



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 PM UTC

PDB ID : 3IN5 / pdb_00003in5
Title : Structure of human DNA polymerase kappa inserting dATP opposite an 8-oxoG DNA lesion
Authors : Silverstein, T.D.; Vasquez-Del Carpio, R.; Aggarwal, A.K.
Deposited on : 2009-08-11
Resolution : 3.20 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 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

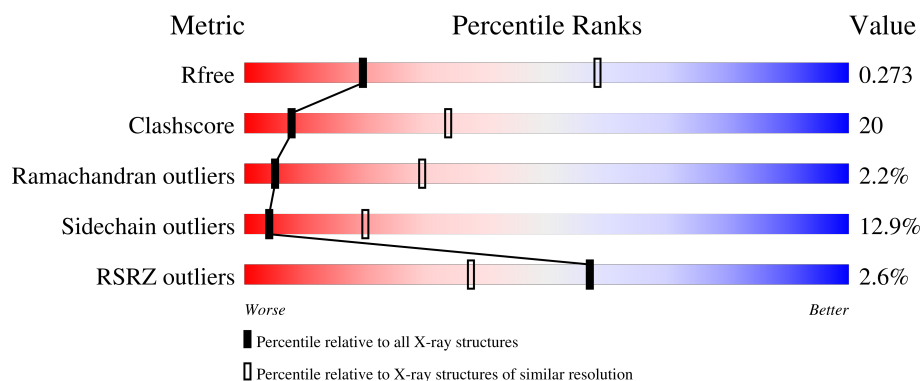
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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	508	8% 50% 31% 5% 14%
1	B	508	3% 53% 27% 6% 14%
2	P	13	8% 8% 69% 8% 15%
2	Q	13	8% 46% 46% 8%
3	T	18	11% 33% 39% 11% 17%

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Mol	Chain	Length	Quality of chain
3	U	18	 A horizontal bar chart showing the quality of chain U. The bar is divided into four segments: green (56%), yellow (11%), orange (11%), and grey (22%).

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7894 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 DNA polymerase kappa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	1	0
			3410	2148	598	643	21			
1	B	437	Total	C	N	O	S	0	0	0
			3346	2106	585	633	22			

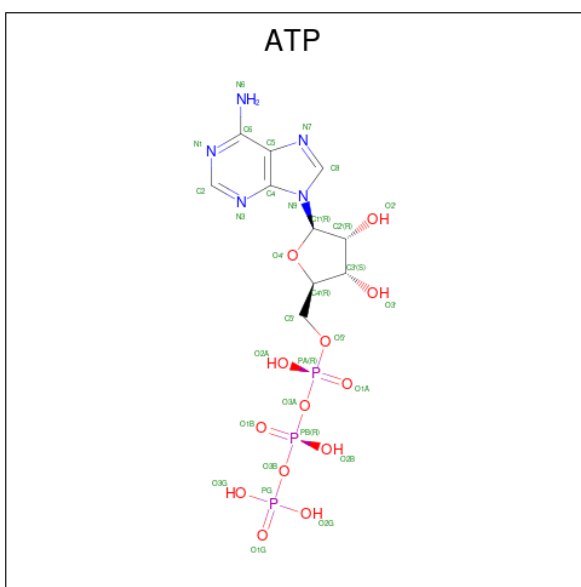
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*G*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			227	108	48	61	10			
2	Q	12	Total	C	N	O	P	0	0	0
			249	118	53	67	11			

- Molecule 3 is a DNA chain called DNA (5'-D(*C*CP*TP*AP*(8OG)P*GP*AP*GP*TP*C P*CP*TP*TP*CP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			300	144	51	91	14			
3	U	14	Total	C	N	O	P	0	0	0
			280	134	49	84	13			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

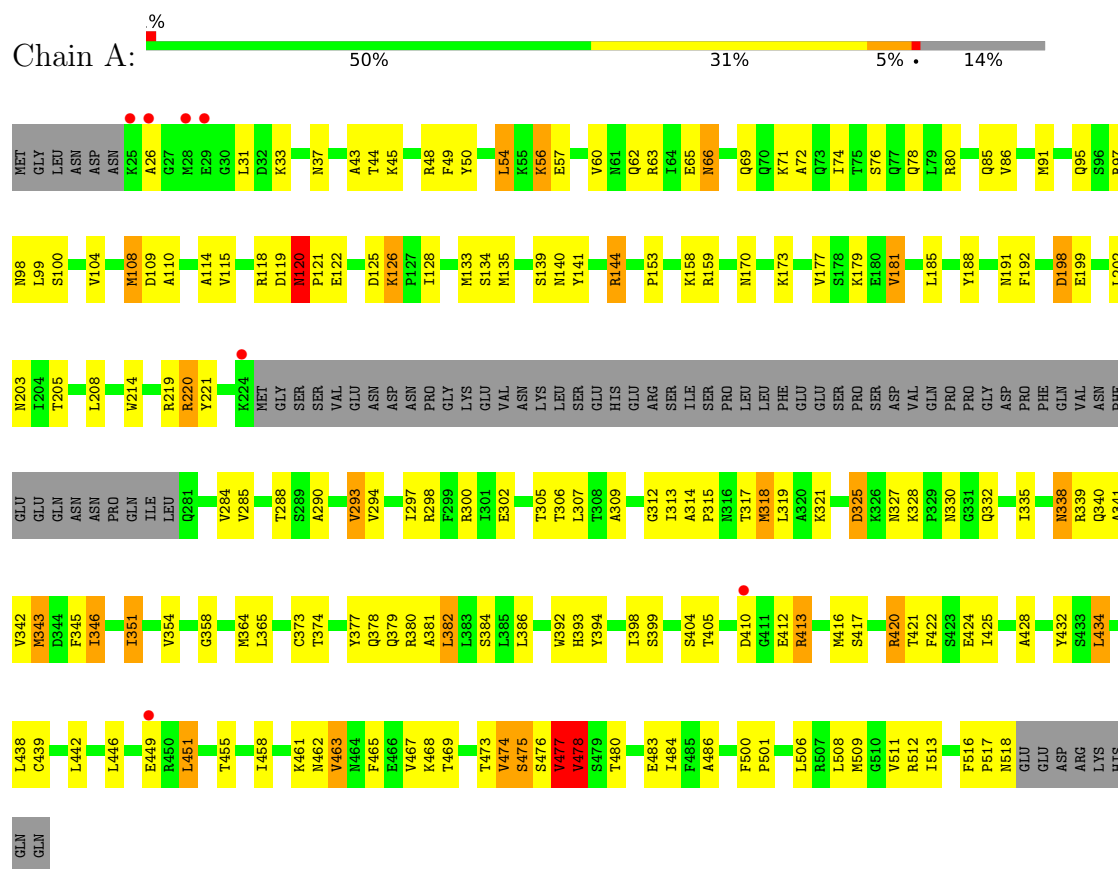
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	7	Total	O	0	0
			7	7		
6	U	1	Total	O	0	0
			1	1		

