



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:34 PM UTC

PDB ID : 3F5M / pdb_00003f5m
Title : Crystal Structure of ATP-Bound Phosphofructokinase from Trypanosoma brucei
Authors : McNae, I.W.; Martinez-Oyanedel, J.; Keillor, J.W.; Michels, P.A.M.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.
Deposited on : 2008-11-04
Resolution : 2.70 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

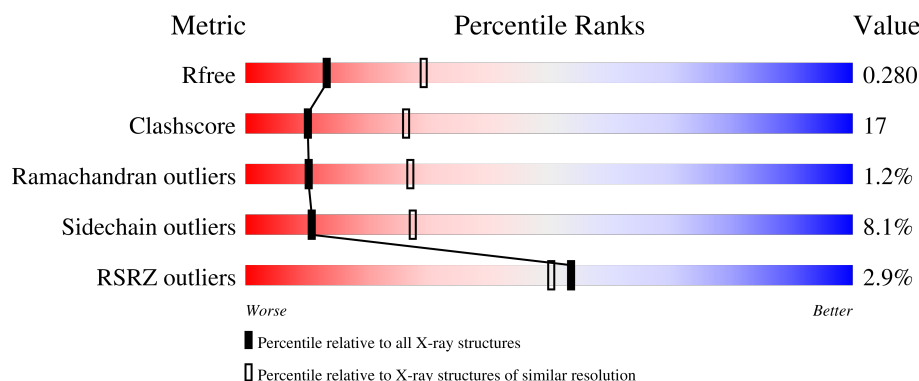
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	487	2% 64% 27% • 6%
1	B	487	2% 62% 28% • 5%
1	C	487	5% 62% 28% • 5%
1	D	487	2% 62% 28% • 6%

2 Entry composition [i](#)

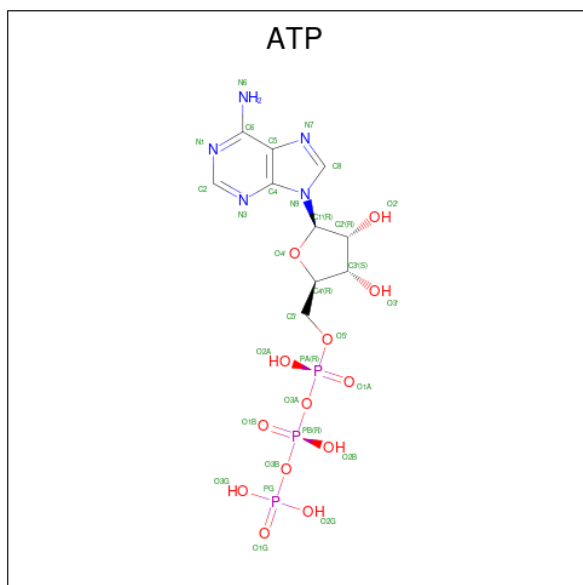
There are 7 unique types of molecules in this entry. The entry contains 14783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-phospho-1-fructokinase (ATP-dependent phosphofructokinase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3536	2218	652	649	17			
1	B	462	Total	C	N	O	S	0	0	0
			3569	2234	659	659	17			
1	C	461	Total	C	N	O	S	0	0	0
			3562	2233	658	654	17			
1	D	458	Total	C	N	O	S	0	0	0
			3540	2219	655	649	17			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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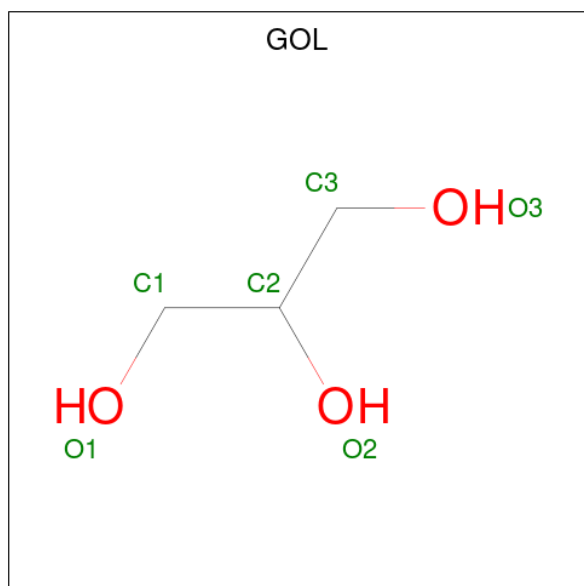
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Na 2	0	0
5	B	1	Total 1	Na 1	0	0
5	C	1	Total 1	Na 1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 5	O 4	S 1	0	0

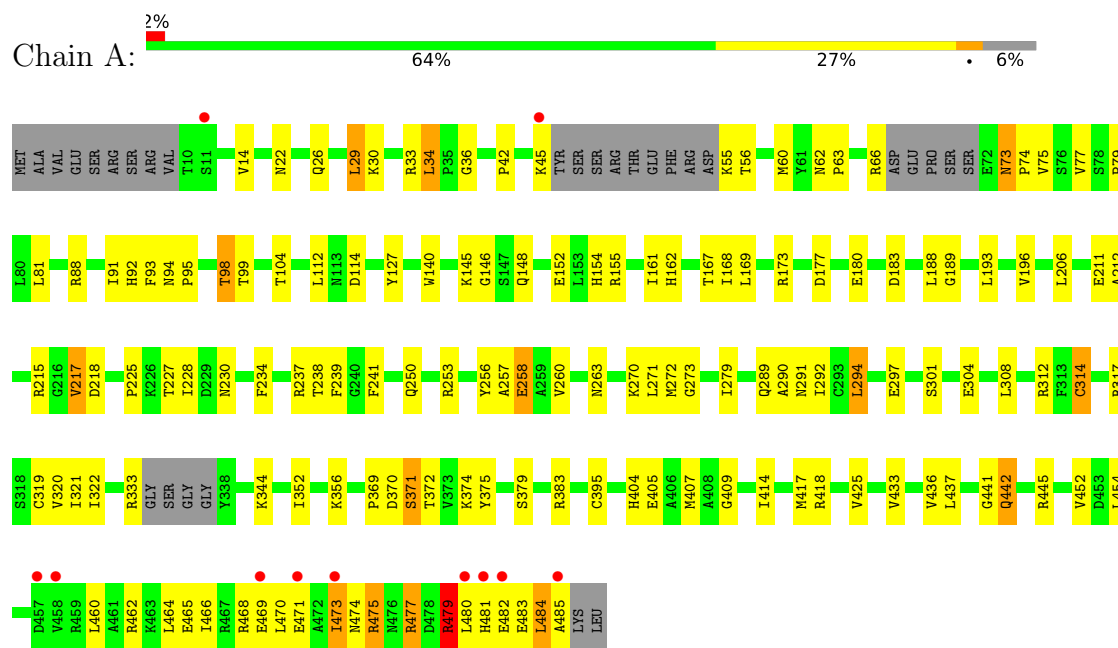
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total 102	O 102	0	0
7	B	103	Total 103	O 103	0	0
7	C	100	Total 100	O 100	0	0
7	D	123	Total 123	O 123	0	0

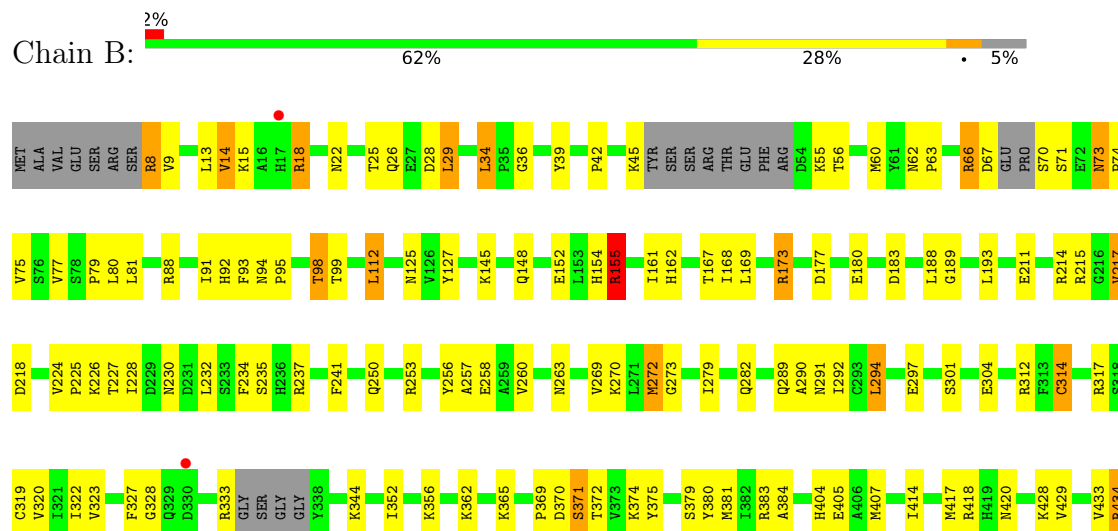
3 Residue-property plots

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 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: 6-phospho-1-fructokinase (ATP-dependent phosphofructokinase)

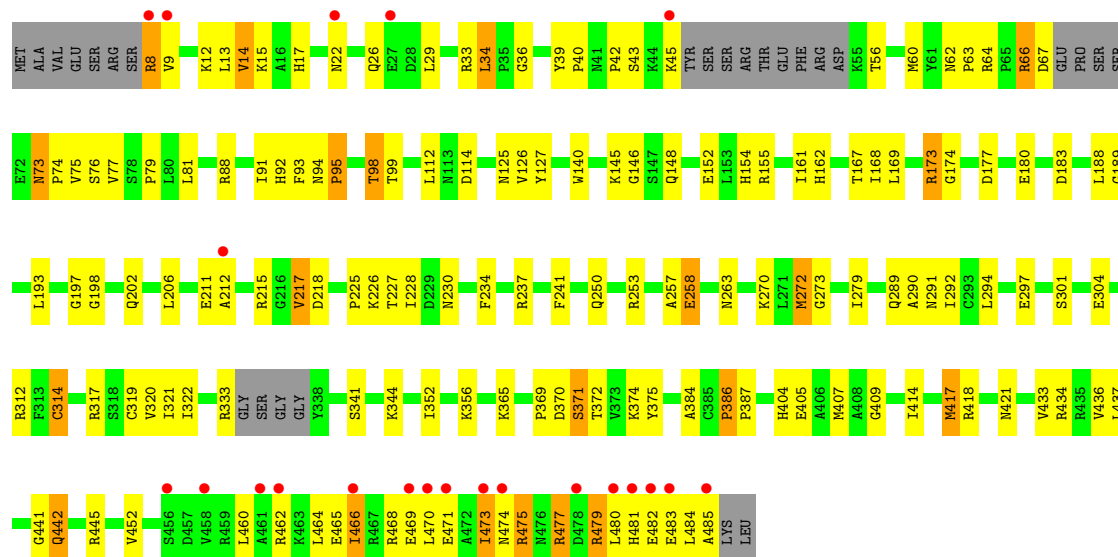


- Molecule 1: 6-phospho-1-fructokinase (ATP-dependent phosphofructokinase)

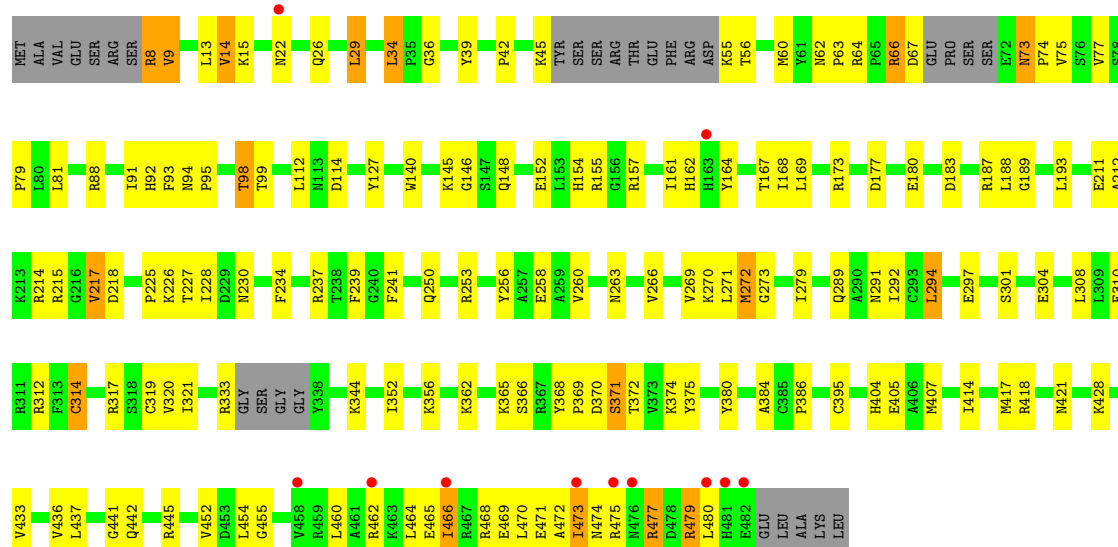




- Molecule 1: 6-phospho-1-fructokinase (ATP-dependent phosphofructokinase)



