



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:02 am BST

PDB ID : 3F5M
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

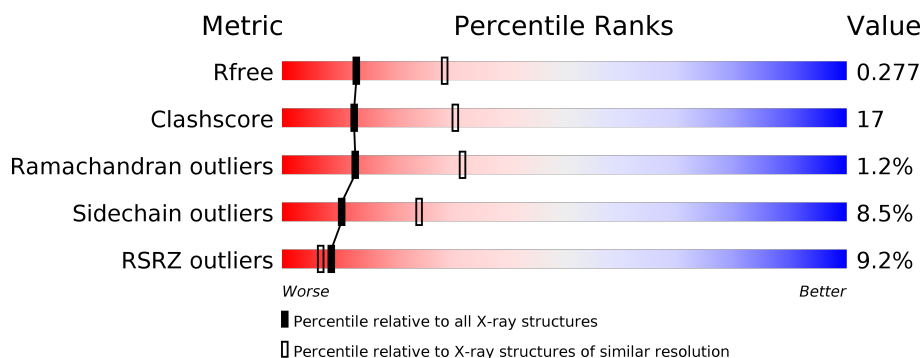
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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	<div> <div>8%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>• 6%</div> </div> </div>
1	B	487	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>27%</div> <div>5% 5%</div> </div> </div>
1	C	487	<div> <div>10%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>• 5%</div> </div> </div>
1	D	487	<div> <div>9%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>• 6%</div> </div> </div>

2 Entry composition [i](#)

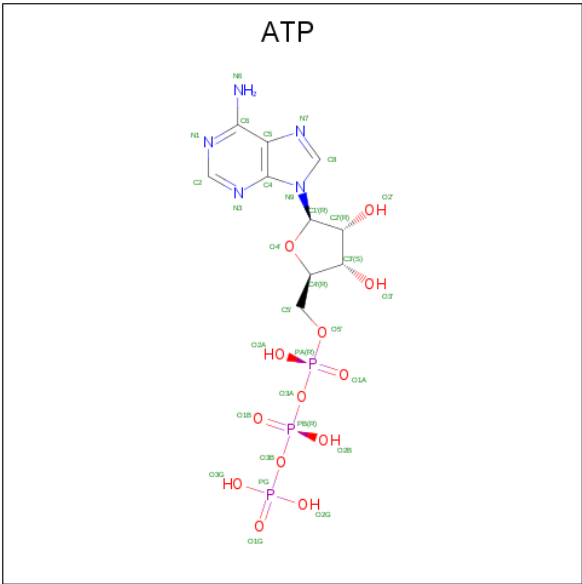
There are 7 unique types of molecules in this entry. The entry contains 14783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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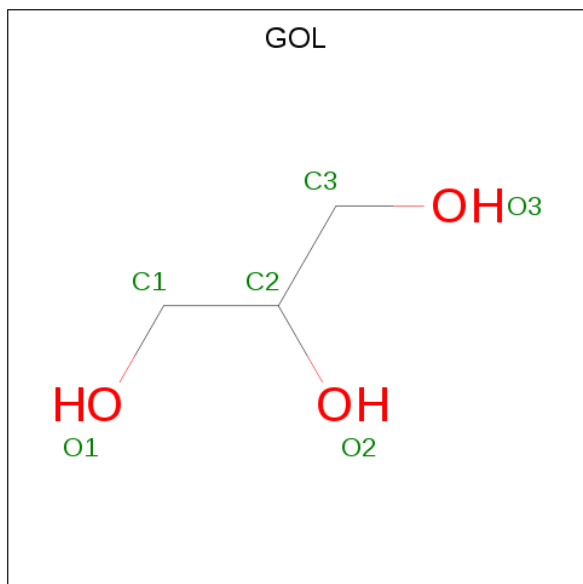
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

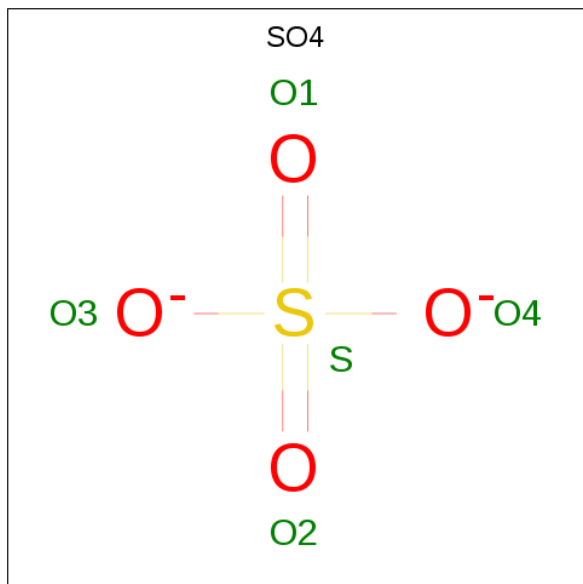


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

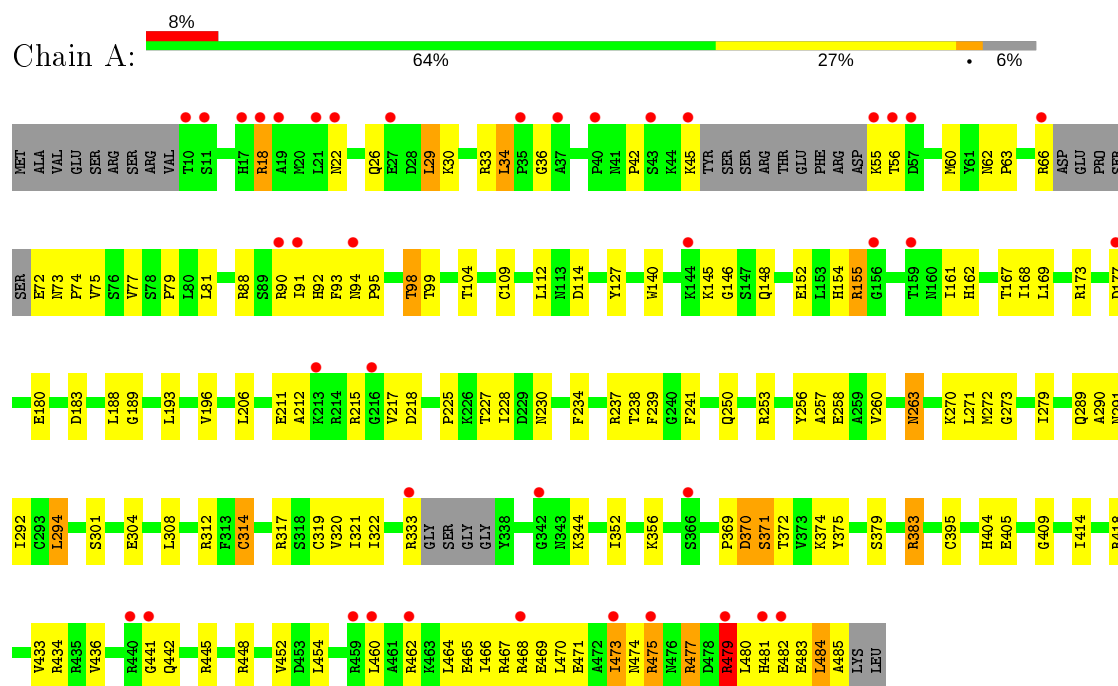
- Molecule 7 is water.

