



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:24 PM UTC

PDB ID : 2CCH / pdb_00002cch
Title : The crystal structure of CDK2 cyclin A in complex with a substrate peptide derived from CDC modified with a gamma-linked ATP analogue
Authors : Cheng, K.Y.; Noble, M.E.M.; Skamnaki, V.; Brown, N.R.; Lowe, E.D.; Kontogiannis, L.; Shen, K.; Cole, P.A.; Siligardi, G.; Johnson, L.N.
Deposited on : 2006-01-16
Resolution : 1.70 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)
Xtrriage (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

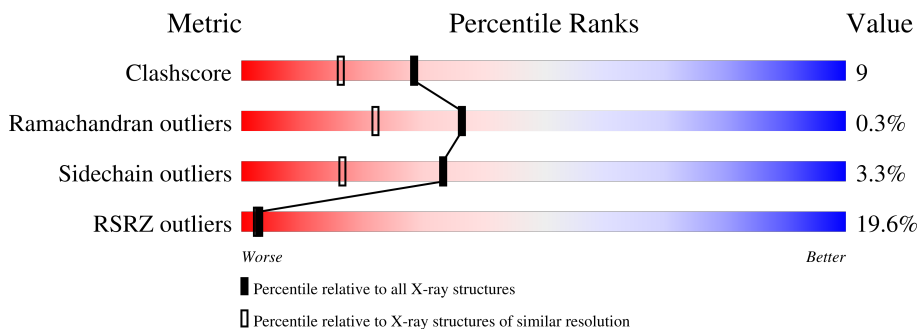
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	299	
1	C	299	
2	B	260	
2	D	260	
3	E	12	
3	F	12	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10526 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	297	Total	C	N	O	P	S	0	9	0
			2460	1592	415	443	1	9			
1	C	297	Total	C	N	O	P	S	0	3	0
			2408	1560	407	431	1	9			

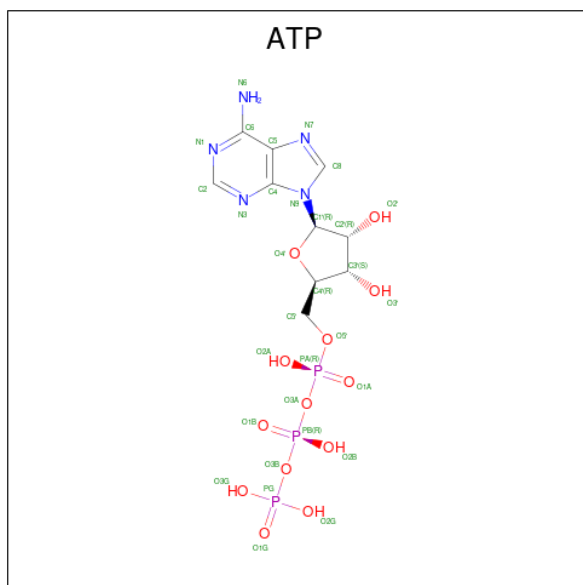
- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	260	Total	C	N	O	S	0	11	0
			2180	1407	354	405	14			
2	D	256	Total	C	N	O	S	0	3	0
			2088	1351	340	384	13			

- Molecule 3 is a protein called CELL DIVISION CONTROL PROTEIN 6 HOMOLOG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	12	Total	C	N	O	0	0	0
			102	64	22	16			
3	F	12	Total	C	N	O	0	0	0
			102	64	22	16			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
4	A	1	Total	62	20	10	26	6	0	1
4	C	1	Total	62	20	10	26	6	0	1

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

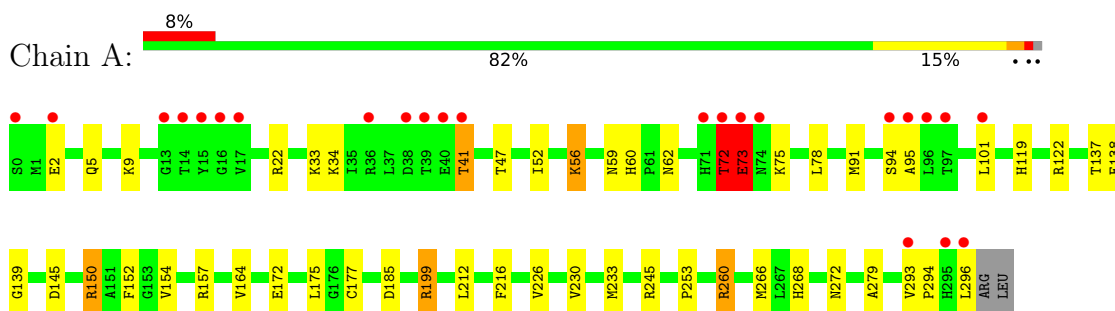
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	390	Total O 390 390	0	0
7	B	327	Total O 327 327	0	0
7	C	144	Total O 144 144	0	0
7	D	160	Total O 160 160	0	0
7	E	17	Total O 17 17	0	0
7	F	7	Total O 7 7	0	0

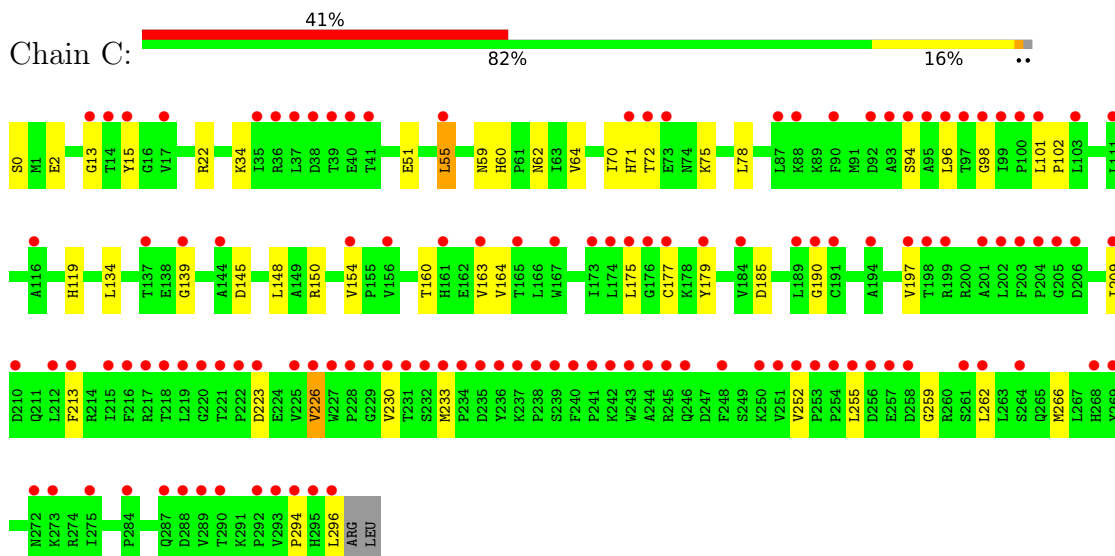
3 Residue-property plots i

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

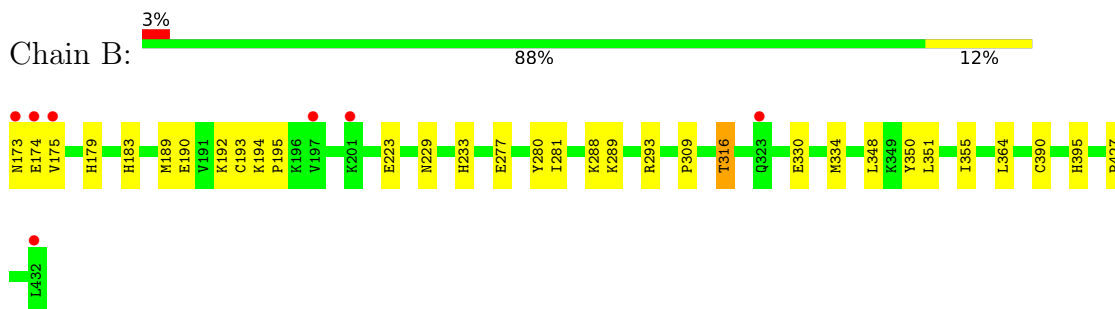
- Molecule 1: CELL DIVISION PROTEIN KINASE 2



