	L	2	GLN
1	L	28	LEU
1	L	57	LEU
1	L	80	GLU
1	L	116	LEU
1	L	123	GLN
1	L	139	LYS
1	L	150	ILE
1	L	156	LYS
1	A	2	GLN
1	A	53	LYS
1	A	66	GLU
1	A	79	LYS
1	A	107	LYS
1	A	116	LEU
1	A	123	GLN
1	A	153	LEU
1	B	2	GLN
1	B	4	ILE
1	B	28	LEU
1	B	50	GLU
1	B	64	ASN
1	B	79	LYS
1	B	99	GLU
1	B	109	LEU
1	B	150	ILE

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Mol	Chain	Res	Type
1	B	156	LYS
1	C	4	ILE
1	C	24	ARG
1	C	39	SER
1	C	42	LYS
1	C	47	SER
1	C	59	THR
1	C	73	LEU
1	C	80	GLU
1	C	81	TYR
1	C	129	SER
1	C	131	ILE
1	C	148	LYS
1	C	152	PRO
1	C	153	LEU
1	C	154	ILE
1	D	27	GLU
1	D	31	LYS
1	D	57	LEU
1	D	63	LYS
1	D	71	GLU
1	D	131	ILE
1	E	1	MET
1	E	2	GLN
1	E	28	LEU
1	E	55	ILE
1	E	71	GLU
1	E	73	LEU
1	E	80	GLU
1	E	112	GLU
1	E	149	GLU
1	E	154	ILE
1	F	3	LYS
1	F	4	ILE
1	F	28	LEU
1	F	31	LYS
1	F	39	SER
1	F	63	LYS
1	F	71	GLU
1	G	1	MET
1	G	4	ILE
1	G	31	LYS

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Mol	Chain	Res	Type
1	G	57	LEU
1	G	76	ASN
1	G	84	LYS
1	G	109	LEU
1	G	112	GLU
1	G	130	SER
1	G	134	SER
1	G	148	LYS
1	G	153	LEU
1	H	60	LYS
1	H	66	GLU
1	H	71	GLU
1	H	74	LEU
1	H	79	LYS
1	H	131	ILE
1	H	139	LYS
1	H	148	LYS
1	H	153	LEU
1	H	154	ILE
1	K	63	LYS
1	K	90	LEU
1	K	156	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	43	ASN
1	I	106	ASN
1	I	111	HIS
1	J	56	GLN
1	J	101	GLN
1	J	124	ASN
1	L	18	HIS
1	L	56	GLN
1	L	106	ASN
1	L	111	HIS
1	L	138	HIS
1	A	38	HIS
1	A	43	ASN
1	A	124	ASN
1	A	138	HIS
1	B	16	ASN

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Mol	Chain	Res	Type
1	B	18	HIS
1	B	64	ASN
1	B	106	ASN
1	C	18	HIS
1	C	23	HIS
1	C	38	HIS
1	C	43	ASN
1	C	138	HIS
1	D	18	HIS
1	D	23	HIS
1	D	123	GLN
1	E	76	ASN
1	F	18	HIS
1	F	106	ASN
1	F	123	GLN
1	F	138	HIS
1	F	144	HIS
1	G	18	HIS
1	G	23	HIS
1	H	43	ASN
1	H	56	GLN
1	H	76	ASN
1	H	101	GLN
1	K	18	HIS