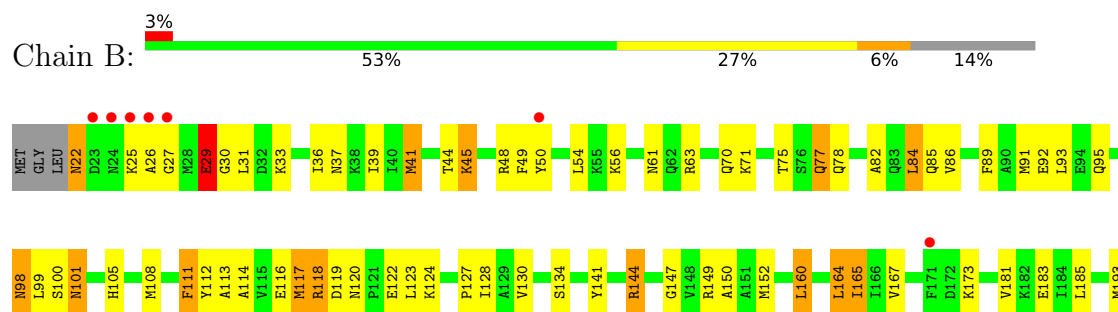
3 Residue-property plots

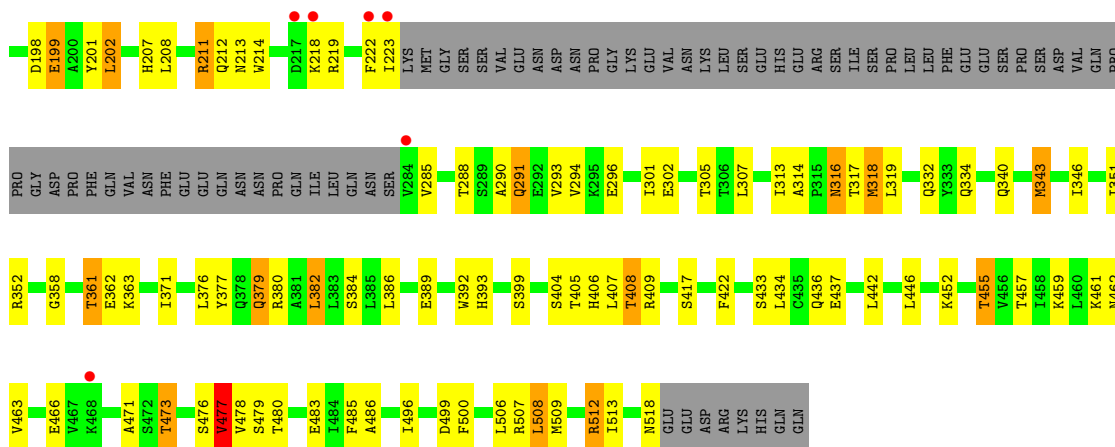
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase kappa

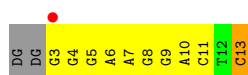
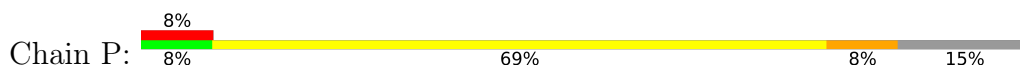


• Molecule 1: DNA polymerase kappa

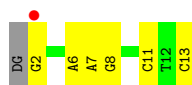




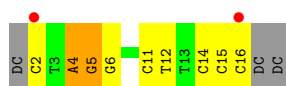
- Molecule 2: DNA (5'-D(*GP*G*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*(DOC))-3')



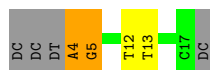
- Molecule 2: DNA (5'-D(*GP*G*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*(DOC))-3')



- Molecule 3: DNA (5'-D(*C*CP*TP*AP*(8OG)P*GP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3')



- Molecule 3: DNA (5'-D(*C*CP*TP*AP*(8OG)P*GP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	116.85Å 154.48Å 217.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 3.20 47.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.12-3.20) 99.9 (47.12-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.225 , 0.274 0.223 , 0.273	Depositor DCC
R_{free} test set	1640 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7894	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 8OG, MG, DOC