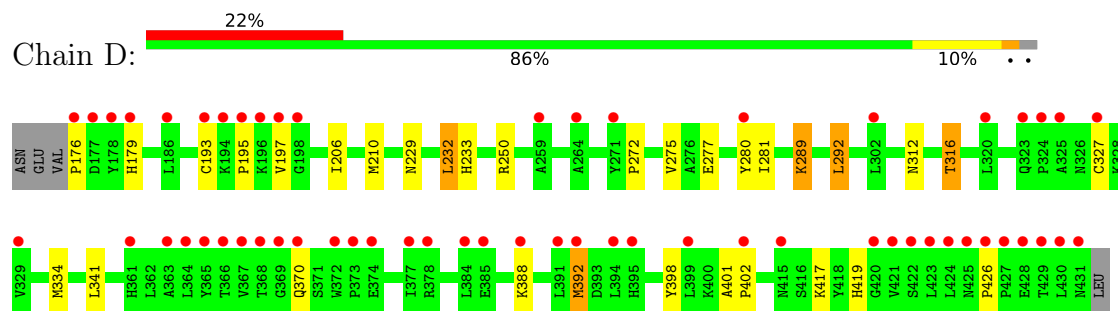
- Molecule 1: CELL DIVISION PROTEIN KINASE 2



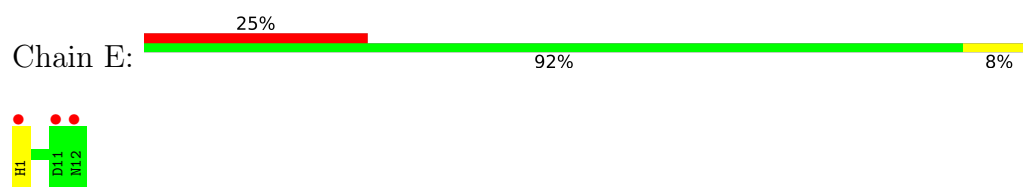
- Molecule 2: CYCLIN A2



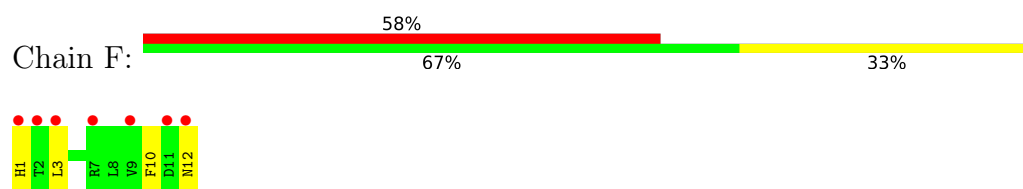
- Molecule 2: CYCLIN A2



- Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG



- Molecule 3: CELL DIVISION CONTROL PROTEIN 6 HOMOLOG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.53Å 114.48Å 181.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.67 – 1.70 96.67 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (96.67-1.70) 98.0 (96.67-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.148 , 0.182 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10526	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: GOL, SO4, TPO, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.09	7/2511 (0.3%)	1.05	9/3407 (0.3%)
1	C	0.80	0/2458	0.88	0/3335
2	B	0.98	1/2230 (0.0%)	0.90	0/3027
2	D	0.78	1/2138 (0.0%)	0.86	0/2902
3	E	0.98	0/103	0.75	0/136
3	F	0.81	0/103	0.82	0/136
All	All	0.93	9/9543 (0.1%)	0.93	9/12943 (0.1%)

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	C	0	1
2	B	1	0
All	All	1	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ARG	CZ-NH1	7.30	1.43	1.32
1	A	91	MET	SD-CE	-6.91	1.62	1.79
1	A	266	MET	C-O	6.54	1.32	1.24
2	B	316	THR	CB-CG2	-6.46	1.31	1.52
1	A	150	ARG	CB-CG	-5.32	1.36	1.52
1	A	260	ARG	CZ-NH2	-5.25	1.26	1.33
2	D	272	PRO	CA-C	5.14	1.54	1.51
1	A	279	ALA	CA-C	-5.13	1.46	1.52
1	A	157	ARG	CB-CG	-5.05	1.37	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	NE-CZ-NH2	-10.60	109.66	119.20
1	A	260	ARG	NE-CZ-NH2	-9.97	110.23	119.20
1	A	72	THR	CB-CA-C	-8.33	100.18	112.09
1	A	199	ARG	NE-CZ-NH1	6.92	128.41	121.50
1	A	260	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	A	199	ARG	CG-CD-NE	-6.44	97.83	112.00
1	A	150	ARG	CA-CB-CG	5.68	125.45	114.10
1	A	199	ARG	CD-NE-CZ	5.67	132.34	124.40
1	A	253	PRO	N-CA-C	5.46	117.36	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	316	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	71	HIS	Peptide

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	2460	0	2484	58	0
1	C	2408	0	2441	37	0
2	B	2180	0	2189	32	0
2	D	2088	0	2106	42	0
3	E	102	0	108	1	0
3	F	102	0	108	5	0
4	A	62	0	24	7	0
4	C	62	0	24	4	0
5	A	5	0	0	1	0
6	A	12	0	15	0	0
7	A	390	0	0	23	1
7	B	327	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	144	0	0	6	0
7	D	160	0	0	11	0
7	E	17	0	0	0	0
7	F	7	0	0	0	0
All	All	10526	0	9499	168	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 9.

