



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:03 pm BST

PDB ID : 2YXU
Title : Human Pyridoxal Kinase
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Deposited on : 2007-04-27
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

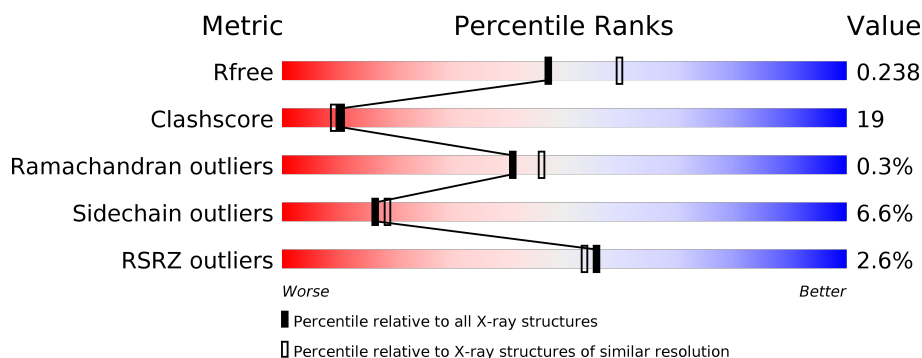
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	312	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>• •</div> </div> </div>
1	B	312	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5503 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 Pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2414	1522	422	455	15			
1	B	307	Total	C	N	O	S	0	0	0
			2428	1531	427	455	15			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

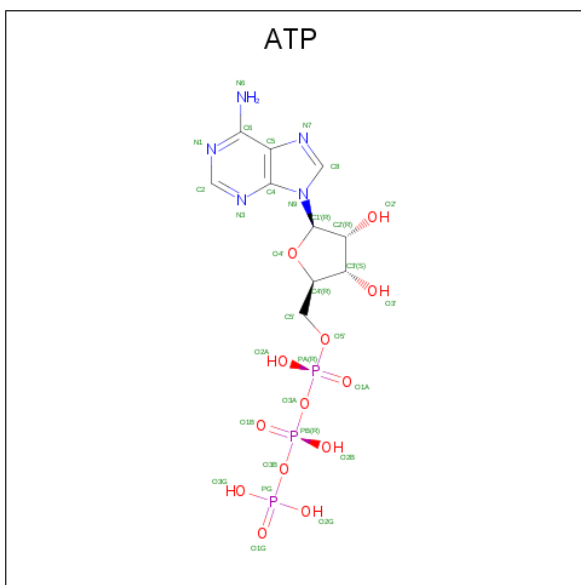
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



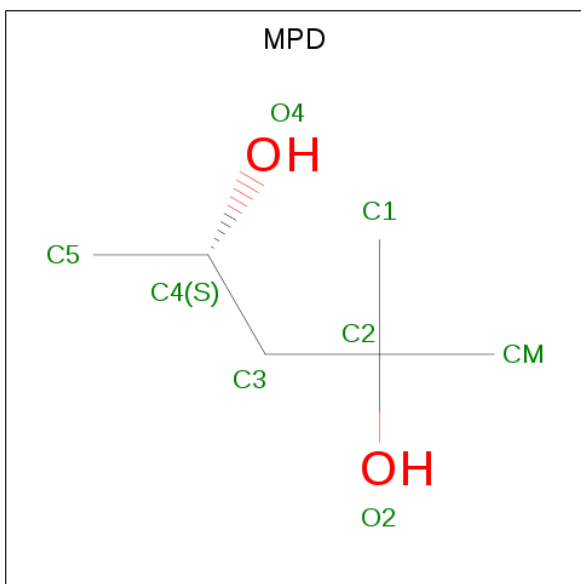
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

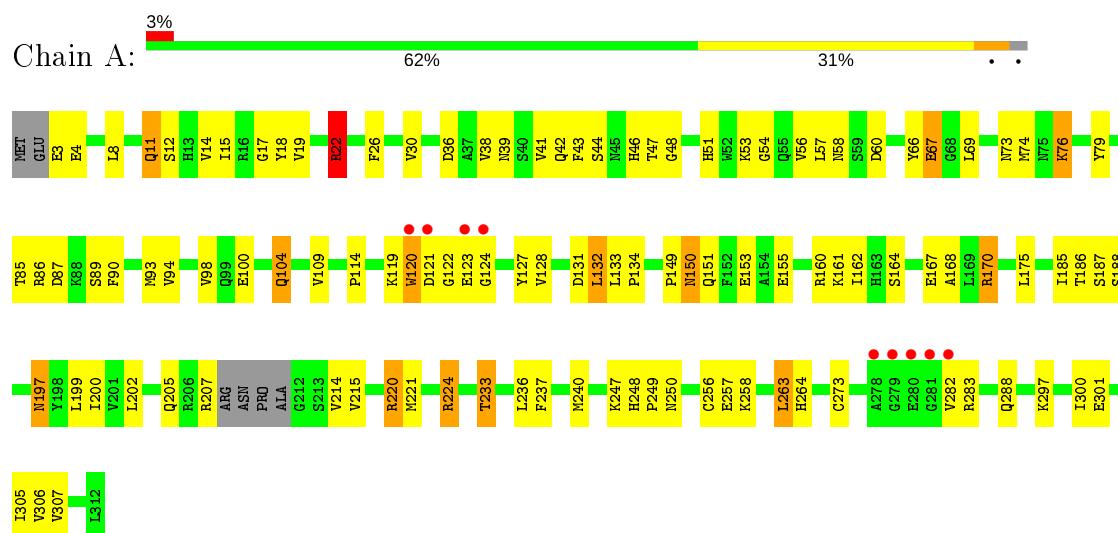
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	226	Total	O	0	0
			226	226		
7	B	248	Total	O	0	0
			248	248		