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

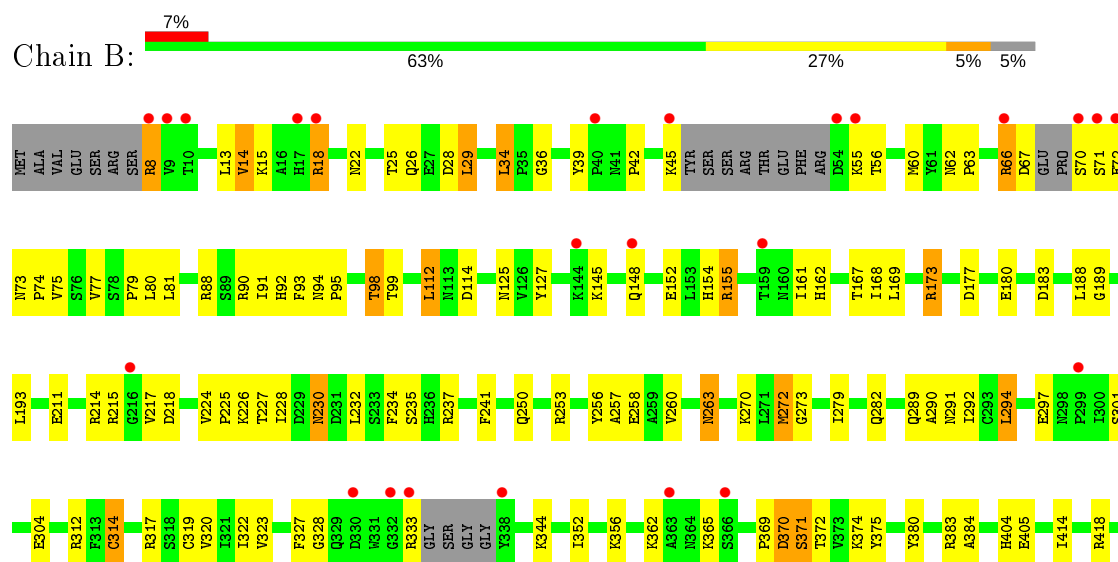
3 Residue-property plots [i](#)

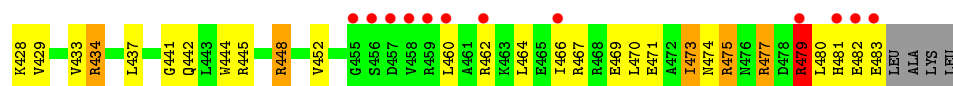
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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)

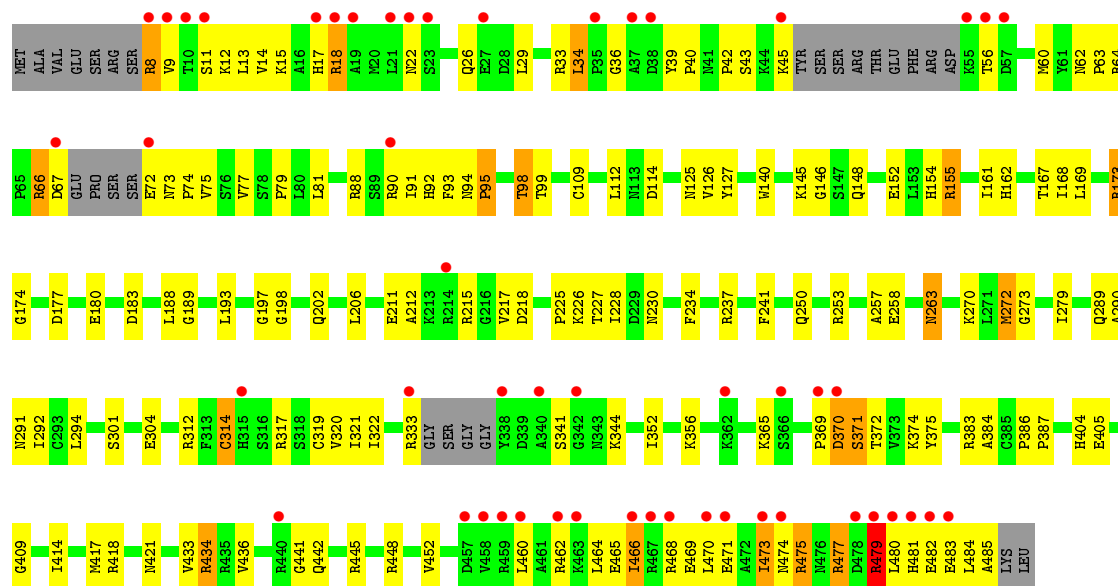


- Molecule 1: 6-phospho-1-fructokinase (ATP-dependent phosphofructokinase)

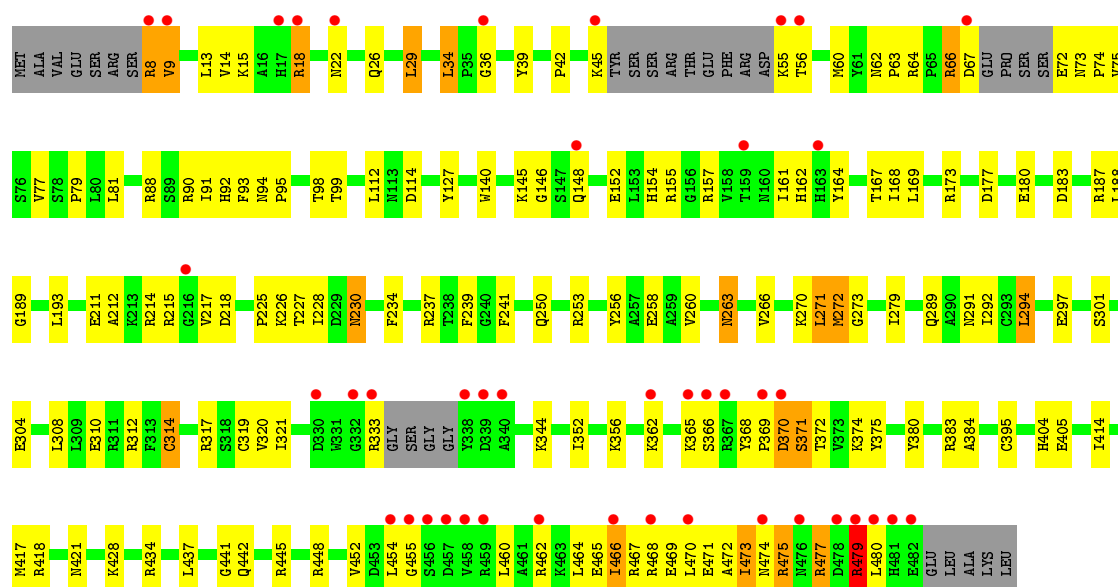




- Molecule 1: 6-phospho-1-fructokinase (ATP-dependent phosphofructokinase)