All (168) 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:177[A]:CYS:HB3	7:A:2213:HOH:O	1.35	1.25
1:C:64:VAL:HB	7:C:2065:HOH:O	1.43	1.16
1:A:177[B]:CYS:HB2	7:A:2213:HOH:O	1.54	1.07
2:D:210:MET:HE3	3:F:10:PHE:HB3	1.37	1.05
1:A:175:LEU:HD13	1:A:233:MET:CE	1.93	0.99
2:D:334:MET:HG2	7:D:2105:HOH:O	1.61	0.99
1:A:101:LEU:HB3	7:A:2143:HOH:O	1.62	0.98
1:A:175:LEU:HD13	1:A:233:MET:HE1	1.46	0.97
1:A:94:SER:O	1:A:199:ARG:HD3	1.66	0.95
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:C5'	2.19	0.89
1:A:101:LEU:HD12	7:A:2039:HOH:O	1.72	0.89
1:C:190:GLY:HA2	1:C:266:MET:HE3	1.57	0.86
2:D:210:MET:HE1	2:D:250:ARG:CB	2.06	0.86
1:A:175:LEU:CD1	1:A:233:MET:HE1	2.05	0.86
2:D:334:MET:HE3	7:D:2105:HOH:O	1.75	0.85
1:C:154:VAL:O	2:D:316:THR:HG23	1.77	0.84
1:A:60:HIS:HD2	1:A:62:ASN:H	1.26	0.82
1:A:154:VAL:O	2:B:316:THR:HG23	1.80	0.81
5:A:1298:SO4:O3	7:A:2386:HOH:O	1.98	0.80
2:D:210:MET:HE1	2:D:250:ARG:HB3	1.63	0.79
1:A:101:LEU:HB3	7:A:2041:HOH:O	1.82	0.79
2:B:193[B]:CYS:HB3	7:B:2130:HOH:O	1.80	0.79
2:B:316:THR:HG21	7:B:2025:HOH:O	1.83	0.78
1:C:190:GLY:HA2	1:C:266:MET:CE	2.14	0.77
2:D:316:THR:HG21	7:D:2008:HOH:O	1.82	0.77
2:B:195:PRO:HD3	7:B:2127:HOH:O	1.85	0.76
1:A:172:GLU:O	1:A:177[B]:CYS:SG	2.43	0.75
2:D:210:MET:HE3	3:F:10:PHE:CB	2.16	0.74
2:D:197:VAL:N	7:D:2021:HOH:O	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CD2	1:A:62:ASN:H	2.06	0.74
1:A:59:ASN:ND2	7:A:2076:HOH:O	2.20	0.73
1:A:230:VAL:HG23	1:A:233:MET:CE	2.17	0.73
2:D:232:LEU:C	2:D:232:LEU:HD13	2.14	0.72
2:D:229:ASN:HD22	2:D:334:MET:HE1	1.54	0.72
2:B:350:TYR:HB2	2:B:355[B]:ILE:HD11	1.73	0.70
2:D:229:ASN:HD22	2:D:334:MET:CE	2.04	0.70
1:A:22:ARG:HD3	7:A:2007:HOH:O	1.92	0.69
1:C:154:VAL:O	2:D:316:THR:CG2	2.39	0.69
2:D:210:MET:CE	2:D:250:ARG:HB2	2.23	0.69
1:C:64:VAL:HG21	1:C:134:LEU:HD12	1.74	0.68
2:B:229:ASN:HD22	2:B:334[A]:MET:CE	2.06	0.68
4:A:1297[B]:ATP:H3'	7:A:2379:HOH:O	1.93	0.68
1:C:60:HIS:HD2	1:C:62:ASN:H	1.41	0.67
1:C:190:GLY:CA	1:C:266:MET:HE3	2.24	0.67
2:B:334[B]:MET:HE3	7:B:2220:HOH:O	1.94	0.67
1:A:94:SER:O	1:A:199:ARG:CD	2.41	0.66
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.76	0.65
1:C:51:GLU:OE2	7:C:2052:HOH:O	2.15	0.64
1:A:41:THR:HG22	2:B:288:LYS:HE2	1.80	0.63
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.80	0.63
1:A:268:HIS:ND1	7:A:2338:HOH:O	2.31	0.63
1:A:230:VAL:HG23	1:A:233:MET:HE2	1.80	0.62
1:C:60:HIS:CD2	1:C:62:ASN:H	2.18	0.62
4:A:1297[B]:ATP:O1G	7:A:2380:HOH:O	2.16	0.61
2:B:229:ASN:HD22	2:B:334[B]:MET:HE2	1.66	0.61
1:A:119:HIS:HD2	7:B:2062:HOH:O	1.82	0.60
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.79	0.60
1:A:272[B]:ASN:OD1	2:B:175:VAL:HB	2.00	0.60
2:B:229:ASN:HD22	2:B:334[A]:MET:HE2	1.66	0.60
1:A:145[B]:ASP:CG	4:A:1297[B]:ATP:O2B	2.45	0.60
1:A:101:LEU:HD13	7:A:2041:HOH:O	2.02	0.59
2:B:355[B]:ILE:HD13	2:B:390:CYS:SG	2.43	0.59
1:C:34:LYS:HE2	1:C:75:LYS:HD3	1.83	0.59
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:O5'	2.21	0.59
2:D:388:LYS:O	2:D:392:MET:HG2	2.03	0.59
1:A:230:VAL:CG2	1:A:233:MET:HE2	2.32	0.59
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:H5'1	2.02	0.58
1:A:33:LYS:NZ	7:A:2037:HOH:O	2.36	0.58
1:A:101:LEU:CB	7:A:2041:HOH:O	2.44	0.57
2:B:395:HIS:HE1	2:B:427:PRO:O	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193[B]:CYS:SG	2:B:309:PRO:HD2	2.45	0.57
2:D:210:MET:CE	3:F:10:PHE:HB3	2.25	0.57
2:D:232:LEU:CD1	2:D:341:LEU:HD13	2.34	0.57
2:D:232:LEU:HD11	2:D:341:LEU:HD13	1.86	0.57
2:B:189:MET:O	2:B:193[B]:CYS:SG	2.64	0.56
1:C:70:ILE:HG22	1:C:72:THR:OG1	2.06	0.56
2:B:183:HIS:HD2	7:B:2072:HOH:O	1.88	0.55
1:C:22:ARG:HD3	7:C:2030:HOH:O	2.06	0.55
2:D:277:GLU:OE1	3:F:1:HIS:HE1	1.89	0.55
1:A:34:LYS:HZ1	1:A:75:LYS:HE3	1.71	0.55
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.88	0.54
1:A:230:VAL:HG23	1:A:233:MET:HE1	1.86	0.54
4:A:1297[B]:ATP:C3'	7:A:2379:HOH:O	2.51	0.54
2:D:289:LYS:HE2	7:D:2080:HOH:O	2.08	0.54
1:C:119:HIS:HD2	7:C:2136:HOH:O	1.90	0.53
1:A:212[B]:LEU:HG	1:A:216:PHE:CZ	2.45	0.53
1:A:145[B]:ASP:OD2	4:A:1297[B]:ATP:O3B	2.27	0.52
1:C:0:SER:N	7:C:2003:HOH:O	2.18	0.52
2:D:289:LYS:HD3	7:D:2084:HOH:O	2.10	0.52
2:B:277:GLU:OE1	3:E:1:HIS:HE1	1.91	0.52
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.40	0.52
1:A:73:GLU:N	7:A:2102:HOH:O	2.42	0.52
2:B:229:ASN:HD22	2:B:334[B]:MET:CE	2.23	0.51
2:B:229:ASN:HD22	2:B:334[A]:MET:HE1	1.74	0.51
2:D:176:PRO:HA	2:D:179:HIS:CG	2.47	0.50
2:B:233:HIS:HE1	7:B:2220:HOH:O	1.93	0.50
2:B:233:HIS:HD2	7:B:2193:HOH:O	1.94	0.50
1:C:223:ASP:OD1	1:C:226:VAL:HG12	2.11	0.50
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.94	0.50
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.94	0.49
1:A:52:ILE:O	1:A:56:LYS:HG3	2.11	0.49
1:C:177[B]:CYS:SG	1:C:179:TYR:O	2.67	0.49
2:D:232:LEU:CD1	2:D:341:LEU:CD1	2.90	0.49
1:A:101:LEU:HG	7:A:2142:HOH:O	2.13	0.49
1:C:94:SER:O	1:C:98:GLY:N	2.44	0.49
2:B:190:GLU:HA	2:B:193[B]:CYS:SG	2.53	0.49
2:B:223:GLU:OE1	7:B:2108:HOH:O	2.20	0.49
2:B:194:LYS:HE2	2:B:351:LEU:HD23	1.94	0.48
2:B:289:LYS:HE2	2:B:293:ARG:CZ	2.43	0.48
1:A:47[B]:THR:HG23	7:A:2054:HOH:O	2.13	0.48
1:A:145[B]:ASP:OD2	4:A:1297[B]:ATP:PB	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145[B]:ASP:OD2	4:C:1297[B]:ATP:H5'2	2.09	0.48
1:A:175:LEU:CD1	1:A:233:MET:CE	2.72	0.48
1:C:175:LEU:HD13	1:C:233:MET:CE	2.43	0.48
2:B:192:LYS:O	7:B:2080:HOH:O	2.20	0.47
2:D:327[B]:CYS:HB3	2:D:419:HIS:CE1	2.49	0.47
1:A:101:LEU:CD1	7:A:2039:HOH:O	2.46	0.47
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.96	0.47
1:A:101:LEU:CD1	7:A:2041:HOH:O	2.61	0.47
2:B:174:GLU:OE2	2:B:179:HIS:HE1	1.97	0.47
1:A:145[B]:ASP:OD1	4:A:1297[B]:ATP:O2B	2.31	0.47
1:C:175:LEU:HB3	1:C:233:MET:HE3	1.96	0.47
1:A:34:LYS:HE2	1:A:75:LYS:HD3	1.97	0.47
2:D:193[B]:CYS:O	2:D:193[B]:CYS:SG	2.73	0.46
2:D:232:LEU:HD11	2:D:341:LEU:CD1	2.45	0.46
1:C:175:LEU:HD13	1:C:233:MET:HE1	1.98	0.46
2:D:233:HIS:HE1	7:D:2115:HOH:O	1.98	0.46
1:A:47[B]:THR:HG22	7:A:2052:HOH:O	2.15	0.46
2:B:280:TYR:CD2	2:B:280:TYR:C	2.94	0.45
2:B:330:GLU:O	2:B:334[A]:MET:HG3	2.15	0.45
2:B:174:GLU:OE2	2:B:179:HIS:CE1	2.69	0.45
2:D:232:LEU:C	2:D:232:LEU:CD1	2.85	0.45
1:A:230:VAL:O	1:A:233:MET:HE2	2.17	0.45
1:C:262:LEU:O	1:C:266:MET:HG3	2.17	0.45
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.99	0.45
1:A:34:LYS:HZ3	1:A:75:LYS:HG2	1.83	0.44
2:D:232:LEU:HD13	2:D:232:LEU:O	2.16	0.44
1:A:5:GLN:HG2	7:A:2007:HOH:O	2.16	0.44
1:C:13:GLY:N	1:C:15:TYR:CE2	2.86	0.44
1:C:209:ILE:HD11	1:C:213:PHE:CE1	2.52	0.44
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.33	0.44
2:D:233:HIS:HD2	7:D:2102:HOH:O	2.00	0.44
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.99	0.44
1:A:137:THR:HA	1:A:296:LEU:HD11	2.00	0.43
2:D:280:TYR:CD2	2:D:280:TYR:C	2.95	0.43
1:A:22:ARG:HH11	1:A:22:ARG:HG3	1.82	0.43
2:D:281:ILE:HD11	3:F:3:LEU:HD23	2.00	0.43
1:C:255:LEU:HG	1:C:259:GLY:HA3	2.00	0.43
1:C:230:VAL:HG23	1:C:233:MET:HE2	2.01	0.43
2:D:195:PRO:HD3	7:D:2049:HOH:O	2.18	0.43
2:D:334:MET:CE	7:D:2105:HOH:O	2.47	0.43
1:C:51:GLU:O	1:C:55:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:LYS:NZ	7:D:2080:HOH:O	2.52	0.42
1:A:175:LEU:HD12	1:A:233:MET:HE1	1.93	0.42
1:A:137:THR:HG22	1:A:296:LEU:CD1	2.50	0.42
1:C:145[B]:ASP:OD1	7:C:2094:HOH:O	2.22	0.42
1:A:72:THR:O	1:A:73:GLU:HB2	2.20	0.42
2:B:183:HIS:HE1	7:B:2201:HOH:O	2.03	0.41
2:D:206:ILE:HA	2:D:210:MET:SD	2.60	0.41
2:D:401:ALA:N	2:D:402:PRO:CD	2.84	0.41
2:B:194:LYS:HE2	2:B:351:LEU:HA	2.03	0.41
1:A:138:GLU:HG3	7:A:2162:HOH:O	2.20	0.41
1:A:94:SER:C	1:A:199:ARG:HD3	2.41	0.40
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.56	0.40
2:D:312:ASN:O	2:D:316:THR:HB	2.21	0.40
1:C:101:LEU:N	1:C:102:PRO:CD	2.84	0.40
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.04	0.40
2:D:398:TYR:CD2	2:D:426:PRO:HB3	2.56	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)
7:A:2235:HOH:O	7:A:2386:HOH:O[4_555]	1.99	0.21