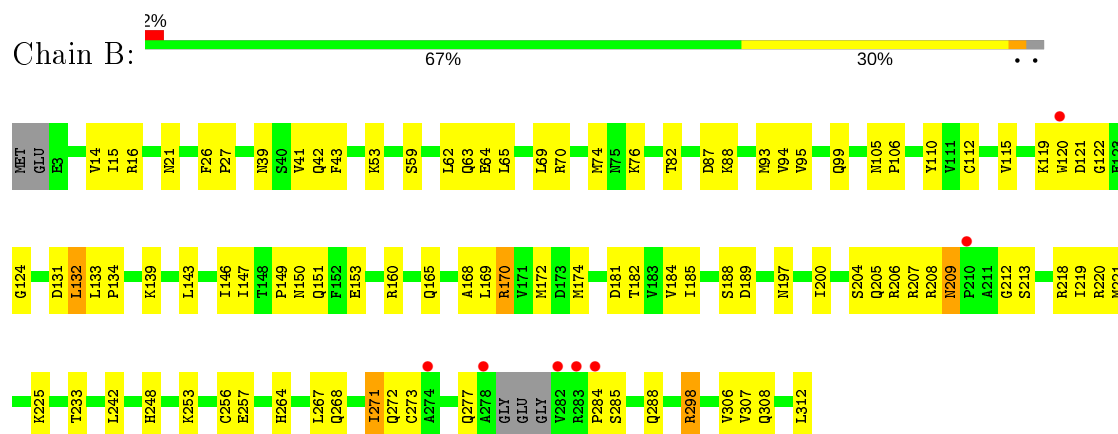
3 Residue-property plots [i](#)

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: Pyridoxal kinase



• Molecule 1: Pyridoxal kinase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.46Å 115.12Å 170.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 27.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.20) 97.6 (27.29-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.21 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.243 0.187 , 0.238	Depositor DCC
R_{free} test set	2238 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5503	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, PO4, ATP, MPD

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	0.72	0/2458	0.87	1/3330 (0.0%)
1	B	0.70	0/2473	0.86	1/3352 (0.0%)
All	All	0.71	0/4931	0.87	2/6682 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	22	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	B	16	ARG	NE-CZ-NH2	-5.38	117.61	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2414	0	2420	100	0
1	B	2428	0	2439	89	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
6	A	24	0	42	5	0
6	B	72	0	125	9	0
7	A	226	0	0	12	0
7	B	248	0	0	11	0
All	All	5503	0	5050	187	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 19.

