



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:32 AM UTC

PDB ID : 2CJM / pdb_00002cjm
Title : Mechanism of CDK inhibition by active site phosphorylation: CDK2 Y15p
T160p in complex with cyclin A structure
Authors : Welburn, J.P.I.; Tucker, J.; Johnson, T.; Lindert, L.; Morgan, M.; Willis, A.;
Noble, M.E.M.; Endicott, J.A.
Deposited on : 2006-04-05
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

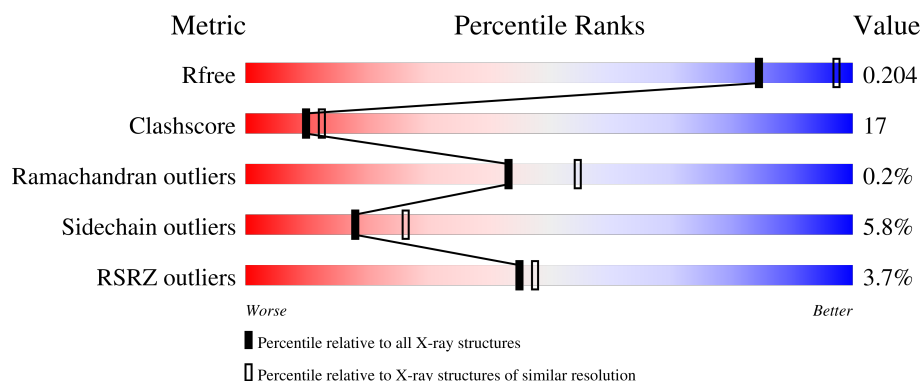
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	298	4% 65% 26% ...
1	C	298	5% 63% 31% 5%
2	B	258	2% 80% 17% .
2	D	258	3% 76% 22% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9528 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.

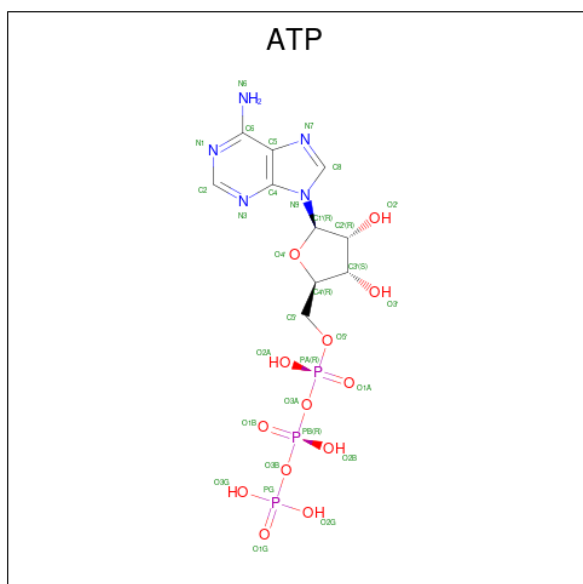
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	P	S	0	0	0
			2315	1502	392	411	2	8			
1	C	297	Total	C	N	O	P	S	0	0	1
			2387	1547	404	426	2	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2077	1345	338	383	11			
2	D	257	Total	C	N	O	S	0	0	0
			2077	1345	338	383	11			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

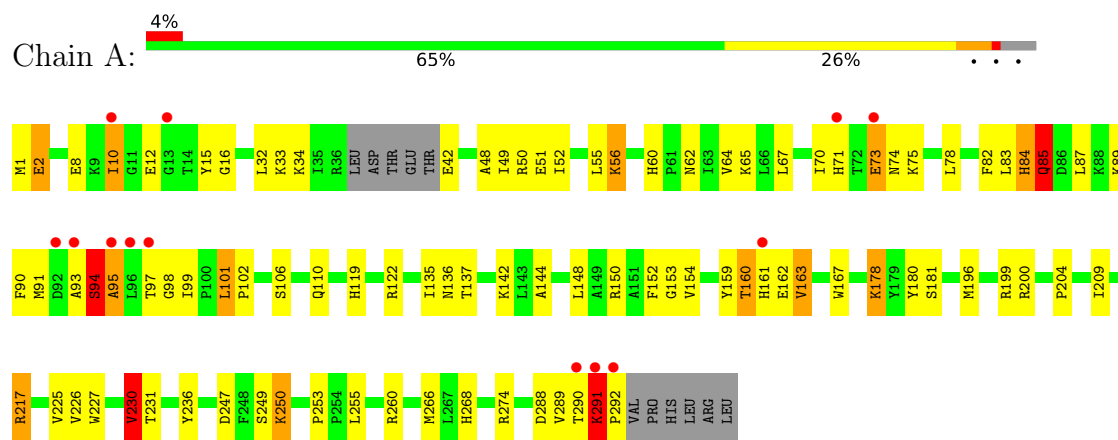
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	152	Total	O	0	0
			152	152		
5	C	156	Total	O	0	0
			156	156		
5	D	125	Total	O	0	0
			125	125		

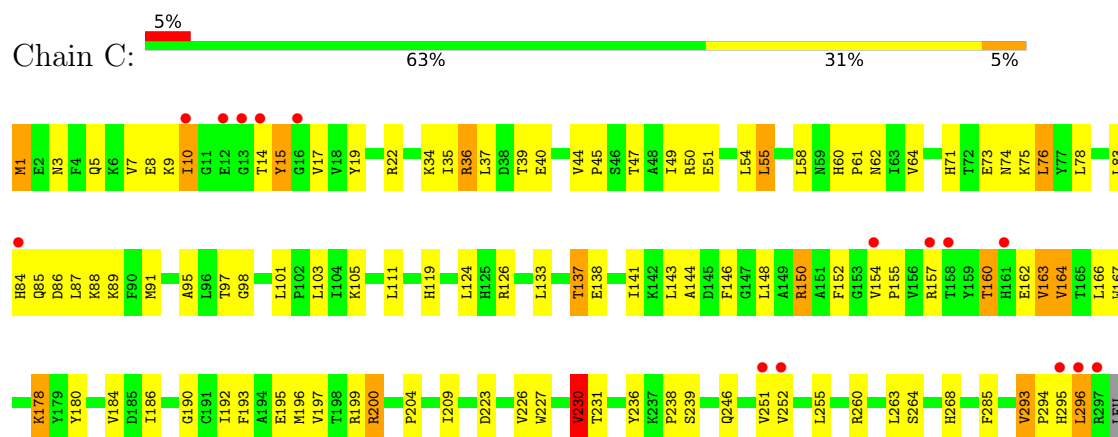
3 Residue-property plots [i](#)

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.