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	0.79	0/3465	0.97	5/4677 (0.1%)
1	B	0.74	0/3397	0.95	2/4591 (0.0%)
2	P	0.57	0/236	1.28	1/364 (0.3%)
2	Q	0.54	0/261	1.20	2/403 (0.5%)
3	T	0.52	0/307	1.34	3/468 (0.6%)
3	U	0.52	0/285	1.20	2/434 (0.5%)
All	All	0.74	0/7951	1.01	15/10937 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	2	DG	P-O3'-C3'	6.88	130.52	120.20
1	A	120	ASN	CA-C-N	5.81	125.95	119.32
1	A	120	ASN	C-N-CA	5.81	125.95	119.32
1	A	342	VAL	N-CA-C	-5.81	104.19	110.23
3	T	2	DC	P-O3'-C3'	5.76	128.83	120.20
3	T	4	DA	C4'-C3'-O3'	-5.68	101.48	110.00
1	B	314	ALA	CA-C-N	5.66	126.91	119.84
1	B	314	ALA	C-N-CA	5.66	126.91	119.84
2	P	3	DG	P-O3'-C3'	5.53	128.50	120.20
1	A	327	ASN	N-CA-C	5.49	119.61	111.87
3	T	2	DC	O4'-C1'-N1	5.47	116.61	108.40
2	Q	2	DG	C4'-C3'-O3'	5.41	118.12	110.00
1	A	424	GLU	N-CA-C	5.22	117.66	110.35
3	U	4	DA	O4'-C4'-C3'	-5.17	97.64	105.40
3	U	4	DA	O5'-C5'-C4'	5.17	118.55	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3410	0	3394	152	0
1	B	3346	0	3281	137	0
2	P	227	0	124	15	0
2	Q	249	0	135	6	0
3	T	300	0	171	6	0
3	U	280	0	159	4	0
4	A	30	0	10	4	0
4	B	30	0	10	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	10	0	0	1	0
6	B	7	0	0	0	0
6	U	1	0	0	0	0
All	All	7894	0	7284	301	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 20.