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	304/299 (102%)	297 (98%)	5 (2%)	2 (1%)	18 7
1	C	297/299 (99%)	287 (97%)	9 (3%)	1 (0%)	36 22
2	B	269/260 (104%)	267 (99%)	2 (1%)	0	100 100
2	D	257/260 (99%)	255 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	10/12 (83%)	10 (100%)	0	0	100	100
3	F	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
All	All	1147/1142 (100%)	1125 (98%)	19 (2%)	3 (0%)	36	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	164	VAL
1	C	164	VAL

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	271/263 (103%)	260 (96%)	11 (4%)	27	11
1	C	264/263 (100%)	254 (96%)	10 (4%)	29	13
2	B	245/234 (105%)	240 (98%)	5 (2%)	48	32
2	D	233/234 (100%)	226 (97%)	7 (3%)	36	19
3	E	11/11 (100%)	11 (100%)	0	100	100
3	F	11/11 (100%)	10 (91%)	1 (9%)	9	2
All	All	1035/1016 (102%)	1001 (97%)	34 (3%)	33	17

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	LYS
1	A	41	THR
1	A	56	LYS
1	A	72	THR
1	A	73	GLU
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	150	ARG
1	A	226	VAL
1	A	260	ARG
1	A	293	VAL
2	B	173	ASN
2	B	281	ILE
2	B	348[A]	LEU
2	B	348[B]	LEU
2	B	364	LEU
1	C	2	GLU
1	C	55	LEU
1	C	59	ASN
1	C	78	LEU
1	C	96	LEU
1	C	148	LEU
1	C	150	ARG
1	C	163	VAL
1	C	226	VAL
1	C	296	LEU
2	D	232	LEU
2	D	289	LYS
2	D	292	LEU
2	D	316	THR
2	D	370	GLN
2	D	392	MET
2	D	417	LYS
3	F	12	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	85	GLN
1	A	119	HIS
1	A	265	GLN
2	B	179	HIS
2	B	183	HIS
2	B	229	ASN
2	B	233	HIS
2	B	313	GLN
2	B	317	GLN

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Mol	Chain	Res	Type
2	B	395	HIS
2	B	425	ASN
1	C	60	HIS
1	C	62	ASN
1	C	113	GLN
1	C	119	HIS
1	C	287	GLN
2	D	183	HIS
2	D	229	ASN
2	D	233	HIS
2	D	313	GLN
2	D	317	GLN
2	D	370	GLN
2	D	395	HIS
2	D	419	HIS
2	D	425	ASN
2	D	431	ASN
3	E	1	HIS
3	F	1	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	C	160	1	8,10,11	1.29	1 (12%)	10,14,16	1.19	1 (10%)
1	TPO	A	160	1	8,10,11	0.84	0	10,14,16	0.80	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
1	TPO	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	2.67	1.64	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	P-OG1-CB	-2.37	116.88	123.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	A	1297[B]	-	32,33,33	1.49	6 (18%)	48,52,52	1.88	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	1297[A]	-	32,33,33	1.50	7 (21%)	48,52,52	1.72	9 (18%)
5	SO4	A	1298	-	4,4,4	0.43	0	6,6,6	0.68	0
6	GOL	A	1299	-	5,5,5	1.21	1 (20%)	5,5,5	0.56	0
4	ATP	C	1297[B]	-	32,33,33	1.61	6 (18%)	48,52,52	1.79	9 (18%)
4	ATP	C	1297[A]	-	32,33,33	1.44	5 (15%)	48,52,52	1.70	10 (20%)
6	GOL	A	1300	-	5,5,5	0.50	0	5,5,5	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
4	ATP	A	1297[B]	-	-	0/22/38/38	0/3/3/3
4	ATP	A	1297[A]	-	-	6/22/38/38	0/3/3/3
6	GOL	A	1299	-	-	0/4/4/4	-
4	ATP	C	1297[B]	-	-	9/22/38/38	0/3/3/3
4	ATP	C	1297[A]	-	-	4/22/38/38	0/3/3/3
6	GOL	A	1300	-	-	0/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297[B]	ATP	C5-C4	4.99	1.48	1.39
4	C	1297[B]	ATP	C5-C4	4.93	1.47	1.39
4	C	1297[A]	ATP	C5-C4	4.92	1.47	1.39
4	A	1297[A]	ATP	C5-C4	4.92	1.47	1.39
4	C	1297[B]	ATP	PA-O3A	3.54	1.63	1.59
4	C	1297[B]	ATP	PB-O3A	3.32	1.63	1.59
4	A	1297[A]	ATP	C5-C6	3.14	1.49	1.41
4	A	1297[B]	ATP	C5-C6	2.87	1.49	1.41
4	C	1297[A]	ATP	C5-C6	2.82	1.48	1.41
4	C	1297[B]	ATP	C5-C6	2.77	1.48	1.41
4	C	1297[A]	ATP	C8-N7	2.68	1.36	1.31
4	A	1297[A]	ATP	C8-N7	2.63	1.36	1.31
4	A	1297[B]	ATP	C5-N7	-2.50	1.34	1.39
4	C	1297[B]	ATP	C8-N7	2.49	1.36	1.31
4	A	1297[A]	ATP	PB-O3A	2.35	1.62	1.59
4	C	1297[B]	ATP	C5-N7	-2.27	1.34	1.39
4	C	1297[A]	ATP	C4-N9	-2.24	1.33	1.37
4	A	1297[A]	ATP	PA-O3A	2.21	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297[A]	ATP	C4-N9	-2.14	1.33	1.37
4	A	1297[A]	ATP	C5-N7	-2.14	1.35	1.39
4	A	1297[B]	ATP	PB-O3A	2.12	1.61	1.59
4	C	1297[A]	ATP	C5-N7	-2.08	1.35	1.39
4	A	1297[B]	ATP	C8-N7	2.05	1.35	1.31
6	A	1299	GOL	O2-C2	2.03	1.49	1.43
4	A	1297[B]	ATP	PB-O3B	2.01	1.61	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1297[B]	ATP	C5-C4-N3	-6.40	117.90	126.72
4	C	1297[B]	ATP	C5-C4-N3	-5.76	118.78	126.72
4	A	1297[B]	ATP	N3-C4-N9	5.57	136.65	127.17
4	A	1297[A]	ATP	C5-C4-N3	-5.50	119.15	126.72
4	C	1297[A]	ATP	C5-C4-N3	-5.06	119.75	126.72
4	C	1297[B]	ATP	N3-C4-N9	4.60	134.99	127.17
4	A	1297[A]	ATP	N3-C4-N9	4.07	134.09	127.17
4	C	1297[A]	ATP	N3-C4-N9	3.93	133.86	127.17
4	A	1297[A]	ATP	C4-C5-N7	-3.84	106.19	110.58
4	C	1297[B]	ATP	C2-N3-C4	3.79	121.09	111.83
4	A	1297[B]	ATP	C2-N3-C4	3.76	121.01	111.83
4	A	1297[A]	ATP	C2-N3-C4	3.68	120.82	111.83
4	C	1297[A]	ATP	C2-N3-C4	3.55	120.51	111.83
4	C	1297[A]	ATP	C4-C5-N7	-3.41	106.68	110.58
4	C	1297[B]	ATP	N3-C2-N1	-3.33	123.54	128.58
4	C	1297[A]	ATP	N3-C2-N1	-3.31	123.56	128.58
4	A	1297[B]	ATP	C4-C5-N7	-3.16	106.97	110.58
4	A	1297[A]	ATP	N3-C2-N1	-3.14	123.82	128.58
4	C	1297[B]	ATP	C4-C5-N7	-3.09	107.05	110.58
4	C	1297[A]	ATP	C4-N9-C8	2.99	108.88	105.74
4	A	1297[B]	ATP	N3-C2-N1	-2.98	124.07	128.58
4	A	1297[B]	ATP	C4-N9-C8	2.85	108.73	105.74
4	A	1297[A]	ATP	C4-N9-C8	2.75	108.63	105.74
4	A	1297[A]	ATP	C5-N7-C8	2.70	107.69	103.45
4	A	1297[B]	ATP	C5-N7-C8	2.68	107.66	103.45
4	A	1297[A]	ATP	C6-C5-N7	2.60	137.11	132.09
4	C	1297[A]	ATP	C6-C5-N7	2.56	137.02	132.09
4	C	1297[A]	ATP	C5-N7-C8	2.41	107.24	103.45
4	C	1297[B]	ATP	C5-N7-C8	2.36	107.17	103.45
4	A	1297[B]	ATP	C2'-C3'-C4'	2.29	107.04	102.61
4	C	1297[B]	ATP	C4-N9-C8	2.27	108.12	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1297[A]	ATP	N9-C8-N7	-2.26	110.73	113.94
4	C	1297[A]	ATP	N9-C8-N7	-2.21	110.81	113.94
4	C	1297[B]	ATP	C6-C5-N7	2.15	136.23	132.09
4	C	1297[A]	ATP	C2-N1-C6	2.04	122.08	118.73
4	C	1297[B]	ATP	O2B-PB-O1B	2.00	121.76	112.44