- 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) 97.9 (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 0.213 , 0.277	Depositor DCC
R_{free} test set	2775 reflections (5.09%)	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)	0.41 , 77.3	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	0.95	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, MG, SO4, ATP, 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	0.47	0/3593	0.80	17/4856 (0.4%)
1	B	0.48	0/3626	1.14	22/4900 (0.4%)
1	C	0.46	0/3619	0.73	13/4891 (0.3%)
1	D	0.47	0/3597	0.73	16/4861 (0.3%)
All	All	0.47	0/14435	0.87	68/19508 (0.3%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	NE-CZ-NH1	-20.03	110.28	120.30
1	B	383	ARG	NE-CZ-NH1	-19.32	110.64	120.30
1	B	155	ARG	NE-CZ-NH2	18.89	129.75	120.30
1	B	383	ARG	NE-CZ-NH2	18.87	129.74	120.30
1	B	18	ARG	NE-CZ-NH2	-18.76	110.92	120.30
1	B	434	ARG	NE-CZ-NH1	-17.78	111.41	120.30
1	B	434	ARG	NE-CZ-NH2	17.59	129.09	120.30
1	A	479	ARG	NE-CZ-NH2	17.48	129.04	120.30
1	B	18	ARG	NE-CZ-NH1	17.47	129.04	120.30
1	B	448	ARG	NE-CZ-NH2	17.24	128.92	120.30
1	B	448	ARG	NE-CZ-NH1	-16.96	111.82	120.30
1	A	479	ARG	NE-CZ-NH1	-15.69	112.45	120.30
1	B	467	ARG	NE-CZ-NH1	-14.84	112.88	120.30
1	B	467	ARG	NE-CZ-NH2	14.25	127.42	120.30
1	B	66	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	C	66	ARG	NE-CZ-NH2	-12.05	114.28	120.30
1	D	66	ARG	NE-CZ-NH1	-11.67	114.46	120.30
1	C	66	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	B	66	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	66	ARG	NE-CZ-NH1	-11.40	114.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	ARG	NE-CZ-NH2	10.80	125.70	120.30
1	A	66	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	B	155	ARG	CD-NE-CZ	9.29	136.61	123.60
1	B	434	ARG	CD-NE-CZ	8.98	136.17	123.60
1	B	18	ARG	CD-NE-CZ	8.72	135.80	123.60
1	B	448	ARG	CD-NE-CZ	8.64	135.69	123.60
1	B	383	ARG	CD-NE-CZ	8.62	135.67	123.60
1	C	383	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	383	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	D	383	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	434	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	383	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	479	ARG	CD-NE-CZ	6.99	133.38	123.60
1	C	383	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	434	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	D	434	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	C	155	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	155	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	D	18	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	D	434	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	18	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	A	155	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	434	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	434	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	155	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	155	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	467	ARG	CD-NE-CZ	6.12	132.17	123.60
1	C	18	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	A	18	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	D	18	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	18	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	D	155	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	479	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	479	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	271	LEU	CB-CG-CD1	5.67	120.64	111.00
1	A	448	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	479	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	66	ARG	CD-NE-CZ	5.59	131.42	123.60
1	A	66	ARG	CD-NE-CZ	5.57	131.39	123.60
1	B	66	ARG	CD-NE-CZ	5.55	131.37	123.60
1	D	383	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	66	ARG	CD-NE-CZ	5.53	131.33	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	448	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	448	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	448	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	467	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	467	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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	145	0
1	B	3569	0	3632	142	1
1	C	3562	0	3634	148	1
1	D	3540	0	3612	135	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	479	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 (479) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:8:ARG:CZ	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
1:D:475:ARG:NH2	1:D:479:ARG:NH1	2.35	0.73
1:B:480:LEU:HD13	1:D:473:ILE:HG22	1.70	0.73
1:B:473:ILE:HG22	1:D:480:LEU:HD13	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:370:ASP:O	1:B:371:SER:HB3	1.96	0.65
1:B:66:ARG:HG2	1:B:67:ASP:H	1.61	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:370:ASP:O	1:A:371:SER:HB3	1.94	0.64
1:A:88:ARG:NH1	1:A:405:GLU:OE1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:481:HIS:C	1:B:483:GLU:H	2.02	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:460:LEU:O	1:A:464:LEU:HG	2.02	0.60
1:A:91:ILE:HD11	1:A:95:PRO:HG3	1.84	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: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:D:258:GLU:CG	1:D:374:LYS:HG3	2.28	0.58
1:B:473:ILE:HG21	1:D:480:LEU:CB	2.33	0.58
1:B:480:LEU:CB	1:D:473:ILE:HG21	2.32	0.58
1:C:145:LYS:O	1:C:148:GLN:HG2	2.02	0.58
1:C:66:ARG:CG	1:C:67:ASP:H	2.15	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:370:ASP:O	1:D:371:SER:HB3	2.02	0.58
1:D:312:ARG:HB2	1:D:452:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:HB2	1:C:217:VAL:CG2	2.34	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: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:C:481:HIS:C	1:C:483:GLU:H	2.08	0.55
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: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:473:ILE:HG22	1:C:480:LEU:HD13	1.89	0.53
1:A:470:LEU:CD2	1:C:481:HIS:HA	2.35	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:A:481:HIS:C	1:A:483:GLU:H	2.13	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:480:LEU:HD13	1:C:473:ILE:HG22	1.90	0.52
1:A:477:ARG:NE	1:C:474:ASN:ND2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:MET:HE3	1:C:272:MET:HA	1.92	0.52
1:C:475:ARG:NH2	1:C:479:ARG:HD2	2.24	0.52
1:D:230:ASN:HD21	1:D:237:ARG:HA	1.75	0.52
1:D:93:PHE:O	1:D:95:PRO:HD3	2.09	0.52
1:A:294:LEU:HA	7:A:582:HOH:O	2.09	0.51
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:B:481:HIS:C	1:B:483:GLU:N	2.64	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
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:480:LEU:O	1:D:470:LEU:HD21	2.12	0.50
1:B:66:ARG:CG	1:B:67:ASP:H	2.24	0.50
1:B:225:PRO:HG3	1:B:414:ILE:HB	1.93	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:A:79:PRO:O	1:B:70:SER:HB2	2.12	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:477:ARG:CB	1:D:477:ARG:HG3	2.42	0.49
1:B:475:ARG:NH2	1:B:479:ARG:HD2	2.27	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:352:ILE:O	1:D:356:LYS:HG2	2.13	0.49
1:D:60:MET:HA	1:D:81:LEU:HD23	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:238:THR:HB	7:A:563:HOH:O	2.13	0.48
1:A:60:MET:HA	1:A:81:LEU:HD23	1.96	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:C:161:ILE:HG21	1:C:168:ILE:HD13	1.96	0.48
1:B:480:LEU:CD1	1:D:473:ILE:CG2	2.90	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:C:211:GLU:O	1:C:215:ARG:HG3	2.13	0.47
1:D:162:HIS:CD2	1:D:162:HIS:H	2.32	0.47
1:B:483:GLU:OE1	1:D:466:ILE:HG22	2.14	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: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:D:8:ARG:NE	1:D:8:ARG:HA	2.29	0.47
1:C:92:HIS:HE1	1:C:218:ASP:OD1	1.98	0.47
1:D:314:CYS:HB3	1:D:462:ARG:HH21	1.80	0.47
1:B:480:LEU:CD1	1:D:473:ILE:HG21	2.44	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: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:481:HIS:C	1:C:483:GLU:N	2.68	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:140:TRP:O	1:C:146:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:MET:HA	1:C:81:LEU:HD23	1.96	0.46
1:B:272:MET:HA	1:B:272:MET:HE3	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: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
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: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: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:A:484:LEU:HD23	1:C:470:LEU:HD12	1.97	0.46
1:D:214:ARG:NH2	7:D:542:HOH:O	2.46	0.46
1:B:470:LEU:HD21	1:D:480:LEU:O	2.16	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:428:LYS:HG3	7:B:567:HOH:O	2.16	0.46
1:B:8:ARG:HA	1:B:8:ARG:NE	2.30	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:B:39:TYR:CZ	1:B:94:ASN:HB2	2.52	0.45
1:B:36:GLY:O	1:B:92:HIS:HD2	1.99	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:297:GLU:CD	1:D:437:LEU:HB2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:484:LEU:CD1	1:A:484:LEU:C	2.86	0.44
1:C:484:LEU:HG	1:C:485:ALA:N	2.32	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
1:D:55:LYS:HB3	1:D:55:LYS:HE2	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:B:473:ILE:HG21	1:D:480:LEU:HB3	1.99	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:C:386:PRO:HA	1:C:387:PRO:HD3	1.83	0.44
1:D:253:ARG:HH11	1:D:253:ARG:HG2	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:D:140:TRP:O	1:D:146:GLY:HA3	2.17	0.43
1:A:154:HIS:O	1:A:155:ARG:C	2.56	0.43
1:A:314:CYS:HB3	1:A:462:ARG:HH21	1.83	0.43
1:A:481:HIS:C	1:A:483:GLU:N	2.71	0.43
1:B:473:ILE:HG12	1:B:474:ASN:N	2.33	0.43
1:C:22:ASN:HA	1:C:22:ASN:HD22	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:257:ALA:HB3	1:D:384:ALA:HB1	1.99	0.43
1:B:480:LEU:HB3	1:D:473:ILE:HG21	1.99	0.43
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.80	0.43
1:B:22:ASN:HA	1:B:22:ASN:HD22	1.63	0.43
1:B:352:ILE:O	1:B:356:LYS:HG2	2.18	0.43
1:B:73:ASN:HD22	1:B:73:ASN:N	2.16	0.43
1:C:34:LEU:HD23	1:C:93:PHE:CZ	2.52	0.43
1:C:33:ARG:HA	1:C:409:GLY:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:297:GLU:CD	1:B:437:LEU:HB2	2.39	0.43
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:477:ARG:HG3	1:D:477:ARG:HB2	2.01	0.43
1:B:92:HIS:HE1	1:B:218:ASP:OD1	2.01	0.43
1:C:228:ILE:O	1:C:279:ILE:HD11	2.19	0.43
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.83	0.42
1:A:95:PRO:O	1:A:98:THR:HG23	2.18	0.42
1:B:362:LYS:O	1:B:365:LYS:HG3	2.19	0.42
1:A:473:ILE:HD12	1:C:480:LEU:HB2	2.00	0.42
1:B:125:ASN:HD21	1:B:155:ARG:NH2	2.17	0.42
1:B:99:THR:HB	1:B:189:GLY:O	2.18	0.42
1:C:263:ASN:ND2	1:C:317:ARG:HH11	2.11	0.42
1:D:272:MET:HE3	1:D:272:MET:HA	2.01	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: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:HE2	1:B:55:LYS:HB3	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:A:62:ASN:C	1:A:62:ASN:OD1	2.58	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: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:D:73:ASN:HA	1:D:74:PRO:HD3	1.78	0.42
1:A:253:ARG:HA	1:A:289:GLN:HE22	1.85	0.42
1:A:73:ASN:HA	1:A:74:PRO:HD3	1.78	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:228:ILE:O	1:A:279:ILE:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:HA	1:A:409:GLY:O	2.20	0.41
1:B:270:LYS:HA	1:B:323:VAL:O	2.20	0.41
1:B:94:ASN:O	1:B:98:THR:HG22	2.19	0.41
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:292:ILE:HB	1:D:321:ILE:HG12	2.02	0.41
1:D:66:ARG:HG2	1:D:67:ASP:N	2.29	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:164:TYR:HB3	7:D:493:HOH:O	2.19	0.41
1:D:34:LEU:HB3	1:D:92:HIS:NE2	2.35	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:212:ALA:O	1:C:217:VAL:HG23	2.21	0.41
1:C:26:GLN:NE2	1:C:81:LEU:H	2.13	0.41
1:D:310:GLU:HG3	1:D:368:TYR:OH	2.20	0.41
1:D:9:VAL:HG13	1:D:64:ARG:NH2	2.36	0.41
1:B:253:ARG:HA	1:B:289:GLN:HE22	1.85	0.41
1:B:228:ILE:O	1:B:279:ILE:HD11	2.20	0.41
1:B:62:ASN:HA	1:B:63:PRO:HD3	1.78	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:272:MET:HB2	1:D:279:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:NH1	7:D:522:HOH:O	2.39	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
1:A:29:LEU:HA	1:A:29:LEU:HD12	1.96	0.40
1:C:465:GLU:O	1:C:468:ARG:HB2	2.21	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: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:A:473:ILE:HG12	1:A:474:ASN:N	2.35	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:417:MET:HG2	1:C:421:ASN:O	2.21	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:D:472:ALA:HB3	7:D:563:HOH:O	2.22	0.40
1:A:22:ASN:HA	1:A:22:ASN:HD22	1.59	0.40
1:A:256:TYR:CZ	1:A:260:VAL:HG21	2.56	0.40
1:B:230:ASN:HB2	1:B:241:PHE:CD2	2.56	0.40
1:B:26:GLN:NE2	1:B:80:LEU:HA	2.36	0.40
1:B:272:MET:CE	1:B:272:MET:HA	2.50	0.40
1:B:29:LEU:HD12	1:B:429:VAL:HG21	2.04	0.40
1:C:15:LYS:HE3	1:C:22:ASN:ND2	2.37	0.40
1:C:62:ASN:OD1	1:C:62:ASN:C	2.60	0.40
1:D:157:ARG:HG3	7:D:595:HOH:O	2.22	0.40
1:D:29:LEU:HA	1:D:29:LEU:HD12	1.96	0.40
1:A:480:LEU:HB2	1:C:473:ILE:HD12	2.03	0.40
1:A:79:PRO:HB3	1:B:73:ASN:ND2	2.36	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%)	14	34
1	B	454/487 (93%)	426 (94%)	23 (5%)	5 (1%)	14	34
1	C	453/487 (93%)	425 (94%)	22 (5%)	6 (1%)	12	30
1	D	450/487 (92%)	425 (94%)	20 (4%)	5 (1%)	14	34
All	All	1807/1948 (93%)	1701 (94%)	85 (5%)	21 (1%)	13	32