All (301) 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:B:351:ILE:HD11	1:B:376:LEU:HD22	1.15	1.11
1:B:361:THR:HG22	2:Q:11:DC:OP1	1.50	1.09
1:A:108:MET:HE3	1:A:309:ALA:HB2	1.42	1.01
1:B:147:GLY:O	1:B:152:MET:HE1	1.72	0.90
1:B:351:ILE:CD1	1:B:376:LEU:HD22	2.00	0.90
1:B:408:THR:HG23	1:B:408:THR:O	1.71	0.87
1:A:128:ILE:HG12	1:A:140:ASN:ND2	1.90	0.86
1:A:185:LEU:HD13	1:A:202:LEU:HD11	1.57	0.86
1:B:29:GLU:OE2	1:B:31:LEU:HD12	1.79	0.82
1:A:318:MET:HE1	1:A:319:LEU:HD23	1.61	0.81
1:B:318:MET:C	1:B:318:MET:HE2	2.06	0.81
2:P:5:DG:H2''	2:P:6:DA:C5'	2.11	0.81
1:A:108:MET:CE	1:A:309:ALA:HB2	2.09	0.81
1:B:408:THR:O	1:B:408:THR:CG2	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASN:ND2	1:A:205:THR:HG22	1.97	0.80
1:B:294:VAL:HG12	1:B:332:GLN:OE1	1.83	0.79
1:B:185:LEU:HD22	1:B:202:LEU:HD21	1.66	0.78
2:P:4:DG:H2''	2:P:5:DG:O5'	1.84	0.77
1:A:305:THR:O	1:A:306:THR:HB	1.83	0.77
1:A:108:MET:HE3	1:A:309:ALA:CB	2.15	0.77
1:B:214:TRP:O	1:B:219:ARG:NH2	2.18	0.76
1:A:128:ILE:HG12	1:A:140:ASN:HD22	1.50	0.75
2:P:5:DG:H2''	2:P:6:DA:H5'	1.68	0.75
1:B:117:MET:HE2	1:B:124:LYS:HA	1.67	0.75
1:B:39:ILE:HG21	1:B:160:LEU:HD12	1.67	0.75
1:A:170:ASN:HD22	1:A:173:LYS:HE2	1.53	0.73
1:A:120:ASN:C	1:A:120:ASN:HD22	1.95	0.73
1:A:394:TYR:O	1:A:398:ILE:HD12	1.88	0.73
1:A:44:THR:HG22	1:A:50:TYR:HB2	1.71	0.73
1:A:48:ARG:HD3	1:A:463:VAL:HG13	1.73	0.71
1:B:457:THR:HG23	1:B:471:ALA:HB2	1.72	0.71
1:A:141:TYR:HA	1:A:144:ARG:HD3	1.74	0.70
1:A:91:MET:SD	1:B:91:MET:HE1	2.33	0.69
1:A:455:THR:OG1	1:A:473:THR:HB	1.93	0.69
1:A:338:ASN:ND2	1:A:341:ALA:H	1.91	0.69
1:B:352:ARG:HD3	1:B:362:GLU:CD	2.18	0.69
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.57	0.69
1:A:343:MET:HE3	1:A:343:MET:HA	1.74	0.68
2:P:5:DG:C2'	2:P:6:DA:H5'	2.24	0.68
1:A:480:THR:HG22	1:A:483:GLU:HG2	1.74	0.67
1:A:43:ALA:HB2	1:A:159:ARG:HH11	1.59	0.67
1:B:33:LYS:HG2	1:B:37:ASN:HD21	1.59	0.67
1:A:43:ALA:HB2	1:A:159:ARG:NH1	2.10	0.67
1:A:473:THR:HG22	2:P:6:DA:OP1	1.96	0.66
1:B:26:ALA:HB1	1:B:144:ARG:NH2	2.11	0.66
1:A:91:MET:HE3	1:B:84:LEU:HD13	1.76	0.66
1:A:328:LYS:HE2	4:A:1:ATP:PG	2.35	0.66
2:P:5:DG:H2''	2:P:6:DA:H5''	1.76	0.66
1:B:483:GLU:O	1:B:486:ALA:HB3	1.96	0.65
1:B:211:ARG:HH11	1:B:211:ARG:CG	2.09	0.65
1:A:133:MET:HE1	1:A:158:LYS:NZ	2.11	0.65
1:A:208:LEU:HD11	1:A:290:ALA:HB2	1.78	0.65
1:A:177:VAL:O	1:A:181:VAL:HG13	1.96	0.65
1:B:41:MET:HA	1:B:41:MET:HE2	1.79	0.64
1:A:473:THR:HG22	2:P:6:DA:P	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LEU:HD22	1:B:513:ILE:HG21	1.78	0.64
1:B:29:GLU:HG2	1:B:30:GLY:H	1.63	0.63
1:A:318:MET:HE2	1:A:319:LEU:N	2.14	0.63
1:A:318:MET:CE	1:A:319:LEU:HD23	2.27	0.63
1:A:338:ASN:HD21	1:A:341:ALA:H	1.44	0.63
1:A:76:SER:O	1:A:80:ARG:HG3	1.99	0.63
1:B:316:ASN:C	1:B:316:ASN:HD22	2.06	0.62
1:A:480:THR:CG2	1:A:483:GLU:HG2	2.29	0.62
1:A:50:TYR:CE2	1:A:54:LEU:HD22	2.34	0.62
1:A:461:LYS:HB3	1:A:508:LEU:HB3	1.82	0.62
1:B:98:ASN:C	1:B:98:ASN:HD22	2.07	0.62
1:B:316:ASN:ND2	1:B:319:LEU:H	1.96	0.62
1:B:71:LYS:HD2	1:B:382:LEU:HD11	1.81	0.61
1:B:455:THR:HG23	1:B:473:THR:HB	1.81	0.61
1:A:214:TRP:O	1:A:219:ARG:NH1	2.34	0.61
1:B:316:ASN:HD21	1:B:319:LEU:H	1.49	0.61
1:B:193:MET:HE3	1:B:407:LEU:HB3	1.82	0.61
1:A:133:MET:HE1	1:A:158:LYS:HD2	1.82	0.61
1:B:101:ASN:N	1:B:101:ASN:HD22	1.99	0.61
1:B:77:GLN:HG2	1:B:78:GLN:N	2.14	0.61
1:A:91:MET:SD	1:B:91:MET:CE	2.89	0.60
3:U:12:DT:C6	3:U:13:DT:H72	2.36	0.60
1:A:335:ILE:HD11	1:A:345:PHE:CG	2.36	0.60
1:B:39:ILE:CG2	1:B:160:LEU:HD12	2.32	0.60
1:A:203:ASN:CG	1:A:205:THR:HG22	2.25	0.60
1:B:478:VAL:HG13	1:B:483:GLU:HB2	1.82	0.60
1:B:480:THR:HG23	1:B:483:GLU:OE1	2.02	0.59
3:U:12:DT:H6	3:U:13:DT:H72	1.66	0.59
1:B:193:MET:HE1	1:B:408:THR:N	2.17	0.59
1:A:203:ASN:ND2	1:A:205:THR:CG2	2.65	0.59
1:A:335:ILE:HD11	1:A:345:PHE:CD2	2.38	0.59
1:B:291:GLN:NE2	1:B:334:GLN:OE1	2.36	0.58
1:B:219:ARG:O	1:B:285:VAL:HA	2.03	0.58
1:B:478:VAL:HG13	1:B:483:GLU:CB	2.33	0.58
1:A:305:THR:O	1:A:306:THR:CB	2.52	0.58
1:B:507:ARG:NH1	3:U:5:8OG:OP1	2.37	0.57
1:B:208:LEU:HD11	1:B:290:ALA:HB2	1.86	0.57
1:B:211:ARG:NH2	1:B:296:GLU:OE2	2.36	0.57
1:B:291:GLN:HE22	1:B:334:GLN:HB3	1.69	0.57
1:B:111:PHE:O	1:B:112:TYR:C	2.47	0.57
2:Q:7:DA:H2"	2:Q:8:DG:OP2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:THR:HG22	1:A:306:THR:O	2.05	0.57
1:B:105:HIS:CE1	1:B:199:GLU:HG2	2.40	0.57
1:B:201:TYR:C	1:B:202:LEU:HD12	2.30	0.57
3:T:5:8OG:H2'	3:T:6:DG:H5'	1.87	0.57
1:A:170:ASN:ND2	1:A:173:LYS:HB2	2.20	0.56
1:A:420:ARG:O	1:A:508:LEU:HD22	2.05	0.56
1:B:480:THR:OG1	1:B:483:GLU:HG3	2.05	0.56
1:B:508:LEU:HD13	1:B:509:MET:N	2.19	0.56