All (187) 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:224:ARG:HD3	1:A:224:ARG:H	0.96	1.10
1:A:224:ARG:HD3	1:A:224:ARG:N	1.68	1.08
1:B:298:ARG:HH11	1:B:298:ARG:HG2	1.18	1.05
1:A:46:HIS:HD2	1:A:48:GLY:H	0.95	0.94
1:A:224:ARG:CD	1:A:224:ARG:H	1.68	0.94
6:B:1015:MPD:H4	7:B:2438:HOH:O	1.66	0.94
1:A:46:HIS:CD2	1:A:48:GLY:H	1.85	0.93
1:A:170:ARG:HH11	1:A:170:ARG:HG2	1.39	0.86
1:A:224:ARG:HH21	1:A:307:VAL:HG23	1.44	0.81
1:B:272:GLN:HE21	1:B:272:GLN:HA	1.44	0.81
1:A:46:HIS:HD2	1:A:48:GLY:N	1.77	0.80
1:A:128:VAL:CG2	1:A:132:LEU:HG	2.14	0.78
1:A:119:LYS:HA	1:A:124:GLY:HA2	1.63	0.78
1:A:150:ASN:HD22	1:A:150:ASN:C	1.88	0.77
1:A:197:ASN:HD22	1:A:197:ASN:H	1.31	0.77
1:B:205:GLN:HE21	1:B:207:ARG:HH11	1.30	0.77
1:A:150:ASN:ND2	1:A:153:GLU:H	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:NE2	1:B:220:ARG:HH11	1.85	0.74
1:A:205:GLN:HE21	1:A:207:ARG:HH11	1.34	0.74
1:A:39:ASN:H	1:B:42:GLN:HE22	1.36	0.73
1:A:120:TRP:O	7:A:1511:HOH:O	2.06	0.72
1:A:273:CYS:SG	7:B:2570:HOH:O	2.47	0.72
1:A:221:MET:CE	1:A:256:CYS:HB3	2.20	0.71
1:A:160:ARG:HG2	1:A:160:ARG:HH11	1.56	0.70
1:A:42:GLN:HE22	1:B:39:ASN:H	1.37	0.70
1:B:268:GLN:O	1:B:272:GLN:HG2	1.92	0.70
1:A:87:ASP:OD2	1:A:90:PHE:HB2	1.91	0.69
1:B:298:ARG:NH1	1:B:298:ARG:HG2	1.92	0.69
1:A:224:ARG:HH21	1:A:307:VAL:CG2	2.07	0.68
1:B:209:ASN:HD21	1:B:213:SER:H	1.39	0.68
1:A:150:ASN:HD21	1:A:153:GLU:H	1.41	0.67
1:B:160:ARG:HE	1:B:174:MET:HE1	1.61	0.66
1:B:248:HIS:HD1	6:B:1025:MPD:H4	1.60	0.66
1:B:119:LYS:HA	1:B:124:GLY:HA2	1.76	0.66
1:B:133:LEU:HB3	1:B:134:PRO:HD3	1.77	0.66
1:A:128:VAL:HG22	1:A:132:LEU:HG	1.77	0.66
1:B:253:LYS:NZ	1:B:308:GLN:HE21	1.94	0.65
1:B:218:ARG:HB3	1:B:312:LEU:HB2	1.79	0.65
1:A:15:ILE:HD11	1:B:65:LEU:HD22	1.78	0.65
1:A:15:ILE:HD12	1:A:44:SER:HA	1.80	0.64
1:A:94:VAL:O	1:A:98:VAL:HG23	1.98	0.64
1:A:221:MET:HE2	1:A:256:CYS:HB3	1.79	0.63
1:A:53:LYS:NZ	7:A:1586:HOH:O	2.31	0.63
1:B:43:PHE:CE2	6:B:1031:MPD:H53	2.33	0.63
1:A:15:ILE:CD1	1:B:65:LEU:HD22	2.29	0.62
1:A:133:LEU:HB3	1:A:134:PRO:HD3	1.82	0.62
1:B:209:ASN:ND2	1:B:213:SER:H	1.98	0.61
1:B:272:GLN:NE2	1:B:272:GLN:HA	2.12	0.61
1:A:297:LYS:O	1:A:301:GLU:HG3	2.00	0.61
1:A:160:ARG:HG2	1:A:160:ARG:NH1	2.13	0.61
1:B:82:THR:HG21	1:B:94:VAL:HG11	1.82	0.61
1:A:11:GLN:NE2	7:A:1520:HOH:O	2.31	0.61
6:B:1025:MPD:H51	7:B:2546:HOH:O	2.00	0.60
1:B:151:GLN:HE22	1:B:189:ASP:H	1.50	0.60
1:B:209:ASN:HD22	1:B:212:GLY:H	1.49	0.59
1:B:151:GLN:NE2	1:B:189:ASP:H	1.99	0.59
1:A:282:VAL:HG11	7:A:1719:HOH:O	2.03	0.59
1:A:162:ILE:HD13	1:A:168:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLN:HE21	1:B:207:ARG:NH1	2.01	0.59
1:B:307:VAL:HG13	1:B:307:VAL:O	2.02	0.59
1:B:150:ASN:OD1	1:B:153:GLU:HG3	2.04	0.58
1:A:221:MET:HE1	1:A:256:CYS:HB3	1.85	0.57
1:A:93:MET:CE	6:A:1011:MPD:H12	2.35	0.57
1:A:240:MET:HE1	1:A:300:ILE:HG23	1.85	0.56
1:A:3:GLU:N	7:A:1661:HOH:O	2.37	0.56
1:B:209:ASN:HD22	1:B:209:ASN:C	2.09	0.56
7:A:1584:HOH:O	1:B:53:LYS:HE3	2.06	0.56
1:A:128:VAL:HG21	1:A:132:LEU:HG	1.88	0.56
1:A:56:VAL:HG12	1:A:57:LEU:N	2.21	0.56
1:B:165:GLN:HE21	1:B:220:ARG:HH11	1.51	0.56
1:B:62:LEU:HD23	1:B:93:MET:HG3	1.87	0.56
1:A:197:ASN:HD22	1:A:197:ASN:N	2.03	0.55
1:B:253:LYS:HZ1	1:B:308:GLN:HE21	1.54	0.55
1:A:26:PHE:O	1:A:30:VAL:HG23	2.07	0.55
1:B:99:GLN:HG2	1:B:143:LEU:HD11	1.89	0.55
1:A:85:THR:HG22	1:A:87:ASP:H	1.73	0.54
1:A:86:ARG:NH1	7:A:1569:HOH:O	2.40	0.54
1:B:43:PHE:HE2	6:B:1031:MPD:H53	1.73	0.54
1:A:155:GLU:HG2	1:A:162:ILE:HG13	1.88	0.53
1:A:257:GLU:HG2	1:A:307:VAL:O	2.08	0.53
1:B:115:VAL:HA	1:B:153:GLU:OE2	2.09	0.53
1:A:149:PRO:O	1:A:185:ILE:HA	2.09	0.52
1:B:253:LYS:O	1:B:257:GLU:HG3	2.09	0.52
1:B:76:LYS:HA	7:B:2482:HOH:O	2.09	0.52
1:A:150:ASN:ND2	1:A:150:ASN:C	2.61	0.52
1:B:146:ILE:HG12	1:B:182:THR:HB	1.92	0.52
1:A:43:PHE:CD1	1:A:54:GLY:HA3	2.45	0.51
1:B:181:ASP:OD2	6:B:1021:MPD:HM3	2.10	0.51
1:B:298:ARG:NH1	1:B:298:ARG:CG	2.70	0.51
1:A:214:VAL:HG22	1:A:214:VAL:O	2.11	0.50
1:A:207:ARG:HG3	1:A:215:VAL:HG22	1.94	0.50
1:B:169:LEU:HD23	1:B:172:MET:CE	2.41	0.50
1:B:70:ARG:HD2	7:B:2484:HOH:O	2.11	0.50
6:B:1015:MPD:H12	7:B:2438:HOH:O	2.11	0.49