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%)	348 (92%)	32 (8%)	11	25
1	B	385/405 (95%)	352 (91%)	33 (9%)	10	24
1	C	383/405 (95%)	349 (91%)	34 (9%)	9	22
1	D	381/405 (94%)	350 (92%)	31 (8%)	11	27
All	All	1529/1620 (94%)	1399 (92%)	130 (8%)	10	24

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	29	LEU
1	A	34	LEU
1	A	72	GLU
1	A	77	VAL
1	A	90	ARG
1	A	98	THR
1	A	109	CYS
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	227	THR
1	A	263	ASN
1	A	272	MET
1	A	294	LEU
1	A	314	CYS
1	A	333	ARG
1	A	344	LYS
1	A	370	ASP
1	A	372	THR

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Mol	Chain	Res	Type
1	A	433	VAL
1	A	436	VAL
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	14	VAL
1	B	18	ARG
1	B	29	LEU
1	B	34	LEU
1	B	72	GLU
1	B	77	VAL
1	B	90	ARG
1	B	98	THR
1	B	112	LEU
1	B	114	ASP
1	B	167	THR
1	B	169	LEU
1	B	173	ARG
1	B	188	LEU
1	B	193	LEU
1	B	227	THR
1	B	230	ASN
1	B	263	ASN
1	B	272	MET
1	B	294	LEU
1	B	314	CYS
1	B	333	ARG
1	B	344	LYS
1	B	370	ASP
1	B	372	THR
1	B	433	VAL
1	B	434	ARG
1	B	466	ILE
1	B	473	ILE
1	B	475	ARG
1	B	477	ARG
1	B	479	ARG
1	C	8	ARG

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Mol	Chain	Res	Type
1	C	9	VAL
1	C	11	SER
1	C	18	ARG
1	C	29	LEU
1	C	34	LEU
1	C	72	GLU
1	C	77	VAL
1	C	90	ARG
1	C	98	THR
1	C	109	CYS
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	227	THR
1	C	263	ASN
1	C	272	MET
1	C	294	LEU
1	C	314	CYS
1	C	333	ARG
1	C	344	LYS
1	C	370	ASP
1	C	372	THR
1	C	433	VAL
1	C	436	VAL
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	18	ARG
1	D	29	LEU
1	D	34	LEU
1	D	72	GLU
1	D	77	VAL
1	D	90	ARG
1	D	98	THR
1	D	112	LEU

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Mol	Chain	Res	Type
1	D	114	ASP
1	D	167	THR
1	D	169	LEU
1	D	173	ARG
1	D	188	LEU
1	D	193	LEU
1	D	227	THR
1	D	230	ASN
1	D	263	ASN
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	370	ASP
1	D	372	THR
1	D	466	ILE
1	D	473	ILE
1	D	475	ARG
1	D	477	ARG
1	D	479	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	26	GLN
1	A	73	ASN
1	A	92	HIS
1	A	94	ASN
1	A	128	ASN
1	A	162	HIS
1	A	163	HIS
1	A	176	GLN
1	A	210	GLN
1	A	230	ASN
1	A	242	GLN
1	A	250	GLN
1	A	263	ASN
1	A	282	GLN
1	A	289	GLN

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Mol	Chain	Res	Type
1	A	291	ASN
1	A	298	ASN
1	A	404	HIS
1	A	421	ASN
1	A	442	GLN
1	A	474	ASN
1	B	22	ASN
1	B	26	GLN
1	B	73	ASN
1	B	92	HIS
1	B	94	ASN
1	B	128	ASN
1	B	154	HIS
1	B	162	HIS
1	B	176	GLN
1	B	210	GLN
1	B	230	ASN
1	B	242	GLN
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	419	HIS
1	B	442	GLN
1	B	474	ASN
1	B	481	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	162	HIS
1	C	176	GLN
1	C	210	GLN
1	C	230	ASN
1	C	242	GLN
1	C	250	GLN
1	C	263	ASN

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Mol	Chain	Res	Type
1	C	282	GLN
1	C	289	GLN
1	C	291	ASN
1	C	298	ASN
1	C	404	HIS
1	C	419	HIS
1	C	442	GLN
1	C	474	ASN
1	D	22	ASN
1	D	26	GLN
1	D	73	ASN
1	D	92	HIS
1	D	128	ASN
1	D	148	GLN
1	D	154	HIS
1	D	162	HIS
1	D	176	GLN
1	D	210	GLN
1	D	230	ASN
1	D	242	GLN
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	419	HIS
1	D	442	GLN
1	D	474	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
4	GOL	C	488	-	5,5,5	0.23	0	5,5,5	1.33	1 (20%)
4	GOL	A	488	-	5,5,5	0.39	0	5,5,5	1.01	0
6	SO4	C	489	-	4,4,4	0.19	0	6,6,6	0.27	0
2	ATP	B	1001	3	26,33,33	0.99	2 (7%)	31,52,52	1.54	6 (19%)
2	ATP	A	1001	-	26,33,33	0.92	2 (7%)	31,52,52	1.43	6 (19%)
2	ATP	C	1001	-	26,33,33	0.95	2 (7%)	31,52,52	1.40	4 (12%)
2	ATP	D	1001	3	26,33,33	1.05	2 (7%)	31,52,52	1.36	4 (12%)