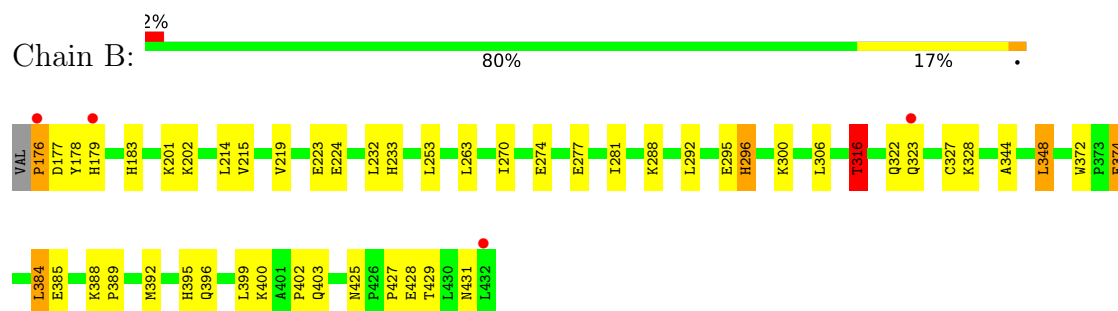
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



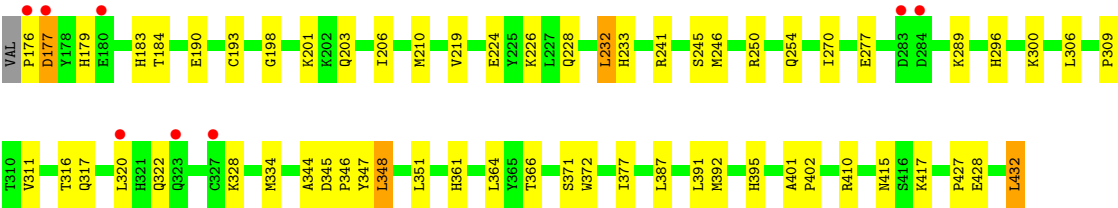
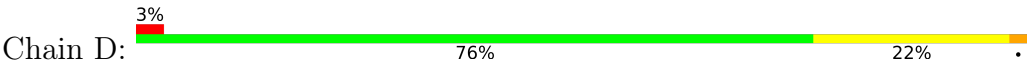
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 2: CYCLIN A2



● Molecule 2: CYCLIN A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.80Å 133.20Å 147.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 98.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (100.00-2.30) 88.6 (98.88-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.201 , 0.265 0.200 , 0.204	Depositor DCC
R_{free} test set	3195 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9528	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: ATP, PTR, TPO, MG

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	1.20	5/2344 (0.2%)	1.33	8/3174 (0.3%)
1	C	1.09	4/2419 (0.2%)	1.20	4/3281 (0.1%)
2	B	1.13	0/2127	1.18	1/2886 (0.0%)
2	D	1.00	0/2127	1.14	4/2886 (0.1%)
All	All	1.11	9/9017 (0.1%)	1.22	17/12227 (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	A	1	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	209	ILE	CA-CB	9.14	1.65	1.54
1	A	180	TYR	CA-C	6.94	1.61	1.52
1	A	93	ALA	CA-CB	6.50	1.63	1.53
1	C	186	ILE	CA-CB	6.41	1.62	1.54
1	A	291	LYS	CA-C	5.99	1.60	1.52
1	C	296	LEU	C-N	-5.93	1.25	1.33
1	A	204	PRO	CA-C	5.34	1.58	1.53
1	C	164	VAL	CA-CB	5.31	1.61	1.54
1	A	209	ILE	CA-CB	5.10	1.60	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	SER	N-CA-C	19.14	133.72	111.71
1	A	93	ALA	N-CA-C	10.54	122.52	111.14
1	A	85	GLN	N-CA-C	8.38	120.31	108.74
1	A	253	PRO	N-CA-C	6.64	118.80	110.70
1	A	217	ARG	NE-CZ-NH2	-6.54	113.31	119.20
1	C	230	VAL	N-CA-CB	6.52	117.75	110.51
2	D	347	TYR	N-CA-C	6.30	118.96	111.71
1	C	230	VAL	CB-CA-C	-6.15	104.00	111.88
1	C	74	ASN	N-CA-C	6.11	121.48	113.30
1	A	163	VAL	N-CA-C	5.84	121.48	109.34
1	A	217	ARG	CG-CD-NE	-5.55	99.78	112.00
2	B	316	THR	N-CA-CB	-5.47	102.08	110.12
2	D	311	VAL	CA-C-N	5.43	127.56	120.28
2	D	311	VAL	C-N-CA	5.43	127.56	120.28
2	D	364	LEU	N-CA-C	-5.19	105.54	111.14
1	A	230	VAL	CB-CA-C	-5.14	102.86	111.29
1	C	166	LEU	N-CA-C	5.09	117.22	111.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	94	SER	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	VAL	Peptide
1	A	94	SER	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	2315	0	2353	111	0
1	C	2387	0	2423	110	0
2	B	2077	0	2099	56	0
2	D	2077	0	2099	54	0
3	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	0	12	1	0
4	A	1	0	0	0	0
5	A	176	0	0	46	0
5	B	152	0	0	29	0
5	C	156	0	0	42	0
5	D	125	0	0	19	0
All	All	9528	0	8998	311	0