1:A:26:ALA:HB1	1:A:325:ASP:OD2	2.06	0.56
1:B:455:THR:HG23	1:B:473:THR:CB	2.36	0.56
1:B:26:ALA:HB1	1:B:144:ARG:HH21	1.71	0.55
1:B:211:ARG:HH11	1:B:211:ARG:HG3	1.70	0.55
1:A:379:GLN:HG2	1:B:340:GLN:NE2	2.22	0.55
1:A:413:ARG:NH2	1:A:449:GLU:OE1	2.40	0.55
1:B:185:LEU:CD2	1:B:202:LEU:HD21	2.36	0.55
1:B:114:ALA:HA	1:B:117:MET:HG3	1.88	0.55
1:A:318:MET:HE2	1:A:318:MET:C	2.31	0.55
1:B:202:LEU:HD12	1:B:202:LEU:N	2.22	0.55
1:A:65:GLU:OE2	1:A:65:GLU:HA	2.06	0.54
1:A:351:ILE:CD1	1:A:365:LEU:HD12	2.37	0.54
1:B:291:GLN:HE22	1:B:334:GLN:CB	2.20	0.54
1:A:86:VAL:HG11	1:A:380:ARG:HB2	1.89	0.54
1:A:474:VAL:O	1:A:475:SER:HB3	2.07	0.54
1:B:114:ALA:HB1	1:B:307:LEU:HD22	1.88	0.54
1:A:220:ARG:HB2	1:A:285:VAL:HG12	1.87	0.54
1:A:516:PHE:HB3	1:A:517:PRO:HD2	1.89	0.54
1:B:384:SER:HA	1:B:392:TRP:CD1	2.43	0.54
1:B:417:SER:HB3	1:B:512:ARG:HG3	1.90	0.54
1:B:98:ASN:C	1:B:98:ASN:ND2	2.67	0.53
1:B:113:ALA:O	1:B:117:MET:HG2	2.07	0.53
1:A:451:LEU:HD23	1:A:516:PHE:CE2	2.43	0.53
1:A:294:VAL:HG12	1:A:332:GLN:OE1	2.07	0.53
1:B:48:ARG:NH1	1:B:463:VAL:HG11	2.24	0.53
1:A:115:VAL:HG22	1:A:177:VAL:HG21	1.91	0.53
1:A:306:THR:O	1:A:306:THR:CG2	2.56	0.53
1:B:108:MET:HB2	1:B:198:ASP:HB2	1.90	0.53
1:A:500:PHE:CG	1:A:501:PRO:HA	2.44	0.53
1:B:119:ASP:OD2	1:B:173:LYS:NZ	2.39	0.52
3:T:4:DA:H2''	3:T:5:8OG:OP2	2.10	0.52
1:B:39:ILE:CG2	1:B:160:LEU:CD1	2.88	0.52
1:A:144:ARG:NH2	4:A:1:ATP:O2G	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:VAL:O	1:A:478:VAL:HB	2.09	0.52
1:B:318:MET:HE2	1:B:319:LEU:N	2.24	0.52
1:A:56:LYS:O	1:A:60:VAL:HG23	2.10	0.51
1:A:420:ARG:HG3	1:A:420:ARG:HH11	1.75	0.51
1:B:128:ILE:HG22	1:B:165:ILE:HG23	1.93	0.51
1:B:211:ARG:HH22	1:B:296:GLU:CD	2.17	0.51
1:A:364:MET:HE1	6:A:9:HOH:O	2.10	0.51
1:B:105:HIS:HD2	1:B:201:TYR:CE1	2.29	0.51
1:A:298:ARG:HH21	1:A:330:ASN:ND2	2.09	0.51
1:A:135:MET:HA	1:A:153:PRO:HA	1.92	0.51
1:B:318:MET:HE2	1:B:318:MET:O	2.10	0.51
1:A:97:ARG:HG2	1:A:99:LEU:CD1	2.41	0.50
1:A:382:LEU:HD22	1:A:386:LEU:HG	1.92	0.50
1:B:382:LEU:HD22	1:B:386:LEU:HG	1.92	0.50
1:A:108:MET:HB2	1:A:198:ASP:HB2	1.93	0.50
1:A:302:GLU:HA	1:A:307:LEU:O	2.12	0.50
1:A:318:MET:HE2	1:A:319:LEU:CA	2.41	0.50
1:B:111:PHE:CD2	1:B:198:ASP:HB3	2.46	0.50
1:A:422:PHE:CE2	1:A:434:LEU:HD11	2.48	0.49
1:A:473:THR:N	2:P:6:DA:OP1	2.42	0.49
1:A:98:ASN:ND2	1:A:100:SER:H	2.10	0.49
1:A:192:PHE:CD1	1:A:192:PHE:C	2.89	0.49
1:A:483:GLU:O	1:A:486:ALA:HB3	2.12	0.49
1:A:422:PHE:HE2	1:A:434:LEU:HD11	1.78	0.49
1:A:199:GLU:OE2	1:A:321:LYS:NZ	2.46	0.49
1:A:477:VAL:O	1:A:478:VAL:CB	2.60	0.49
1:A:97:ARG:CD	1:A:99:LEU:HD11	2.43	0.49
1:A:314:ALA:HB1	1:A:315:PRO:HD2	1.95	0.49
1:A:384:SER:HA	1:A:392:TRP:CD1	2.48	0.48
1:B:476:SER:O	1:B:477:VAL:HB	2.12	0.48
1:A:438:LEU:O	1:A:439:CYS:C	2.55	0.48
1:B:111:PHE:O	1:B:114:ALA:N	2.46	0.48
1:B:44:THR:HG22	1:B:50:TYR:HB2	1.94	0.48
1:A:120:ASN:HD21	1:A:122:GLU:HG3	1.79	0.48
1:A:325:ASP:HA	1:A:328:LYS:HG3	1.96	0.48
1:B:117:MET:CE	1:B:124:LYS:HA	2.42	0.48
1:A:98:ASN:C	1:A:98:ASN:HD22	2.22	0.47
1:B:75:THR:HG1	1:B:78:GLN:H	1.61	0.47
1:B:433:SER:O	1:B:437:GLU:HG3	2.14	0.47
1:B:343:MET:O	1:B:346:ILE:HG22	2.14	0.47
1:B:29:GLU:CG	1:B:30:GLY:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:C	1:B:316:ASN:ND2	2.72	0.47
1:A:108:MET:CE	1:A:108:MET:HA	2.44	0.47
1:B:422:PHE:CE2	1:B:434:LEU:HD11	2.49	0.47
1:B:316:ASN:HD21	1:B:319:LEU:HG	1.78	0.47
1:A:340:GLN:HE22	1:B:379:GLN:HG2	1.80	0.47
1:A:434:LEU:HD22	1:A:438:LEU:HG	1.97	0.47
1:B:123:LEU:HD23	1:B:165:ILE:HD13	1.97	0.47
1:A:109:ASP:O	1:A:110:ALA:C	2.58	0.46
1:B:141:TYR:OH	4:B:2:ATP:O3G	2.09	0.46
1:B:417:SER:HA	1:B:442:LEU:HD13	1.98	0.46
1:B:499:ASP:O	1:B:500:PHE:C	2.59	0.46
1:B:508:LEU:HD13	1:B:508:LEU:C	2.40	0.46
1:A:416:MET:HE1	1:A:449:GLU:HG3	1.97	0.46
1:B:317:THR:HG21	1:B:404:SER:HB2	1.98	0.46
1:B:377:TYR:HB2	1:B:399:SER:HB2	1.98	0.46
1:B:294:VAL:HG11	1:B:313:ILE:HD11	1.96	0.46
1:B:70:GLN:O	1:B:71:LYS:C	2.58	0.46
1:A:474:VAL:HG23	1:A:475:SER:H	1.81	0.45
1:B:100:SER:HB2	1:B:101:ASN:HD22	1.81	0.45
1:B:317:THR:CG2	1:B:404:SER:HB2	2.45	0.45
1:A:328:LYS:HE2	4:A:1:ATP:O1G	2.16	0.45
1:A:422:PHE:CE1	1:A:425:ILE:HD12	2.51	0.45
1:A:442:LEU:CD2	1:A:511:VAL:HG12	2.47	0.45
1:A:461:LYS:HD3	1:A:467:VAL:HG22	1.98	0.45
2:P:8:DG:H1'	2:P:9:DG:H5''	1.97	0.45
1:A:377:TYR:HB2	1:A:399:SER:HB2	1.98	0.45
1:B:86:VAL:HG11	1:B:380:ARG:HB2	1.99	0.45
1:A:478:VAL:HG22	1:A:483:GLU:HG3	1.98	0.45
1:B:49:PHE:CE2	3:U:4:DA:C5	3.04	0.45
1:A:434:LEU:HD13	1:A:509:MET:SD	2.56	0.45
1:B:127:PRO:C	1:B:164:LEU:HD12	2.41	0.45
1:B:389:GLU:HG3	1:B:393:HIS:CE1	2.52	0.45