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
4	GOL	C	488	-	-	2/4/4/4	-
4	GOL	A	488	-	-	2/4/4/4	-
2	ATP	B	1001	3	-	0/18/38/38	0/3/3/3
2	ATP	A	1001	-	-	1/18/38/38	0/3/3/3
2	ATP	C	1001	-	-	4/18/38/38	0/3/3/3
2	ATP	D	1001	3	-	0/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ATP	C5-C4	2.89	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	ATP	C5-C4	2.59	1.47	1.40
2	B	1001	ATP	O4'-C1'	2.43	1.44	1.41
2	A	1001	ATP	C5-C4	2.43	1.47	1.40
2	B	1001	ATP	C5-C4	2.41	1.47	1.40
2	C	1001	ATP	O4'-C1'	2.11	1.44	1.41
2	D	1001	ATP	O4'-C1'	2.08	1.44	1.41
2	A	1001	ATP	O4'-C1'	2.04	1.43	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ATP	N3-C2-N1	-3.60	123.04	128.68
2	B	1001	ATP	N3-C2-N1	-3.54	123.14	128.68
2	D	1001	ATP	N3-C2-N1	-3.45	123.29	128.68
2	B	1001	ATP	N6-C6-N1	3.25	125.32	118.57
2	A	1001	ATP	N3-C2-N1	-3.05	123.91	128.68
2	C	1001	ATP	PB-O3B-PG	-2.74	123.43	132.83
2	A	1001	ATP	PB-O3B-PG	-2.63	123.80	132.83
2	B	1001	ATP	PB-O3B-PG	-2.57	124.02	132.83
2	A	1001	ATP	C4-C5-N7	-2.56	106.73	109.40
2	B	1001	ATP	O3'-C3'-C4'	-2.54	103.70	111.05
2	D	1001	ATP	N6-C6-N1	2.54	123.84	118.57
4	C	488	GOL	C3-C2-C1	-2.54	101.85	111.70
2	D	1001	ATP	C2-N1-C6	2.40	122.87	118.75
2	B	1001	ATP	PA-O3A-PB	-2.39	124.62	132.83
2	D	1001	ATP	O3'-C3'-C4'	-2.38	104.15	111.05
2	A	1001	ATP	PA-O3A-PB	-2.38	124.67	132.83
2	A	1001	ATP	C3'-C2'-C1'	2.35	104.51	100.98
2	C	1001	ATP	N6-C6-N1	2.28	123.31	118.57
2	C	1001	ATP	C2-N1-C6	2.19	122.50	118.75
2	B	1001	ATP	C2-N1-C6	2.17	122.46	118.75
2	A	1001	ATP	O3G-PG-O2G	2.00	115.29	107.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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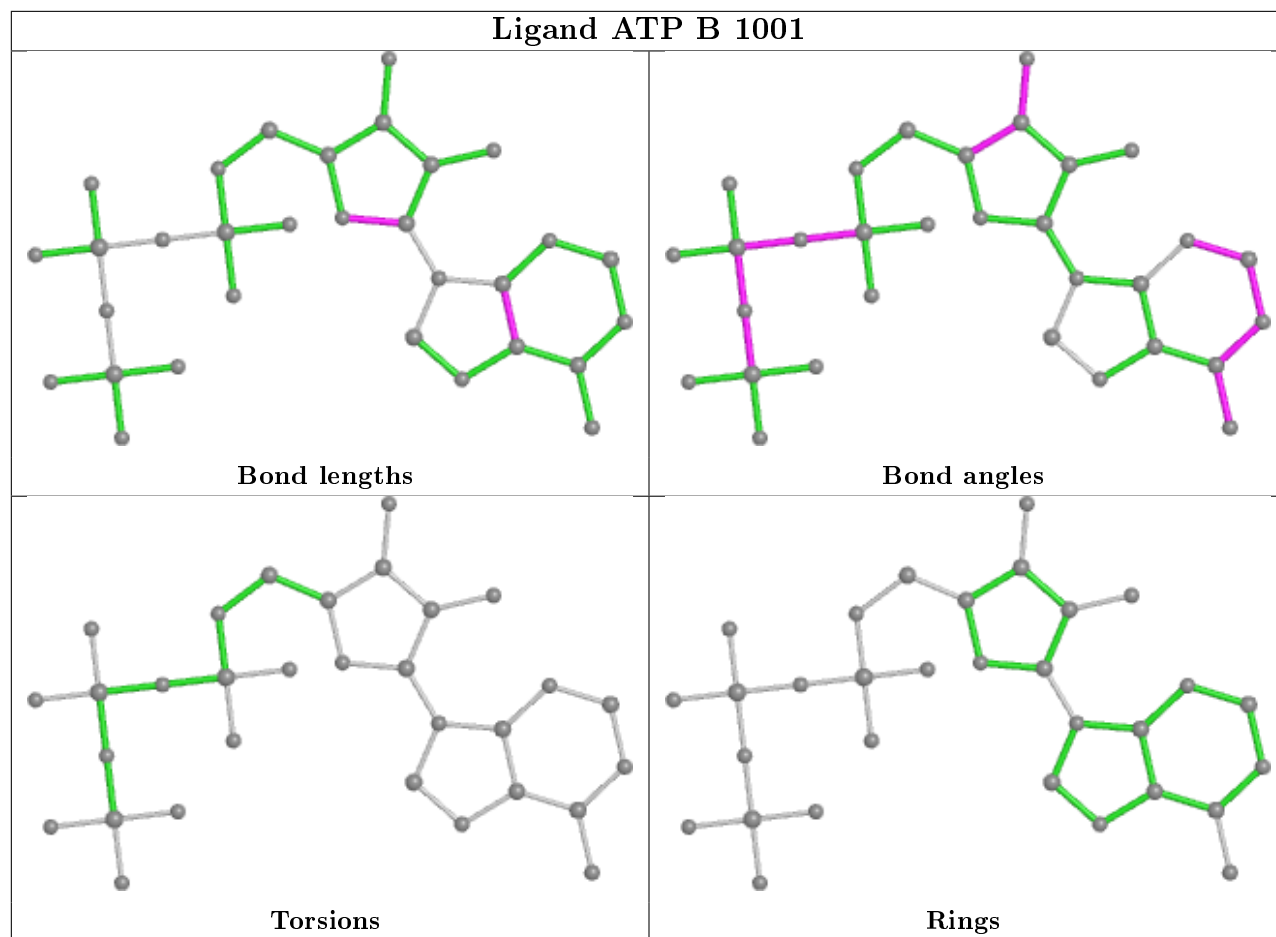
Mol	Chain	Res	Type	Atoms
2	C	1001	ATP	PB-O3B-PG-O2G
2	C	1001	ATP	PA-O3A-PB-O1B
2	C	1001	ATP	PA-O3A-PB-O2B
2	C	1001	ATP	PB-O3A-PA-O2A

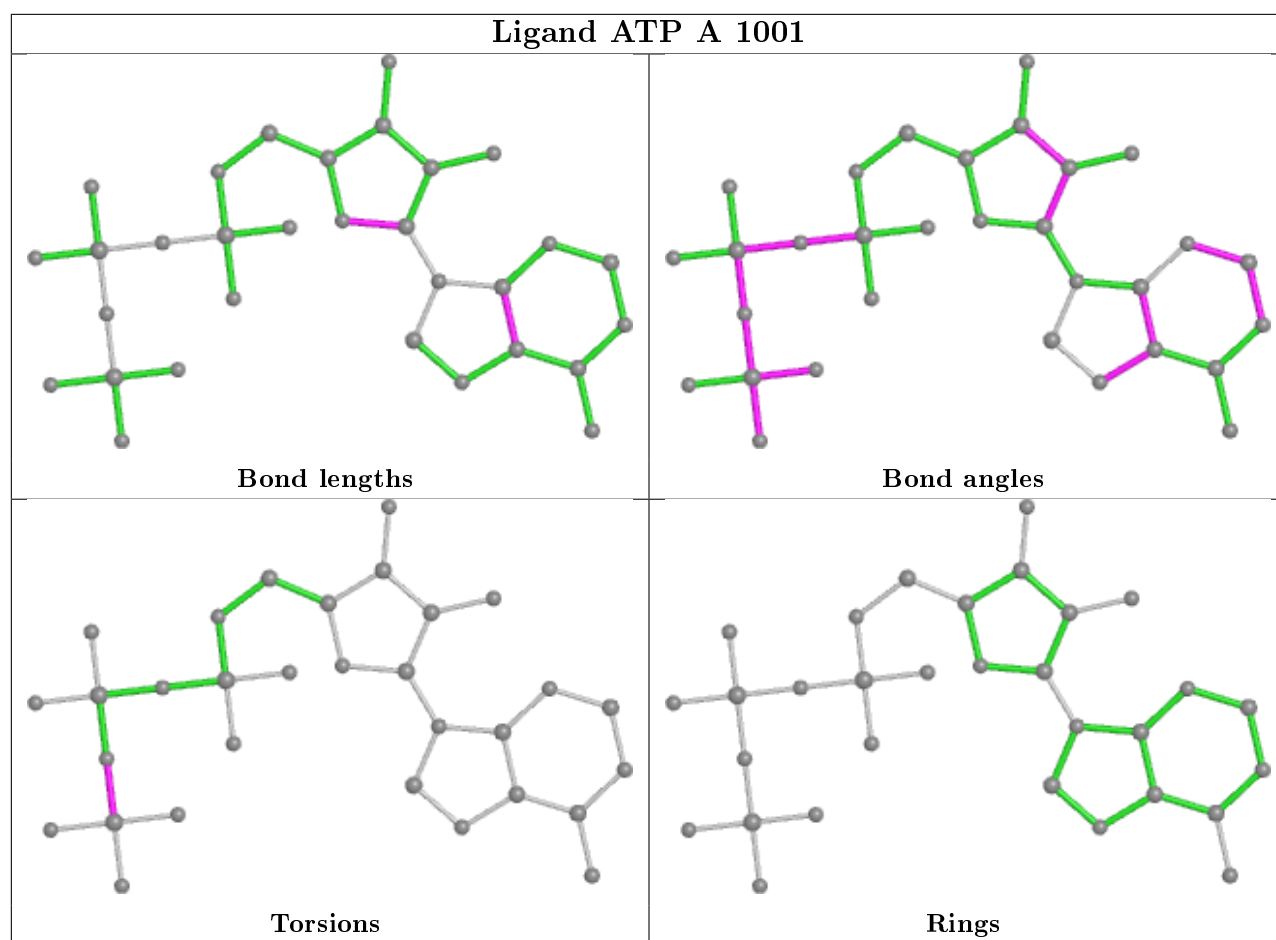
There are no ring outliers.