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 (311) 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)
2:B:176:PRO:HB3	5:B:2008:HOH:O	1.29	1.32
1:C:111:LEU:HD23	5:C:2078:HOH:O	1.30	1.25
2:B:327:CYS:HB2	5:B:2086:HOH:O	1.36	1.25
1:C:238:PRO:HD3	5:C:2127:HOH:O	1.35	1.23
1:A:71:HIS:HD2	2:B:296:HIS:CE1	1.60	1.20
1:A:73:GLU:HA	5:A:2036:HOH:O	1.38	1.19
1:A:10:ILE:HG21	5:A:2175:HOH:O	1.38	1.19
1:C:97:THR:HB	5:C:2062:HOH:O	1.41	1.17
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.63	1.17
2:D:250:ARG:HD2	5:D:2050:HOH:O	1.45	1.15
1:A:91:MET:HE1	1:A:196:MET:HA	1.22	1.15
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.67	1.10
1:A:71:HIS:CD2	2:B:296:HIS:HE1	1.72	1.08
1:C:268:HIS:HD2	5:C:2137:HOH:O	1.39	1.05
1:A:49:ILE:HD13	5:B:2050:HOH:O	1.56	1.04
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.38	1.03
1:A:181:SER:HB3	5:A:2102:HOH:O	1.58	1.02
1:A:78:LEU:HG	5:A:2039:HOH:O	1.59	1.02
1:C:146:PHE:HB3	5:C:2080:HOH:O	1.60	1.01
1:C:87:LEU:HB2	5:C:2075:HOH:O	1.60	1.01
1:A:290:THR:O	1:A:292:PRO:HD3	1.62	0.98
2:B:202:LYS:HD2	5:B:2023:HOH:O	1.62	0.98
1:A:167:TRP:HD1	5:A:2118:HOH:O	1.46	0.97
2:B:402:PRO:HD2	5:B:2128:HOH:O	1.64	0.96
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.51	0.95
1:C:19:TYR:CE1	5:C:2029:HOH:O	2.22	0.92
1:A:154:VAL:O	2:B:316:THR:HG22	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PRO:HA	2:B:179:HIS:CE1	2.07	0.90
1:C:154:VAL:O	2:D:316:THR:HG22	1.75	0.87
1:C:137:THR:HB	5:C:2077:HOH:O	1.75	0.86
2:B:374:GLU:HG3	5:B:2116:HOH:O	1.75	0.85
2:B:323:GLN:HB2	5:B:2112:HOH:O	1.76	0.85
1:C:252:VAL:HB	5:C:2133:HOH:O	1.77	0.85
1:C:10:ILE:HD11	5:C:2058:HOH:O	1.77	0.83
5:C:2070:HOH:O	2:D:309:PRO:HG3	1.78	0.83
1:C:148:LEU:HD22	5:C:2072:HOH:O	1.78	0.82
1:C:268:HIS:CD2	5:C:2137:HOH:O	2.22	0.82
1:A:161:HIS:HB2	5:A:2088:HOH:O	1.79	0.82
1:A:85:GLN:HE21	1:A:89:LYS:HE3	1.45	0.82
1:A:290:THR:HG22	5:A:2169:HOH:O	1.80	0.82
1:A:153:GLY:HA3	5:A:2075:HOH:O	1.80	0.81
2:D:334:MET:HG3	5:D:2088:HOH:O	1.80	0.81
1:C:1:MET:HG3	5:C:2009:HOH:O	1.79	0.80
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.12	0.80
2:B:263:LEU:HD23	5:B:2050:HOH:O	1.81	0.79
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.63	0.78
1:A:87:LEU:O	1:A:91:MET:HG3	1.84	0.78
1:A:95:ALA:O	1:A:199:ARG:HD2	1.83	0.78
1:A:290:THR:HA	5:A:2172:HOH:O	1.83	0.77
2:B:396:GLN:NE2	5:B:2125:HOH:O	2.17	0.77
1:A:227:TRP:O	1:A:230:VAL:HG22	1.85	0.77
2:D:277:GLU:HG3	5:D:2062:HOH:O	1.84	0.77
2:B:399:LEU:HD12	5:B:2125:HOH:O	1.85	0.76
2:D:428:GLU:HB3	5:D:2123:HOH:O	1.85	0.76
1:A:178:LYS:H	1:A:178:LYS:HZ2	1.32	0.76
1:A:71:HIS:HD2	2:B:296:HIS:HE1	0.85	0.76
1:A:91:MET:CE	1:A:196:MET:HA	2.12	0.76
2:B:403:GLN:HB3	5:B:2130:HOH:O	1.86	0.76
1:C:150:ARG:HD2	5:C:2082:HOH:O	1.85	0.75
1:C:36:ARG:HH21	1:C:75:LYS:HE2	1.52	0.75
1:A:119:HIS:HD2	5:B:2010:HOH:O	1.69	0.74
2:D:210:MET:CE	2:D:250:ARG:HB2	2.16	0.74
1:A:94:SER:OG	5:A:2048:HOH:O	2.06	0.74
1:C:239:SER:HB3	5:C:2130:HOH:O	1.87	0.73
2:D:328:LYS:HG3	5:D:2087:HOH:O	1.89	0.72
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.71	0.72
1:C:162:GLU:HG2	5:C:2092:HOH:O	1.88	0.72
2:B:176:PRO:HA	2:B:179:HIS:NE2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLY:CA	5:A:2075:HOH:O	2.37	0.71
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.55	0.71
1:A:161:HIS:NE2	1:A:162:GLU:OE1	2.23	0.71
1:C:3:ASN:HA	5:C:2004:HOH:O	1.91	0.71
2:B:277:GLU:HG3	5:B:2056:HOH:O	1.91	0.70
1:A:85:GLN:NE2	1:A:89:LYS:HE3	2.05	0.70
1:C:141:ILE:HD11	5:C:2075:HOH:O	1.90	0.70
1:A:288:ASP:HB3	5:A:2168:HOH:O	1.92	0.70
1:A:225:VAL:HG23	5:A:2127:HOH:O	1.91	0.69
1:A:60:HIS:HE1	5:A:2027:HOH:O	1.74	0.69
1:C:64:VAL:HG23	1:C:143:LEU:O	1.93	0.68
1:A:16:GLY:N	5:A:2007:HOH:O	2.26	0.68
1:C:119:HIS:HD2	5:D:2011:HOH:O	1.74	0.68
1:C:195:GLU:O	1:C:199:ARG:HA	1.94	0.68
2:B:224:GLU:HG3	5:B:2033:HOH:O	1.93	0.67
1:A:84:HIS:HB2	5:A:2042:HOH:O	1.95	0.67
1:C:227:TRP:CE3	1:C:230:VAL:HG13	2.29	0.67
1:A:95:ALA:O	1:A:199:ARG:CD	2.42	0.67
2:D:177:ASP:HB2	5:D:2009:HOH:O	1.95	0.67
1:A:78:LEU:CG	5:A:2039:HOH:O	2.30	0.66
2:D:176:PRO:HA	2:D:179:HIS:CG	2.30	0.66
1:A:291:LYS:O	5:A:2173:HOH:O	2.13	0.66
1:C:60:HIS:HD2	1:C:62:ASN:H	1.43	0.66
1:C:178:LYS:H	1:C:178:LYS:HD3	1.61	0.66
2:B:263:LEU:CD2	5:B:2050:HOH:O	2.40	0.65
1:A:90:PHE:O	1:A:95:ALA:HB2	1.96	0.65
2:B:395:HIS:HE1	2:B:427:PRO:O	1.78	0.65
2:B:399:LEU:CD1	5:B:2125:HOH:O	2.44	0.65
1:A:98:GLY:HA2	1:A:199:ARG:CZ	2.27	0.65
1:A:64:VAL:HB	5:A:2031:HOH:O	1.95	0.65
1:A:217:ARG:NH2	5:A:2121:HOH:O	2.21	0.65
2:D:322:GLN:HB2	5:D:2082:HOH:O	1.97	0.65
1:C:39:THR:HG22	1:C:40:GLU:OE2	1.97	0.64
2:D:210:MET:HE1	2:D:250:ARG:CB	2.23	0.64
1:A:290:THR:CG2	5:A:2169:HOH:O	2.40	0.64