1:A:317:THR:HG23	1:A:404:SER:HB2	1.98	0.45
1:B:436:GLN:HA	1:B:485:PHE:CD1	2.52	0.45
1:B:61:ASN:OD1	1:B:363:LYS:NZ	2.50	0.45
1:B:446:LEU:CD2	1:B:513:ILE:HG21	2.47	0.45
1:B:473:THR:HB	2:Q:6:DA:OP2	2.17	0.45
1:A:177:VAL:HG11	1:A:307:LEU:HD12	1.99	0.45
1:B:512:ARG:HG3	1:B:512:ARG:NH1	2.27	0.44
1:A:74:ILE:HG23	1:A:78:GLN:HE21	1.83	0.44
1:A:134:SER:O	1:A:135:MET:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ALA:HB1	1:A:315:PRO:CD	2.48	0.44
3:T:14:DC:C4	3:T:15:DC:N4	2.85	0.44
1:B:112:TYR:HB3	1:B:130:VAL:HG21	1.99	0.44
1:A:290:ALA:HA	1:A:293:VAL:HG13	2.00	0.44
1:A:177:VAL:HG11	1:A:307:LEU:CD1	2.48	0.44
1:A:417:SER:HB2	1:A:512:ARG:NH1	2.32	0.44
1:A:421:THR:N	3:T:6:DG:OP1	2.38	0.44
1:B:22:ASN:N	1:B:22:ASN:HD22	2.16	0.44
1:B:25:LYS:O	1:B:26:ALA:HB3	2.18	0.44
1:B:358:GLY:HA3	2:Q:11:DC:O5'	2.17	0.44
1:A:63:ARG:HH12	2:P:10:DA:H5''	1.81	0.44
1:A:294:VAL:HG21	1:A:313:ILE:HG12	1.99	0.44
1:B:317:THR:HG22	1:B:404:SER:H	1.83	0.44
1:B:508:LEU:C	1:B:508:LEU:CD1	2.90	0.44
2:P:6:DA:C6	2:P:7:DA:N6	2.86	0.44
1:A:48:ARG:HD3	1:A:463:VAL:CG1	2.45	0.44
1:A:54:LEU:HD12	1:A:57:GLU:OE2	2.18	0.43
1:A:358:GLY:HA3	2:P:11:DC:O5'	2.18	0.43
1:A:382:LEU:HD22	1:A:386:LEU:CD1	2.47	0.43
1:B:141:TYR:HA	1:B:144:ARG:HD3	2.00	0.43
3:T:15:DC:H2''	3:T:16:DC:C5	2.53	0.43
1:A:461:LYS:HD3	1:A:467:VAL:CG2	2.48	0.43
1:B:149:ARG:HG3	1:B:150:ALA:O	2.17	0.43
1:A:66:ASN:N	1:A:66:ASN:ND2	2.66	0.43
1:A:97:ARG:HG2	1:A:99:LEU:HD11	2.00	0.43
1:A:346:ILE:HG23	1:A:373:CYS:HB3	2.00	0.43
1:A:428:ALA:O	1:A:432:TYR:HD1	2.02	0.43
1:B:452:LYS:HG2	1:B:479:SER:HB3	2.01	0.43
1:A:354:VAL:HG11	1:A:398:ILE:HG12	2.00	0.43
1:B:116:GLU:OE2	1:B:167:VAL:HG11	2.18	0.43
1:B:207:HIS:NE2	1:B:211:ARG:NH1	2.66	0.43
1:B:288:THR:HG22	1:B:288:THR:O	2.17	0.43
1:B:358:GLY:HA3	2:Q:11:DC:P	2.59	0.43
1:A:480:THR:HG22	1:A:483:GLU:CG	2.44	0.43
1:A:98:ASN:HD22	1:A:99:LEU:N	2.16	0.43
1:A:203:ASN:HD21	1:A:205:THR:CG2	2.31	0.43
1:B:118:ARG:HD3	1:B:119:ASP:OD1	2.19	0.43
1:A:120:ASN:HA	1:A:121:PRO:HD2	1.80	0.42
1:A:478:VAL:HG23	1:A:483:GLU:HB2	2.01	0.42
1:B:39:ILE:HB	1:B:160:LEU:HD11	2.00	0.42
3:T:11:DC:H2''	3:T:12:DT:H71	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1:ATP:C8	2:P:13:DOC:H2'	2.54	0.42
1:B:120:ASN:OD1	1:B:122:GLU:N	2.52	0.42
1:B:202:LEU:N	1:B:202:LEU:CD1	2.82	0.42
2:P:6:DA:C6	2:P:7:DA:C6	3.07	0.42
1:A:49:PHE:HA	1:A:465:PHE:CE1	2.53	0.42
1:A:74:ILE:HA	1:A:78:GLN:NE2	2.35	0.42
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.89	0.42
1:A:346:ILE:HG23	1:A:373:CYS:CB	2.48	0.42
1:B:461:LYS:HB3	1:B:508:LEU:HB3	2.02	0.42
1:A:71:LYS:HG3	1:A:382:LEU:HD21	2.02	0.42
1:A:104:VAL:HA	1:A:312:GLY:O	2.20	0.42
1:A:346:ILE:O	1:A:373:CYS:HB2	2.19	0.42
1:A:125:ASP:HB3	1:A:126:LYS:NZ	2.34	0.42
1:A:80:ARG:NH2	1:B:95:GLN:O	2.49	0.41
2:P:5:DG:C6	2:P:6:DA:C6	3.08	0.41
1:A:378[A]:GLN:OE1	1:A:378[A]:GLN:HA	2.21	0.41
1:B:92:GLU:O	1:B:93:LEU:C	2.63	0.41
1:A:139:SER:O	1:A:144:ARG:HD2	2.20	0.41
1:A:446:LEU:CD2	1:A:513:ILE:HD13	2.50	0.41
1:B:181:VAL:HG13	1:B:301:ILE:CD1	2.50	0.41
1:B:352:ARG:HD3	1:B:362:GLU:OE1	2.20	0.41
1:A:125:ASP:HB3	1:A:126:LYS:HZ3	1.84	0.41
1:A:318:MET:HE2	1:A:319:LEU:HA	2.01	0.41
1:B:212:GLN:HG3	1:B:213:ASN:N	2.34	0.41
2:Q:8:DG:OP2	2:Q:8:DG:H2'	2.21	0.41
1:A:338:ASN:O	1:A:339:ARG:C	2.63	0.41
1:B:222:PHE:O	1:B:223:ILE:CB	2.69	0.41
1:A:188:TYR:CE1	1:A:297:ILE:HG12	2.55	0.41
1:B:44:THR:O	1:B:45:LYS:C	2.63	0.41
1:A:33:LYS:O	1:A:37:ASN:HB2	2.21	0.41
1:A:343:MET:HA	1:A:343:MET:CE	2.48	0.41
1:A:221:TYR:CE2	1:A:300:ARG:HD2	2.56	0.41
1:A:340:GLN:NE2	1:B:379:GLN:HG2	2.35	0.41
1:B:82:ALA:O	1:B:86:VAL:HG23	2.20	0.41
1:B:89:PHE:HE2	1:B:93:LEU:HD11	1.85	0.41
1:A:208:LEU:HD11	1:A:290:ALA:CB	2.50	0.40
1:B:181:VAL:C	1:B:183:GLU:N	2.78	0.40
1:A:219:ARG:O	1:A:285:VAL:HA	2.21	0.40
1:B:105:HIS:CD2	1:B:201:TYR:CE1	3.09	0.40
1:A:43:ALA:CB	1:A:159:ARG:NH1	2.84	0.40
1:A:114:ALA:HB1	1:A:307:LEU:HD22	2.02	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	435/508 (86%)	390 (90%)	33 (8%)	12 (3%)	4	25
1	B	433/508 (85%)	385 (89%)	41 (10%)	7 (2%)	7	36
All	All	868/1016 (85%)	775 (89%)	74 (8%)	19 (2%)	5	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	SER
1	A	477	VAL
1	B	29	GLU
1	B	45	LYS
1	B	111	PHE
1	B	477	VAL
1	A	478	VAL
1	B	409	ARG
1	A	410	ASP
1	B	27	GLY
1	B	462	ASN
1	A	72	ALA
1	A	346	ILE
1	A	412	GLU
1	A	476	SER
1	A	45	LYS
1	A	381	ALA
1	A	462	ASN
1	A	474	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/454 (80%)	321 (88%)	44 (12%)	5	22
1	B	350/454 (77%)	302 (86%)	48 (14%)	3	18
All	All	715/908 (79%)	623 (87%)	92 (13%)	4	20