- Molecule 1: 6-phospho-1-fructokinase (ATP-dependent phosphofructokinase)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.58Å 117.57Å 176.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.88 – 2.70 15.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.88-2.70) 97.4 (15.88-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.224 , 0.286 0.214 , 0.280	Depositor DCC
R_{free} test set	2775 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14783	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 57.84 % 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 2.2323e-05. 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: GOL, ATP, MG, SO4, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/3593	0.92	10/4856 (0.2%)
1	B	0.62	0/3626	1.07	23/4900 (0.5%)
1	C	0.60	0/3619	0.91	8/4891 (0.2%)
1	D	0.62	0/3597	0.92	8/4861 (0.2%)
All	All	0.61	0/14435	0.96	49/19508 (0.3%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	NE-CZ-NH2	11.72	129.75	119.20
1	B	383	ARG	NE-CZ-NH2	11.71	129.74	119.20
1	B	155	ARG	NE-CZ-NH1	-11.21	110.28	121.50
1	B	434	ARG	NE-CZ-NH2	10.99	129.09	119.20
1	A	479	ARG	NE-CZ-NH2	10.94	129.04	119.20
1	B	383	ARG	NE-CZ-NH1	-10.86	110.64	121.50
1	B	448	ARG	NE-CZ-NH2	10.80	128.92	119.20
1	B	434	ARG	NE-CZ-NH1	-10.09	111.41	121.50
1	B	448	ARG	NE-CZ-NH1	-9.68	111.82	121.50
1	B	18	ARG	NE-CZ-NH2	-9.20	110.92	119.20
1	B	467	ARG	NE-CZ-NH2	9.14	127.42	119.20
1	A	479	ARG	NE-CZ-NH1	-9.05	112.45	121.50
1	B	155	ARG	CD-NE-CZ	8.72	136.61	124.40
1	B	467	ARG	NE-CZ-NH1	-8.62	112.88	121.50
1	B	434	ARG	CD-NE-CZ	8.41	136.17	124.40
1	B	18	ARG	CD-NE-CZ	8.14	135.80	124.40
1	B	448	ARG	CD-NE-CZ	8.07	135.69	124.40
1	B	383	ARG	CD-NE-CZ	8.05	135.67	124.40
1	B	18	ARG	NE-CZ-NH1	7.54	129.04	121.50
1	D	66	ARG	NE-CZ-NH2	7.22	125.70	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	D	66	ARG	NE-CZ-NH1	-7.04	114.46	121.50
1	A	66	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	D	73	ASN	N-CA-C	6.60	117.19	109.60
1	C	73	ASN	CA-C-N	6.52	126.48	119.76
1	C	73	ASN	C-N-CA	6.52	126.48	119.76
1	A	479	ARG	CD-NE-CZ	6.41	133.38	124.40
1	B	73	ASN	CA-C-N	6.33	126.28	119.76
1	B	73	ASN	C-N-CA	6.33	126.28	119.76
1	B	73	ASN	N-CA-C	6.20	116.72	109.60
1	A	73	ASN	CA-C-N	6.10	126.05	119.76
1	A	73	ASN	C-N-CA	6.10	126.05	119.76
1	C	386	PRO	CA-C-N	6.04	125.80	119.76
1	C	386	PRO	C-N-CA	6.04	125.80	119.76
1	D	73	ASN	CA-C-N	5.99	125.93	119.76
1	D	73	ASN	C-N-CA	5.99	125.93	119.76
1	B	379	SER	N-CA-C	5.82	118.12	111.02
1	D	386	PRO	O-C-N	5.81	123.88	121.15
1	B	66	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	C	386	PRO	O-C-N	5.62	123.79	121.15
1	B	467	ARG	CD-NE-CZ	5.55	132.17	124.40
1	C	66	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	C	73	ASN	N-CA-C	5.28	115.68	109.60
1	D	386	PRO	CA-C-N	5.18	124.94	119.76
1	D	386	PRO	C-N-CA	5.18	124.94	119.76
1	A	73	ASN	N-CA-C	5.09	115.45	109.60
1	C	66	ARG	CD-NE-CZ	5.02	131.42	124.40
1	A	425	VAL	CA-C-N	5.01	124.92	119.76
1	A	425	VAL	C-N-CA	5.01	124.92	119.76

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	3536	0	3608	147	0
1	B	3569	0	3632	147	1
1	C	3562	0	3634	153	1
1	D	3540	0	3612	139	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
2	C	31	0	12	2	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	C	5	0	0	0	0
7	A	102	0	0	5	0
7	B	103	0	0	7	0
7	C	100	0	0	5	0
7	D	123	0	0	12	0
All	All	14783	0	14550	494	1

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 17.