1	K	123	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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
2	ATP	L	201	-	32,33,33	2.03	7 (21%)	48,52,52	1.95	15 (31%)
2	ATP	J	201	-	32,33,33	2.03	7 (21%)	48,52,52	1.84	11 (22%)
2	ATP	I	201	-	32,33,33	2.01	6 (18%)	48,52,52	2.11	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
2	ATP	L	201	-	-	5/22/38/38	0/3/3/3
2	ATP	J	201	-	-	6/22/38/38	0/3/3/3
2	ATP	I	201	-	-	6/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	ATP	PB-O3B	7.70	1.67	1.59
2	J	201	ATP	PB-O3B	6.40	1.66	1.59
2	I	201	ATP	PB-O3B	6.26	1.66	1.59
2	L	201	ATP	C5-C4	5.15	1.48	1.39
2	J	201	ATP	C5-C4	5.03	1.48	1.39
2	I	201	ATP	PB-O3A	4.54	1.64	1.59
2	I	201	ATP	PA-O3A	4.35	1.64	1.59
2	I	201	ATP	C5-C4	4.27	1.46	1.39
2	J	201	ATP	PA-O3A	3.75	1.63	1.59
2	J	201	ATP	PB-O3A	3.47	1.63	1.59
2	J	201	ATP	C5-C6	3.28	1.50	1.41
2	I	201	ATP	C8-N7	3.20	1.37	1.31
2	I	201	ATP	C5-C6	3.00	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	ATP	C8-N7	2.98	1.37	1.31
2	L	201	ATP	C5-C6	2.89	1.49	1.41
2	J	201	ATP	C8-N7	2.70	1.36	1.31
2	L	201	ATP	PA-O3A	2.59	1.62	1.59
2	L	201	ATP	C4-N9	-2.54	1.32	1.37
2	J	201	ATP	C4-N9	-2.40	1.32	1.37
2	L	201	ATP	PB-O3A	2.01	1.61	1.59

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	ATP	C5-C4-N3	-6.42	117.88	126.72
2	J	201	ATP	C5-C4-N3	-4.89	119.98	126.72
2	I	201	ATP	C2-N3-C4	4.53	122.88	111.83
2	L	201	ATP	N3-C2-N1	-4.38	121.95	128.58
2	I	201	ATP	N3-C4-N9	4.25	134.40	127.17
2	I	201	ATP	N3-C2-N1	-4.19	122.23	128.58
2	J	201	ATP	C4-C5-N7	-4.09	105.91	110.58
2	L	201	ATP	C5-C4-N3	-3.94	121.29	126.72
2	L	201	ATP	C2-N1-C6	3.84	125.04	118.73
2	J	201	ATP	O4'-C1'-N9	3.82	115.43	108.09
2	J	201	ATP	N3-C2-N1	-3.80	122.83	128.58
2	I	201	ATP	C4-C5-N7	-3.70	106.35	110.58
2	J	201	ATP	C2-N3-C4	3.65	120.75	111.83