1:A:51:HIS:ND1	7:A:1516:HOH:O	2.35	0.49
1:A:123:GLU:O	1:A:123:GLU:HG3	2.11	0.49
1:B:242:LEU:HD23	1:B:242:LEU:C	2.33	0.49
1:A:186:THR:O	1:A:187:SER:HB3	2.13	0.49
1:A:19:VAL:O	1:A:22:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:HG23	6:A:1013:MPD:H4	1.95	0.49
1:A:69:LEU:HD23	1:A:74:MET:CE	2.43	0.48
1:A:236:LEU:HD23	1:A:263:LEU:HD13	1.94	0.48
1:A:12:SER:HB2	1:A:41:VAL:HG22	1.96	0.48
1:B:221:MET:CE	1:B:256:CYS:HB3	2.44	0.48
1:A:100:GLU:HG3	6:A:1011:MPD:HM2	1.96	0.47
1:A:69:LEU:HD23	1:A:74:MET:HE3	1.95	0.47
1:B:188:SER:OG	1:B:200:ILE:HB	2.13	0.47
1:A:224:ARG:NH2	1:A:306:VAL:HG23	2.29	0.47
1:A:247:LYS:C	1:A:249:PRO:HD3	2.35	0.47
1:A:120:TRP:C	1:A:120:TRP:HE3	2.18	0.47
1:B:165:GLN:NE2	1:B:220:ARG:NH1	2.59	0.47
1:A:4:GLU:HA	7:A:1605:HOH:O	2.14	0.46
1:B:110:TYR:CZ	1:B:112:CYS:HB2	2.50	0.46
1:B:160:ARG:HE	1:B:174:MET:CE	2.26	0.46
1:A:104:GLN:HE21	1:A:104:GLN:HA	1.80	0.46
1:A:12:SER:CB	1:A:41:VAL:HG22	2.45	0.46
1:A:186:THR:HG22	1:A:237:PHE:CE2	2.50	0.46
1:B:285:SER:HB3	7:B:2565:HOH:O	2.15	0.46
1:B:264:HIS:CD2	1:B:306:VAL:HG21	2.50	0.46
1:A:224:ARG:N	1:A:224:ARG:CD	2.43	0.46
1:B:272:GLN:CA	1:B:272:GLN:HE21	2.15	0.46
1:A:79:TYR:CD2	1:A:109:VAL:HB	2.50	0.46
1:A:17:GLY:O	1:A:22:ARG:HD2	2.16	0.45
1:B:209:ASN:ND2	1:B:212:GLY:H	2.14	0.45
1:A:214:VAL:HG13	1:A:214:VAL:O	2.16	0.45
1:B:284:PRO:HA	1:B:288:GLN:OE1	2.16	0.45
1:A:164:SER:OG	1:A:167:GLU:HG3	2.17	0.45
1:B:253:LYS:HZ1	1:B:308:GLN:NE2	2.13	0.45
1:A:86:ARG:HH21	1:A:86:ARG:HG2	1.81	0.45
1:B:298:ARG:NH1	7:B:2427:HOH:O	2.49	0.45
1:B:271:ILE:HD13	1:B:271:ILE:HA	1.65	0.44
1:B:95:VAL:O	1:B:99:GLN:HG3	2.17	0.44
1:B:208:ARG:HA	1:B:213:SER:O	2.17	0.44
1:A:233:THR:HG22	1:A:263:LEU:CD1	2.46	0.44
1:B:174:MET:HB2	1:B:174:MET:HE2	1.47	0.44
1:B:119:LYS:HE2	1:B:119:LYS:HB3	1.61	0.44
1:A:18:TYR:HA	1:A:22:ARG:HB3	1.99	0.44
1:A:14:VAL:HA	1:A:43:PHE:O	2.18	0.44
1:B:88:LYS:N	1:B:132:LEU:HD11	2.33	0.44
1:B:63:GLN:HB2	1:B:93:MET:CE	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HD23	1:B:74:MET:CE	2.48	0.43
1:A:58:ASN:OD1	1:A:60:ASP:HB2	2.18	0.43
1:A:76:LYS:NZ	1:A:104:GLN:OE1	2.50	0.43
1:B:160:ARG:NE	1:B:170:ARG:HD3	2.34	0.43
1:A:46:HIS:HB2	6:A:1013:MPD:C1	2.47	0.43
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.88	0.43
1:A:202:LEU:HD23	1:A:220:ARG:HB2	2.00	0.43
1:A:17:GLY:O	1:A:22:ARG:CD	2.67	0.43
1:B:209:ASN:O	1:B:212:GLY:N	2.47	0.43
1:A:248:HIS:N	1:A:249:PRO:HD3	2.33	0.42
1:B:149:PRO:O	1:B:185:ILE:HA	2.19	0.42
1:B:139:LYS:HD3	1:B:139:LYS:HA	1.83	0.42
1:B:105:ASN:HA	1:B:106:PRO:HD3	1.78	0.42
1:B:169:LEU:HD23	1:B:172:MET:HE1	2.00	0.42
1:B:165:GLN:O	1:B:168:ALA:HB3	2.19	0.42
1:A:250:ASN:N	7:A:1641:HOH:O	2.40	0.42
1:B:112:CYS:O	1:B:147:ILE:HA	2.19	0.42
1:A:151:GLN:OE1	1:A:188:SER:HB2	2.19	0.42
1:A:56:VAL:CG1	1:A:57:LEU:N	2.83	0.42
1:A:67:GLU:HG3	7:A:1727:HOH:O	2.19	0.42
1:A:8:LEU:HD11	1:A:38:VAL:CG2	2.49	0.42
1:B:131:ASP:OD2	7:B:2502:HOH:O	2.22	0.42
1:B:14:VAL:HA	1:B:43:PHE:O	2.20	0.42
1:B:70:ARG:CD	7:B:2484:HOH:O	2.67	0.41
1:B:149:PRO:HD2	1:B:184:VAL:O	2.20	0.41
1:B:209:ASN:ND2	1:B:212:GLY:N	2.68	0.41
1:B:206:ARG:HD3	1:B:206:ARG:HH11	1.61	0.41
1:A:46:HIS:HB2	6:A:1013:MPD:H13	2.02	0.41
1:B:219:ILE:C	1:B:219:ILE:HD12	2.41	0.41
1:B:233:THR:HG21	1:B:267:LEU:HD21	2.02	0.41
1:A:161:LYS:NZ	7:A:1593:HOH:O	2.31	0.41
1:A:38:VAL:HG22	1:B:15:ILE:HD12	2.03	0.41
1:B:69:LEU:HA	1:B:74:MET:HE3	2.03	0.41
1:A:258:LYS:HG2	1:A:305:ILE:HD11	2.02	0.41
1:B:26:PHE:N	1:B:27:PRO:CD	2.83	0.41
1:A:36:ASP:HB3	1:B:15:ILE:HG22	2.02	0.40
1:A:8:LEU:HD11	1:A:38:VAL:HG23	2.03	0.40
1:B:197:ASN:HA	1:B:225:LYS:HE3	2.02	0.40
1:B:221:MET:HE1	1:B:256:CYS:HB3	2.03	0.40
1:A:200:ILE:HD13	1:A:220:ARG:NH1	2.37	0.40
6:B:1025:MPD:C5	7:B:2546:HOH:O	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLN:CA	1:B:272:GLN:NE2	2.77	0.40
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.87	0.40
1:B:273:CYS:O	1:B:277:GLN:HG3	2.21	0.40
1:A:297:LYS:O	1:A:301:GLU:CG	2.66	0.40
1:A:264:HIS:CD2	1:A:306:VAL:HG21	2.56	0.40
1:B:248:HIS:HD1	6:B:1025:MPD:C4	2.31	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:170:ARG:NH1	1:B:170:ARG:NH1[3_555]	1.94	0.26