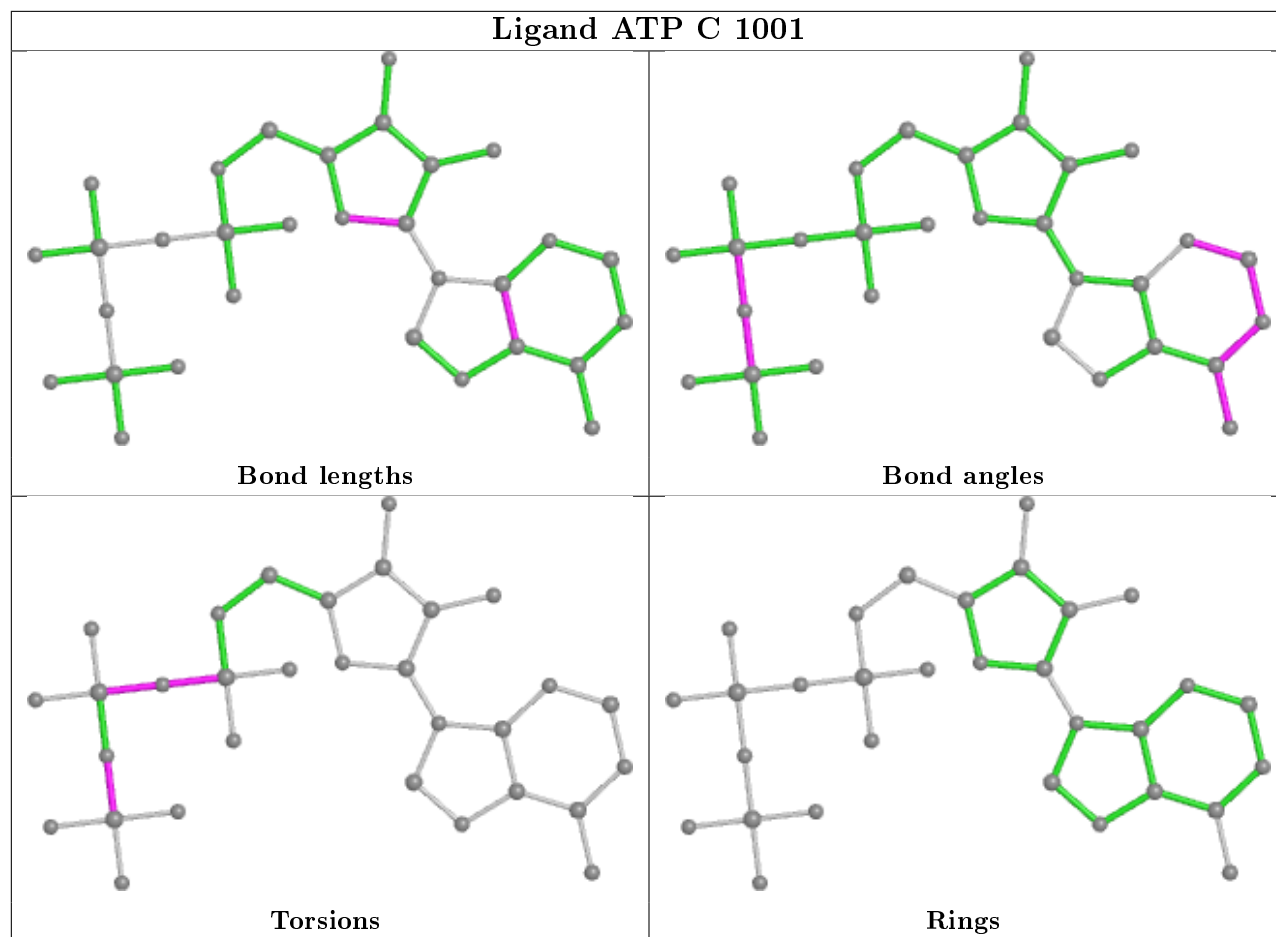
2 monomers are involved in 3 short contacts:

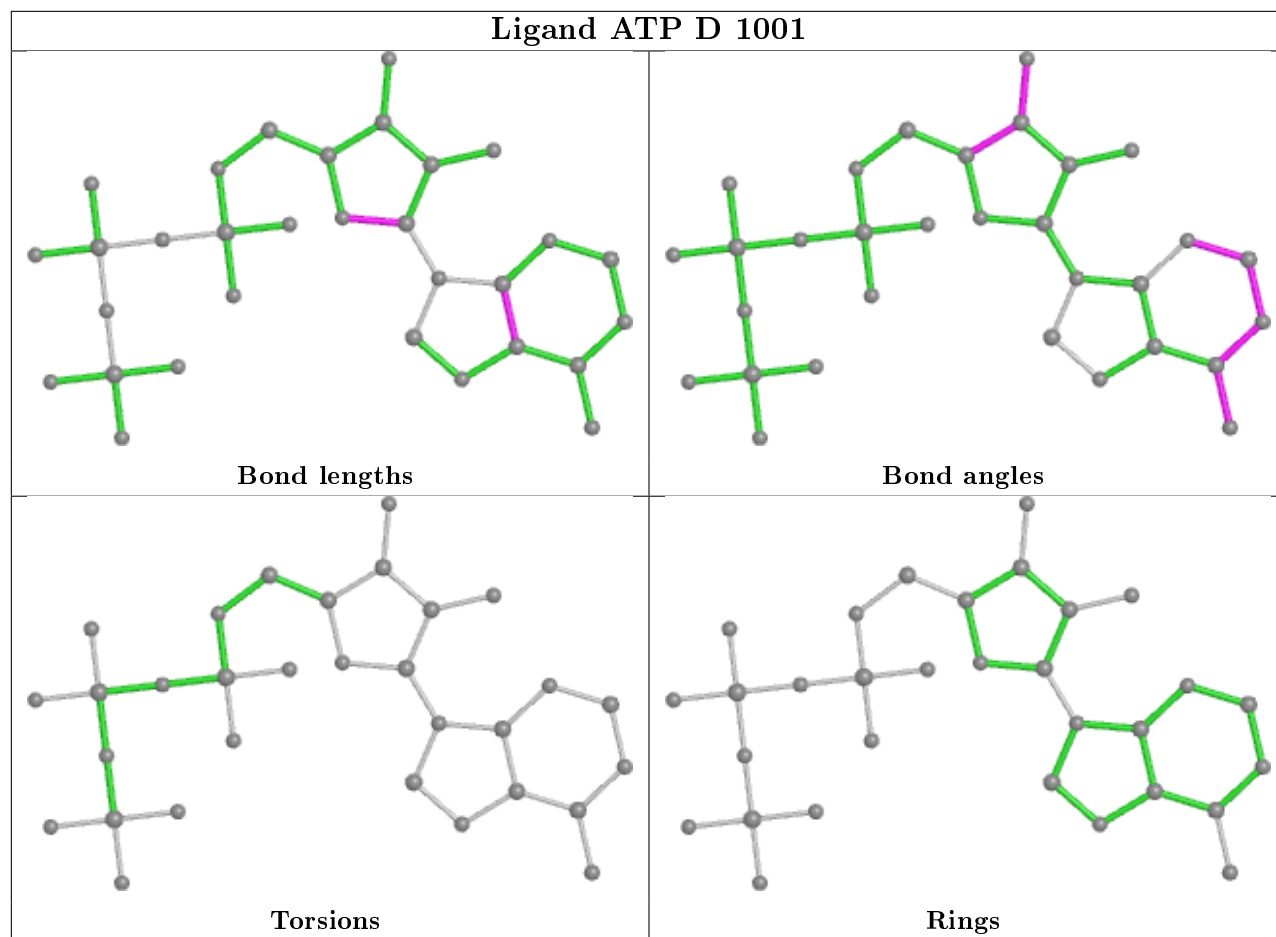
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	ATP	1	0
2	C	1001	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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%)	0.20	40 (8%) 10 8	12, 29, 77, 111	0
1	B	462/487 (94%)	0.19	36 (7%) 13 11	12, 28, 80, 111	0
1	C	461/487 (94%)	0.29	51 (11%) 5 4	12, 29, 80, 111	0
1	D	458/487 (94%)	0.19	43 (9%) 8 6	12, 28, 81, 113	0
All	All	1839/1948 (94%)	0.22	170 (9%) 9 7	12, 29, 80, 113	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	480	LEU	7.7
1	D	455	GLY	7.1
1	B	45	LYS	6.2
1	C	55	LYS	6.0
1	A	45	LYS	6.0
1	C	482	GLU	5.9
1	D	457	ASP	5.9
1	D	8	ARG	5.8
1	C	17	HIS	5.8
1	D	45	LYS	5.6
1	C	22	ASN	5.5
1	A	482	GLU	5.2
1	B	457	ASP	5.1
1	B	9	VAL	5.1
1	C	480	LEU	5.0
1	C	9	VAL	5.0
1	B	54	ASP	5.0
1	B	460	LEU	5.0
1	C	473	ILE	4.9
1	B	482	GLU	4.9
1	C	45	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	460	LEU	4.6
1	D	9	VAL	4.6
1	C	457	ASP	4.6
1	B	456	SER	4.6
1	C	8	ARG	4.6
1	B	455	GLY	4.5
1	A	366	SER	4.4
1	C	459	ARG	4.4
1	C	478	ASP	4.3
1	A	17	HIS	4.3
1	D	370	ASP	4.2
1	D	163	HIS	4.1
1	B	363	ALA	4.0
1	D	456	SER	4.0
1	B	8	ARG	3.9
1	D	340	ALA	3.9
1	D	476	ASN	3.9
1	B	462	ARG	3.9
1	D	36	GLY	3.9
1	C	483	GLU	3.9
1	C	366	SER	3.9
1	D	17	HIS	3.8
1	C	481	HIS	3.8
1	D	479	ARG	3.8
1	A	459	ARG	3.8
1	D	458	VAL	3.8
1	A	333	ARG	3.8
1	D	481	HIS	3.8
1	A	216	GLY	3.7
1	B	330	ASP	3.7
1	C	27	GLU	3.6
1	A	55	LYS	3.6
1	B	17	HIS	3.6
1	C	479	ARG	3.5
1	A	19	ALA	3.5
1	A	11	SER	3.5
1	C	463	LYS	3.5
1	B	333	ARG	3.5
1	A	43	SER	3.5
1	C	90	ARG	3.4
1	C	18	ARG	3.4
1	D	466	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	90	ARG	3.3
1	B	72	GLU	3.3
1	C	214	ARG	3.3
1	C	460	LEU	3.2
1	C	56	THR	3.2
1	C	333	ARG	3.2
1	C	57	ASP	3.2
1	B	458	VAL	3.1
1	B	71	SER	3.1
1	D	22	ASN	3.1
1	D	333	ARG	3.1
1	A	18	ARG	3.1
1	A	473	ILE	3.1
1	C	471	GLU	3.1
1	D	478	ASP	3.1
1	A	342	GLY	3.0
1	A	213	LYS	3.0
1	A	441	GLY	3.0
1	B	299	PRO	3.0
1	C	38	ASP	3.0
1	D	216	GLY	3.0
1	A	177	ASP	2.9
1	D	338	TYR	2.9
1	C	458	VAL	2.9
1	A	479	ARG	2.9
1	A	40	PRO	2.9
1	D	55	LYS	2.9
1	B	148	GLN	2.9
1	C	21	LEU	2.9
1	B	144	LYS	2.9
1	D	332	GLY	2.9
1	B	466	ILE	2.9
1	D	468	ARG	2.9
1	D	459	ARG	2.8
1	C	474	ASN	2.8
1	D	159	THR	2.8
1	C	23	SER	2.8
1	A	27	GLU	2.8
1	C	470	LEU	2.8
1	A	22	ASN	2.8
1	A	481	HIS	2.7
1	A	440	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	365	LYS	2.7
1	A	57	ASP	2.7
1	C	338	TYR	2.7
1	A	56	THR	2.7
1	D	454	LEU	2.6
1	B	55	LYS	2.6
1	B	479	ARG	2.6
1	A	10	THR	2.6
1	C	19	ALA	2.6
1	A	66	ARG	2.6
1	C	462	ARG	2.5
1	D	367	ARG	2.5
1	D	366	SER	2.5
1	C	466	ILE	2.5
1	A	21	LEU	2.5
1	A	144	LYS	2.5
1	A	35	PRO	2.5
1	A	91	ILE	2.5
1	D	18	ARG	2.4
1	C	72	GLU	2.4
1	D	369	PRO	2.4
1	A	159	THR	2.4
1	D	362	LYS	2.4
1	C	35	PRO	2.4
1	C	315	HIS	2.4
1	C	362	LYS	2.4
1	C	10	THR	2.4
1	D	462	ARG	2.4
1	C	340	ALA	2.3
1	D	470	LEU	2.3
1	B	18	ARG	2.3
1	C	467	ARG	2.3
1	D	330	ASP	2.3
1	C	468	ARG	2.3
1	A	37	ALA	2.3
1	C	37	ALA	2.3
1	B	366	SER	2.3
1	A	462	ARG	2.3
1	A	475	ARG	2.3
1	B	70	SER	2.2
1	C	369	PRO	2.2
1	B	459	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	440	ARG	2.2
1	B	40	PRO	2.2
1	B	159	THR	2.2
1	A	156	GLY	2.2
1	D	474	ASN	2.2
1	B	481	HIS	2.2
1	C	11	SER	2.2
1	B	10	THR	2.2
1	D	56	THR	2.1
1	B	66	ARG	2.1
1	D	482	GLU	2.1
1	B	332	GLY	2.1
1	C	67	ASP	2.1
1	C	342	GLY	2.1
1	B	483	GLU	2.1
1	C	370	ASP	2.1
1	D	339	ASP	2.1
1	B	216	GLY	2.1
1	D	67	ASP	2.0
1	D	148	GLN	2.0
1	A	468	ARG	2.0
1	B	338	TYR	2.0
1	A	94	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 carbohydrates in this entry.