2	I	201	ATP	C3'-C2'-C1'	3.47	108.02	101.46
2	L	201	ATP	C2-N3-C4	3.47	120.30	111.83
2	J	201	ATP	N3-C4-N9	3.33	132.83	127.17
2	L	201	ATP	C6-C5-N7	3.32	138.49	132.09
2	L	201	ATP	O2A-PA-O3A	-3.18	98.67	107.27
2	L	201	ATP	C4-C5-N7	-3.17	106.96	110.58
2	J	201	ATP	C6-C5-N7	3.12	138.11	132.09
2	I	201	ATP	C6-C5-N7	3.01	137.89	132.09
2	I	201	ATP	O2'-C2'-C3'	-2.87	102.60	111.82
2	I	201	ATP	O3A-PA-O1A	2.75	118.97	110.70
2	L	201	ATP	O3G-PG-O3B	2.72	113.76	104.64
2	L	201	ATP	N3-C4-N9	2.71	131.78	127.17
2	L	201	ATP	O3B-PG-O1G	-2.71	96.78	111.04
2	L	201	ATP	O4'-C4'-C5'	2.70	117.97	109.33
2	J	201	ATP	C2-N1-C6	2.68	123.13	118.73
2	J	201	ATP	C4-N9-C8	2.61	108.48	105.74
2	I	201	ATP	C2'-C1'-N9	2.56	119.67	113.30
2	L	201	ATP	C4-N9-C8	2.52	108.39	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	ATP	O4'-C1'-N9	-2.48	103.32	108.09
2	J	201	ATP	C5-N7-C8	2.43	107.27	103.45
2	L	201	ATP	O4'-C1'-N9	2.38	112.66	108.09
2	I	201	ATP	C5-N7-C8	2.35	107.15	103.45
2	L	201	ATP	C4-N9-C1'	-2.35	121.13	126.63
2	L	201	ATP	O3'-C3'-C4'	-2.28	104.55	111.08
2	I	201	ATP	O2A-PA-O3A	-2.26	101.18	107.27
2	I	201	ATP	C2-N1-C6	2.22	122.38	118.73
2	I	201	ATP	O3B-PG-O1G	-2.12	99.91	111.04
2	J	201	ATP	O3B-PG-O1G	-2.05	100.28	111.04

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	201	ATP	PB-O3B-PG-O3G
2	I	201	ATP	C5'-O5'-PA-O2A
2	I	201	ATP	C5'-O5'-PA-O3A
2	J	201	ATP	PB-O3A-PA-O5'
2	J	201	ATP	C5'-O5'-PA-O3A
2	L	201	ATP	C5'-O5'-PA-O3A
2	L	201	ATP	C2'-C1'-N9-C8
2	I	201	ATP	PA-O3A-PB-O1B
2	I	201	ATP	C5'-O5'-PA-O1A
2	J	201	ATP	C5'-O5'-PA-O1A
2	L	201	ATP	C5'-O5'-PA-O1A
2	J	201	ATP	PA-O3A-PB-O2B
2	I	201	ATP	PB-O3B-PG-O1G
2	J	201	ATP	O4'-C1'-N9-C8
2	L	201	ATP	O4'-C1'-N9-C8
2	J	201	ATP	C2'-C1'-N9-C8
2	L	201	ATP	PA-O3A-PB-O2B

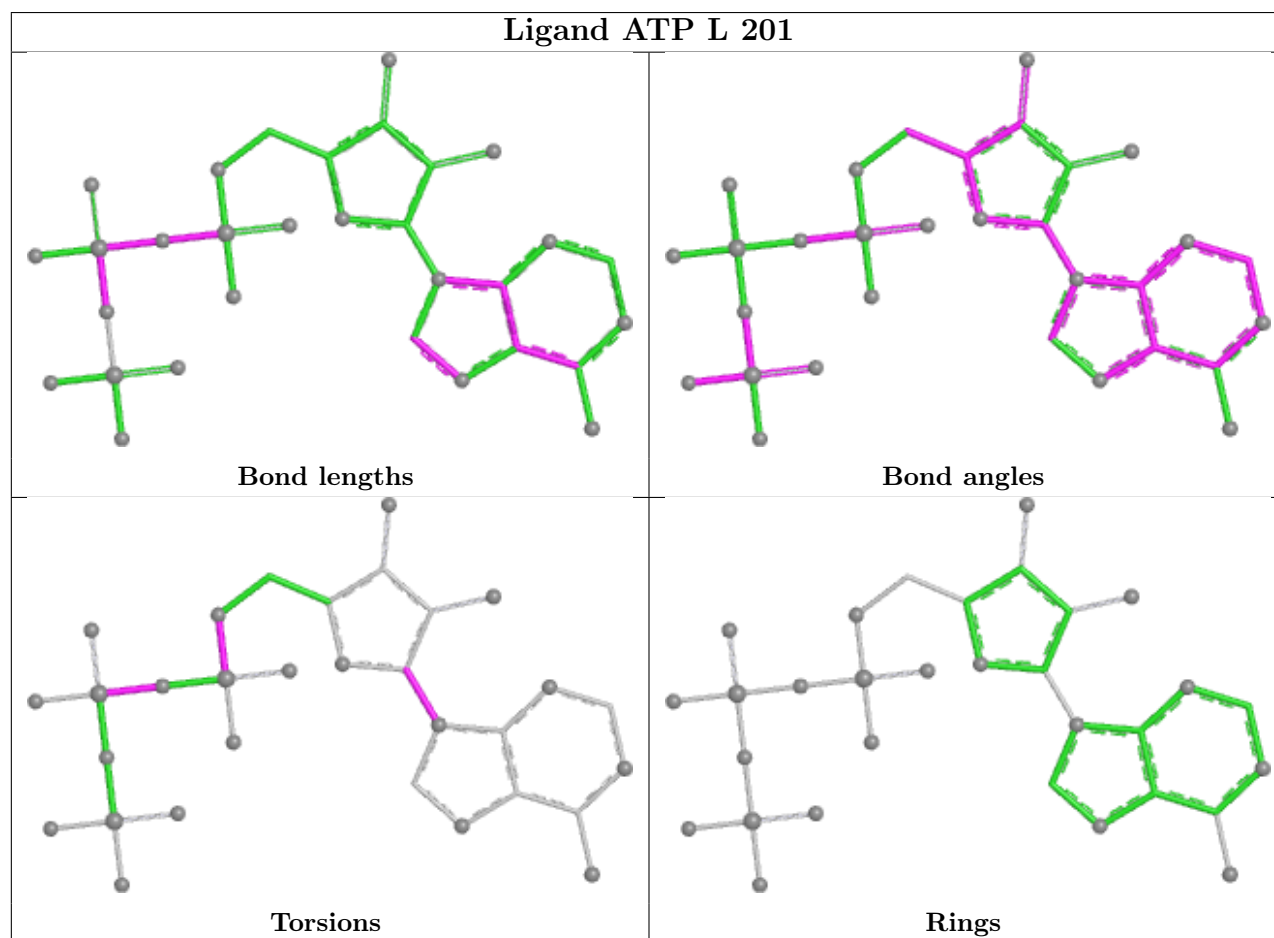
There are no ring outliers.