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	302/312 (97%)	286 (95%)	15 (5%)	1 (0%)	41	46
1	B	303/312 (97%)	289 (95%)	13 (4%)	1 (0%)	41	46
All	All	605/624 (97%)	575 (95%)	28 (5%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLY
1	B	122	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	270/275 (98%)	247 (92%)	23 (8%)	10	10
1	B	272/275 (99%)	259 (95%)	13 (5%)	25	32
All	All	542/550 (98%)	506 (93%)	36 (7%)	16	19

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	22	ARG
1	A	67	GLU
1	A	73	ASN
1	A	76	LYS
1	A	89	SER
1	A	104	GLN
1	A	114	PRO
1	A	120	TRP
1	A	121	ASP
1	A	127	TYR
1	A	131	ASP
1	A	132	LEU
1	A	150	ASN
1	A	170	ARG
1	A	197	ASN
1	A	199	LEU
1	A	220	ARG
1	A	224	ARG
1	A	233	THR
1	A	263	LEU
1	A	283	ARG
1	A	288	GLN
1	B	21	ASN
1	B	41	VAL
1	B	59	SER
1	B	64	GLU
1	B	87	ASP
1	B	120	TRP
1	B	121	ASP
1	B	132	LEU

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Mol	Chain	Res	Type
1	B	170	ARG
1	B	204	SER
1	B	209	ASN
1	B	271	ILE
1	B	298	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	42	GLN
1	A	46	HIS
1	A	99	GLN
1	A	103	GLN
1	A	150	ASN
1	A	197	ASN
1	A	205	GLN
1	A	264	HIS
1	B	21	ASN
1	B	42	GLN
1	B	45	ASN
1	B	73	ASN
1	B	151	GLN
1	B	163	HIS
1	B	165	GLN
1	B	205	GLN
1	B	209	ASN
1	B	250	ASN
1	B	264	HIS
1	B	272	GLN
1	B	308	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	PO4	B	1527	-	4,4,4	1.60	0	6,6,6	0.44	0
6	MPD	B	1015	-	7,7,7	0.77	0	9,10,10	0.40	0
6	MPD	A	1011	-	7,7,7	0.62	0	9,10,10	0.31	0
6	MPD	B	1039	-	7,7,7	0.85	0	9,10,10	0.44	0
6	MPD	B	1021	-	7,7,7	0.91	0	9,10,10	0.46	0
6	MPD	A	1013	-	7,7,7	0.58	0	9,10,10	0.29	0
4	PO4	B	1517	-	4,4,4	1.36	0	6,6,6	0.43	0
6	MPD	B	1025	-	7,7,7	0.88	0	9,10,10	0.46	0
6	MPD	B	1019	-	7,7,7	0.73	0	9,10,10	0.38	0
6	MPD	B	1031	-	7,7,7	0.43	0	9,10,10	0.44	0
6	MPD	B	1029	-	7,7,7	0.83	0	9,10,10	0.36	0
5	ATP	B	2410	-	26,33,33	2.06	10 (38%)	31,52,52	1.72	7 (22%)
6	MPD	B	1023	-	7,7,7	0.81	0	9,10,10	0.60	0
4	PO4	A	1505	-	4,4,4	1.52	0	6,6,6	0.44	0
4	PO4	B	1503	-	4,4,4	1.56	0	6,6,6	0.41	0
6	MPD	B	1041	-	7,7,7	0.89	1 (14%)	9,10,10	0.47	0
5	ATP	A	1410	-	26,33,33	2.00	9 (34%)	31,52,52	1.66	10 (32%)
4	PO4	A	1501	-	4,4,4	1.60	0	6,6,6	0.41	0
6	MPD	A	1037	-	7,7,7	0.89	0	9,10,10	0.47	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
6	MPD	A	1037	-	-	0/5/5/5	-
6	MPD	B	1039	-	-	0/5/5/5	-
6	MPD	B	1021	-	-	3/5/5/5	-
6	MPD	A	1011	-	-	4/5/5/5	-
6	MPD	B	1025	-	-	2/5/5/5	-
6	MPD	B	1019	-	-	3/5/5/5	-
6	MPD	B	1031	-	-	2/5/5/5	-
6	MPD	B	1029	-	-	3/5/5/5	-
6	MPD	B	1023	-	-	1/5/5/5	-
6	MPD	A	1013	-	-	1/5/5/5	-
6	MPD	B	1015	-	-	2/5/5/5	-
6	MPD	B	1041	-	-	0/5/5/5	-
5	ATP	A	1410	-	-	5/18/38/38	0/3/3/3
5	ATP	B	2410	-	-	6/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1410	ATP	O4'-C1'	4.99	1.48	1.41
5	B	2410	ATP	O4'-C1'	4.24	1.47	1.41
5	B	2410	ATP	C2'-C3'	-3.97	1.42	1.53
5	B	2410	ATP	PG-O1G	3.70	1.62	1.50
5	A	1410	ATP	C3'-C4'	3.41	1.61	1.53
5	B	2410	ATP	C3'-C4'	3.37	1.61	1.53
5	A	1410	ATP	C8-N7	-3.35	1.28	1.34
5	A	1410	ATP	C2'-C1'	3.17	1.58	1.53
5	B	2410	ATP	PB-O2B	-2.89	1.41	1.55
5	A	1410	ATP	O4'-C4'	-2.89	1.38	1.45
5	A	1410	ATP	PG-O1G	2.87	1.59	1.50
5	B	2410	ATP	C2-N3	2.62	1.36	1.32
5	A	1410	ATP	C2'-C3'	-2.47	1.46	1.53
5	A	1410	ATP	PB-O2B	-2.46	1.43	1.55
5	B	2410	ATP	C8-N7	-2.46	1.30	1.34
5	B	2410	ATP	C4-N3	2.40	1.39	1.35
5	B	2410	ATP	PA-O2A	-2.33	1.44	1.55
5	B	2410	ATP	C2'-C1'	2.16	1.57	1.53
5	A	1410	ATP	PA-O2A	-2.09	1.45	1.55
6	B	1041	MPD	C3-C2	2.00	1.59	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2410	ATP	PB-O3B-PG	3.64	145.32	132.83
5	A	1410	ATP	PB-O3B-PG	3.41	144.52	132.83
5	B	2410	ATP	O4'-C4'-C5'	3.25	120.05	109.37
5	B	2410	ATP	C2'-C3'-C4'	-3.04	96.74	102.64
5	A	1410	ATP	O3'-C3'-C2'	2.76	120.75	111.82
5	B	2410	ATP	N3-C2-N1	-2.73	124.41	128.68
5	B	2410	ATP	C4-C5-N7	2.67	112.18	109.40
5	B	2410	ATP	O3'-C3'-C2'	2.62	120.30	111.82
5	A	1410	ATP	O4'-C4'-C5'	2.58	117.86	109.37
5	A	1410	ATP	N3-C2-N1	-2.47	124.81	128.68
5	A	1410	ATP	C4-C5-N7	2.38	111.88	109.40
5	A	1410	ATP	O2B-PB-O1B	2.35	123.87	112.24
5	A	1410	ATP	O5'-C5'-C4'	-2.28	101.14	108.99
5	A	1410	ATP	PA-O5'-C5'	2.21	134.62	121.68
5	A	1410	ATP	C2'-C3'-C4'	-2.13	98.50	102.64
5	A	1410	ATP	O5'-PA-O1A	2.12	117.34	109.07
5	B	2410	ATP	O2G-PG-O3B	2.10	111.67	104.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1031	MPD	C2-C3-C4-O4
6	A	1011	MPD	C2-C3-C4-O4
5	A	1410	ATP	PB-O3B-PG-O3G
5	B	2410	ATP	PB-O3B-PG-O2G
6	B	1029	MPD	O2-C2-C3-C4
6	B	1019	MPD	O2-C2-C3-C4
6	B	1023	MPD	O2-C2-C3-C4
5	A	1410	ATP	PG-O3B-PB-O1B
5	B	2410	ATP	PG-O3B-PB-O1B
6	B	1031	MPD	C2-C3-C4-C5
6	B	1015	MPD	C2-C3-C4-C5
6	B	1015	MPD	C2-C3-C4-O4
6	A	1011	MPD	C1-C2-C3-C4
6	B	1019	MPD	C1-C2-C3-C4
6	B	1019	MPD	CM-C2-C3-C4
6	B	1021	MPD	C1-C2-C3-C4
6	B	1021	MPD	CM-C2-C3-C4
5	A	1410	ATP	PB-O3A-PA-O1A
6	A	1011	MPD	O2-C2-C3-C4
6	B	1021	MPD	O2-C2-C3-C4
5	A	1410	ATP	PB-O3B-PG-O1G