All (494) 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:A:473:ILE:HG13	1:C:477:ARG:HG2	1.40	1.03
1:A:477:ARG:HG2	1:C:473:ILE:HG13	1.38	1.02
1:B:477:ARG:HG3	1:D:477:ARG:HG3	1.44	0.98
1:C:258:GLU:HG2	1:C:374:LYS:HG3	1.45	0.97
1:C:475:ARG:HH22	1:C:479:ARG:HH11	1.00	0.97
1:B:258:GLU:HG2	1:B:374:LYS:HG3	1.43	0.97
1:A:291:ASN:ND2	1:A:320:VAL:H	1.62	0.96
1:C:291:ASN:HD22	1:C:320:VAL:H	1.02	0.95
1:A:258:GLU:HG2	1:A:374:LYS:HG3	1.47	0.95
1:D:475:ARG:HH22	1:D:479:ARG:HH11	0.96	0.95
1:B:475:ARG:HH22	1:B:479:ARG:HH11	0.97	0.94
1:B:291:ASN:HD22	1:B:320:VAL:H	1.09	0.93
1:C:291:ASN:ND2	1:C:320:VAL:H	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ASN:HD22	1:D:320:VAL:H	1.11	0.92
1:A:474:ASN:HD21	1:C:477:ARG:HE	1.13	0.91
1:A:291:ASN:HD22	1:A:320:VAL:H	1.03	0.91
1:D:291:ASN:ND2	1:D:320:VAL:H	1.68	0.91
1:A:477:ARG:HE	1:C:474:ASN:HD21	1.18	0.89
1:B:291:ASN:ND2	1:B:320:VAL:H	1.68	0.89
1:A:75:VAL:HG22	1:B:75:VAL:HG22	1.51	0.89
1:D:56:THR:HG22	1:D:88:ARG:HH21	1.35	0.89
1:B:480:LEU:HB2	1:D:473:ILE:HD12	1.54	0.89
1:C:56:THR:HG22	1:C:88:ARG:HH21	1.37	0.89
1:D:475:ARG:HH22	1:D:479:ARG:NH1	1.70	0.89
1:B:475:ARG:HH22	1:B:479:ARG:NH1	1.71	0.88
1:D:258:GLU:HG2	1:D:374:LYS:HG3	1.55	0.87
1:C:75:VAL:HG22	1:D:75:VAL:HG22	1.55	0.87
1:A:56:THR:HG22	1:A:88:ARG:HH21	1.40	0.86
1:B:473:ILE:HD12	1:D:480:LEU:HB2	1.54	0.86
1:D:428:LYS:HD2	7:D:601:HOH:O	1.77	0.85
1:D:475:ARG:NH2	1:D:479:ARG:HH11	1.75	0.85
1:A:474:ASN:ND2	1:C:477:ARG:HE	1.75	0.85
1:A:484:LEU:HB2	1:C:470:LEU:HD11	1.59	0.84
1:C:475:ARG:HH22	1:C:479:ARG:NH1	1.74	0.84
1:A:481:HIS:HA	1:C:470:LEU:HD21	1.57	0.84
1:B:56:THR:HG22	1:B:88:ARG:HH21	1.42	0.84
1:A:477:ARG:HE	1:C:474:ASN:ND2	1.75	0.83
1:B:475:ARG:NH2	1:B:479:ARG:HH11	1.76	0.83
1:A:291:ASN:HD22	1:A:320:VAL:N	1.76	0.82
1:A:475:ARG:HH22	1:A:479:ARG:HH11	1.23	0.82
1:A:470:LEU:HD21	1:C:481:HIS:HA	1.60	0.81
1:C:291:ASN:HD22	1:C:320:VAL:N	1.77	0.81
1:C:475:ARG:NH2	1:C:479:ARG:HH11	1.78	0.81
1:B:291:ASN:HD22	1:B:320:VAL:N	1.80	0.78
1:B:480:LEU:HD13	1:D:473:ILE:CG2	2.13	0.78
1:B:473:ILE:CG2	1:D:480:LEU:HD13	2.12	0.78
1:D:291:ASN:HD22	1:D:320:VAL:N	1.82	0.77
1:B:263:ASN:HD21	1:B:317:ARG:HH11	1.31	0.77
1:D:66:ARG:HG2	1:D:67:ASP:H	1.50	0.76
1:B:8:ARG:CZ	1:B:8:ARG:HA	2.16	0.75
1:D:263:ASN:HD21	1:D:317:ARG:HH11	1.34	0.74
1:C:263:ASN:HD21	1:C:317:ARG:HH11	1.35	0.74
1:B:26:GLN:HE22	1:B:81:LEU:H	1.36	0.74
1:A:474:ASN:HD21	1:C:477:ARG:NE	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:ARG:NH2	1:D:479:ARG:NH1	2.35	0.73
1:B:473:ILE:HG22	1:D:480:LEU:HD13	1.69	0.73
1:B:480:LEU:HD13	1:D:473:ILE:HG22	1.70	0.73
1:A:483:GLU:HG2	1:C:466:ILE:HG21	1.71	0.72
1:A:263:ASN:HD21	1:A:317:ARG:HH11	1.32	0.72
1:B:477:ARG:CG	1:D:477:ARG:HG3	2.19	0.72
1:A:477:ARG:NE	1:C:474:ASN:HD21	1.88	0.72
1:B:475:ARG:NH2	1:B:479:ARG:NH1	2.35	0.72
1:C:475:ARG:NH2	1:C:479:ARG:NH1	2.37	0.72
1:C:270:LYS:HE2	1:C:375:TYR:OH	1.90	0.72
1:D:469:GLU:O	1:D:473:ILE:HG23	1.90	0.71
1:A:26:GLN:HE22	1:A:81:LEU:H	1.39	0.71
1:A:127:TYR:OH	1:A:404:HIS:HD2	1.74	0.71
1:B:88:ARG:NH1	1:B:405:GLU:OE1	2.24	0.70
1:D:26:GLN:HE22	1:D:81:LEU:H	1.38	0.70
1:C:64:ARG:NH1	7:C:586:HOH:O	2.23	0.70
1:A:469:GLU:O	1:A:473:ILE:HG23	1.92	0.70
1:D:56:THR:HG22	1:D:88:ARG:NH2	2.07	0.70
1:B:477:ARG:HG3	1:D:477:ARG:CG	2.19	0.70
1:D:88:ARG:NH1	1:D:405:GLU:OE1	2.25	0.69
1:D:291:ASN:ND2	1:D:319:CYS:HA	2.06	0.69
1:B:469:GLU:O	1:B:473:ILE:HG23	1.91	0.69
1:C:66:ARG:HG2	1:C:67:ASP:H	1.56	0.69
1:B:291:ASN:ND2	1:B:319:CYS:HA	2.07	0.68
1:A:473:ILE:CG2	1:C:480:LEU:HD13	2.23	0.68
1:C:469:GLU:O	1:C:473:ILE:HG23	1.94	0.68
1:B:215:ARG:HB2	1:B:217:VAL:HG23	1.76	0.68
1:B:481:HIS:C	1:B:483:GLU:H	2.02	0.68
1:C:480:LEU:HD23	1:C:483:GLU:OE1	1.92	0.68
1:C:8:ARG:CZ	1:C:8:ARG:HA	2.22	0.67
1:C:26:GLN:HE22	1:C:81:LEU:H	1.39	0.67
1:A:480:LEU:HD13	1:C:473:ILE:CG2	2.24	0.67
1:A:291:ASN:ND2	1:A:319:CYS:HA	2.10	0.67
1:C:215:ARG:HB2	1:C:217:VAL:HG23	1.77	0.66
1:C:370:ASP:O	1:C:371:SER:HB3	1.96	0.66
1:B:66:ARG:HG2	1:B:67:ASP:H	1.61	0.65
1:B:370:ASP:O	1:B:371:SER:HB3	1.96	0.65
1:C:56:THR:HG22	1:C:88:ARG:NH2	2.11	0.65
1:D:215:ARG:HB2	1:D:217:VAL:HG23	1.79	0.65
1:B:301:SER:OG	1:B:304:GLU:HG3	1.97	0.64
1:A:88:ARG:NH1	1:A:405:GLU:OE1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ASP:O	1:A:371:SER:HB3	1.94	0.64
1:A:473:ILE:HG21	1:C:480:LEU:CD1	2.28	0.64
1:D:301:SER:OG	1:D:304:GLU:HG3	1.97	0.64
1:C:127:TYR:OH	1:C:404:HIS:HD2	1.79	0.64
1:A:475:ARG:NH2	1:A:479:ARG:HH11	1.93	0.64
1:A:480:LEU:CD1	1:C:473:ILE:HG21	2.28	0.64
1:B:480:LEU:HB2	1:D:473:ILE:CD1	2.28	0.64
1:D:127:TYR:OH	1:D:404:HIS:HD2	1.80	0.63
1:D:291:ASN:HD22	1:D:319:CYS:HA	1.63	0.63
1:A:263:ASN:ND2	1:A:317:ARG:HD3	2.14	0.63
1:B:127:TYR:OH	1:B:404:HIS:HD2	1.82	0.63
1:D:177:ASP:HB3	1:D:180:GLU:HG3	1.78	0.63
1:D:8:ARG:HA	1:D:8:ARG:CZ	2.28	0.63
1:A:215:ARG:HB2	1:A:217:VAL:HG23	1.80	0.62
1:B:270:LYS:HE2	1:B:375:TYR:OH	1.99	0.62
1:B:460:LEU:O	1:B:464:LEU:HG	1.99	0.62
1:D:270:LYS:HE2	1:D:375:TYR:OH	1.98	0.62
1:A:177:ASP:HB3	1:A:180:GLU:HG3	1.80	0.62
1:C:312:ARG:HB2	1:C:452:VAL:HG21	1.80	0.62
1:A:270:LYS:HE2	1:A:375:TYR:OH	1.99	0.62
1:C:291:ASN:ND2	1:C:319:CYS:HA	2.15	0.62
1:A:475:ARG:HH22	1:A:479:ARG:NH1	1.95	0.62
1:B:258:GLU:CG	1:B:374:LYS:HG3	2.26	0.62
1:A:250:GLN:HE22	1:D:250:GLN:HE22	1.45	0.62
1:A:30:LYS:HG3	7:A:530:HOH:O	1.98	0.62
1:A:473:ILE:HG21	1:C:480:LEU:HD13	1.82	0.62
1:B:258:GLU:HG2	1:B:374:LYS:CG	2.27	0.61
1:B:473:ILE:CD1	1:D:480:LEU:HB2	2.29	0.61
1:A:301:SER:OG	1:A:304:GLU:HG3	2.00	0.61
1:D:263:ASN:ND2	1:D:317:ARG:HD3	2.15	0.61
1:A:74:PRO:HD3	1:B:79:PRO:HA	1.83	0.61
1:A:93:PHE:O	1:A:95:PRO:HD3	2.00	0.61
1:B:250:GLN:HE22	1:C:250:GLN:HE22	1.49	0.61
1:C:88:ARG:NH1	1:C:405:GLU:OE1	2.32	0.61
1:B:177:ASP:HB3	1:B:180:GLU:HG3	1.81	0.61
1:D:460:LEU:O	1:D:464:LEU:HG	2.01	0.60
1:C:93:PHE:O	1:C:95:PRO:HD3	2.01	0.60
1:A:145:LYS:O	1:A:148:GLN:HG2	2.02	0.60
1:A:312:ARG:HB2	1:A:452:VAL:HG21	1.83	0.60
1:A:481:HIS:HA	1:C:470:LEU:CD2	2.31	0.60
1:A:91:ILE:HD11	1:A:95:PRO:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:O	1:A:464:LEU:HG	2.02	0.60
1:A:475:ARG:NH1	1:B:152:GLU:H	1.99	0.60
1:C:74:PRO:HD3	1:D:79:PRO:HA	1.84	0.59
1:B:56:THR:HG22	1:B:88:ARG:NH2	2.16	0.59
1:C:460:LEU:O	1:C:464:LEU:HG	2.02	0.59
1:C:481:HIS:C	1:C:483:GLU:H	2.08	0.59
1:B:441:GLY:O	1:B:445:ARG:HG3	2.02	0.59
1:D:145:LYS:O	1:D:148:GLN:HG2	2.02	0.59
1:A:56:THR:HG22	1:A:88:ARG:NH2	2.13	0.59
1:B:263:ASN:ND2	1:B:317:ARG:HD3	2.17	0.59
1:B:145:LYS:O	1:B:148:GLN:HG2	2.02	0.59
1:B:473:ILE:HG21	1:D:480:LEU:CB	2.33	0.58
1:D:258:GLU:CG	1:D:374:LYS:HG3	2.28	0.58
1:B:480:LEU:CB	1:D:473:ILE:HG21	2.32	0.58
1:C:66:ARG:CG	1:C:67:ASP:H	2.15	0.58
1:C:145:LYS:O	1:C:148:GLN:HG2	2.02	0.58
1:C:154:HIS:HB2	7:C:562:HOH:O	2.03	0.58
1:B:291:ASN:HD22	1:B:319:CYS:HA	1.67	0.58
1:D:91:ILE:HD11	1:D:95:PRO:HG3	1.86	0.58
1:A:258:GLU:HG2	1:A:374:LYS:CG	2.30	0.58
1:B:480:LEU:HD13	1:D:473:ILE:HG21	1.85	0.58
1:C:301:SER:OG	1:C:304:GLU:HG3	2.03	0.58
1:B:91:ILE:HD11	1:B:95:PRO:HG3	1.84	0.58
1:D:312:ARG:HB2	1:D:452:VAL:HG21	1.86	0.58
1:D:370:ASP:O	1:D:371:SER:HB3	2.02	0.58
1:C:215:ARG:HB2	1:C:217:VAL:CG2	2.34	0.57
1:D:98:THR:HG21	1:D:407:MET:HE1	1.85	0.57
1:A:481:HIS:C	1:A:483:GLU:H	2.13	0.57
1:A:230:ASN:HD21	1:A:237:ARG:HA	1.70	0.57
1:B:312:ARG:HB2	1:B:452:VAL:HG21	1.87	0.57
1:A:215:ARG:HB2	1:A:217:VAL:CG2	2.36	0.56
1:A:79:PRO:HA	1:B:74:PRO:HD3	1.88	0.56
1:C:177:ASP:HB3	1:C:180:GLU:HG3	1.86	0.56
1:D:66:ARG:O	1:D:67:ASP:HB2	2.04	0.56
1:A:26:GLN:HG2	1:B:70:SER:HB3	1.87	0.56
1:B:481:HIS:C	1:B:483:GLU:N	2.64	0.56
1:C:475:ARG:HG2	7:D:600:HOH:O	2.05	0.56
1:A:475:ARG:NH2	1:A:479:ARG:HE	2.04	0.55
1:C:263:ASN:ND2	1:C:317:ARG:HD3	2.22	0.55
1:D:441:GLY:O	1:D:445:ARG:HG3	2.06	0.55
1:B:98:THR:HG21	1:B:407:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ILE:HG21	1:D:480:LEU:HD13	1.86	0.55
1:A:480:LEU:HD13	1:C:473:ILE:HG21	1.84	0.55
1:A:473:ILE:CG2	1:C:480:LEU:CD1	2.85	0.55
1:C:98:THR:HG21	1:C:407:MET:HE1	1.88	0.55
1:A:258:GLU:CG	1:A:374:LYS:HG3	2.31	0.54
1:C:258:GLU:CG	1:C:374:LYS:HG3	2.29	0.54
1:C:475:ARG:NH1	1:D:152:GLU:H	2.06	0.54
1:D:258:GLU:HG2	1:D:374:LYS:CG	2.33	0.54
1:A:481:HIS:CA	1:C:470:LEU:HD21	2.34	0.54
1:D:187:ARG:NH1	7:D:499:HOH:O	2.41	0.54
1:A:291:ASN:ND2	1:A:320:VAL:N	2.43	0.53
1:A:475:ARG:NH2	1:A:479:ARG:NH1	2.55	0.53
1:A:98:THR:HG21	1:A:407:MET:HE1	1.90	0.53
1:A:470:LEU:CD2	1:C:481:HIS:HA	2.35	0.53
1:A:473:ILE:HG22	1:C:480:LEU:HD13	1.89	0.53
1:A:234:PHE:HA	1:A:418:ARG:HD2	1.91	0.53
1:A:480:LEU:CD1	1:C:473:ILE:CG2	2.86	0.53
1:C:91:ILE:HD11	1:C:95:PRO:HG3	1.90	0.53
1:D:475:ARG:NH2	1:D:479:ARG:HD2	2.23	0.53
1:B:215:ARG:HB2	1:B:217:VAL:CG2	2.39	0.53
1:B:214:ARG:NH2	7:B:514:HOH:O	2.42	0.53
1:C:230:ASN:HD21	1:C:237:ARG:HA	1.74	0.52
1:D:215:ARG:HB2	1:D:217:VAL:CG2	2.39	0.52
1:A:477:ARG:NE	1:C:474:ASN:ND2	2.51	0.52
1:A:480:LEU:HD13	1:C:473:ILE:HG22	1.90	0.52
1:A:480:LEU:HD23	1:A:483:GLU:OE1	2.09	0.52
1:D:42:PRO:O	1:D:45:LYS:HG2	2.10	0.52
1:B:230:ASN:HD21	1:B:237:ARG:HA	1.75	0.52
1:C:441:GLY:O	1:C:445:ARG:HG3	2.10	0.52
1:C:475:ARG:NH2	1:C:479:ARG:HD2	2.24	0.52
1:D:93:PHE:O	1:D:95:PRO:HD3	2.09	0.52
1:D:230:ASN:HD21	1:D:237:ARG:HA	1.75	0.52
1:A:30:LYS:CG	7:A:530:HOH:O	2.56	0.51
1:A:291:ASN:HD22	1:A:319:CYS:HA	1.72	0.51
1:A:294:LEU:HA	7:A:582:HOH:O	2.09	0.51
1:C:481:HIS:C	1:C:483:GLU:N	2.68	0.51
1:D:234:PHE:HA	1:D:418:ARG:HD2	1.93	0.51
1:A:263:ASN:ND2	1:A:317:ARG:HH11	2.07	0.51
1:A:477:ARG:HA	1:C:473:ILE:HD12	1.93	0.51
1:A:94:ASN:O	1:A:98:THR:HG22	2.11	0.51
1:B:180:GLU:O	1:B:183:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG21	1:A:168:ILE:HD13	1.93	0.50
1:C:234:PHE:HA	1:C:418:ARG:HD2	1.93	0.50
1:B:93:PHE:O	1:B:95:PRO:HD3	2.10	0.50
1:C:79:PRO:HA	1:D:74:PRO:HD3	1.94	0.50
1:B:66:ARG:CG	1:B:67:ASP:H	2.24	0.50
1:B:480:LEU:O	1:D:470:LEU:HD21	2.12	0.50
1:B:225:PRO:HG3	1:B:414:ILE:HB	1.93	0.50
1:A:79:PRO:O	1:B:70:SER:HB2	2.12	0.50
1:A:470:LEU:HD21	1:C:481:HIS:CA	2.38	0.50
1:B:263:ASN:ND2	1:B:317:ARG:HH11	2.04	0.50
1:B:161:ILE:HG21	1:B:168:ILE:HD13	1.94	0.50
1:C:258:GLU:HG2	1:C:374:LYS:CG	2.29	0.50
1:C:291:ASN:HD22	1:C:319:CYS:HA	1.75	0.50
1:B:234:PHE:HA	1:B:418:ARG:HD2	1.94	0.49
1:B:475:ARG:NH2	1:B:479:ARG:HD2	2.27	0.49
1:B:477:ARG:CB	1:D:477:ARG:HG3	2.42	0.49
1:D:297:GLU:CD	1:D:437:LEU:HB2	2.37	0.49
1:D:13:LEU:O	1:D:14:VAL:HG23	2.11	0.49
1:A:26:GLN:CG	1:B:70:SER:HB3	2.42	0.49
1:B:235:SER:HB3	7:B:565:HOH:O	2.12	0.49
1:C:8:ARG:HA	1:C:8:ARG:NH1	2.27	0.49
1:D:60:MET:HA	1:D:81:LEU:HD23	1.94	0.49
1:D:352:ILE:O	1:D:356:LYS:HG2	2.13	0.49
1:A:442:GLN:HE22	1:A:445:ARG:NH2	2.10	0.49
1:B:42:PRO:O	1:B:45:LYS:HG2	2.12	0.49
1:B:477:ARG:HG3	1:D:477:ARG:CB	2.42	0.49
1:A:152:GLU:H	1:B:475:ARG:NH1	2.11	0.49