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1297[A]	ATP	C5'-O5'-PA-O2A
4	A	1297[A]	ATP	C5'-O5'-PA-O3A
4	C	1297[A]	ATP	PB-O3A-PA-O5'
4	C	1297[A]	ATP	O4'-C4'-C5'-O5'
4	C	1297[B]	ATP	PB-O3B-PG-O3G
4	C	1297[B]	ATP	C5'-O5'-PA-O3A
4	C	1297[A]	ATP	C3'-C4'-C5'-O5'
4	C	1297[B]	ATP	C3'-C4'-C5'-O5'
4	C	1297[B]	ATP	O4'-C4'-C5'-O5'
4	A	1297[A]	ATP	PB-O3A-PA-O5'
4	C	1297[B]	ATP	C4'-C5'-O5'-PA
4	A	1297[A]	ATP	C5'-O5'-PA-O1A
4	C	1297[B]	ATP	C5'-O5'-PA-O1A
4	A	1297[A]	ATP	O4'-C4'-C5'-O5'
4	C	1297[B]	ATP	PB-O3B-PG-O1G
4	A	1297[A]	ATP	PB-O3A-PA-O1A
4	C	1297[A]	ATP	PG-O3B-PB-O2B
4	C	1297[B]	ATP	PA-O3A-PB-O1B
4	C	1297[B]	ATP	PA-O3A-PB-O2B

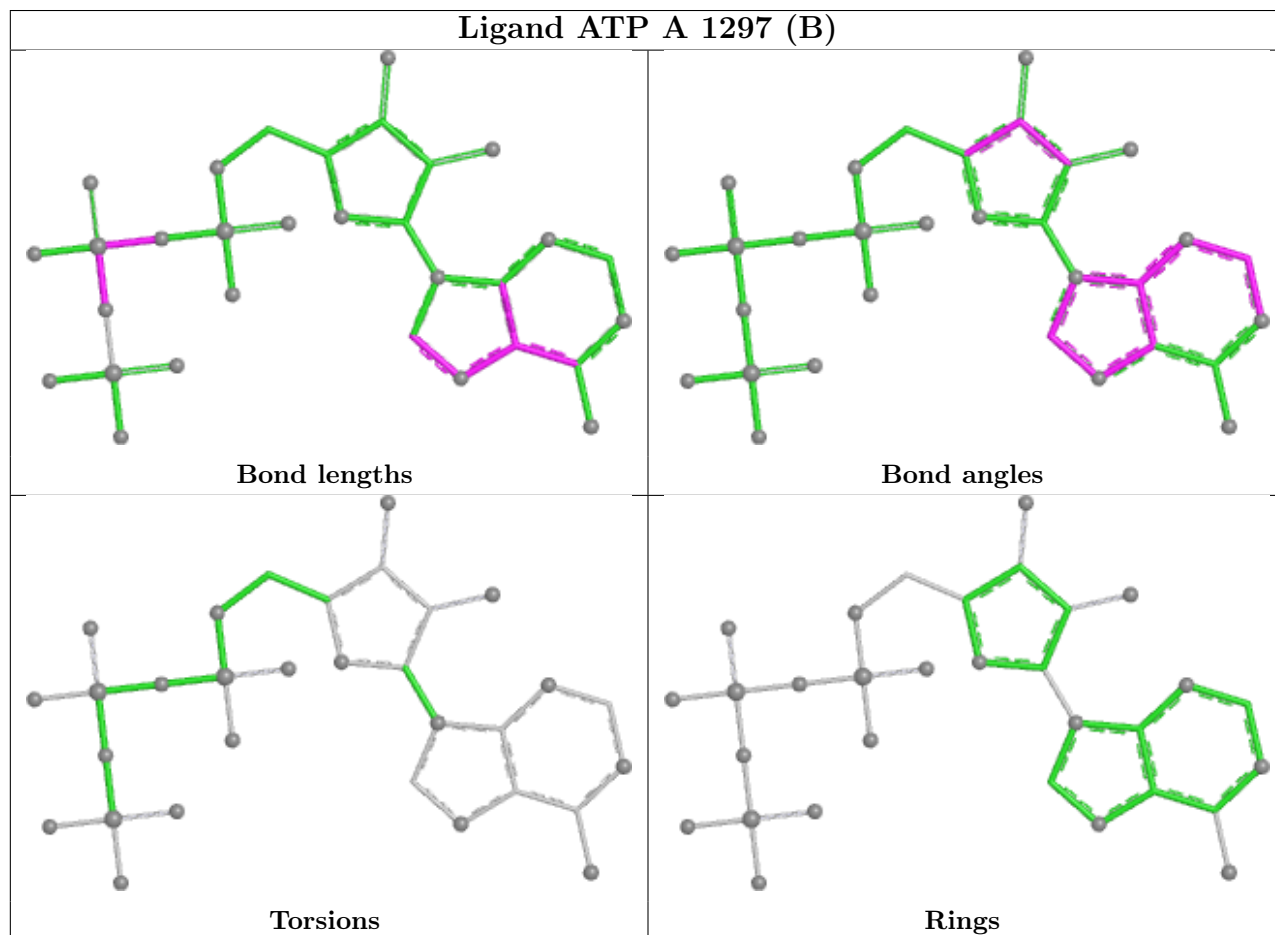
There are no ring outliers.

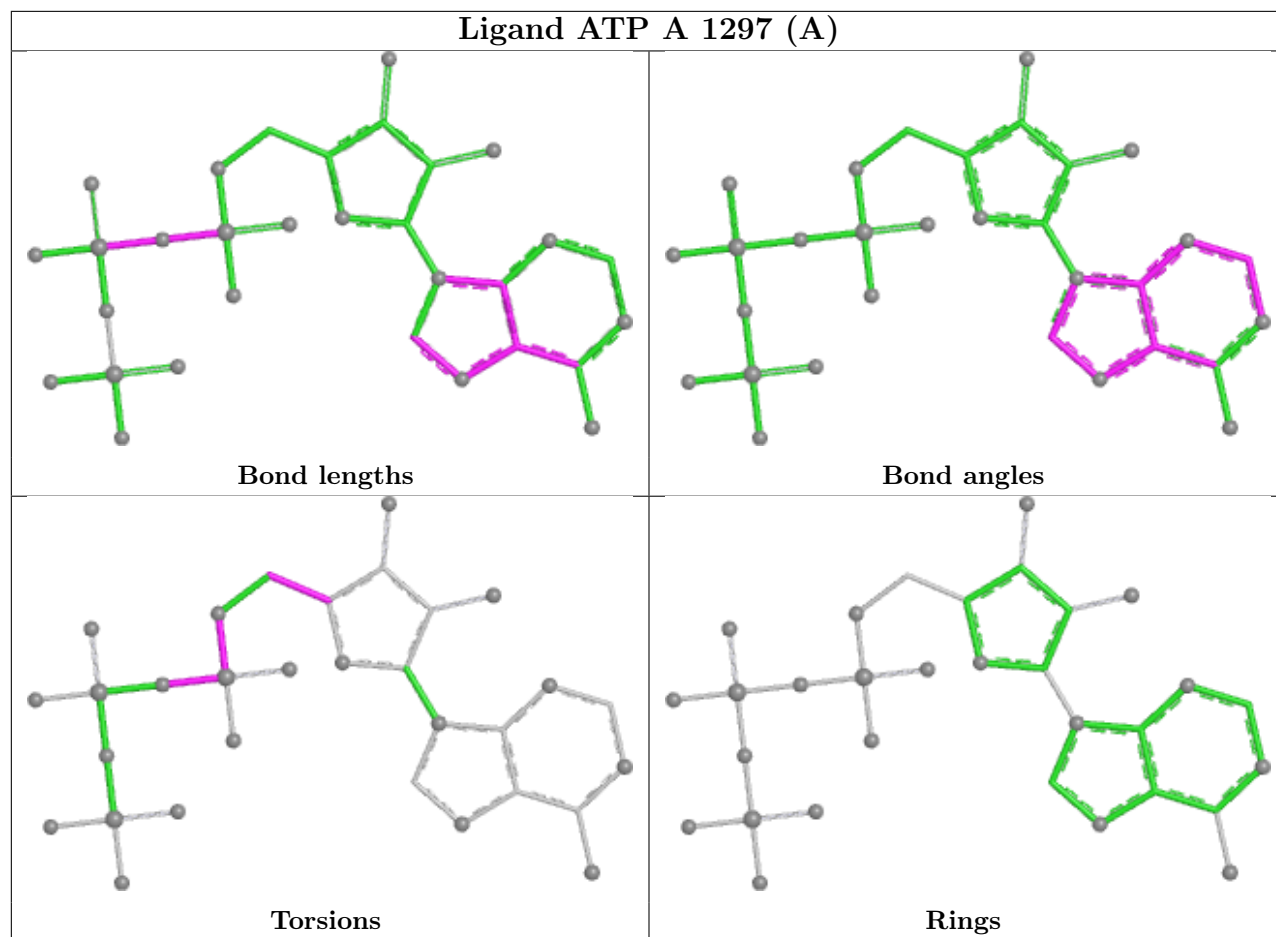
3 monomers are involved in 12 short contacts:

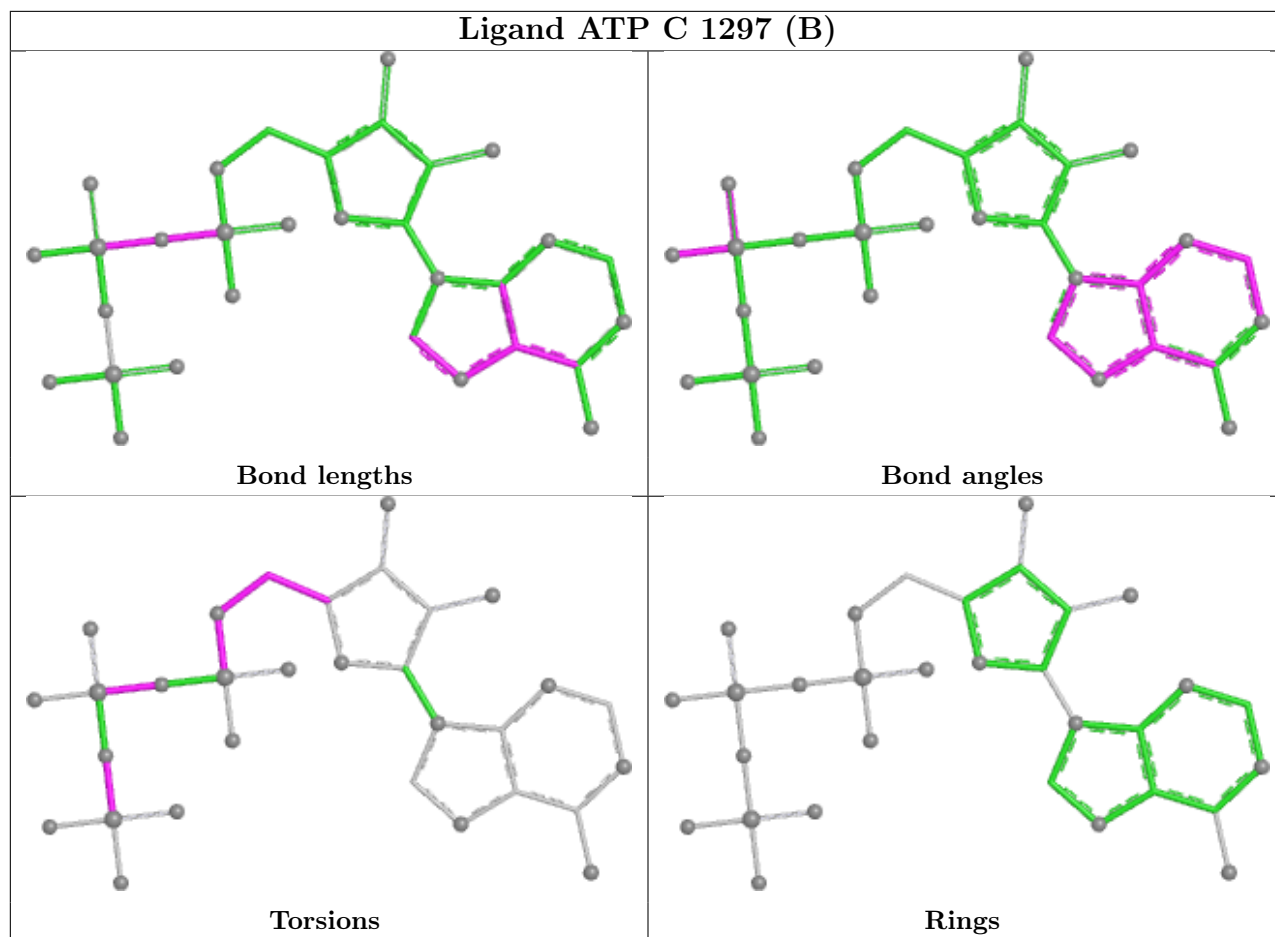
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1297[B]	ATP	7	0
5	A	1298	SO4	1	0
4	C	1297[B]	ATP	4	0

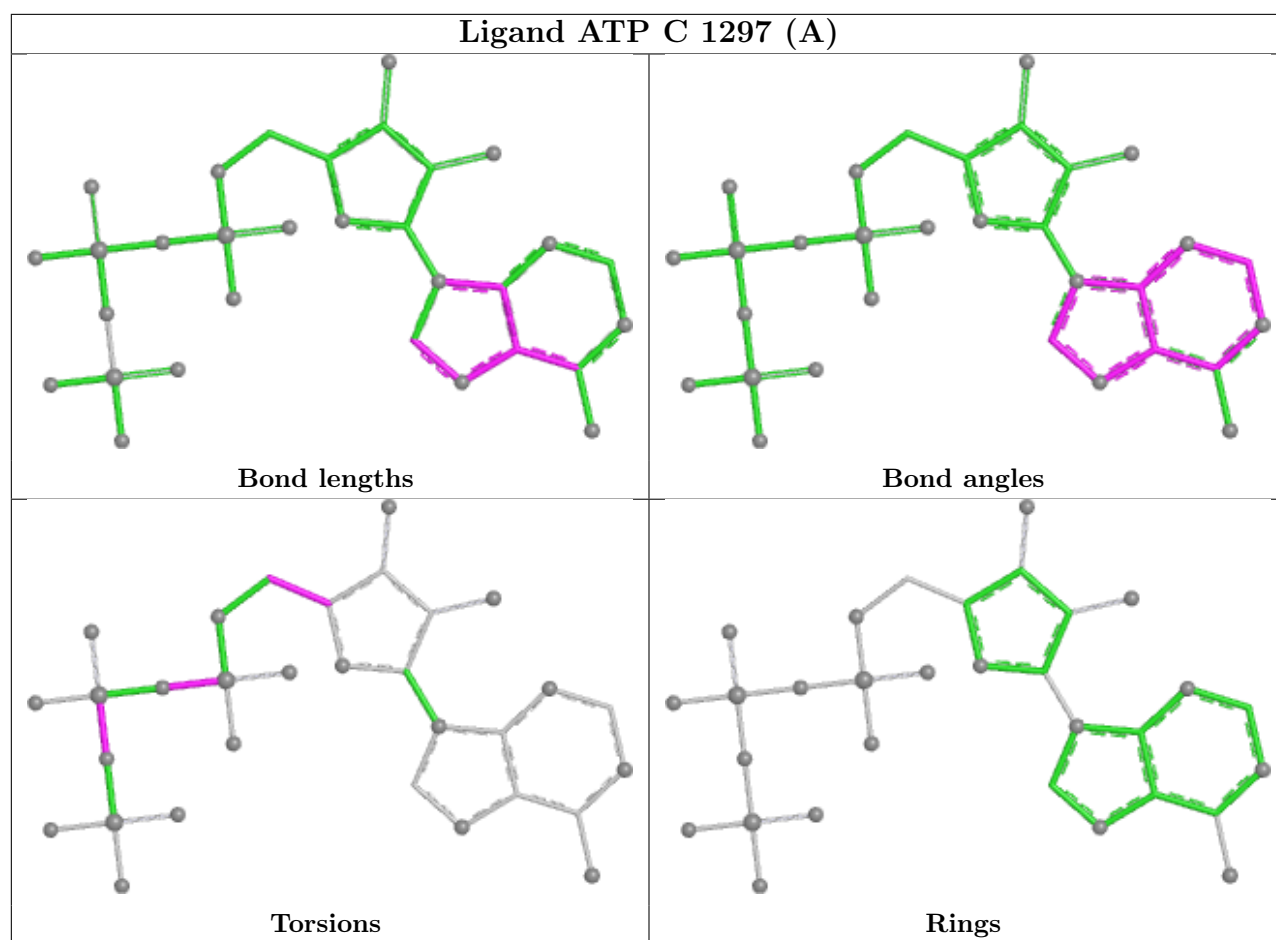
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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	296/299 (98%)	0.26	24 (8%) 18 19	5, 14, 36, 46	9 (3%)
1	C	296/299 (98%)	1.95	123 (41%) 0 0	13, 31, 44, 60	3 (1%)
2	B	260/260 (100%)	0.12	7 (2%) 56 60	5, 14, 26, 44	11 (4%)
2	D	256/260 (98%)	1.33	58 (22%) 2 2	14, 25, 37, 53	3 (1%)
3	E	12/12 (100%)	1.07	3 (25%) 2 1	18, 28, 41, 48	0
3	F	12/12 (100%)	2.30	7 (58%) 0 0	32, 41, 49, 54	0
All	All	1132/1142 (99%)	0.94	222 (19%) 3 2	5, 21, 41, 60	26 (2%)