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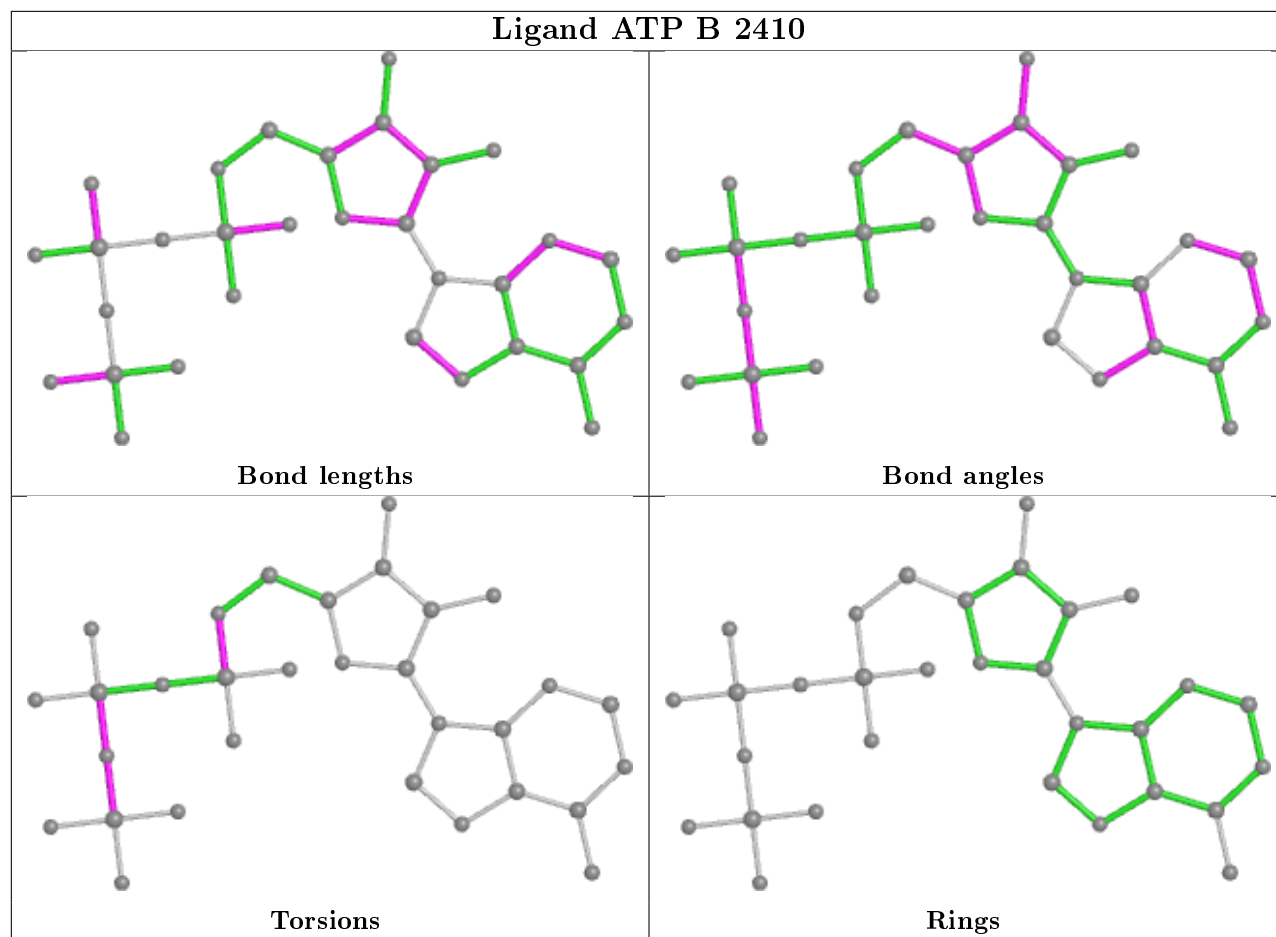
Mol	Chain	Res	Type	Atoms
5	B	2410	ATP	PB-O3B-PG-O1G
5	B	2410	ATP	PB-O3B-PG-O3G
5	B	2410	ATP	PG-O3B-PB-O2B
6	B	1025	MPD	C2-C3-C4-C5
6	B	1029	MPD	C2-C3-C4-C5
6	A	1011	MPD	C2-C3-C4-C5
5	A	1410	ATP	C5'-O5'-PA-O1A
5	B	2410	ATP	C5'-O5'-PA-O1A
6	B	1025	MPD	C2-C3-C4-O4
6	B	1029	MPD	C2-C3-C4-O4
6	A	1013	MPD	C2-C3-C4-O4