1:A:484:LEU:C	1:A:484:LEU:CD1	2.86	0.49
1:B:290:ALA:CB	1:B:322:ILE:HD13	2.42	0.49
1:A:475:ARG:HH22	1:A:479:ARG:HE	1.60	0.48
1:B:272:MET:HB2	1:B:279:ILE:HD12	1.95	0.48
1:D:26:GLN:NE2	1:D:81:LEU:H	2.07	0.48
1:A:60:MET:HA	1:A:81:LEU:HD23	1.96	0.48
1:A:238:THR:HB	7:A:563:HOH:O	2.13	0.48
1:C:162:HIS:H	1:C:162:HIS:CD2	2.31	0.48
1:A:34:LEU:HB3	1:A:92:HIS:NE2	2.29	0.48
1:A:477:ARG:CG	1:C:473:ILE:HG13	2.26	0.48
1:B:297:GLU:CD	1:B:437:LEU:HB2	2.39	0.48
1:A:154:HIS:O	1:A:155:ARG:C	2.56	0.48
1:B:480:LEU:CD1	1:D:473:ILE:CG2	2.90	0.48
1:C:161:ILE:HG21	1:C:168:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:HIS:C	1:A:483:GLU:N	2.71	0.48
1:C:253:ARG:HG2	1:C:289:GLN:HE22	1.79	0.48
1:D:36:GLY:O	1:D:92:HIS:HD2	1.97	0.48
1:A:230:ASN:HB2	1:A:241:PHE:CD2	2.48	0.48
1:C:442:GLN:HE22	1:C:445:ARG:NH2	2.12	0.48
1:B:483:GLU:OE1	1:D:466:ILE:HG22	2.14	0.47
1:C:211:GLU:O	1:C:215:ARG:HG3	2.13	0.47
1:D:162:HIS:H	1:D:162:HIS:CD2	2.32	0.47
1:C:173:ARG:NH1	2:C:1001:ATP:O1G	2.48	0.47
1:C:314:CYS:HB3	1:C:462:ARG:HH21	1.79	0.47
1:B:13:LEU:O	1:B:14:VAL:HG23	2.15	0.47
1:B:60:MET:HA	1:B:81:LEU:HD23	1.95	0.47
1:A:42:PRO:O	1:A:45:LYS:HG2	2.15	0.47
1:A:473:ILE:HD12	1:C:477:ARG:HA	1.97	0.47
1:D:180:GLU:O	1:D:183:ASP:HB2	2.14	0.47
1:B:480:LEU:CD1	1:D:473:ILE:HG21	2.44	0.47
1:C:42:PRO:O	1:C:45:LYS:HG2	2.15	0.47
1:C:66:ARG:HG2	1:C:67:ASP:N	2.27	0.47
1:C:92:HIS:HE1	1:C:218:ASP:OD1	1.98	0.47
1:D:8:ARG:HA	1:D:8:ARG:NE	2.29	0.47
1:D:314:CYS:HB3	1:D:462:ARG:HH21	1.80	0.47
1:A:441:GLY:O	1:A:445:ARG:HG3	2.14	0.47
1:D:225:PRO:HG3	1:D:414:ILE:HB	1.95	0.47
1:A:62:ASN:OD1	1:A:62:ASN:C	2.58	0.47
1:A:484:LEU:HD13	1:A:485:ALA:N	2.30	0.47
1:B:314:CYS:HB3	1:B:462:ARG:HH21	1.79	0.47
1:C:99:THR:HB	1:C:189:GLY:O	2.14	0.47
1:A:225:PRO:HG3	1:A:414:ILE:HB	1.95	0.47
1:A:180:GLU:O	1:A:183:ASP:HB2	2.15	0.46
1:B:26:GLN:NE2	1:B:81:LEU:H	2.07	0.46
1:D:15:LYS:HE3	1:D:22:ASN:ND2	2.30	0.46
1:B:70:SER:OG	1:B:71:SER:N	2.48	0.46
1:C:60:MET:HA	1:C:81:LEU:HD23	1.96	0.46
1:C:140:TRP:O	1:C:146:GLY:HA3	2.15	0.46
1:B:272:MET:HE3	1:B:272:MET:HA	1.97	0.46
1:B:384:ALA:HB1	1:C:257:ALA:HB3	1.97	0.46
1:B:442:GLN:HE22	1:B:445:ARG:NH2	2.13	0.46
1:C:79:PRO:HB3	1:D:73:ASN:ND2	2.30	0.46
1:D:92:HIS:HE1	1:D:218:ASP:OD1	1.98	0.46
1:D:417:MET:HG2	1:D:421:ASN:O	2.16	0.46
1:D:442:GLN:HE22	1:D:445:ARG:NH2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ARG:NH1	7:B:523:HOH:O	2.47	0.46
1:C:292:ILE:HB	1:C:321:ILE:HG12	1.98	0.46
1:A:484:LEU:HD23	1:C:470:LEU:HD12	1.97	0.46
1:B:470:LEU:HD21	1:D:480:LEU:O	2.16	0.46
1:C:152:GLU:H	1:D:475:ARG:NH1	2.12	0.46
1:C:352:ILE:O	1:C:356:LYS:HG2	2.15	0.46
1:D:214:ARG:NH2	7:D:542:HOH:O	2.46	0.46
1:B:15:LYS:HE3	1:B:22:ASN:ND2	2.30	0.46
1:B:232:LEU:HB3	7:B:565:HOH:O	2.14	0.46
1:D:226:LYS:HA	7:D:553:HOH:O	2.15	0.46
1:B:66:ARG:O	1:B:67:ASP:HB2	2.15	0.46
1:D:366:SER:HB3	7:D:579:HOH:O	2.16	0.46
1:B:8:ARG:HA	1:B:8:ARG:NE	2.30	0.46
1:B:428:LYS:HG3	7:B:567:HOH:O	2.16	0.46
1:A:473:ILE:HG13	1:C:477:ARG:CG	2.29	0.46
1:C:12:LYS:HE2	7:C:542:HOH:O	2.15	0.46
1:C:365:LYS:HD3	7:C:499:HOH:O	2.15	0.46
1:A:253:ARG:NH2	7:A:522:HOH:O	2.48	0.45
1:D:211:GLU:O	1:D:215:ARG:HG3	2.16	0.45
1:B:162:HIS:CD2	1:B:162:HIS:H	2.35	0.45
1:B:444:TRP:O	1:B:448:ARG:HG3	2.16	0.45
1:C:36:GLY:O	1:C:92:HIS:HD2	1.98	0.45
1:A:162:HIS:H	1:A:162:HIS:CD2	2.33	0.45
1:A:212:ALA:O	1:A:217:VAL:HG23	2.16	0.45
1:D:272:MET:HE3	1:D:272:MET:HA	1.98	0.45
1:B:36:GLY:O	1:B:92:HIS:HD2	1.99	0.45
1:B:39:TYR:CZ	1:B:94:ASN:HB2	2.52	0.45
1:C:62:ASN:OD1	1:C:62:ASN:C	2.60	0.45
1:B:473:ILE:HG21	1:D:480:LEU:CD1	2.46	0.45
1:B:127:TYR:OH	1:B:404:HIS:CD2	2.67	0.45
1:D:362:LYS:O	1:D:365:LYS:HG3	2.17	0.45
1:B:173:ARG:NH1	2:B:1001:ATP:O3G	2.50	0.44
1:C:225:PRO:HG3	1:C:414:ILE:HB	1.98	0.44
1:C:62:ASN:HA	1:C:63:PRO:HD3	1.79	0.44
1:A:62:ASN:HA	1:A:63:PRO:HD3	1.78	0.44
1:B:481:HIS:O	1:B:483:GLU:N	2.50	0.44
1:C:290:ALA:CB	1:C:322:ILE:HD13	2.47	0.44
1:A:104:THR:HG22	1:A:196:VAL:HB	1.99	0.44
1:A:379:SER:O	1:A:383:ARG:HG3	2.17	0.44
1:B:34:LEU:HB3	1:B:92:HIS:NE2	2.32	0.44
1:C:198:GLY:O	1:C:202:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LYS:HE2	1:D:55:LYS:HB3	1.81	0.44
1:B:473:ILE:CG2	1:D:480:LEU:CD1	2.90	0.44
1:C:95:PRO:O	1:C:98:THR:HG23	2.17	0.44
1:C:173:ARG:HG3	1:C:341:SER:HG	1.83	0.44
1:B:381:MET:HE2	1:B:381:MET:HB3	1.94	0.44
1:B:417:MET:HE3	1:B:420:ASN:H	1.83	0.44
1:B:473:ILE:HG21	1:D:480:LEU:HB3	1.99	0.44
1:D:154:HIS:O	1:D:155:ARG:C	2.61	0.44
1:D:263:ASN:ND2	1:D:317:ARG:HH11	2.10	0.44
1:A:140:TRP:O	1:A:146:GLY:HA3	2.18	0.44
1:A:271:LEU:HD12	1:A:322:ILE:HG23	2.00	0.44
1:A:480:LEU:O	1:C:470:LEU:HD21	2.18	0.44
1:C:226:LYS:HA	7:C:564:HOH:O	2.18	0.44
1:A:297:GLU:CD	1:A:437:LEU:HB2	2.43	0.44
1:C:386:PRO:HA	1:C:387:PRO:HD3	1.83	0.44
1:C:154:HIS:O	1:C:155:ARG:C	2.62	0.43
1:D:253:ARG:HG2	1:D:253:ARG:HH11	1.83	0.43
1:A:352:ILE:O	1:A:356:LYS:HG2	2.18	0.43
1:C:34:LEU:HB3	1:C:92:HIS:NE2	2.34	0.43
1:C:272:MET:HA	1:C:272:MET:HE3	2.00	0.43
1:C:297:GLU:CD	1:C:437:LEU:HB2	2.44	0.43
1:D:140:TRP:O	1:D:146:GLY:HA3	2.17	0.43
1:A:314:CYS:HB3	1:A:462:ARG:HH21	1.83	0.43
1:A:257:ALA:HB3	1:D:384:ALA:HB1	1.99	0.43
1:B:473:ILE:HG12	1:B:474:ASN:N	2.33	0.43
1:B:480:LEU:HB3	1:D:473:ILE:HG21	1.99	0.43
1:C:22:ASN:HD22	1:C:22:ASN:HA	1.60	0.43
1:D:212:ALA:O	1:D:217:VAL:HG23	2.18	0.43
1:D:230:ASN:HB2	1:D:241:PHE:CD2	2.53	0.43
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.80	0.43
1:B:22:ASN:HD22	1:B:22:ASN:HA	1.63	0.43
1:B:73:ASN:N	1:B:73:ASN:HD22	2.16	0.43
1:B:352:ILE:O	1:B:356:LYS:HG2	2.18	0.43
1:C:33:ARG:HA	1:C:409:GLY:O	2.18	0.43
1:C:34:LEU:HD23	1:C:93:PHE:CZ	2.52	0.43
1:D:256:TYR:CZ	1:D:260:VAL:HG21	2.53	0.43
1:B:224:VAL:HA	1:B:225:PRO:HD3	1.84	0.43
1:C:197:GLY:HA2	1:C:226:LYS:HB3	2.00	0.43
1:A:211:GLU:O	1:A:215:ARG:HG3	2.19	0.43
1:A:484:LEU:O	1:A:485:ALA:HB3	2.18	0.43
1:B:290:ALA:HB2	1:B:322:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ARG:HB2	1:D:477:ARG:HG3	2.01	0.43
1:D:455:GLY:HA2	7:D:593:HOH:O	2.19	0.43
1:A:127:TYR:OH	1:A:404:HIS:CD2	2.63	0.43
1:C:230:ASN:HB2	1:C:241:PHE:CD2	2.53	0.43
1:D:99:THR:HB	1:D:189:GLY:O	2.19	0.43
1:B:92:HIS:HE1	1:B:218:ASP:OD1	2.01	0.43
1:B:477:ARG:HG3	1:D:477:ARG:HB2	2.01	0.43
1:C:228:ILE:O	1:C:279:ILE:HD11	2.19	0.43
1:D:62:ASN:OD1	1:D:62:ASN:C	2.62	0.43
1:A:55:LYS:HE2	1:A:55:LYS:HB3	1.83	0.42
1:A:95:PRO:O	1:A:98:THR:HG23	2.18	0.42
1:A:473:ILE:HD12	1:C:480:LEU:HB2	2.00	0.42
1:B:362:LYS:O	1:B:365:LYS:HG3	2.19	0.42
1:B:99:THR:HB	1:B:189:GLY:O	2.18	0.42
1:B:125:ASN:HD21	1:B:155:ARG:NH2	2.17	0.42
1:C:263:ASN:ND2	1:C:317:ARG:HH11	2.11	0.42
1:A:470:LEU:HD21	1:C:480:LEU:O	2.20	0.42
1:B:154:HIS:HE1	7:B:580:HOH:O	2.01	0.42
1:B:154:HIS:O	1:B:155:ARG:C	2.62	0.42
1:C:13:LEU:O	1:C:14:VAL:HG23	2.20	0.42
1:A:94:ASN:O	1:A:98:THR:CG2	2.67	0.42
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.81	0.42
1:D:127:TYR:OH	1:D:404:HIS:CD2	2.67	0.42
1:A:239:PHE:HB2	1:A:395:CYS:SG	2.59	0.42
1:C:76:SER:HA	1:D:60:MET:HE1	2.02	0.42
1:B:256:TYR:CZ	1:B:260:VAL:HG21	2.55	0.42
1:B:292:ILE:HG22	1:B:294:LEU:HD13	2.02	0.42
1:D:73:ASN:HA	1:D:74:PRO:HD3	1.78	0.42
1:D:292:ILE:HG22	1:D:294:LEU:HD13	2.01	0.42
1:D:465:GLU:O	1:D:468:ARG:HB2	2.20	0.42
1:A:73:ASN:HA	1:A:74:PRO:HD3	1.78	0.42
1:A:253:ARG:HA	1:A:289:GLN:HE22	1.85	0.42
1:B:226:LYS:HA	7:B:511:HOH:O	2.19	0.42
1:B:380:TYR:CE1	1:C:374:LYS:HD2	2.55	0.42
1:A:230:ASN:HD21	1:A:237:ARG:CA	2.33	0.42
1:D:161:ILE:HG21	1:D:168:ILE:HD13	2.02	0.42
1:D:253:ARG:HA	1:D:289:GLN:HE22	1.83	0.42
1:A:33:ARG:HA	1:A:409:GLY:O	2.20	0.41
1:A:228:ILE:O	1:A:279:ILE:HD11	2.20	0.41
1:B:94:ASN:O	1:B:98:THR:HG22	2.19	0.41
1:B:270:LYS:HA	1:B:323:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:HIS:CE1	1:C:434:ARG:CZ	3.03	0.41
1:A:92:HIS:HE1	1:A:218:ASP:OD1	2.03	0.41
1:A:374:LYS:HD2	1:D:380:TYR:CE1	2.56	0.41
1:D:39:TYR:CZ	1:D:94:ASN:HB2	2.54	0.41
1:A:290:ALA:CB	1:A:322:ILE:HD13	2.50	0.41
1:C:39:TYR:HA	1:C:40:PRO:HD3	1.89	0.41
1:D:66:ARG:HG2	1:D:67:ASP:N	2.29	0.41
1:D:292:ILE:HB	1:D:321:ILE:HG12	2.02	0.41
1:A:473:ILE:CD1	1:C:480:LEU:HB2	2.50	0.41
1:A:474:ASN:ND2	1:C:477:ARG:NE	2.52	0.41
1:B:257:ALA:HB3	1:C:384:ALA:HB1	2.02	0.41
1:C:174:GLY:O	2:C:1001:ATP:O3'	2.37	0.41
1:C:206:LEU:HD23	1:C:206:LEU:HA	1.83	0.41
1:D:228:ILE:O	1:D:279:ILE:HD11	2.21	0.41
1:D:473:ILE:HG12	1:D:474:ASN:N	2.34	0.41
1:D:34:LEU:HB3	1:D:92:HIS:NE2	2.35	0.41
1:D:164:TYR:HB3	7:D:493:HOH:O	2.19	0.41
1:A:292:ILE:HB	1:A:321:ILE:HG12	2.03	0.41
1:D:239:PHE:HB2	1:D:395:CYS:SG	2.60	0.41
1:A:26:GLN:NE2	1:B:70:SER:HB3	2.35	0.41
1:A:308:LEU:HD21	1:A:454:LEU:HG	2.03	0.41
1:A:480:LEU:HB2	1:C:473:ILE:CD1	2.51	0.41
1:A:484:LEU:HB2	1:C:470:LEU:CD1	2.42	0.41
1:C:173:ARG:HG3	1:C:341:SER:OG	2.20	0.41
1:C:180:GLU:O	1:C:183:ASP:HB2	2.19	0.41
1:D:253:ARG:HG2	1:D:289:GLN:HE22	1.86	0.41
1:D:308:LEU:HD21	1:D:454:LEU:HG	2.03	0.41
1:A:465:GLU:O	1:A:468:ARG:HB2	2.21	0.41
1:C:26:GLN:NE2	1:C:81:LEU:H	2.13	0.41
1:C:212:ALA:O	1:C:217:VAL:HG23	2.21	0.41
1:D:9:VAL:HG13	1:D:64:ARG:NH2	2.36	0.41
1:D:310:GLU:HG3	1:D:368:TYR:OH	2.20	0.41
1:B:62:ASN:HA	1:B:63:PRO:HD3	1.78	0.41
1:B:228:ILE:O	1:B:279:ILE:HD11	2.20	0.41
1:B:253:ARG:HA	1:B:289:GLN:HE22	1.85	0.41
1:B:282:GLN:HE21	1:B:282:GLN:HB3	1.67	0.41
1:C:483:GLU:O	1:C:485:ALA:O	2.38	0.41
1:D:64:ARG:NH1	7:D:522:HOH:O	2.39	0.41
1:D:272:MET:HB2	1:D:279:ILE:HD12	2.02	0.41
1:A:99:THR:HB	1:A:189:GLY:O	2.20	0.41
1:B:25:THR:O	1:B:28:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD12	1:A:29:LEU:HA	1.96	0.40
1:C:465:GLU:O	1:C:468:ARG:HB2	2.21	0.40
1:D:62:ASN:HA	1:D:63:PRO:HD3	1.78	0.40
1:D:73:ASN:N	1:D:73:ASN:HD22	2.17	0.40
1:D:154:HIS:CD2	7:D:600:HOH:O	2.73	0.40
1:D:266:VAL:HA	1:D:319:CYS:O	2.21	0.40
1:A:473:ILE:HG12	1:A:474:ASN:N	2.35	0.40
1:B:62:ASN:OD1	1:B:62:ASN:C	2.64	0.40
1:B:112:LEU:HD12	1:B:112:LEU:HA	1.94	0.40
1:B:327:PHE:CG	1:B:328:GLY:N	2.89	0.40
1:A:36:GLY:O	1:A:92:HIS:HD2	2.04	0.40
1:B:211:GLU:O	1:B:215:ARG:HG3	2.21	0.40
1:C:43:SER:HB2	1:C:126:VAL:CG1	2.52	0.40
1:C:73:ASN:N	1:C:73:ASN:HD22	2.19	0.40
1:C:94:ASN:O	1:C:98:THR:HG22	2.21	0.40
1:C:417:MET:HG2	1:C:421:ASN:O	2.21	0.40
1:C:484:LEU:HG	1:C:485:ALA:N	2.32	0.40
1:D:472:ALA:HB3	7:D:563:HOH:O	2.22	0.40
1:A:22:ASN:HD22	1:A:22:ASN:HA	1.59	0.40
1:A:256:TYR:CZ	1:A:260:VAL:HG21	2.56	0.40
1:B:26:GLN:NE2	1:B:80:LEU:HA	2.36	0.40
1:B:29:LEU:HD12	1:B:429:VAL:HG21	2.04	0.40
1:B:230:ASN:HB2	1:B:241:PHE:CD2	2.56	0.40
1:B:272:MET:HA	1:B:272:MET:CE	2.50	0.40
1:C:15:LYS:HE3	1:C:22:ASN:ND2	2.37	0.40
1:D:29:LEU:HD12	1:D:29:LEU:HA	1.96	0.40
1:D:157:ARG:HG3	7:D:595:HOH:O	2.22	0.40
1:A:79:PRO:HB3	1:B:73:ASN:ND2	2.36	0.40
1:A:480:LEU:HB2	1:C:473:ILE:HD12	2.03	0.40
1:C:125:ASN:HD21	1:C:155:ARG:HH21	1.68	0.40