2 monomers are involved in 5 short contacts:

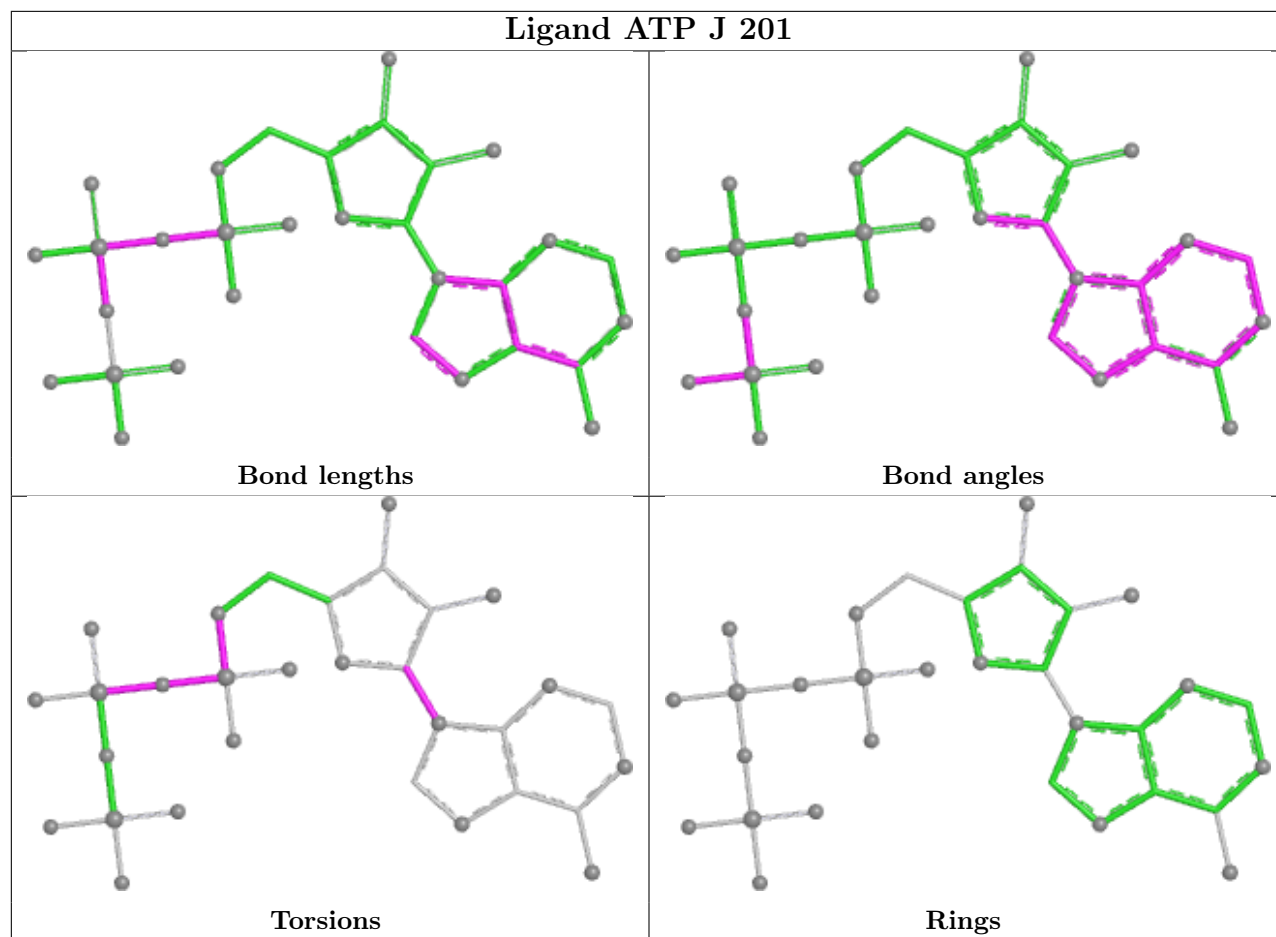
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	201	ATP	2	0
2	I	201	ATP	3	0

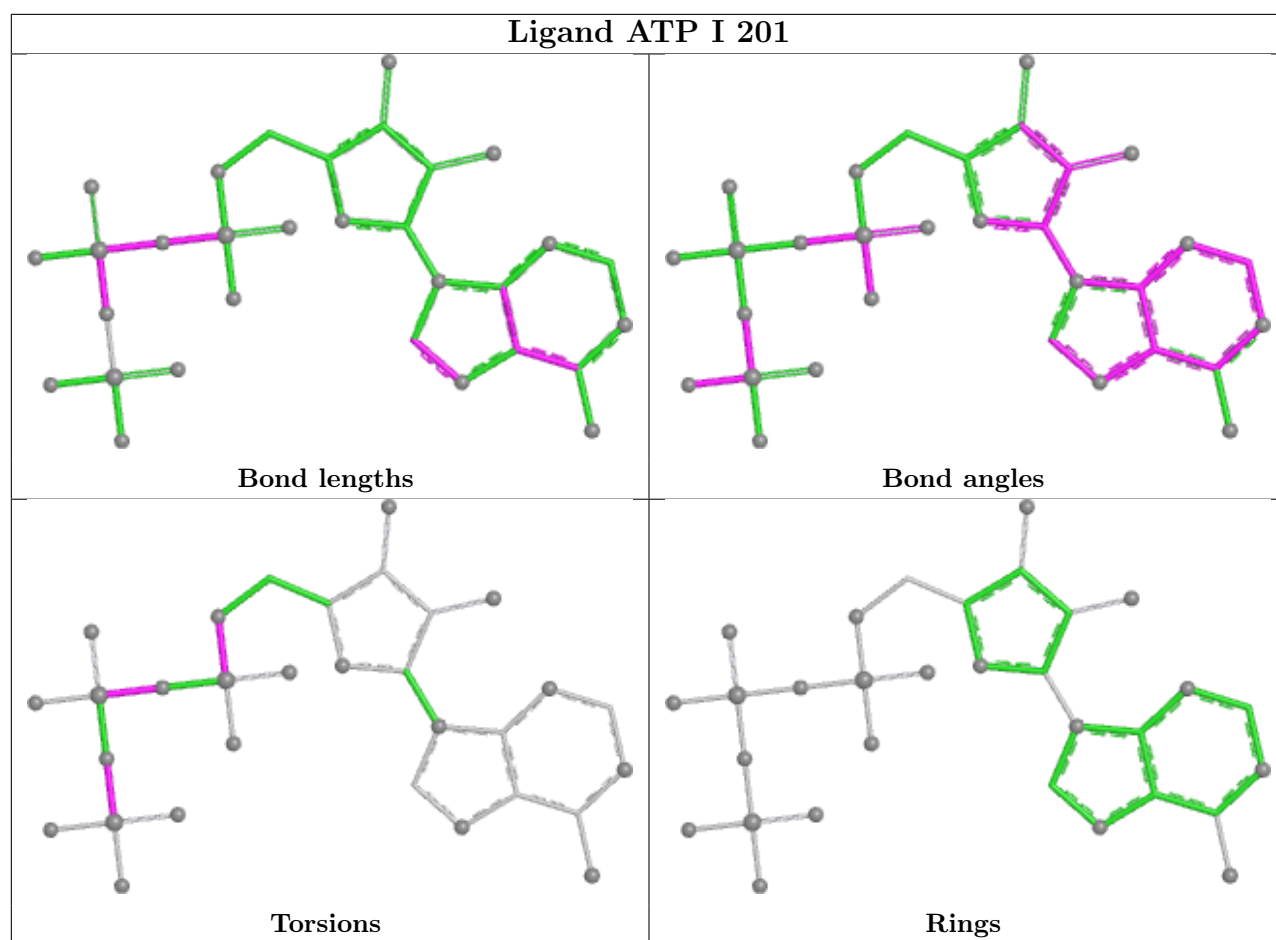
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 J 201





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	157/157 (100%)	0.15	10 (6%) 25 22	23, 34, 75, 112	0
1	B	156/157 (99%)	0.20	5 (3%) 50 47	27, 41, 69, 101	0
1	C	156/157 (99%)	0.86	26 (16%) 4 3	26, 49, 76, 88	0
1	D	156/157 (99%)	-0.07	3 (1%) 66 63	22, 33, 59, 102	0
1	E	156/157 (99%)	0.27	8 (5%) 33 30	25, 41, 90, 121	0
1	F	156/157 (99%)	-0.04	5 (3%) 50 47	23, 36, 59, 100	0
1	G	157/157 (100%)	0.19	7 (4%) 38 35	26, 39, 74, 103	0
1	H	156/157 (99%)	0.13	8 (5%) 33 30	24, 38, 72, 110	0