1:C:260:ARG:HD3	5:C:2135:HOH:O	1.99	0.63
1:A:84:HIS:N	1:A:84:HIS:ND1	2.46	0.63
2:B:224:GLU:CG	5:B:2033:HOH:O	2.47	0.62
1:C:190:GLY:HA2	5:C:2109:HOH:O	1.99	0.62
2:B:431:ASN:O	5:B:2152:HOH:O	2.16	0.62
1:C:54:LEU:HB3	5:C:2038:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLU:HB2	5:C:2093:HOH:O	1.99	0.62
1:A:60:HIS:CD2	1:A:62:ASN:H	2.17	0.62
1:A:94:SER:CA	1:A:95:ALA:HB2	2.31	0.61
5:A:2035:HOH:O	2:B:300:LYS:HE2	2.00	0.61
2:D:226:LYS:HE2	5:D:2042:HOH:O	2.00	0.61
1:A:51:GLU:O	1:A:55:LEU:HB2	2.01	0.60
1:A:163:VAL:HG22	5:A:2090:HOH:O	2.02	0.60
1:C:1:MET:CE	5:C:2009:HOH:O	2.50	0.60
1:C:60:HIS:CD2	1:C:62:ASN:H	2.18	0.60
1:A:10:ILE:O	1:A:10:ILE:HG13	2.00	0.60
1:A:90:PHE:O	1:A:95:ALA:CB	2.50	0.60
2:B:328:LYS:HD3	5:B:2140:HOH:O	2.02	0.60
1:A:159:TYR:CE2	5:A:2084:HOH:O	2.51	0.59
1:A:181:SER:CB	5:A:2102:HOH:O	2.33	0.59
1:C:197:VAL:HG11	1:C:252:VAL:HG12	1.82	0.59
1:A:148:LEU:HD13	5:A:2090:HOH:O	2.00	0.59
1:A:154:VAL:O	2:B:316:THR:CG2	2.46	0.59
2:D:392:MET:HE3	2:D:432:LEU:HD12	1.85	0.59
1:A:60:HIS:HD2	1:A:62:ASN:H	1.51	0.59
2:B:392:MET:HE2	2:B:392:MET:HA	1.85	0.59
2:B:372:TRP:CB	2:B:384:LEU:HD13	2.33	0.59
1:C:85:GLN:HB2	1:C:89:LYS:HD3	1.85	0.59
1:C:294:PRO:HG2	1:C:296:LEU:HD11	1.85	0.59
1:C:51:GLU:O	1:C:55:LEU:HB2	2.02	0.59
2:B:322:GLN:HG2	5:B:2082:HOH:O	2.01	0.58
1:C:239:SER:CB	5:C:2130:HOH:O	2.48	0.58
1:A:33:LYS:NZ	5:A:2015:HOH:O	2.36	0.58
2:B:323:GLN:HG2	5:B:2081:HOH:O	2.04	0.58
1:A:148:LEU:HB3	5:A:2090:HOH:O	2.02	0.58
1:A:91:MET:HE2	1:A:199:ARG:HG3	1.85	0.58
2:D:224:GLU:HG2	5:D:2041:HOH:O	2.02	0.58
2:D:387:LEU:O	2:D:391:LEU:HB2	2.03	0.58
2:B:328:LYS:HE3	5:B:2087:HOH:O	2.03	0.58
1:C:227:TRP:O	1:C:230:VAL:HG22	2.03	0.58
1:A:85:GLN:HE22	1:A:89:LYS:HG2	1.68	0.58
2:D:201:LYS:HD3	5:D:2018:HOH:O	2.03	0.57
2:D:296:HIS:CE1	5:D:2071:HOH:O	2.56	0.57
1:C:22:ARG:HD2	5:C:2023:HOH:O	2.05	0.57
2:B:233:HIS:HD2	5:B:2076:HOH:O	1.85	0.57
1:C:105:LYS:HE2	1:C:285:PHE:O	2.04	0.57
1:C:36:ARG:NH2	1:C:75:LYS:HE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:HD22	1:C:44:VAL:HG22	1.86	0.57
1:A:78:LEU:CD2	5:A:2039:HOH:O	2.50	0.57
1:A:150:ARG:NH2	5:A:2072:HOH:O	2.37	0.57
1:C:295:HIS:HB3	5:C:2151:HOH:O	2.05	0.57
1:A:94:SER:CA	1:A:95:ALA:CB	2.83	0.56
2:D:366:THR:HG23	2:D:427:PRO:HD3	1.87	0.56
3:A:1294:ATP:H5'1	3:A:1294:ATP:H8	1.70	0.56
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.87	0.56
1:C:86:ASP:OD1	1:C:88:LYS:HB3	2.05	0.56
1:A:167:TRP:CD1	5:A:2118:HOH:O	2.33	0.56
2:D:190:GLU:HG3	2:D:351:LEU:HD22	1.88	0.56
1:A:16:GLY:HA3	1:A:34:LYS:O	2.06	0.56
1:C:263:LEU:HD12	5:C:2109:HOH:O	2.06	0.56
1:A:266:MET:O	1:A:274:ARG:HD3	2.05	0.56
1:C:58:LEU:HD12	5:C:2038:HOH:O	2.06	0.56
1:C:83:LEU:O	3:C:1298:ATP:H2	1.89	0.56
1:C:246:GLN:HG3	1:C:251:VAL:CG2	2.36	0.56
1:A:291:LYS:HG2	5:A:2173:HOH:O	2.06	0.55
1:C:164:VAL:HG13	5:C:2073:HOH:O	2.06	0.55
1:C:294:PRO:HG2	1:C:296:LEU:CD1	2.35	0.55
1:C:126:ARG:HB3	1:C:163:VAL:CG2	2.37	0.55
2:D:201:LYS:HE2	5:D:2002:HOH:O	2.06	0.55
2:B:372:TRP:HB3	2:B:384:LEU:HD13	1.87	0.55
1:C:143:LEU:HD23	5:C:2078:HOH:O	2.07	0.54
1:A:84:HIS:CE1	5:A:2066:HOH:O	2.59	0.54
2:D:233:HIS:HD2	5:D:2077:HOH:O	1.90	0.54
1:A:48:ALA:O	1:A:52:ILE:HG13	2.08	0.54
1:A:74:ASN:O	1:A:75:LYS:HG3	2.08	0.54
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.43	0.54
1:C:37:LEU:HD21	1:C:76:LEU:HD22	1.91	0.53
1:C:7:VAL:HG12	1:C:8:GLU:HG2	1.89	0.53
1:C:178:LYS:H	1:C:178:LYS:CD	2.20	0.53
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.89	0.53
1:A:231:THR:HA	1:A:236:TYR:CD1	2.44	0.53
5:A:2072:HOH:O	2:B:270:ILE:HG13	2.07	0.53
2:B:425:ASN:ND2	5:B:2144:HOH:O	2.40	0.53
1:C:180:TYR:HB2	1:C:184:VAL:CG1	2.39	0.53
1:C:178:LYS:HD3	1:C:178:LYS:N	2.24	0.52
1:C:162:GLU:HA	5:C:2095:HOH:O	2.09	0.52
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.75	0.52
1:C:103:LEU:HD21	1:C:294:PRO:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:HB2	1:A:292:PRO:HD2	1.92	0.52
2:B:215:VAL:O	2:B:219:VAL:HG23	2.10	0.52
1:C:58:LEU:CD1	5:C:2038:HOH:O	2.57	0.51
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.92	0.51
5:A:2072:HOH:O	2:B:270:ILE:CG1	2.58	0.51
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.91	0.51
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.91	0.51
1:C:9:LYS:HG3	1:C:17:VAL:CG1	2.41	0.51
2:D:402:PRO:HB2	5:D:2113:HOH:O	2.10	0.51
1:A:91:MET:HA	1:A:95:ALA:HB1	1.92	0.51
1:A:91:MET:HE3	1:A:99:ILE:HD11	1.93	0.51
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.45	0.51
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.40	0.51
1:A:268:HIS:CE1	5:A:2128:HOH:O	2.63	0.51
1:A:150:ARG:CG	5:A:2084:HOH:O	2.59	0.50
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.93	0.50
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.47	0.50