All (1) 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:B:474:ASN:ND2	1:C:477:ARG:NH2[2_554]	2.12	0.08

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	450/487 (92%)	425 (94%)	20 (4%)	5 (1%)	11	29
1	B	454/487 (93%)	426 (94%)	23 (5%)	5 (1%)	11	29
1	C	453/487 (93%)	425 (94%)	22 (5%)	6 (1%)	9	25
1	D	450/487 (92%)	425 (94%)	20 (4%)	5 (1%)	11	29
All	All	1807/1948 (93%)	1701 (94%)	85 (5%)	21 (1%)	10	27

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	GLU
1	A	273	GLY
1	A	371	SER
1	B	371	SER
1	C	273	GLY
1	C	482	GLU
1	D	371	SER
1	A	369	PRO
1	A	482	GLU
1	B	369	PRO
1	C	369	PRO
1	C	371	SER
1	D	369	PRO
1	A	471	GLU
1	B	273	GLY
1	B	471	GLU
1	C	471	GLU
1	D	273	GLY
1	D	471	GLU
1	D	9	VAL
1	C	95	PRO

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	380/405 (94%)	349 (92%)	31 (8%)	10	27
1	B	385/405 (95%)	353 (92%)	32 (8%)	10	26
1	C	383/405 (95%)	351 (92%)	32 (8%)	10	26
1	D	381/405 (94%)	352 (92%)	29 (8%)	12	30
All	All	1529/1620 (94%)	1405 (92%)	124 (8%)	11	27

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	29	LEU
1	A	34	LEU
1	A	77	VAL
1	A	98	THR
1	A	112	LEU
1	A	114	ASP
1	A	167	THR
1	A	169	LEU
1	A	173	ARG
1	A	188	LEU
1	A	193	LEU
1	A	217	VAL
1	A	227	THR
1	A	258	GLU
1	A	272	MET
1	A	294	LEU
1	A	314	CYS
1	A	333	ARG
1	A	344	LYS
1	A	372	THR
1	A	417	MET
1	A	433	VAL
1	A	436	VAL