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	LEU	7.9
1	C	294	PRO	7.1
1	A	72	THR	7.0
1	C	213	PHE	7.0
1	C	243	TRP	6.6
2	B	173	ASN	6.2
1	C	209	ILE	6.2
1	C	96	LEU	6.1
1	C	236	TYR	6.0
2	D	193[A]	CYS	5.9
1	C	248	PHE	5.8
1	C	295	HIS	5.7
1	A	39	THR	5.4
1	C	39	THR	5.2
1	A	95	ALA	5.2
1	C	284	PRO	5.2
1	C	225	VAL	5.1
2	D	324	PRO	5.0
1	C	220	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	238	PRO	4.8
2	B	197	VAL	4.8
1	C	293	VAL	4.7
2	D	176	PRO	4.6
1	A	101	LEU	4.6
1	C	226	VAL	4.5
1	A	15	TYR	4.5
1	C	72	THR	4.4
1	C	93	ALA	4.4
2	D	423	LEU	4.3
1	C	216	PHE	4.3
1	A	38	ASP	4.3
1	C	240	PHE	4.2
1	C	251	VAL	4.2
2	D	365	TYR	4.2
1	C	15	TYR	4.1
1	C	230	VAL	4.1
1	C	227	TRP	4.0
1	C	234	PRO	4.0
1	C	253	PRO	4.0
1	C	88	LYS	4.0
1	C	97	THR	4.0
1	C	228	PRO	4.0
1	A	41	THR	4.0
1	C	244	ALA	4.0
1	A	14	THR	3.9
1	C	201	ALA	3.9
1	C	290	THR	3.9
2	B	175	VAL	3.9
2	D	420	GLY	3.9
1	C	179	TYR	3.9
2	D	327[A]	CYS	3.9
1	C	242	LYS	3.8
1	A	40	GLU	3.8
2	D	323	GLN	3.8
2	B	432	LEU	3.8
1	C	215	ILE	3.8
1	C	229	GLY	3.8
1	C	262	LEU	3.8
1	C	231	THR	3.8
1	A	295	HIS	3.7
1	A	296	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	95	ALA	3.7
2	D	422	SER	3.7
2	D	177	ASP	3.6
1	C	163	VAL	3.6
2	D	178	TYR	3.6
1	C	232	SER	3.6
2	D	364	LEU	3.6
2	D	392	MET	3.6
1	C	245	ARG	3.5
1	C	241	PRO	3.5
2	D	427	PRO	3.5
1	C	222	PRO	3.5
1	C	212	LEU	3.5
3	F	9	VAL	3.5
1	C	221	THR	3.5
1	A	73	GLU	3.4
1	C	197	VAL	3.4
1	C	289	VAL	3.4
2	D	431	ASN	3.4
2	D	198	GLY	3.4
1	C	252	VAL	3.3
3	F	2	THR	3.3
1	C	257	GLU	3.3
1	C	255	LEU	3.3
1	C	206	ASP	3.2
1	C	256	ASP	3.2
1	C	101	LEU	3.2
1	C	198	THR	3.2
1	A	96	LEU	3.2
2	D	428	GLU	3.2
1	C	217	ARG	3.2
2	D	429	THR	3.2
2	D	329	VAL	3.2
1	C	292	PRO	3.1
1	C	233	MET	3.1
1	C	41	THR	3.1
1	C	235	ASP	3.1
2	D	367	VAL	3.0
1	C	287	GLN	3.0
1	C	37	LEU	3.0
1	C	261	SER	3.0
1	C	14	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	378	ARG	2.9
2	D	179	HIS	2.9
2	D	320	LEU	2.9
1	C	210	ASP	2.9
1	C	237	LYS	2.9
1	C	264	SER	2.9
1	A	97	THR	2.9
3	F	12	ASN	2.9
2	D	399	LEU	2.9
1	C	73	GLU	2.9
1	C	223	ASP	2.8
1	C	258	ASP	2.8
2	D	302	LEU	2.8
3	F	3	LEU	2.8
1	C	205	GLY	2.8
1	C	204	PRO	2.8
2	D	372	TRP	2.8
2	D	325	ALA	2.8
2	D	197	VAL	2.7
1	A	94	SER	2.7
1	C	90	PHE	2.7
1	C	103	LEU	2.7
3	F	7	ARG	2.7
2	D	430	LEU	2.7
1	A	36	ARG	2.6
1	A	2	GLU	2.6
3	F	1	HIS	2.6
1	A	13	GLY	2.6
1	C	175	LEU	2.6
1	C	184	VAL	2.6
1	C	167	TRP	2.6
3	E	12	ASN	2.6
2	D	368	THR	2.6
1	C	36	ARG	2.6
1	C	254	PRO	2.6
1	C	13	GLY	2.6
2	D	370	GLN	2.6
1	C	111	LEU	2.6
1	C	219	LEU	2.6
1	C	269	TYR	2.6
1	A	74	ASN	2.6
2	D	363	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	40	GLU	2.5
2	D	366	THR	2.5
1	C	268	HIS	2.5
2	D	395	HIS	2.5
2	D	424	LEU	2.5
1	C	173	ILE	2.5
1	A	71	HIS	2.5
1	C	165	THR	2.5
1	C	71	HIS	2.5
1	A	0	SER	2.5
2	D	425	ASN	2.4
1	C	288	ASP	2.4
1	A	293	VAL	2.4
1	C	38	ASP	2.4
3	F	11	ASP	2.4
1	C	177[A]	CYS	2.4
1	C	98	GLY	2.4
1	C	202	LEU	2.4
1	C	144	ALA	2.4
1	C	239	SER	2.4
2	B	201	LYS	2.4
2	D	374	GLU	2.4
1	C	273	LYS	2.4
1	C	190	GLY	2.3
1	C	100	PRO	2.3
2	D	402	PRO	2.3
1	C	92	ASP	2.3
2	D	186	LEU	2.3
1	C	199	ARG	2.3
1	C	194	ALA	2.3
1	C	55	LEU	2.3
2	D	369	GLY	2.3
2	D	373	PRO	2.3
1	C	161	HIS	2.3
1	C	191	CYS	2.3
1	C	189	LEU	2.3
2	B	174	GLU	2.3
2	D	377	ILE	2.3
1	C	156	VAL	2.3
2	D	415	ASN	2.2
2	D	271	TYR	2.2
2	D	194	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	196	LYS	2.2
3	E	11	ASP	2.2
1	C	246	GLN	2.2
2	B	323	GLN	2.2
1	C	174	LEU	2.2
1	C	250	LYS	2.2
1	C	35	ILE	2.2
1	C	176	GLY	2.1
2	D	388	LYS	2.1
1	C	203	PHE	2.1
2	D	195	PRO	2.1
2	D	385	GLU	2.1
3	E	1	HIS	2.1
1	C	137	THR	2.1
2	D	280	TYR	2.1
1	C	139	GLY	2.1
2	D	421	VAL	2.1
1	C	87	LEU	2.1
2	D	384	LEU	2.1
2	D	394	LEU	2.1
1	C	99	ILE	2.1
1	C	275	ILE	2.1
1	C	272	ASN	2.0
1	C	17	VAL	2.0
1	C	154	VAL	2.0
2	D	391[A]	LEU	2.0
1	C	218	THR	2.0
2	D	426	PRO	2.0
1	A	16	GLY	2.0
1	C	116	ALA	2.0
2	D	259	ALA	2.0
2	D	264	ALA	2.0
1	C	94	SER	2.0
1	A	17	VAL	2.0
2	D	361	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPO	C	160	11/12	0.93	0.10	26,28,30,31	0
1	TPO	A	160	11/12	0.99	0.03	9,10,12,12	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