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	54	LEU
1	A	56	LYS
1	A	62	GLN
1	A	66	ASN
1	A	69	GLN
1	A	85	GLN
1	A	95	GLN
1	A	108	MET
1	A	118	ARG
1	A	119	ASP
1	A	120	ASN
1	A	126	LYS
1	A	144	ARG
1	A	179	LYS
1	A	181	VAL
1	A	191	ASN
1	A	198	ASP
1	A	220	ARG
1	A	284	VAL
1	A	288	THR
1	A	293	VAL
1	A	318	MET
1	A	325	ASP
1	A	338	ASN
1	A	343	MET
1	A	351	ILE

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Mol	Chain	Res	Type
1	A	374	THR
1	A	382	LEU
1	A	393	HIS
1	A	405	THR
1	A	413	ARG
1	A	420	ARG
1	A	434	LEU
1	A	451	LEU
1	A	458	ILE
1	A	463	VAL
1	A	468	LYS
1	A	469	THR
1	A	477	VAL
1	A	478	VAL
1	A	484	ILE
1	A	506	LEU
1	A	518	ASN
1	B	22	ASN
1	B	29	GLU
1	B	36	ILE
1	B	41	MET
1	B	54	LEU
1	B	56	LYS
1	B	63	ARG
1	B	77	GLN
1	B	84	LEU
1	B	85	GLN
1	B	98	ASN
1	B	99	LEU
1	B	101	ASN
1	B	117	MET
1	B	118	ARG
1	B	134	SER
1	B	144	ARG
1	B	160	LEU
1	B	164	LEU
1	B	165	ILE
1	B	199	GLU
1	B	202	LEU
1	B	211	ARG
1	B	218	LYS
1	B	291	GLN