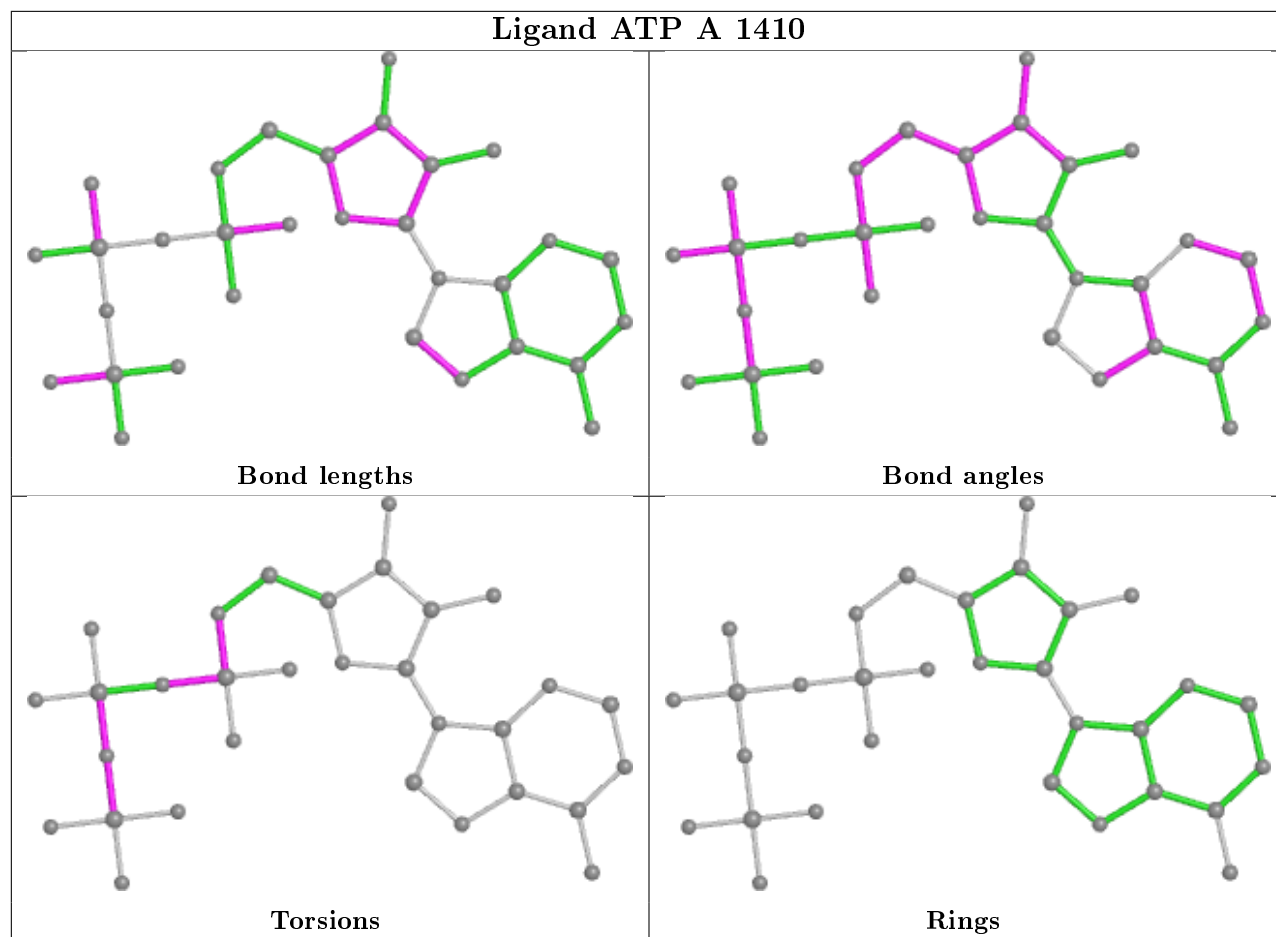
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1015	MPD	2	0
6	A	1011	MPD	2	0
6	B	1021	MPD	1	0
6	A	1013	MPD	3	0
6	B	1025	MPD	4	0
6	B	1031	MPD	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	306/312 (98%)	-0.47	9 (2%) 51 49	19, 35, 68, 98	0
1	B	307/312 (98%)	-0.56	7 (2%) 60 58	18, 32, 65, 102	0
All	All	613/624 (98%)	-0.52	16 (2%) 56 53	18, 34, 68, 102	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	TRP	6.1
1	B	282	VAL	5.1
1	B	274	ALA	4.8
1	A	120	TRP	4.5
1	A	282	VAL	4.3
1	A	280	GLU	4.1
1	A	279	GLY	3.5
1	B	284	PRO	3.3
1	B	278	ALA	3.2
1	B	283	ARG	3.1
1	A	281	GLY	2.9
1	A	121	ASP	2.3
1	A	123	GLU	2.3
1	B	210	PRO	2.2
1	A	278	ALA	2.1
1	A	124	GLY	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