1	I	156/157 (99%)	-0.07	4 (2%) 57 54	21, 32, 55, 106	0
1	J	156/157 (99%)	0.85	19 (12%) 8 6	29, 52, 84, 108	0
1	K	156/157 (99%)	0.09	9 (5%) 29 25	24, 36, 79, 108	0
1	L	156/157 (99%)	0.26	7 (4%) 38 35	24, 39, 73, 115	0
All	All	1874/1884 (99%)	0.23	111 (5%) 28 25	21, 39, 75, 121	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	5.5
1	A	41	ALA	5.4
1	C	77	LEU	5.4
1	J	41	ALA	5.3
1	I	18	HIS	5.0
1	K	41	ALA	5.0
1	C	73	LEU	4.7
1	L	139	LYS	4.7
1	I	1	MET	4.6
1	E	41	ALA	4.5
1	D	71	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	J	48	LEU	4.5
1	K	44	PRO	4.4
1	J	78	ALA	4.3
1	A	38	HIS	4.1
1	J	49	ASP	4.1
1	A	1	MET	3.8
1	C	81	TYR	3.8
1	G	73	LEU	3.6
1	I	17	GLY	3.6
1	J	153	LEU	3.6
1	E	42	LYS	3.6
1	F	1	MET	3.5
1	K	72	GLY	3.5
1	G	1	MET	3.4