1:C:227:TRP:CD2	1:C:230:VAL:HG13	2.47	0.50
2:B:176:PRO:HA	2:B:179:HIS:CD2	2.47	0.50
1:C:5:GLN:HG3	5:C:2008:HOH:O	2.12	0.49
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.47	0.49
1:A:249:SER:HA	1:A:260:ARG:HD2	1.93	0.49
1:C:91:MET:HE3	1:C:196:MET:HG2	1.93	0.49
2:D:392:MET:CE	2:D:432:LEU:HD12	2.42	0.49
2:B:263:LEU:HD21	2:B:295:GLU:HG3	1.94	0.49
1:C:195:GLU:O	1:C:199:ARG:N	2.46	0.49
1:C:154:VAL:HB	2:D:317:GLN:HG2	1.94	0.49
1:C:98:GLY:HA2	1:C:199:ARG:CZ	2.42	0.48
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.94	0.48
1:A:91:MET:HE3	1:A:99:ILE:CD1	2.43	0.48
1:C:95:ALA:HA	5:C:2060:HOH:O	2.12	0.48
2:D:395:HIS:HE1	2:D:427:PRO:O	1.96	0.48
2:D:176:PRO:HA	2:D:179:HIS:CD2	2.48	0.48
1:A:97:THR:HG23	1:A:98:GLY:O	2.13	0.48
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.96	0.48
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.96	0.48
1:C:133:LEU:HB2	5:C:2075:HOH:O	2.14	0.48
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.96	0.48
1:A:2:GLU:HG3	1:C:73:GLU:OE2	2.14	0.47
1:A:85:GLN:HG3	1:A:135:ILE:CG1	2.44	0.47
2:B:396:GLN:CD	5:B:2125:HOH:O	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLU:O	1:C:199:ARG:CA	2.62	0.47
1:A:10:ILE:O	1:A:10:ILE:CG1	2.62	0.47
1:C:180:TYR:HB2	1:C:184:VAL:HG11	1.95	0.47
1:C:15:PTR:CE2	1:C:47:THR:HG21	2.45	0.47
1:C:193:PHE:HD2	5:C:2109:HOH:O	1.98	0.47
2:D:203:GLN:HB3	2:D:206:ILE:HG12	1.96	0.47
1:A:83:LEU:HD21	1:A:142:LYS:HE3	1.96	0.47
1:A:250:LYS:HE3	5:A:2152:HOH:O	2.15	0.47
2:B:388:LYS:O	2:B:392:MET:HG2	2.15	0.47
1:C:152:PHE:HA	5:C:2082:HOH:O	2.15	0.46
1:C:223:ASP:H	1:C:226:VAL:HG12	1.80	0.46
2:D:254:GLN:NE2	5:D:2054:HOH:O	2.42	0.46
1:A:247:ASP:HB3	5:A:2149:HOH:O	2.14	0.46
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.97	0.46
2:B:385:GLU:HG2	5:B:2121:HOH:O	2.14	0.46
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.97	0.46
1:C:154:VAL:C	2:D:316:THR:HG22	2.41	0.46
1:C:197:VAL:CG1	1:C:252:VAL:CG1	2.89	0.46
1:A:161:HIS:CE1	1:A:162:GLU:OE1	2.69	0.46
2:D:344:ALA:HB1	2:D:348:LEU:CD2	2.42	0.46
2:B:431:ASN:N	5:B:2150:HOH:O	2.47	0.46
1:A:91:MET:HB2	5:A:2047:HOH:O	2.15	0.46
2:D:415:ASN:HA	5:D:2119:HOH:O	2.16	0.45
1:A:159:TYR:HA	5:A:2072:HOH:O	2.16	0.45
1:C:138:GLU:HA	1:C:293:VAL:HG22	1.98	0.45
1:A:85:GLN:HE21	1:A:85:GLN:HB2	1.26	0.45
1:C:157:ARG:NH2	2:D:228:GLN:HG3	2.32	0.45
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.47	0.45
1:A:1:MET:HE1	1:A:32:LEU:HD13	1.99	0.45
2:D:361:HIS:C	2:D:361:HIS:CD2	2.95	0.45
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.98	0.45
2:D:345:ASP:HA	2:D:346:PRO:HA	1.80	0.45
2:B:183:HIS:HD2	5:B:2014:HOH:O	2.00	0.45
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.85	0.45
1:A:10:ILE:HG12	3:A:1294:ATP:H1'	1.99	0.44
1:C:197:VAL:CG1	1:C:252:VAL:HG13	2.48	0.44
1:A:73:GLU:O	1:A:74:ASN:CB	2.64	0.44
1:A:10:ILE:HD11	5:A:2041:HOH:O	2.17	0.43
2:B:177:ASP:HB3	2:B:178:TYR:CD2	2.53	0.43
1:A:52:ILE:CD1	1:A:78:LEU:HD21	2.49	0.43
1:A:150:ARG:HG3	5:A:2084:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PRO:HD3	2:D:320:LEU:HD21	2.00	0.43
1:C:50:ARG:O	1:C:54:LEU:HG	2.19	0.43
1:C:111:LEU:HD22	1:C:133:LEU:HD22	1.99	0.43
1:A:65:LYS:HG2	1:A:67:LEU:HD23	2.00	0.43
1:C:126:ARG:HB3	1:C:163:VAL:HG21	1.99	0.43
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.54	0.43
2:B:428:GLU:HG3	2:B:429:THR:H	1.83	0.43
1:C:1:MET:HE3	5:C:2009:HOH:O	2.16	0.43
1:C:64:VAL:HG21	1:C:144:ALA:CB	2.46	0.43
1:C:163:VAL:HG23	5:C:2072:HOH:O	2.19	0.43
5:C:2051:HOH:O	2:D:300:LYS:HE2	2.19	0.42
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.02	0.42
1:C:160:TPO:OG1	2:D:270:ILE:HG23	2.18	0.42
2:B:428:GLU:HG2	5:B:2147:HOH:O	2.18	0.42
1:C:84:HIS:ND1	1:C:84:HIS:N	2.64	0.42
1:C:231:THR:HA	1:C:236:TYR:CD1	2.54	0.42
1:C:97:THR:CG2	5:C:2063:HOH:O	2.67	0.42
2:D:193:CYS:O	2:D:241:ARG:HD2	2.20	0.42
2:D:226:LYS:CE	5:D:2042:HOH:O	2.63	0.42
1:A:50:ARG:HB3	5:A:2070:HOH:O	2.19	0.42
2:D:184:THR:HG22	5:D:2014:HOH:O	2.20	0.41
1:A:82:PHE:HE2	1:A:84:HIS:CD2	2.38	0.41
2:D:371:SER:O	2:D:372:TRP:C	2.63	0.41
1:A:106:SER:O	1:A:110:GLN:HG3	2.19	0.41
1:C:195:GLU:HG3	1:C:200:ARG:C	2.46	0.41
2:B:288:LYS:O	2:B:292:LEU:HG	2.21	0.41
1:A:90:PHE:O	1:A:94:SER:N	2.52	0.41
1:A:247:ASP:CB	5:A:2149:HOH:O	2.68	0.41
1:A:161:HIS:ND1	5:A:2087:HOH:O	2.36	0.41
1:A:178:LYS:H	1:A:178:LYS:CD	2.34	0.41
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.56	0.41
1:A:160:TPO:O1P	2:B:270:ILE:HA	2.21	0.41
2:B:400:LYS:O	2:B:403:GLN:HG2	2.21	0.41
1:A:56:LYS:HE3	1:A:56:LYS:HB3	1.72	0.40
1:A:94:SER:N	1:A:95:ALA:HB3	2.36	0.40
1:C:227:TRP:CE3	1:C:230:VAL:CG1	3.02	0.40
2:D:198:GLY:O	2:D:201:LYS:HG2	2.20	0.40
2:B:428:GLU:HG3	2:B:429:THR:N	2.36	0.40