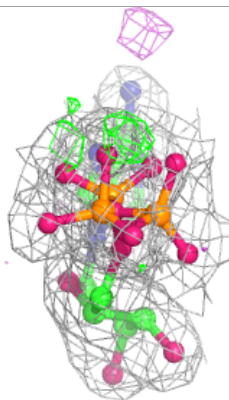
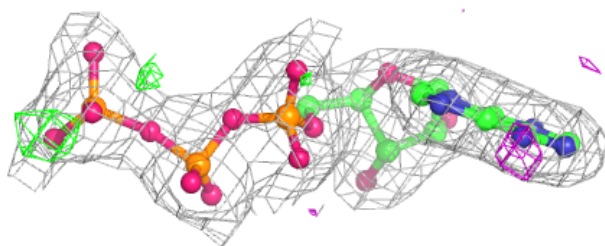
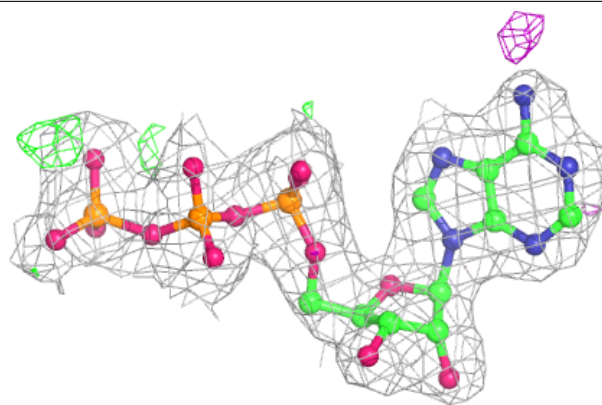
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MPD	B	1041	8/8	0.75	0.24	81,88,92,92	0
6	MPD	B	1015	8/8	0.79	0.27	73,80,88,94	0
6	MPD	A	1011	8/8	0.87	0.20	61,70,77,80	0
6	MPD	B	1029	8/8	0.87	0.22	71,75,84,89	0
6	MPD	B	1031	8/8	0.88	0.22	75,76,85,90	0
6	MPD	A	1013	8/8	0.88	0.22	62,68,72,74	0
6	MPD	B	1025	8/8	0.88	0.42	50,69,81,82	0
6	MPD	A	1037	8/8	0.90	0.13	59,65,74,74	0
6	MPD	B	1023	8/8	0.91	0.18	47,54,63,67	0
6	MPD	B	1039	8/8	0.93	0.13	41,53,56,60	0
4	PO4	B	1503	5/5	0.94	0.23	97,99,100,101	0
4	PO4	A	1501	5/5	0.94	0.15	92,94,96,96	0
4	PO4	B	1517	5/5	0.95	0.18	86,87,89,90	0
4	PO4	A	1505	5/5	0.95	0.30	107,108,109,109	0
6	MPD	B	1019	8/8	0.95	0.15	40,50,53,56	0
4	PO4	B	1527	5/5	0.95	0.11	93,96,98,99	0
6	MPD	B	1021	8/8	0.96	0.14	39,50,65,70	0
3	NA	A	1406	1/1	0.96	0.12	22,22,22,22	0
5	ATP	A	1410	31/31	0.97	0.09	24,32,45,60	0
5	ATP	B	2410	31/31	0.97	0.10	21,30,45,60	0
2	MG	B	2404	1/1	0.98	0.04	28,28,28,28	0
2	MG	A	1404	1/1	0.98	0.08	29,29,29,29	0
3	NA	B	2406	1/1	0.99	0.09	24,24,24,24	0

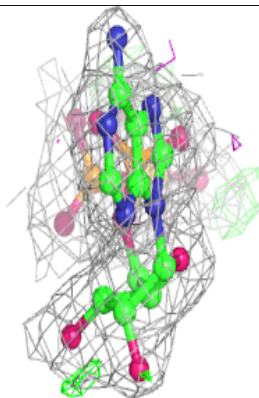
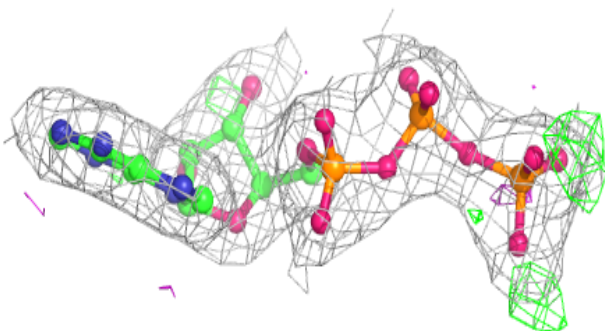
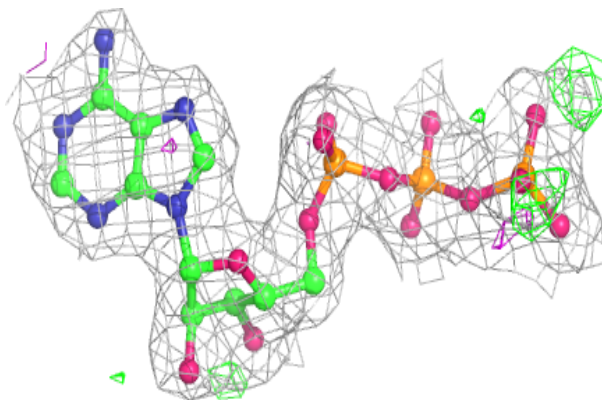
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 1410:

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

**Electron density around ATP B 2410:**

$2mF_o-DF_c$ (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.