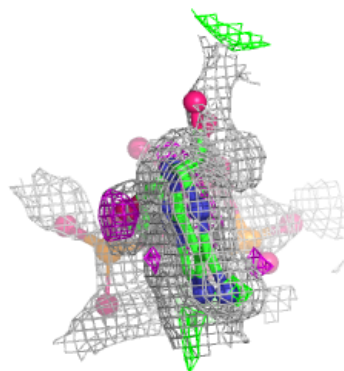
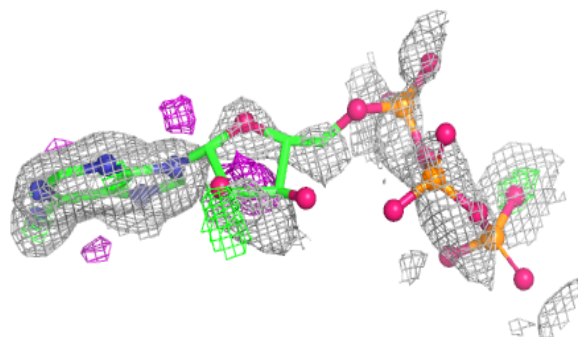
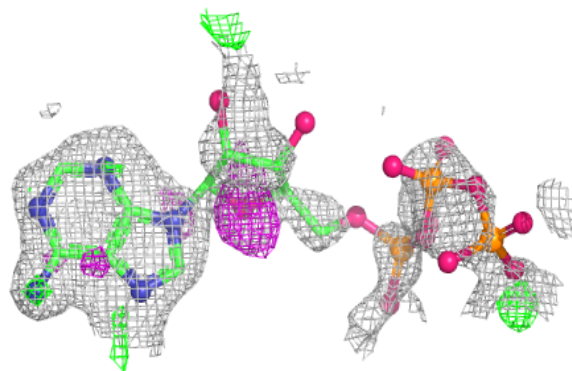
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ATP	C	1297[A]	31/31	0.61	0.23	64,68,78,78	31
4	ATP	C	1297[B]	31/31	0.61	0.23	65,70,79,79	31
4	ATP	A	1297[A]	31/31	0.64	0.30	62,64,74,75	31
4	ATP	A	1297[B]	31/31	0.64	0.30	63,68,79,79	31
6	GOL	A	1299	6/6	0.93	0.09	15,17,21,21	0
5	SO4	A	1298	5/5	0.97	0.16	18,19,20,22	5
6	GOL	A	1300	6/6	0.98	0.06	11,14,15,16	0

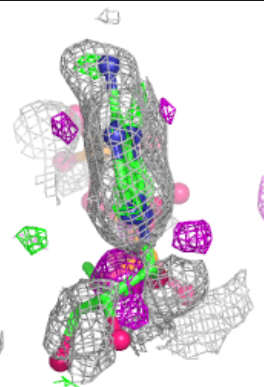
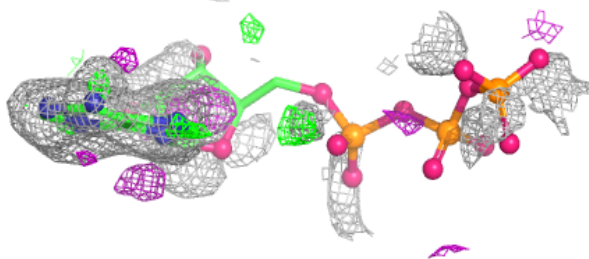
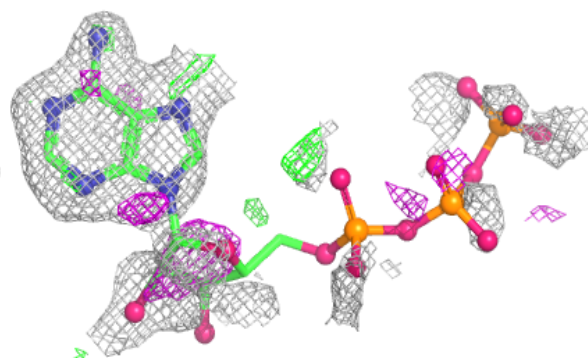
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 1297 (A):

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

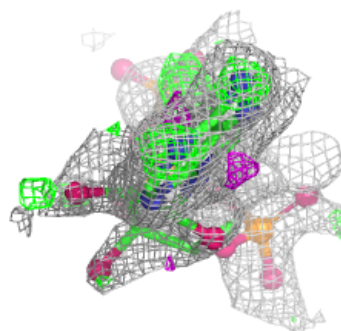
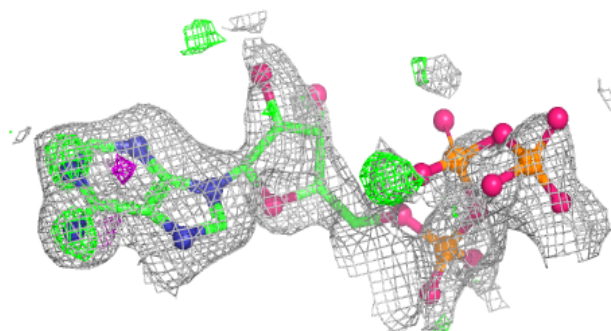
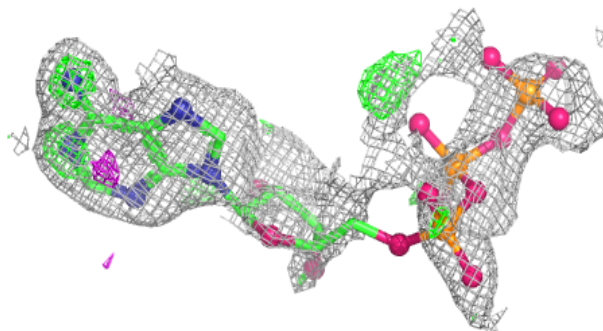
**Electron density around ATP C 1297 (B):**

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

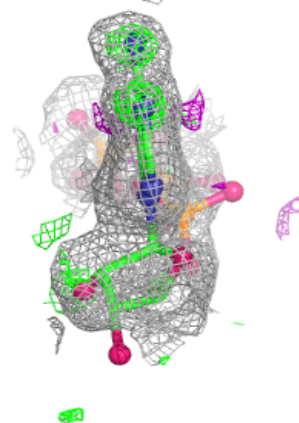
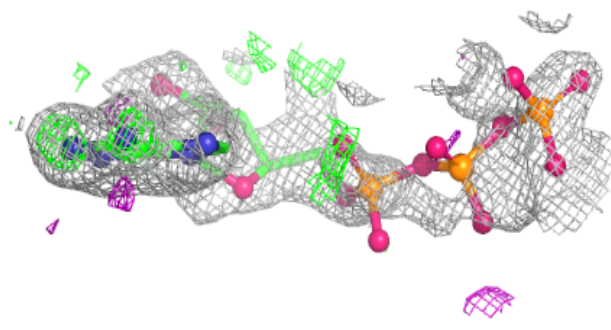
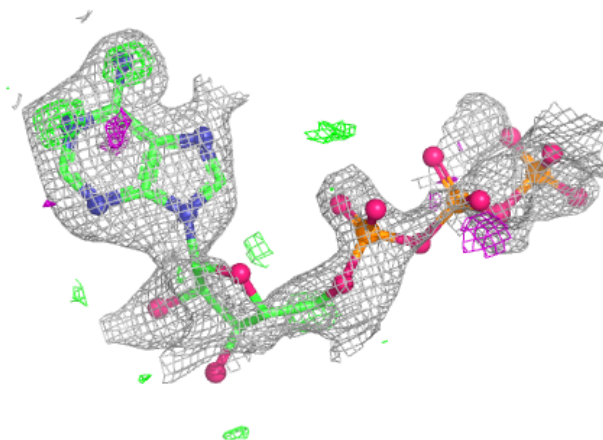


Electron density around ATP A 1297 (A):

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

**Electron density around ATP A 1297 (B):**

$2mF_o-DF_c$ (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.