There are no symmetry-related clashes.

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	281/298 (94%)	263 (94%)	16 (6%)	2 (1%)	18	23
1	C	293/298 (98%)	281 (96%)	12 (4%)	0	100	100
2	B	255/258 (99%)	247 (97%)	8 (3%)	0	100	100
2	D	255/258 (99%)	249 (98%)	6 (2%)	0	100	100
All	All	1084/1112 (98%)	1040 (96%)	42 (4%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ALA
1	A	291	LYS

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	250/261 (96%)	232 (93%)	18 (7%)	13	18
1	C	259/261 (99%)	241 (93%)	18 (7%)	14	20
2	B	231/232 (100%)	220 (95%)	11 (5%)	23	35
2	D	231/232 (100%)	222 (96%)	9 (4%)	28	43
All	All	971/986 (98%)	915 (94%)	56 (6%)	18	26

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	8	GLU
1	A	10	ILE
1	A	12	GLU
1	A	42	GLU
1	A	56	LYS
1	A	70	ILE
1	A	73	GLU
1	A	84	HIS
1	A	85	GLN
1	A	101	LEU
1	A	137	THR
1	A	178	LYS
1	A	200	ARG
1	A	226	VAL
1	A	230	VAL
1	A	250	LYS
1	A	255	LEU
2	B	176	PRO
2	B	201	LYS
2	B	223	GLU
2	B	232	LEU
2	B	274	GLU
2	B	281	ILE
2	B	296	HIS
2	B	316	THR
2	B	348	LEU
2	B	374	GLU
2	B	384	LEU
1	C	1	MET
1	C	10	ILE
1	C	14	THR
1	C	34	LYS
1	C	35	ILE
1	C	36	ARG
1	C	55	LEU
1	C	76	LEU
1	C	78	LEU
1	C	101	LEU
1	C	137	THR
1	C	150	ARG
1	C	163	VAL
1	C	178	LYS

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Mol	Chain	Res	Type
1	C	200	ARG
1	C	230	VAL
1	C	264	SER
1	C	293	VAL
2	D	177	ASP
2	D	232	LEU
2	D	245	SER
2	D	246	MET
2	D	289	LYS
2	D	348	LEU
2	D	377	ILE
2	D	417	LYS
2	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	62	ASN
1	A	71	HIS
1	A	74	ASN
1	A	85	GLN
1	A	119	HIS
1	A	246	GLN
1	A	265	GLN
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	395	HIS
2	B	396	GLN
2	B	425	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	85	GLN
1	C	119	HIS
1	C	265	GLN
2	D	208	ASN
2	D	233	HIS
2	D	254	GLN

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Mol	Chain	Res	Type
2	D	296	HIS
2	D	317	GLN
2	D	395	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	A	160	1	8,10,11	1.77	1 (12%)	10,14,16	1.09	1 (10%)
1	PTR	C	15	1	15,16,17	2.10	2 (13%)	17,22,24	0.61	1 (5%)
1	TPO	C	160	1	8,10,11	1.18	1 (12%)	10,14,16	1.41	2 (20%)
1	PTR	A	15	1	15,16,17	1.95	1 (6%)	17,22,24	0.68	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	A	160	1	-	0/9/11/13	-
1	PTR	C	15	1	-	2/10/11/13	0/1/1/1
1	TPO	C	160	1	-	0/9/11/13	-
1	PTR	A	15	1	-	1/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	PTR	OH-CZ	-7.55	1.23	1.40
1	A	15	PTR	OH-CZ	-7.07	1.24	1.40
1	A	160	TPO	P-OG1	4.14	1.66	1.59
1	C	15	PTR	P-OH	2.26	1.63	1.59
1	C	160	TPO	P-OG1	2.22	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O3P-P-O2P	2.97	118.93	107.80
1	A	160	TPO	O3P-P-O2P	2.08	115.59	107.80
1	C	15	PTR	O2P-P-OH	2.01	111.27	105.32
1	C	160	TPO	O2P-P-OG1	-2.01	98.02	105.85

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	15	PTR	C-CA-CB-CG
1	C	15	PTR	O-C-CA-CB
1	C	15	PTR	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	1	0
1	C	15	PTR	1	0
1	C	160	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
3	ATP	A	1294	4	32,33,33	1.85	6 (18%)	48,52,52	1.69	9 (18%)
3	ATP	C	1298	-	32,33,33	1.87	7 (21%)	48,52,52	1.79	8 (16%)

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
3	ATP	A	1294	4	-	7/22/38/38	0/3/3/3
3	ATP	C	1298	-	-	9/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	ATP	C5-C4	5.28	1.48	1.39
3	A	1294	ATP	C5-C4	5.11	1.48	1.39
3	C	1298	ATP	PB-O3B	4.57	1.64	1.59
3	A	1294	ATP	PB-O3A	4.33	1.64	1.59
3	C	1298	ATP	PB-O3A	4.04	1.63	1.59
3	A	1294	ATP	PA-O3A	4.03	1.63	1.59
3	C	1298	ATP	PA-O3A	3.72	1.63	1.59
3	A	1294	ATP	PB-O3B	3.56	1.63	1.59
3	A	1294	ATP	C5-C6	3.18	1.49	1.41
3	C	1298	ATP	C5-C6	2.95	1.49	1.41
3	C	1298	ATP	C8-N7	2.41	1.36	1.31
3	C	1298	ATP	C5-N7	-2.22	1.35	1.39
3	A	1294	ATP	C5-N7	-2.01	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	ATP	C5-C4-N3	-6.32	118.02	126.72
3	A	1294	ATP	C5-C4-N3	-5.43	119.24	126.72
3	C	1298	ATP	N3-C4-N9	4.77	135.28	127.17
3	A	1294	ATP	N3-C4-N9	4.36	134.59	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	ATP	C2-N3-C4	3.87	121.28	111.83
3	A	1294	ATP	C2-N3-C4	3.51	120.40	111.83
3	C	1298	ATP	C4-C5-N7	-3.46	106.63	110.58
3	A	1294	ATP	O4'-C1'-N9	3.38	114.58	108.09
3	A	1294	ATP	C4-C5-N7	-3.24	106.87	110.58
3	C	1298	ATP	N3-C2-N1	-3.19	123.75	128.58
3	A	1294	ATP	N3-C2-N1	-3.00	124.04	128.58
3	C	1298	ATP	C3'-C2'-C1'	2.56	106.31	101.46
3	C	1298	ATP	C5-N7-C8	2.35	107.15	103.45
3	A	1294	ATP	C5-N7-C8	2.29	107.05	103.45
3	A	1294	ATP	C4-N9-C8	2.24	108.09	105.74
3	A	1294	ATP	C6-C5-N7	2.11	136.16	132.09
3	C	1298	ATP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