6.4 Ligands [i](#)

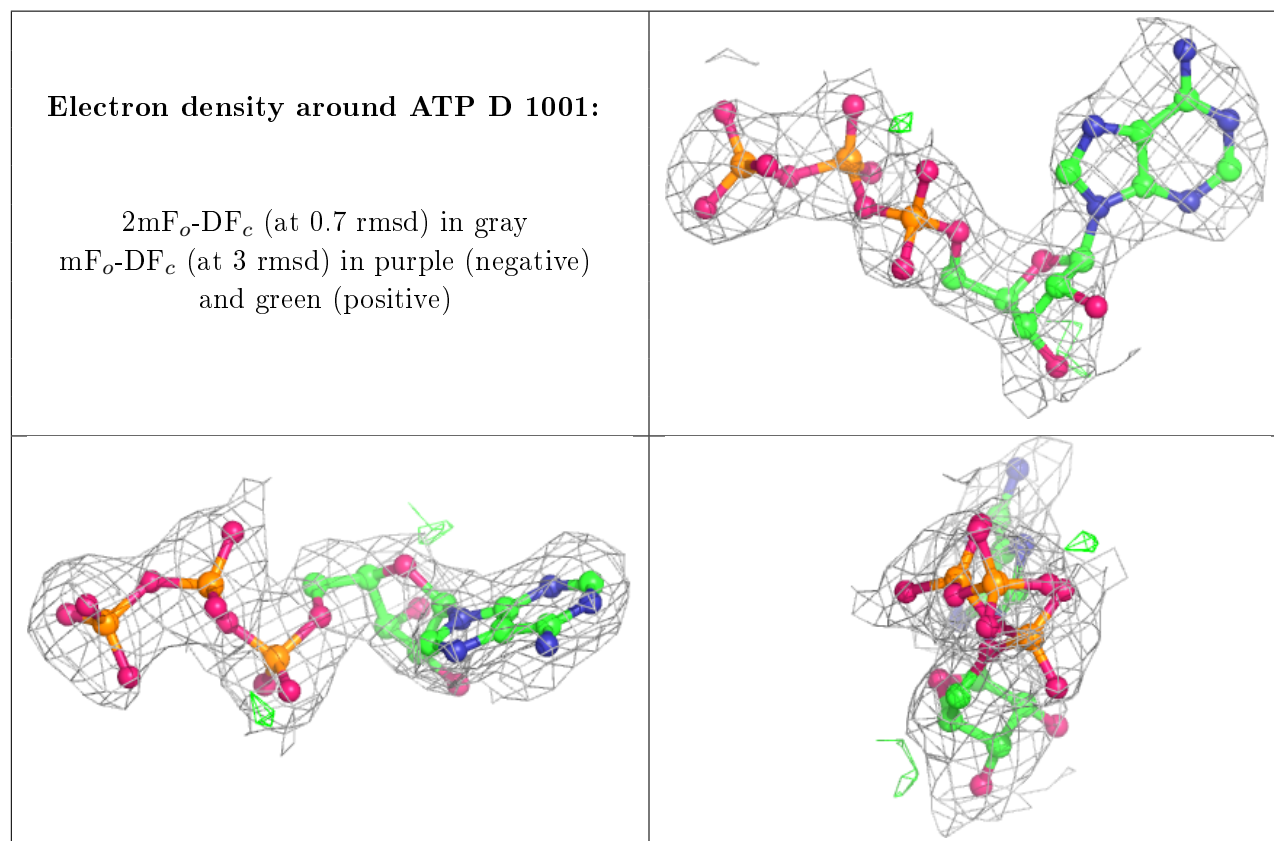
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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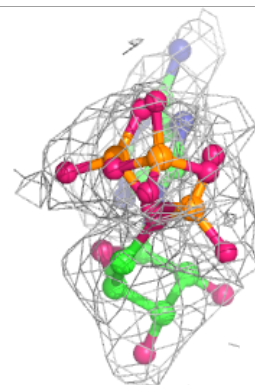
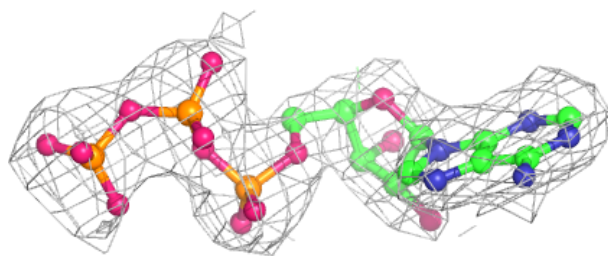
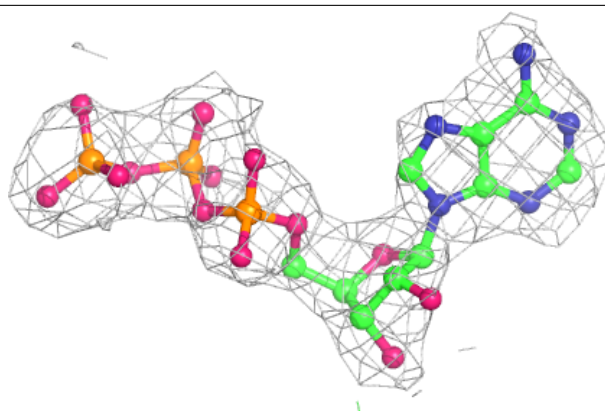
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	1002	1/1	0.76	0.29	49,49,49,49	0
3	MG	D	1002	1/1	0.86	0.24	45,45,45,45	0
5	NA	A	490	1/1	0.89	0.28	43,43,43,43	0
5	NA	B	488	1/1	0.90	0.34	45,45,45,45	0
5	NA	C	490	1/1	0.91	0.19	34,34,34,34	0
3	MG	B	1002	1/1	0.91	0.18	51,51,51,51	0
5	NA	A	489	1/1	0.91	0.16	30,30,30,30	0
6	SO4	C	489	5/5	0.92	0.14	33,41,48,91	0
2	ATP	D	1001	31/31	0.95	0.15	15,29,39,71	0
4	GOL	A	488	6/6	0.96	0.13	5,19,35,41	0
2	ATP	B	1001	31/31	0.96	0.13	14,25,38,66	0
2	ATP	C	1001	31/31	0.96	0.15	17,32,43,62	0
2	ATP	A	1001	31/31	0.97	0.14	19,40,62,73	0
4	GOL	C	488	6/6	0.98	0.11	9,14,28,33	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.

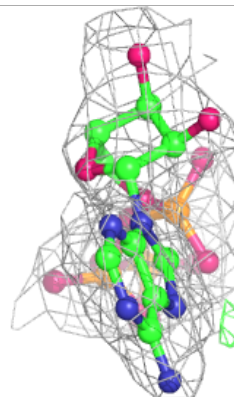
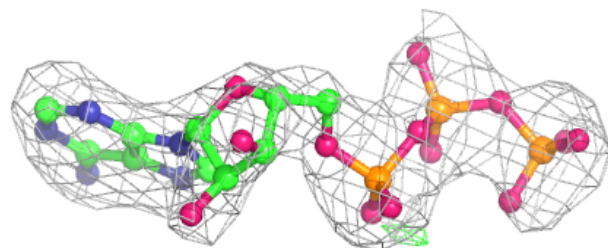
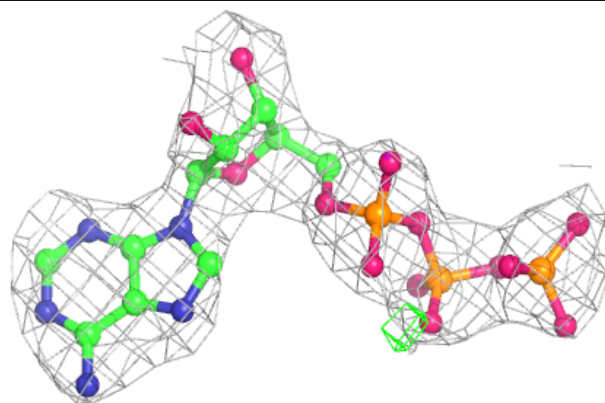


Electron density around ATP B 1001:

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

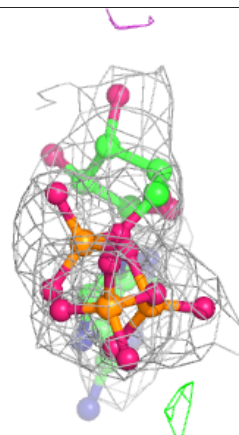
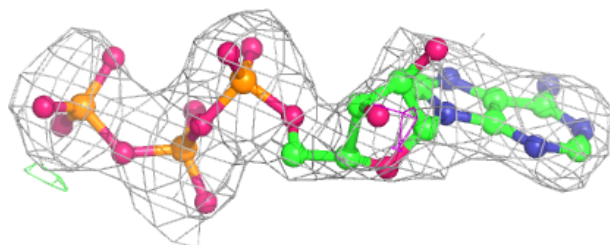
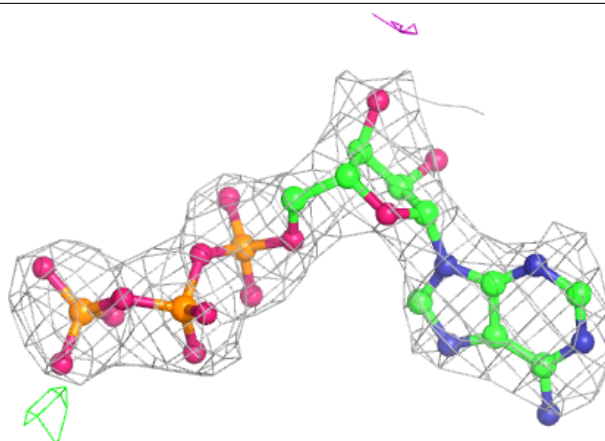
**Electron density around ATP C 1001:**

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



Electron density around ATP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.