1	H	41	ALA	3.4
1	H	155	SER	3.3
1	E	1	MET	3.3
1	C	74	LEU	3.3
1	K	73	LEU	3.3
1	C	75	ALA	3.2
1	C	72	GLY	3.2
1	C	76	ASN	3.2
1	K	71	GLU	3.2
1	C	65	VAL	3.2
1	G	151	TYR	3.2
1	L	1	MET	3.2
1	D	1	MET	3.2
1	C	47	SER	3.1
1	K	39	SER	3.1
1	C	50	GLU	3.1
1	H	154	ILE	3.1
1	L	154	ILE	3.1
1	J	64	ASN	3.0
1	G	72	GLY	3.0
1	C	1	MET	3.0
1	F	71	GLU	2.9
1	J	38	HIS	2.8
1	H	38	HIS	2.8
1	C	153	LEU	2.8
1	F	41	ALA	2.8
1	K	40	SER	2.8
1	E	44	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	2	GLN	2.8
1	C	52	LEU	2.8
1	H	1	MET	2.8
1	I	71	GLU	2.7
1	C	80	GLU	2.7
1	G	157	ALA	2.6
1	E	40	SER	2.6
1	B	41	ALA	2.6
1	C	49	ASP	2.6
1	A	73	LEU	2.6
1	J	76	ASN	2.6
1	A	2	GLN	2.5
1	L	71	GLU	2.5
1	L	130	SER	2.5
1	A	108	SER	2.5
1	A	71	GLU	2.5
1	C	154	ILE	2.5
1	H	2	GLN	2.4
1	E	155	SER	2.4