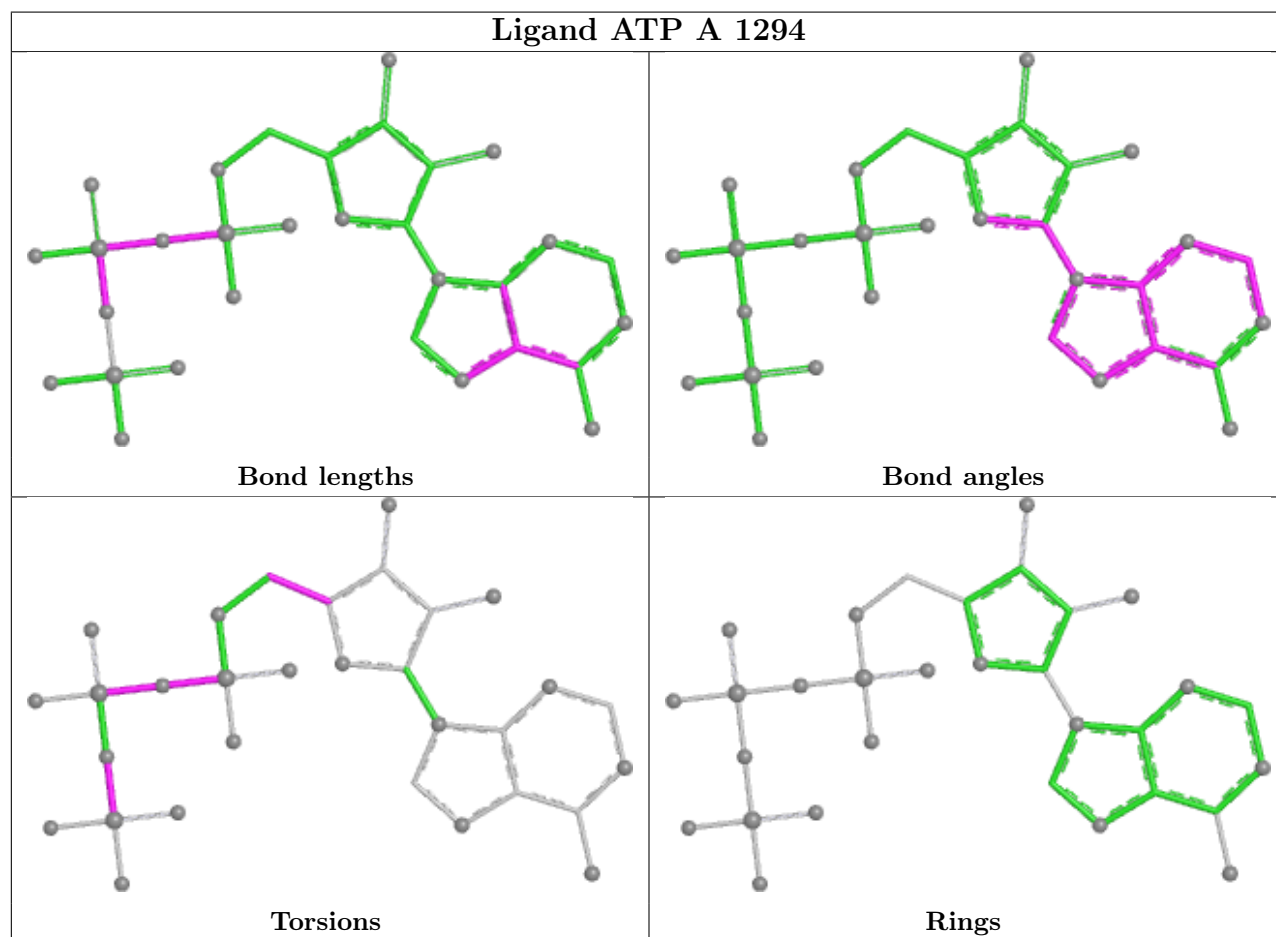
Mol	Chain	Res	Type	Atoms
3	A	1294	ATP	PB-O3B-PG-O2G
3	C	1298	ATP	PB-O3B-PG-O2G
3	C	1298	ATP	C5'-O5'-PA-O1A
3	C	1298	ATP	C5'-O5'-PA-O3A
3	C	1298	ATP	O4'-C4'-C5'-O5'
3	C	1298	ATP	C3'-C4'-C5'-O5'
3	C	1298	ATP	C5'-O5'-PA-O2A
3	A	1294	ATP	PA-O3A-PB-O2B
3	A	1294	ATP	O4'-C4'-C5'-O5'
3	C	1298	ATP	PB-O3B-PG-O1G
3	C	1298	ATP	PB-O3A-PA-O1A
3	A	1294	ATP	PB-O3A-PA-O5'
3	A	1294	ATP	PB-O3B-PG-O1G
3	A	1294	ATP	PB-O3B-PG-O3G
3	A	1294	ATP	PB-O3A-PA-O2A
3	C	1298	ATP	PB-O3A-PA-O2A

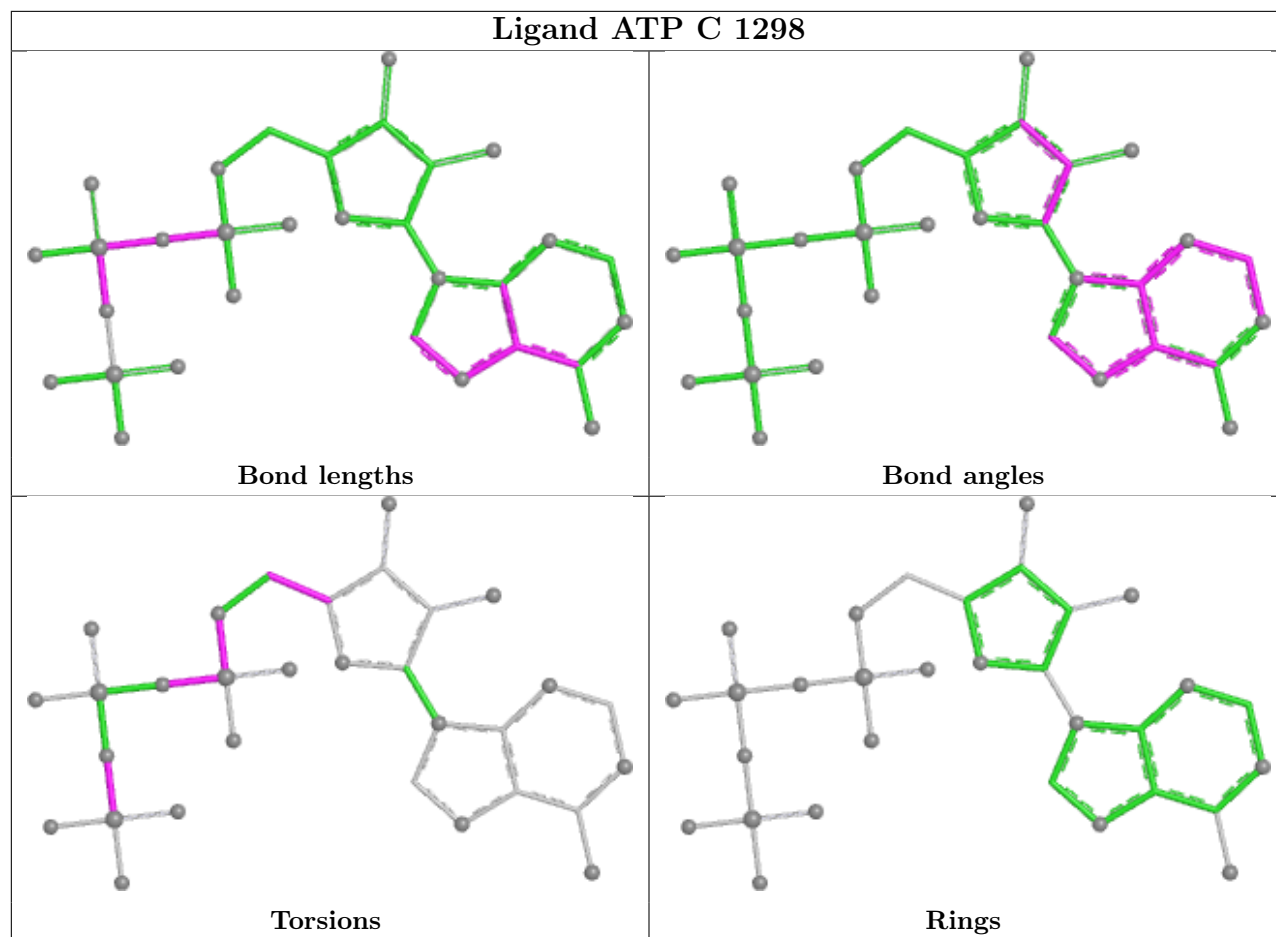
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1294	ATP	2	0
3	C	1298	ATP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/298 (95%)	-0.00	13 (4%) 37 39	14, 26, 52, 62	0
1	C	295/298 (98%)	0.18	15 (5%) 33 35	20, 34, 54, 74	0
2	B	257/258 (99%)	-0.17	4 (1%) 70 72	16, 28, 45, 62	0
2	D	257/258 (99%)	0.15	8 (3%) 51 53	19, 35, 55, 64	0
All	All	1094/1112 (98%)	0.04	40 (3%) 45 48	14, 31, 54, 74	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	5.7
2	D	176	PRO	4.9
1	A	291	LYS	4.5
1	A	290	THR	4.0
2	D	323	GLN	3.9
2	D	327	CYS	3.7
2	B	179	HIS	3.5
1	A	13	GLY	3.4
1	C	10	ILE	3.3
1	C	13	GLY	3.2
1	C	157	ARG	3.2
1	C	297	ARG	3.1
1	A	73	GLU	3.1
1	C	154	VAL	3.1
1	C	158	THR	3.0
1	C	251	VAL	2.9
1	A	95	ALA	2.9
1	C	12	GLU	2.8
1	C	295	HIS	2.8
1	A	97	THR	2.8
2	D	177	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	432	LEU	2.8
1	A	292	PRO	2.6
1	C	16	GLY	2.6
1	A	93	ALA	2.5
2	B	176	PRO	2.5
1	C	161	HIS	2.4
1	A	92	ASP	2.3
2	D	284	ASP	2.3
2	D	283	ASP	2.3
1	C	252	VAL	2.3
1	C	14	THR	2.2
1	A	10	ILE	2.2
2	B	323	GLN	2.2
2	D	180	GLU	2.1
1	A	161	HIS	2.1
1	C	84	HIS	2.1
1	A	71	HIS	2.1
1	C	296	LEU	2.0
2	D	320	LEU	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(Å ²)	Q<0.9
1	PTR	C	15	16/17	0.77	0.20	66,74,87,87	0
1	PTR	A	15	16/17	0.82	0.16	56,61,72,72	0
1	TPO	A	160	11/12	0.94	0.12	33,38,41,41	0
1	TPO	C	160	11/12	0.95	0.19	40,47,51,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