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Mol	Chain	Res	Type
1	A	442	GLN
1	A	466	ILE
1	A	473	ILE
1	A	475	ARG
1	A	477	ARG
1	A	479	ARG
1	A	484	LEU
1	B	8	ARG
1	B	9	VAL
1	B	14	VAL
1	B	18	ARG
1	B	29	LEU
1	B	34	LEU
1	B	77	VAL
1	B	98	THR
1	B	112	LEU
1	B	155	ARG
1	B	167	THR
1	B	169	LEU
1	B	173	ARG
1	B	188	LEU
1	B	193	LEU
1	B	217	VAL
1	B	227	THR
1	B	269	VAL
1	B	272	MET
1	B	294	LEU
1	B	314	CYS
1	B	333	ARG
1	B	344	LYS
1	B	372	THR
1	B	433	VAL
1	B	434	ARG
1	B	436	VAL
1	B	466	ILE
1	B	473	ILE
1	B	475	ARG
1	B	477	ARG
1	B	479	ARG
1	C	8	ARG
1	C	9	VAL
1	C	14	VAL

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	34	LEU
1	C	77	VAL
1	C	98	THR
1	C	112	LEU
1	C	114	ASP
1	C	167	THR
1	C	169	LEU
1	C	173	ARG
1	C	188	LEU
1	C	193	LEU
1	C	217	VAL
1	C	227	THR
1	C	258	GLU
1	C	272	MET
1	C	294	LEU
1	C	314	CYS
1	C	333	ARG
1	C	344	LYS
1	C	372	THR
1	C	417	MET
1	C	433	VAL
1	C	436	VAL
1	C	442	GLN
1	C	466	ILE
1	C	473	ILE
1	C	475	ARG
1	C	477	ARG
1	C	479	ARG
1	D	8	ARG
1	D	14	VAL
1	D	29	LEU
1	D	34	LEU
1	D	77	VAL
1	D	98	THR
1	D	112	LEU
1	D	114	ASP
1	D	167	THR
1	D	169	LEU
1	D	173	ARG
1	D	188	LEU
1	D	193	LEU

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Mol	Chain	Res	Type
1	D	217	VAL
1	D	227	THR
1	D	269	VAL
1	D	271	LEU
1	D	272	MET
1	D	294	LEU
1	D	314	CYS
1	D	333	ARG
1	D	344	LYS
1	D	372	THR
1	D	433	VAL
1	D	436	VAL
1	D	466	ILE
1	D	473	ILE
1	D	477	ARG
1	D	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	ASN
1	A	26	GLN
1	A	73	ASN
1	A	92	HIS
1	A	128	ASN
1	A	154	HIS
1	A	162	HIS
1	A	163	HIS
1	A	176	GLN
1	A	210	GLN
1	A	230	ASN
1	A	250	GLN
1	A	263	ASN
1	A	282	GLN
1	A	289	GLN
1	A	291	ASN
1	A	298	ASN
1	A	404	HIS
1	A	421	ASN
1	A	442	GLN
1	A	474	ASN

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Mol	Chain	Res	Type
1	B	22	ASN
1	B	26	GLN
1	B	73	ASN
1	B	92	HIS
1	B	128	ASN
1	B	148	GLN
1	B	154	HIS
1	B	162	HIS
1	B	176	GLN
1	B	210	GLN
1	B	230	ASN
1	B	250	GLN
1	B	263	ASN
1	B	282	GLN
1	B	289	GLN
1	B	291	ASN
1	B	298	ASN
1	B	404	HIS
1	B	442	GLN
1	B	474	ASN
1	C	17	HIS
1	C	22	ASN
1	C	26	GLN
1	C	73	ASN
1	C	92	HIS
1	C	94	ASN
1	C	128	ASN
1	C	154	HIS
1	C	162	HIS
1	C	163	HIS
1	C	176	GLN
1	C	210	GLN
1	C	230	ASN
1	C	250	GLN
1	C	263	ASN
1	C	282	GLN
1	C	289	GLN
1	C	291	ASN
1	C	298	ASN
1	C	404	HIS
1	C	442	GLN
1	C	474	ASN

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Mol	Chain	Res	Type
1	D	17	HIS
1	D	22	ASN
1	D	26	GLN
1	D	73	ASN
1	D	92	HIS
1	D	128	ASN
1	D	154	HIS
1	D	162	HIS
1	D	176	GLN
1	D	210	GLN
1	D	230	ASN
1	D	236	HIS
1	D	250	GLN
1	D	263	ASN
1	D	282	GLN
1	D	289	GLN
1	D	291	ASN
1	D	298	ASN
1	D	404	HIS
1	D	421	ASN
1	D	442	GLN
1	D	474	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	C	489	-	4,4,4	0.30	0	6,6,6	0.23	0
2	ATP	C	1001	-	32,33,33	1.41	5 (15%)	48,52,52	1.82	10 (20%)
2	ATP	B	1001	3	32,33,33	1.38	4 (12%)	48,52,52	1.89	10 (20%)
2	ATP	A	1001	-	32,33,33	1.35	5 (15%)	48,52,52	1.84	9 (18%)
2	ATP	D	1001	3	32,33,33	1.53	6 (18%)	48,52,52	1.85	11 (22%)
4	GOL	C	488	-	5,5,5	0.23	0	5,5,5	1.42	1 (20%)
4	GOL	A	488	-	5,5,5	0.40	0	5,5,5	1.09	0

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	C	1001	-	-	4/22/38/38	0/3/3/3
2	ATP	B	1001	3	-	0/22/38/38	0/3/3/3
2	ATP	A	1001	-	-	1/22/38/38	0/3/3/3
2	ATP	D	1001	3	-	0/22/38/38	0/3/3/3
4	GOL	C	488	-	-	2/4/4/4	-
4	GOL	A	488	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ATP	C5-C4	5.32	1.48	1.39
2	C	1001	ATP	C5-C4	4.88	1.47	1.39
2	A	1001	ATP	C5-C4	4.63	1.47	1.39
2	B	1001	ATP	C5-C4	4.61	1.47	1.39
2	C	1001	ATP	C8-N7	2.76	1.37	1.31
2	A	1001	ATP	C5-C6	2.72	1.48	1.41
2	D	1001	ATP	PB-O3B	2.61	1.62	1.59
2	B	1001	ATP	PB-O3A	2.56	1.62	1.59
2	D	1001	ATP	C5-C6	2.53	1.48	1.41
2	D	1001	ATP	C8-N7	2.47	1.36	1.31
2	A	1001	ATP	C8-N7	2.44	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ATP	PB-O3A	2.39	1.62	1.59
2	B	1001	ATP	C5-N7	-2.39	1.34	1.39
2	A	1001	ATP	PB-O3B	2.28	1.62	1.59
2	C	1001	ATP	C5-C6	2.28	1.47	1.41
2	D	1001	ATP	C5-N7	-2.23	1.35	1.39
2	C	1001	ATP	C5-N7	-2.19	1.35	1.39
2	C	1001	ATP	PB-O3B	2.18	1.61	1.59
2	B	1001	ATP	C8-N7	2.16	1.35	1.31
2	A	1001	ATP	C5-N7	-2.16	1.35	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ATP	C5-C4-N3	-6.17	118.22	126.72
2	C	1001	ATP	C5-C4-N3	-5.67	118.90	126.72
2	D	1001	ATP	C5-C4-N3	-5.55	119.08	126.72
2	B	1001	ATP	C5-C4-N3	-5.45	119.21	126.72
2	B	1001	ATP	N3-C4-N9	5.37	136.31	127.17
2	D	1001	ATP	N3-C4-N9	5.03	135.72	127.17
2	C	1001	ATP	N3-C4-N9	4.88	135.47	127.17
2	A	1001	ATP	N3-C4-N9	4.68	135.13	127.17
2	A	1001	ATP	C2-N3-C4	3.71	120.89	111.83
2	C	1001	ATP	C2-N3-C4	3.67	120.80	111.83
2	C	1001	ATP	N3-C2-N1	-3.66	123.04	128.58
2	B	1001	ATP	N3-C2-N1	-3.59	123.14	128.58
2	B	1001	ATP	C4-N9-C8	3.55	109.47	105.74
2	D	1001	ATP	N3-C2-N1	-3.50	123.29	128.58
2	B	1001	ATP	C2-N3-C4	3.48	120.32	111.83
2	D	1001	ATP	C2-N3-C4	3.47	120.31	111.83
2	A	1001	ATP	C4-C5-N7	-3.37	106.73	110.58
2	A	1001	ATP	O4'-C1'-N9	3.26	114.34	108.09
2	B	1001	ATP	N6-C6-N1	3.12	125.32	118.38
2	A	1001	ATP	N3-C2-N1	-3.09	123.91	128.58
2	D	1001	ATP	C4-N9-C8	2.83	108.71	105.74
4	C	488	GOL	C3-C2-C1	-2.71	101.85	111.80
2	C	1001	ATP	C4-N9-C8	2.70	108.58	105.74
2	B	1001	ATP	O3'-C3'-C4'	-2.57	103.70	111.08
2	C	1001	ATP	C4-C5-N7	-2.55	107.66	110.58
2	D	1001	ATP	C2-N1-C6	2.52	122.87	118.73
2	D	1001	ATP	O4'-C1'-N9	2.50	112.90	108.09
2	D	1001	ATP	N6-C6-N1	2.45	123.84	118.38
2	D	1001	ATP	C4-C5-N7	-2.44	107.79	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	ATP	O3'-C3'-C4'	-2.41	104.15	111.08
2	A	1001	ATP	C5-N7-C8	2.33	107.12	103.45
2	A	1001	ATP	O2A-PA-O3A	2.31	113.52	107.27
2	B	1001	ATP	C5-C6-N6	-2.30	117.59	123.29
2	C	1001	ATP	C2-N1-C6	2.29	122.50	118.73
2	B	1001	ATP	C2-N1-C6	2.27	122.46	118.73
2	C	1001	ATP	O4'-C1'-N9	2.24	112.39	108.09
2	C	1001	ATP	N6-C6-N1	2.21	123.31	118.38
2	D	1001	ATP	O3A-PA-O1A	-2.04	104.57	110.70
2	B	1001	ATP	N9-C8-N7	-2.03	111.05	113.94
2	C	1001	ATP	C5-N7-C8	2.03	106.64	103.45
2	A	1001	ATP	O3A-PA-O1A	-2.01	104.64	110.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	488	GOL	O1-C1-C2-C3
4	C	488	GOL	C1-C2-C3-O3
4	A	488	GOL	O1-C1-C2-O2
4	C	488	GOL	O2-C2-C3-O3
2	A	1001	ATP	PB-O3B-PG-O3G
2	C	1001	ATP	PB-O3B-PG-O2G
2	C	1001	ATP	PA-O3A-PB-O1B
2	C	1001	ATP	PA-O3A-PB-O2B
2	C	1001	ATP	PB-O3A-PA-O2A