1	C	59	THR	2.4
1	J	70	PHE	2.4
1	B	153	LEU	2.4
1	L	28	LEU	2.4
1	C	71	GLU	2.4
1	K	43	ASN	2.3
1	J	39	SER	2.3
1	E	39	SER	2.3
1	J	4	ILE	2.3
1	C	43	ASN	2.3
1	F	43	ASN	2.3
1	B	155	SER	2.3
1	H	71	GLU	2.3
1	C	156	LYS	2.3
1	C	48	LEU	2.2
1	C	2	GLN	2.2
1	J	1	MET	2.2
1	J	74	LEU	2.2
1	C	55	ILE	2.2
1	G	111	HIS	2.2
1	J	73	LEU	2.1
1	B	1	MET	2.1
1	J	34	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	42	LYS	2.1
1	J	36	VAL	2.1
1	L	3	LYS	2.1
1	E	38	HIS	2.1
1	J	82	HIS	2.1
1	B	75	ALA	2.0
1	C	54	MET	2.0
1	G	41	ALA	2.0
1	H	138	HIS	2.0
1	A	72	GLY	2.0
1	J	47	SER	2.0
1	J	80	GLU	2.0
1	A	39	SER	2.0
1	C	108	SER	2.0
1	C	28	LEU	2.0
1	F	12	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

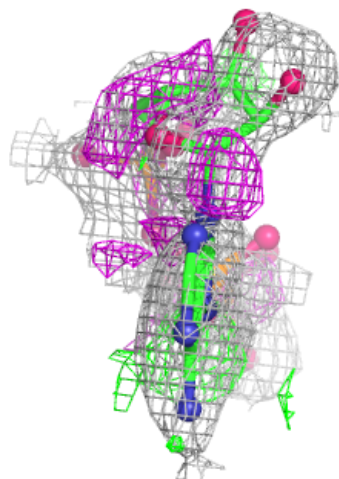
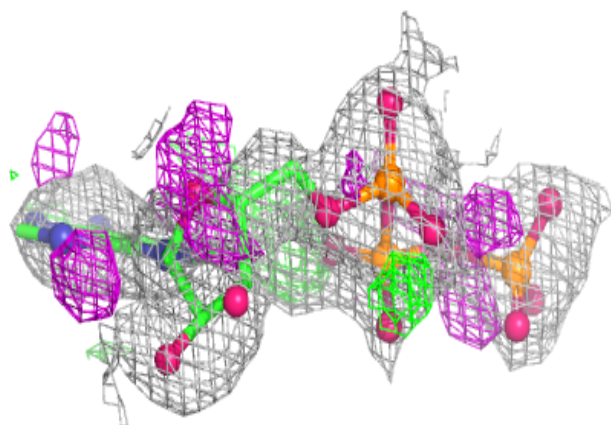