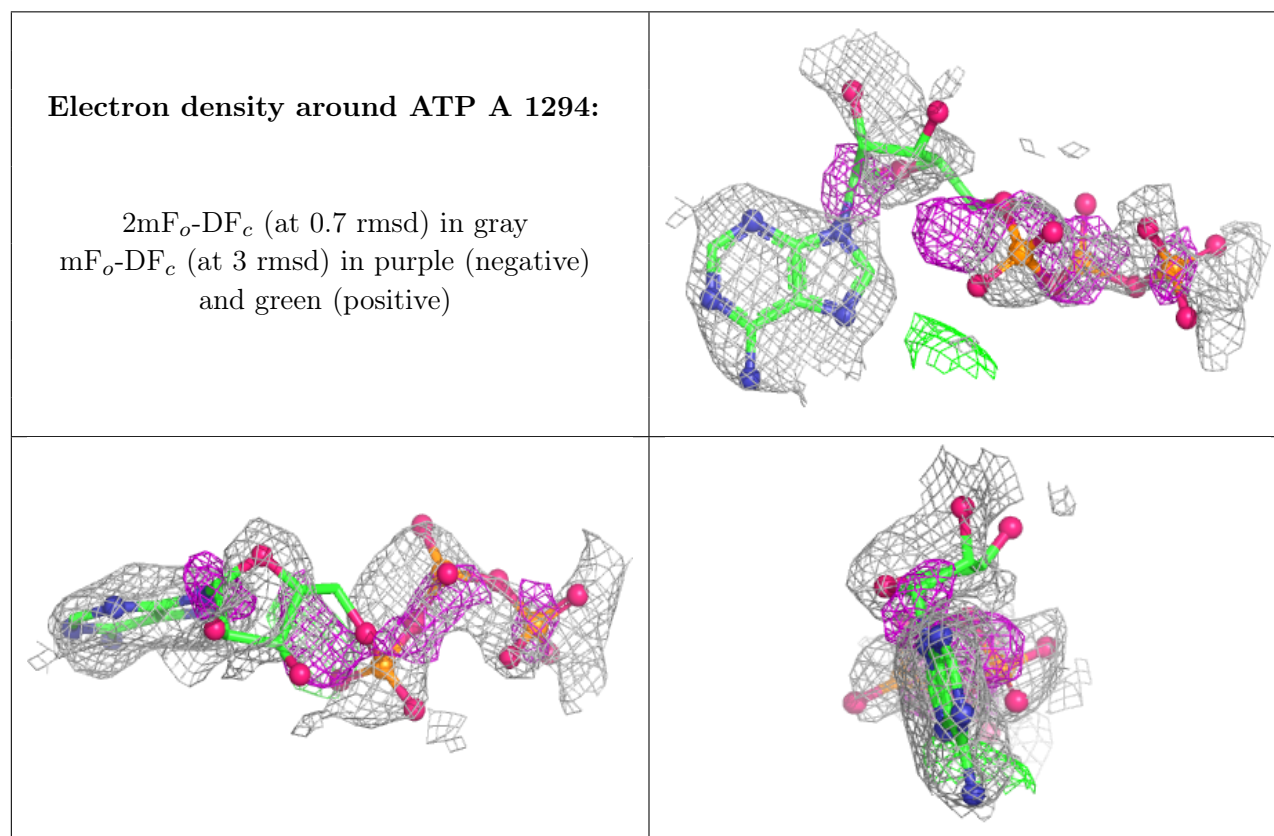
6.4 Ligands [i](#)

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.

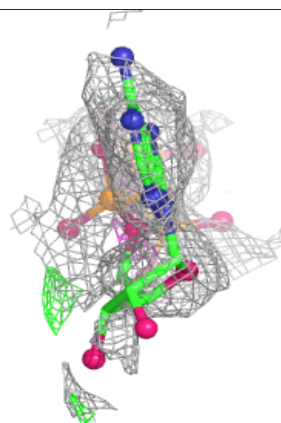
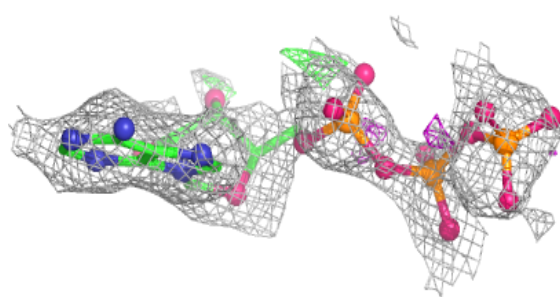
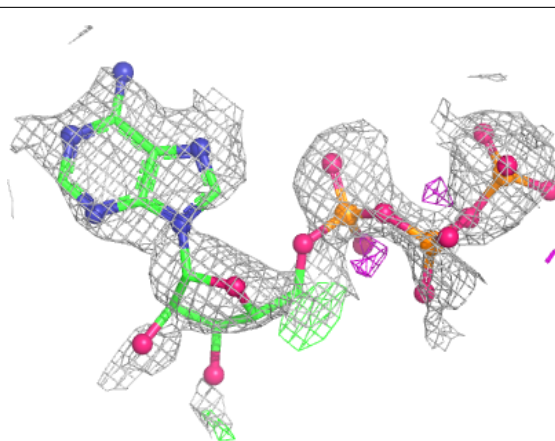
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	A	1294	31/31	0.70	0.17	58,77,103,104	0
3	ATP	C	1298	31/31	0.74	0.19	99,108,115,115	0
4	MG	A	1295	1/1	0.74	0.16	68,68,68,68	0

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 1298:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.