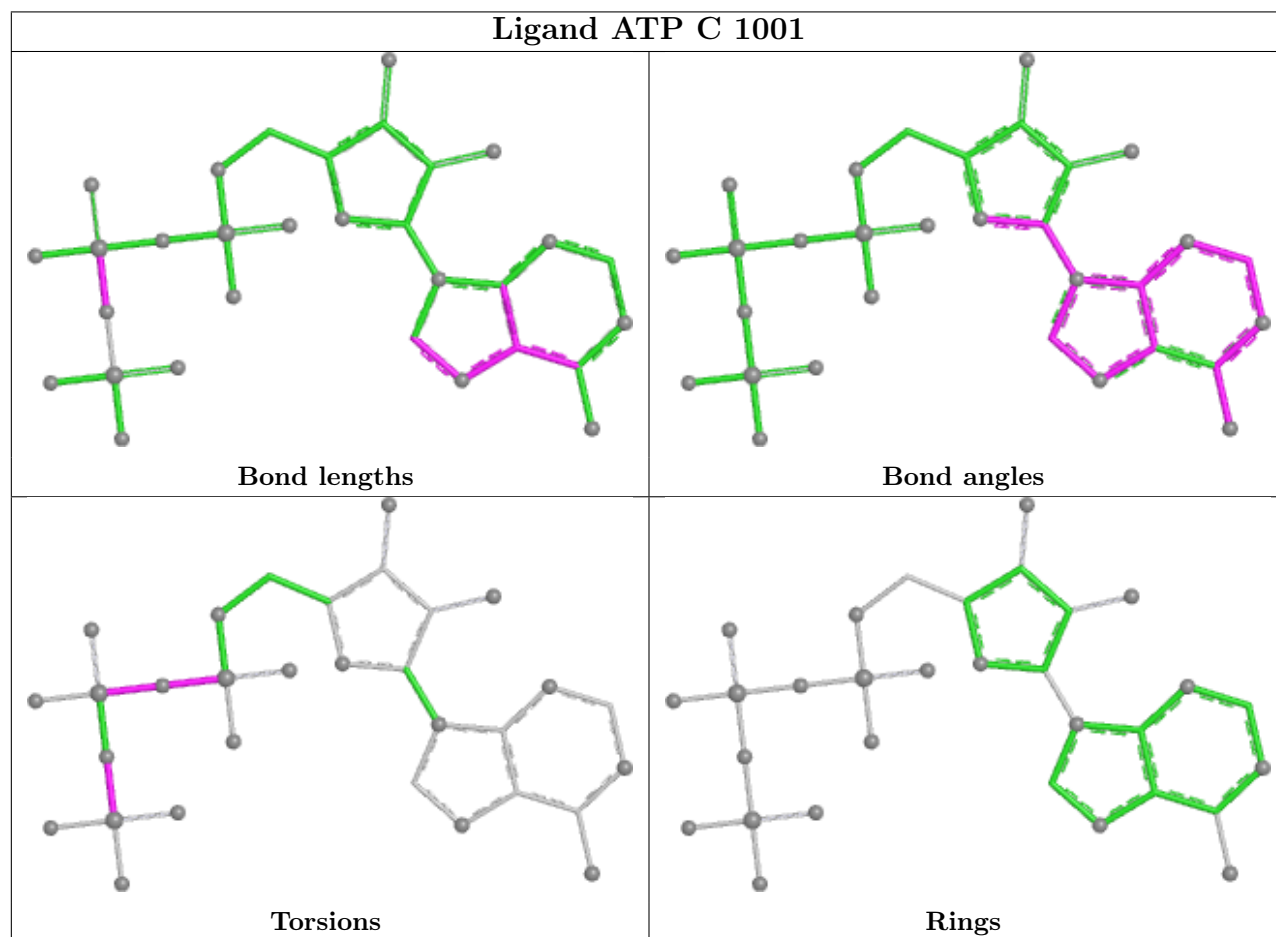
There are no ring outliers.

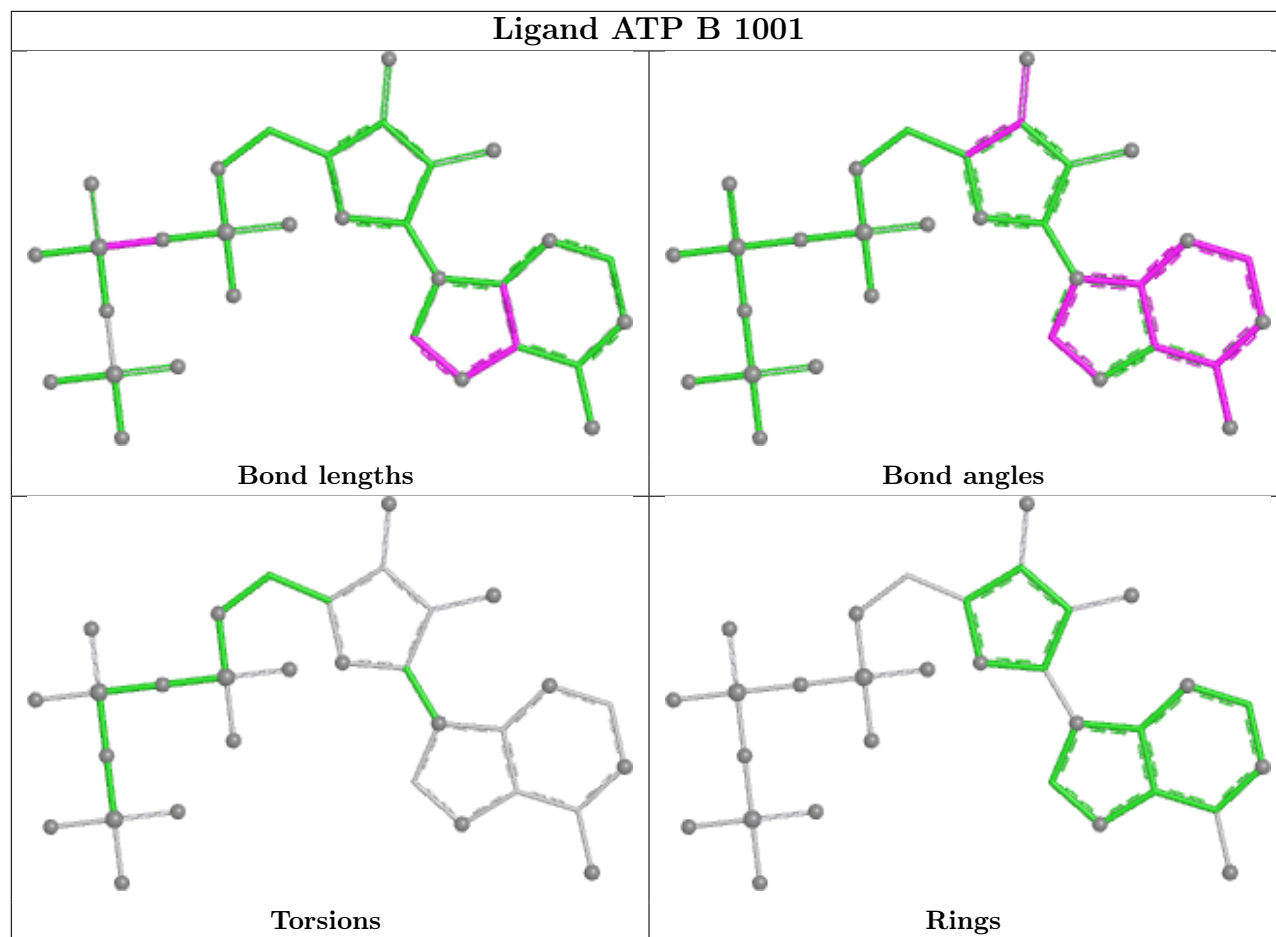
2 monomers are involved in 3 short contacts:

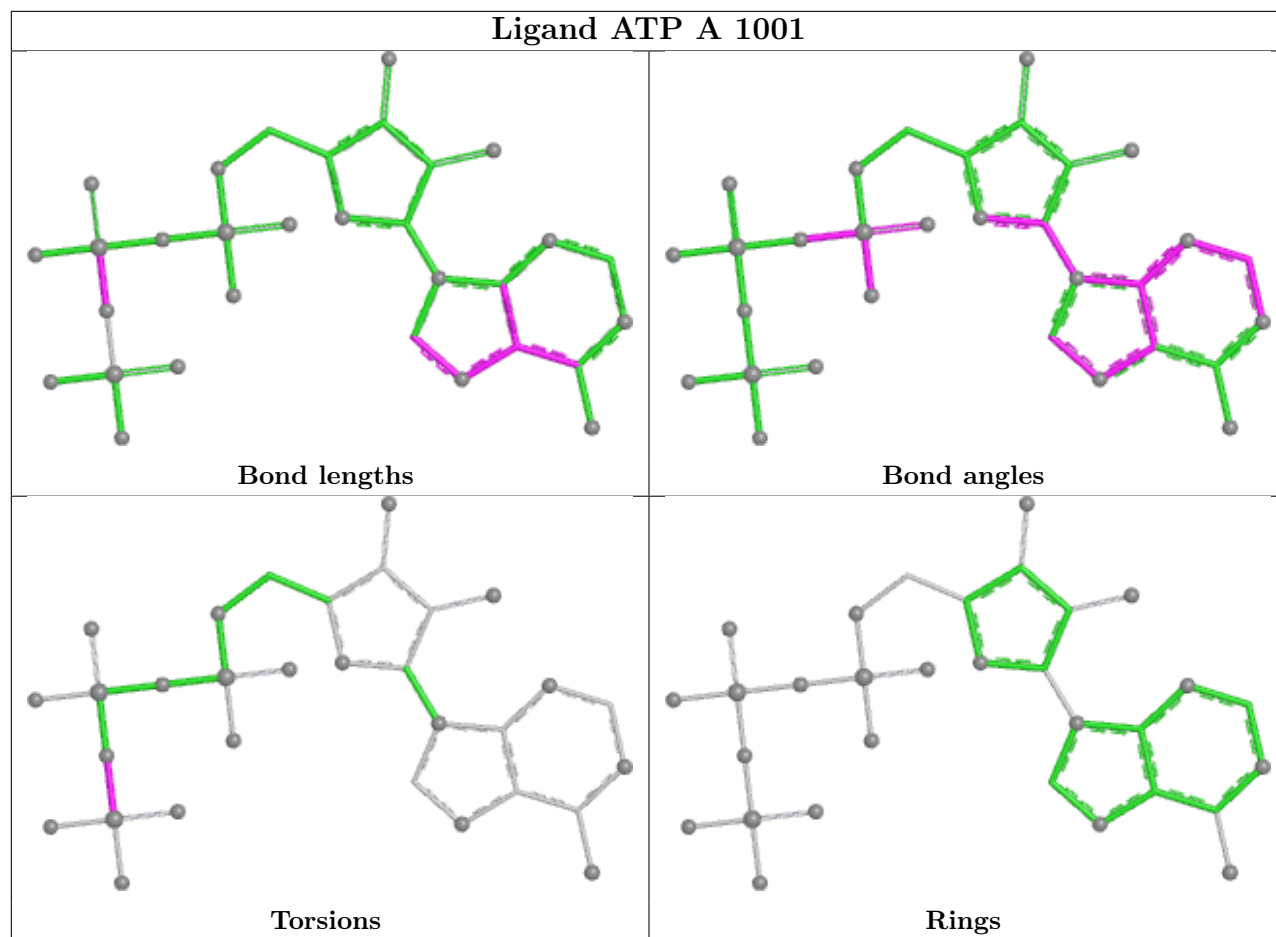
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	ATP	2	0
2	B	1001	ATP	1	0