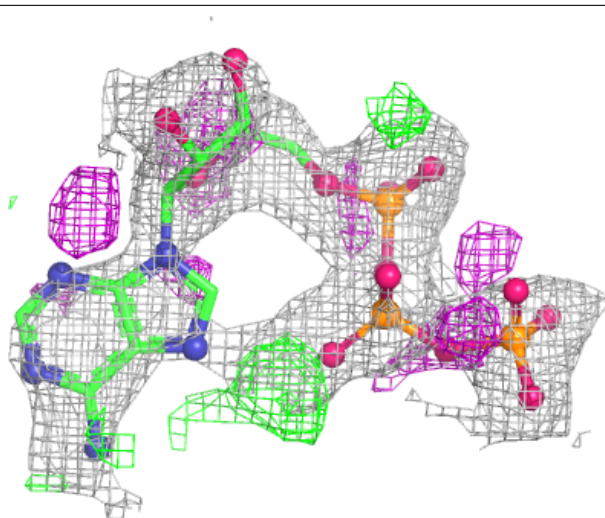
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	I	201	31/31	0.74	0.16	51,72,92,106	0
2	ATP	J	201	31/31	0.76	0.16	79,97,113,114	0
2	ATP	L	201	31/31	0.80	0.13	41,60,82,88	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

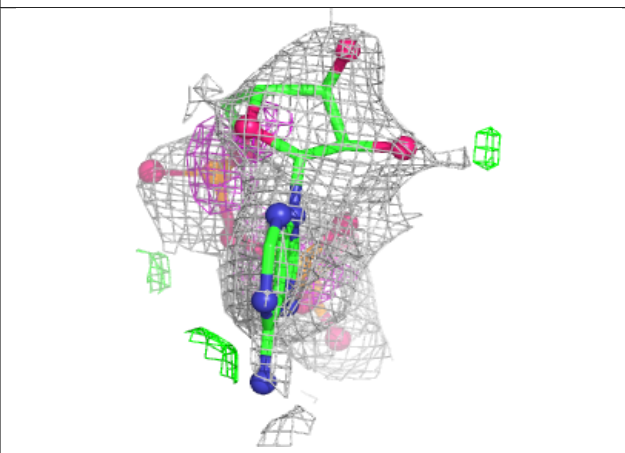
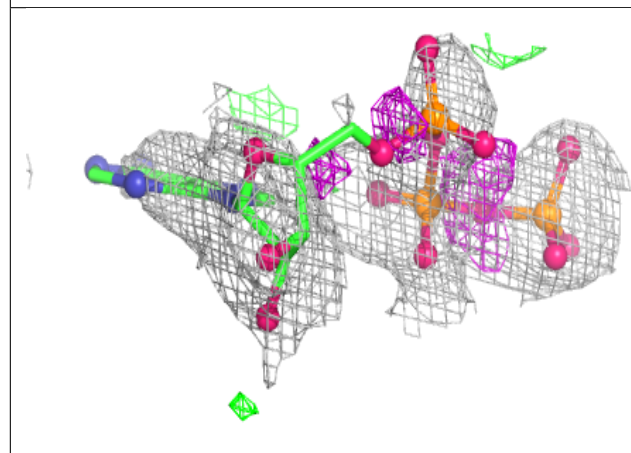
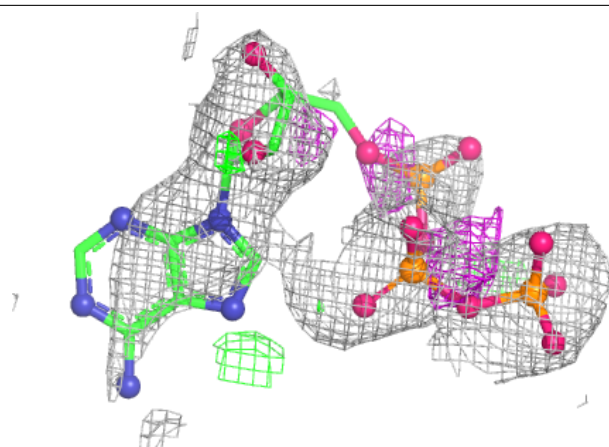
Electron density around ATP I 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



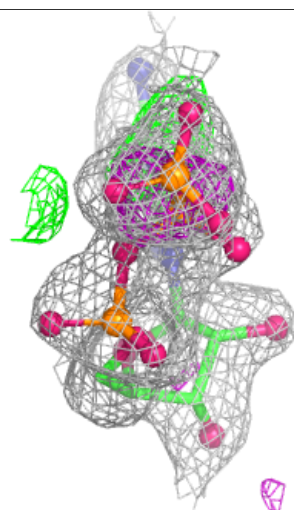
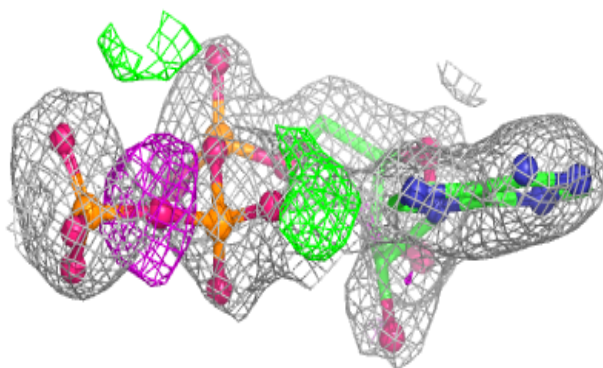
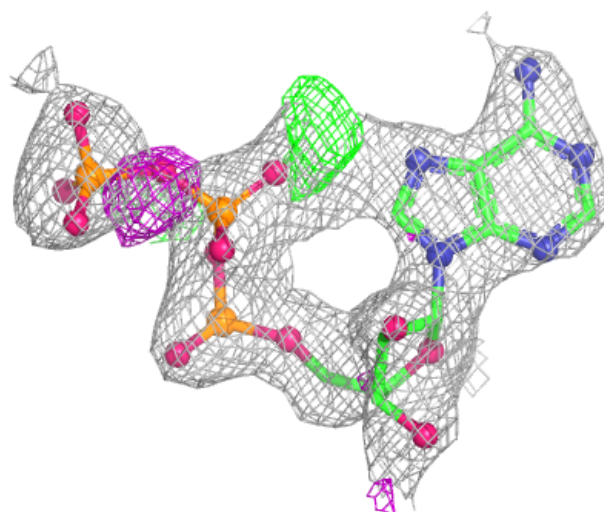
Electron density around ATP J 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP L 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.