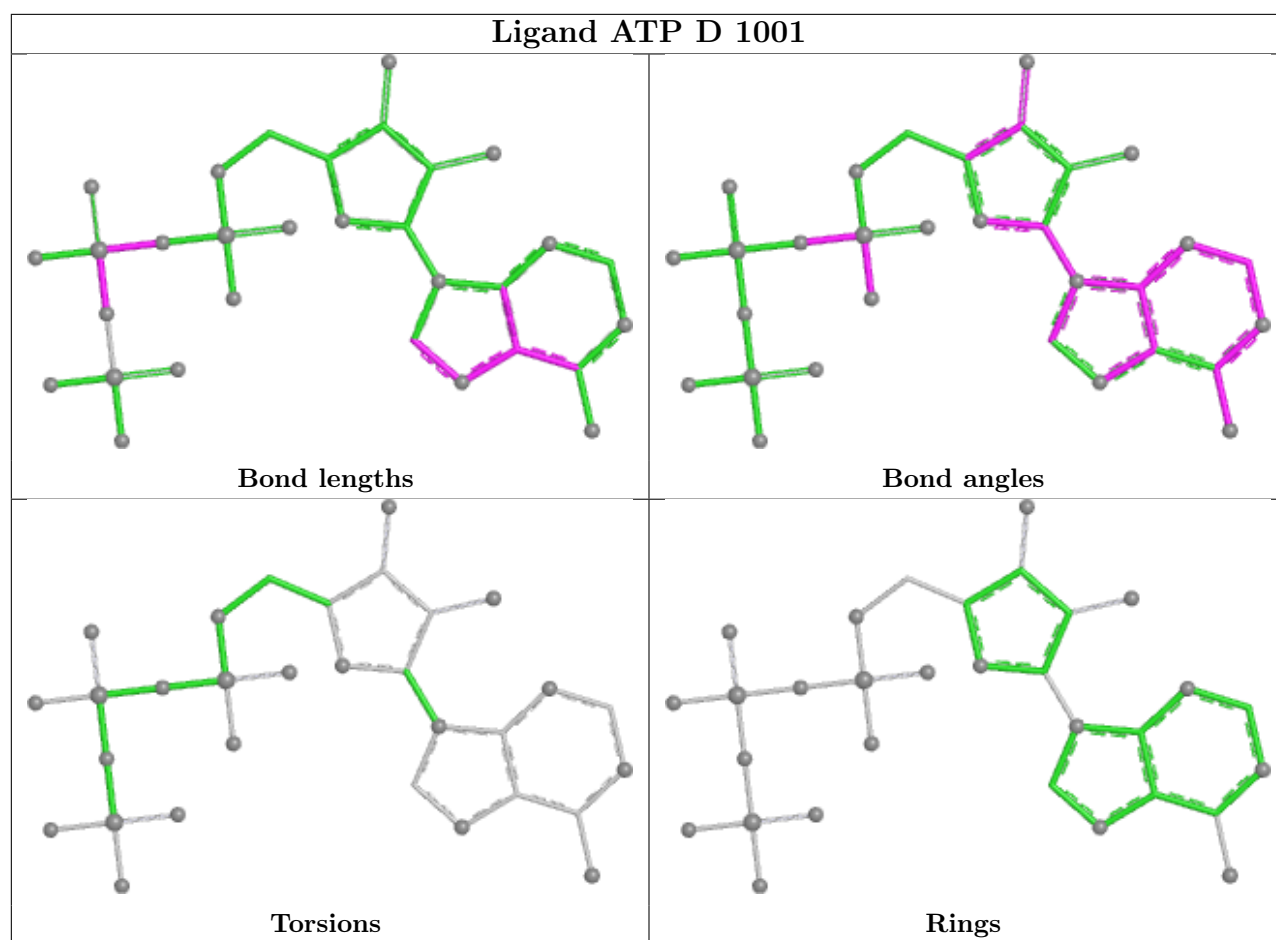
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	458/487 (94%)	-0.13	11 (2%) 59 56	12, 29, 77, 111	0
1	B	462/487 (94%)	-0.19	9 (1%) 66 63	12, 28, 80, 111	0
1	C	461/487 (94%)	-0.11	22 (4%) 35 32	12, 29, 80, 111	0
1	D	458/487 (94%)	-0.18	11 (2%) 59 56	12, 28, 81, 113	0
All	All	1839/1948 (94%)	-0.15	53 (2%) 53 50	12, 29, 80, 113	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	473	ILE	7.4
1	D	466	ILE	4.4
1	D	480	LEU	4.1
1	C	480	LEU	4.0
1	A	473	ILE	4.0
1	D	458	VAL	3.7
1	D	475	ARG	3.7
1	A	480	LEU	3.6
1	C	458	VAL	3.6
1	B	466	ILE	3.4
1	C	481	HIS	3.3
1	C	466	ILE	3.2
1	C	471	GLU	3.2
1	D	473	ILE	3.2
1	C	470	LEU	3.0
1	C	474	ASN	3.0
1	C	469	GLU	2.9
1	D	481	HIS	2.7
1	C	462	ARG	2.7
1	C	212	ALA	2.7
1	A	458	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	9	VAL	2.6
1	B	480	LEU	2.6
1	C	45	LYS	2.6
1	C	22	ASN	2.6
1	C	461	ALA	2.5
1	A	457	ASP	2.5
1	D	462	ARG	2.5
1	C	478	ASP	2.5
1	A	481	HIS	2.5
1	B	462	ARG	2.4
1	C	485	ALA	2.4
1	B	330	ASP	2.4
1	A	485	ALA	2.4
1	A	11	SER	2.3
1	C	8	ARG	2.3
1	A	482	GLU	2.3
1	C	456	SER	2.3
1	B	482	GLU	2.2
1	B	17	HIS	2.2
1	D	476	ASN	2.2
1	A	45	LYS	2.2
1	B	481	HIS	2.1
1	C	483	GLU	2.1
1	D	482	GLU	2.1
1	C	27	GLU	2.1
1	C	482	GLU	2.1
1	D	163	HIS	2.1
1	B	457	ASP	2.0
1	A	471	GLU	2.0
1	D	22	ASN	2.0
1	A	469	GLU	2.0
1	B	476	ASN	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

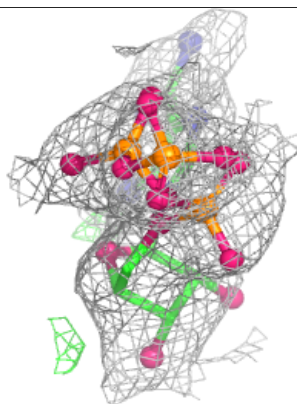
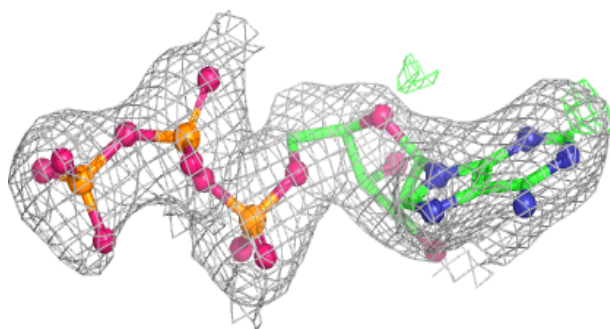
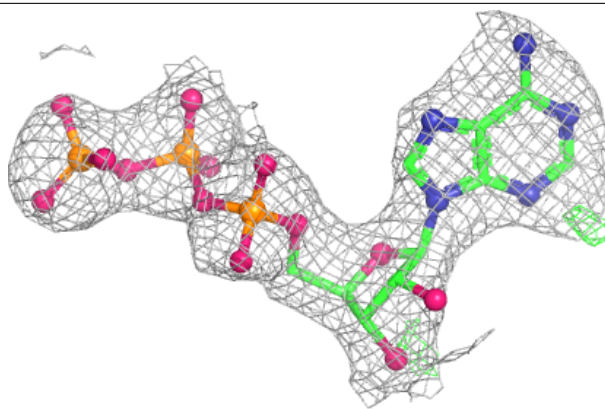
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	NA	A	489	1/1	0.70	0.13	30,30,30,30	0
5	NA	A	490	1/1	0.74	0.17	43,43,43,43	0
5	NA	C	490	1/1	0.79	0.09	34,34,34,34	0
5	NA	B	488	1/1	0.80	0.17	45,45,45,45	0
3	MG	D	1002	1/1	0.81	0.17	45,45,45,45	0
3	MG	B	1002	1/1	0.83	0.15	51,51,51,51	0
3	MG	A	1002	1/1	0.87	0.07	49,49,49,49	0
6	SO4	C	489	5/5	0.90	0.11	33,41,48,91	0
4	GOL	A	488	6/6	0.94	0.09	5,19,35,41	0
2	ATP	D	1001	31/31	0.97	0.06	15,29,39,71	0
2	ATP	A	1001	31/31	0.97	0.07	19,40,62,73	0
4	GOL	C	488	6/6	0.97	0.06	9,14,28,33	0
2	ATP	C	1001	31/31	0.97	0.06	17,32,43,62	0
2	ATP	B	1001	31/31	0.98	0.05	14,25,38,66	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.

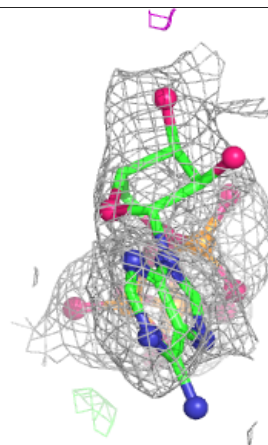
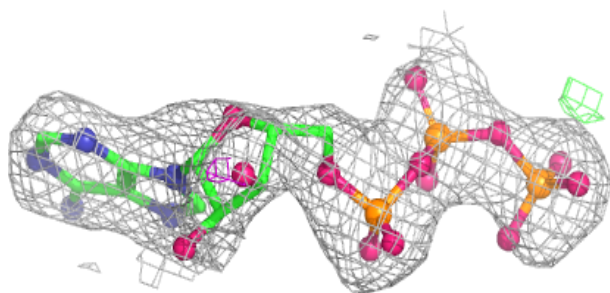
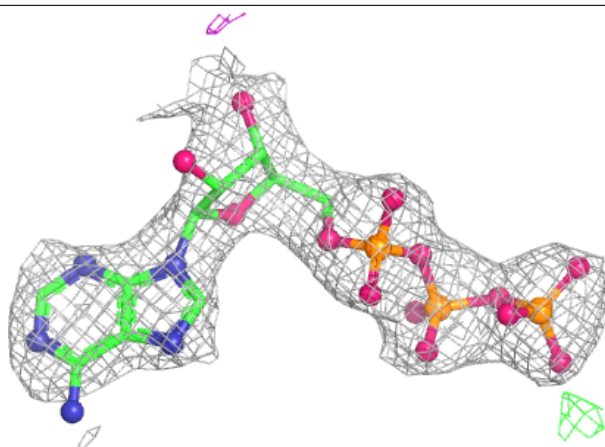
Electron density around ATP D 1001:

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

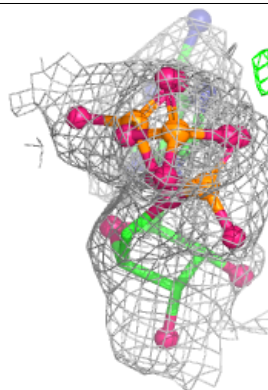
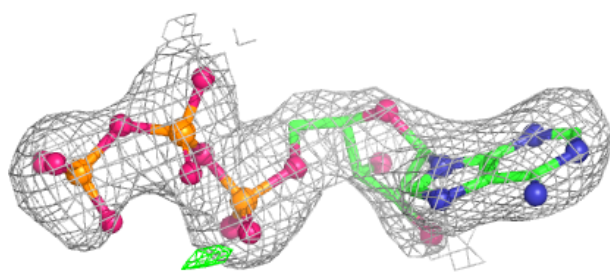
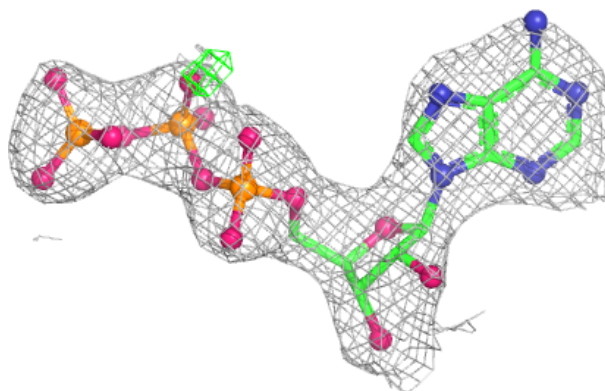


Electron density around ATP A 1001:

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

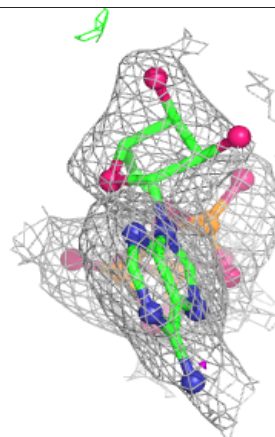
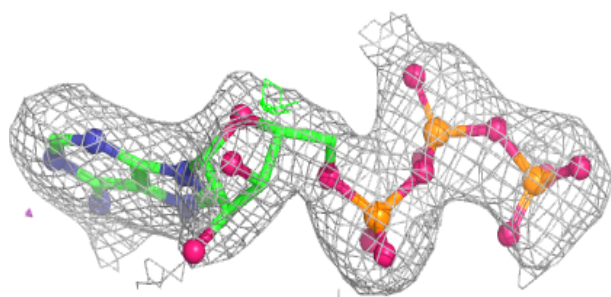
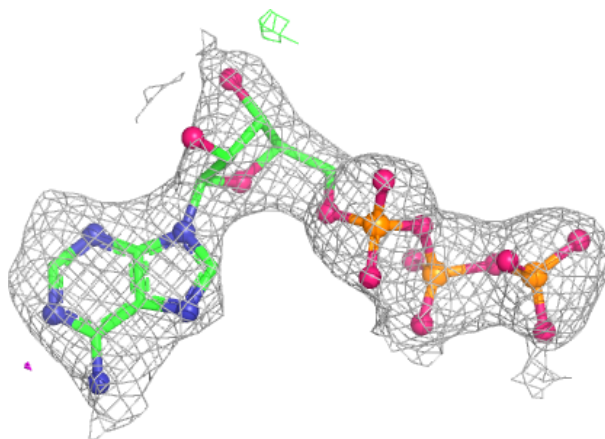
**Electron density around ATP C 1001:**

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



Electron density around ATP B 1001:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.