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Mol	Chain	Res	Type
1	B	293	VAL
1	B	302	GLU
1	B	305	THR
1	B	316	ASN
1	B	318	MET
1	B	343	MET
1	B	361	THR
1	B	371	ILE
1	B	379	GLN
1	B	382	LEU
1	B	405	THR
1	B	406	HIS
1	B	408	THR
1	B	455	THR
1	B	459	LYS
1	B	466	GLU
1	B	473	THR
1	B	477	VAL
1	B	496	ILE
1	B	506	LEU
1	B	508	LEU
1	B	512	ARG
1	B	518	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	69	GLN
1	A	77	GLN
1	A	78	GLN
1	A	83	GLN
1	A	98	ASN
1	A	120	ASN
1	A	170	ASN
1	A	203	ASN
1	A	327	ASN
1	A	330	ASN
1	A	338	ASN
1	A	340	GLN
1	A	379	GLN
1	B	22	ASN

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Mol	Chain	Res	Type
1	B	37	ASN
1	B	66	ASN
1	B	69	GLN
1	B	85	GLN
1	B	95	GLN
1	B	98	ASN
1	B	101	ASN
1	B	142	HIS
1	B	213	ASN
1	B	291	GLN
1	B	316	ASN
1	B	330	ASN
1	B	334	GLN
1	B	340	GLN
1	B	379	GLN
1	B	397	HIS
1	B	431	GLN
1	B	444	GLN
1	B	518	ASN

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
2	DOC	Q	13	3,2	16,19,20	0.93	1 (6%)	20,26,29	1.26	1 (5%)
3	8OG	T	5	3	22,25,26	2.30	8 (36%)	26,37,40	2.48	8 (30%)
3	8OG	U	5	3	22,25,26	2.06	6 (27%)	26,37,40	2.58	8 (30%)
2	DOC	P	13	3,2	16,19,20	0.97	1 (6%)	20,26,29	1.34	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	Q	13	3,2	-	6/7/18/19	0/2/2/2
3	8OG	T	5	3	-	2/7/21/22	0/3/3/3
3	8OG	U	5	3	-	1/7/21/22	0/3/3/3
2	DOC	P	13	3,2	-	2/7/18/19	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	5	8OG	O6-C6	6.47	1.35	1.23
3	U	5	8OG	O6-C6	6.46	1.35	1.23
3	T	5	8OG	C8-N9	-4.36	1.33	1.40
3	U	5	8OG	C8-N9	-3.57	1.34	1.40
3	T	5	8OG	C5-N7	-3.37	1.32	1.37
3	T	5	8OG	O8-C8	3.15	1.28	1.23
3	T	5	8OG	C4-N9	-3.12	1.33	1.39
3	T	5	8OG	C8-N7	-3.05	1.32	1.38
3	U	5	8OG	O8-C8	3.00	1.28	1.23
3	U	5	8OG	C8-N7	-2.64	1.33	1.38
3	U	5	8OG	C4-N9	-2.39	1.34	1.39
3	T	5	8OG	C1'-N9	2.17	1.50	1.47
3	T	5	8OG	C6-N1	-2.08	1.35	1.38
2	P	13	DOC	C6-N1	-2.04	1.33	1.38
2	Q	13	DOC	C6-C5	2.04	1.39	1.35
3	U	5	8OG	C6-N1	-2.02	1.35	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	8OG	N7-C8-N9	7.40	114.85	106.61
3	U	5	8OG	N7-C8-N9	7.02	114.42	106.61
3	U	5	8OG	N9-C4-N3	5.62	133.15	126.13
3	T	5	8OG	C2-N3-C4	4.80	120.57	112.30
3	U	5	8OG	C2-N3-C4	4.75	120.48	112.30
3	U	5	8OG	C5-N7-C8	-4.36	103.47	109.47
3	T	5	8OG	N9-C4-N3	4.17	131.34	126.13
3	T	5	8OG	C5-N7-C8	-3.83	104.19	109.47
3	U	5	8OG	O8-C8-N7	-3.48	119.94	126.47
3	U	5	8OG	O6-C6-C5	-3.26	119.41	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	8OG	O8-C8-N7	-3.15	120.57	126.47
2	P	13	DOC	C3'-C2'-C1'	3.03	106.36	102.87
3	T	5	8OG	C2-N1-C6	-3.00	119.67	125.11
3	U	5	8OG	C5-C6-N1	2.91	120.13	112.13
3	T	5	8OG	O6-C6-C5	-2.90	120.27	127.26
3	T	5	8OG	C5-C6-N1	2.85	119.96	112.13
2	P	13	DOC	C2'-C1'-N1	-2.32	108.01	112.40
2	Q	13	DOC	C3'-C2'-C1'	2.22	105.43	102.87
3	U	5	8OG	C2-N1-C6	-2.10	121.30	125.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	13	DOC	O4'-C4'-C5'-O5'
2	Q	13	DOC	O4'-C4'-C5'-O5'
3	T	5	8OG	O4'-C4'-C5'-O5'
3	T	5	8OG	C3'-C4'-C5'-O5'
3	U	5	8OG	O4'-C4'-C5'-O5'
2	P	13	DOC	C3'-C4'-C5'-O5'
2	Q	13	DOC	C3'-C4'-C5'-O5'
2	Q	13	DOC	C2'-C1'-N1-C6
2	Q	13	DOC	O4'-C1'-N1-C6
2	Q	13	DOC	O4'-C1'-N1-C2
2	Q	13	DOC	C2'-C1'-N1-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	5	8OG	2	0
3	U	5	8OG	1	0
2	P	13	DOC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are 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$
4	ATP	B	2	5	31,32,33	1.41	5 (16%)	46,50,52	1.83	10 (21%)
4	ATP	A	1	5	31,32,33	1.34	3 (9%)	46,50,52	1.95	9 (19%)

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	B	2	5	-	5/22/34/38	0/3/3/3
4	ATP	A	1	5	-	4/22/34/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	ATP	C5-C4	4.29	1.46	1.39
4	A	1	ATP	C5-C4	3.57	1.45	1.39
4	A	1	ATP	C5-N7	-3.03	1.33	1.39
4	B	2	ATP	C5-N7	-2.84	1.33	1.39
4	A	1	ATP	C4-N9	-2.61	1.32	1.37
4	B	2	ATP	C5-C6	2.59	1.48	1.41
4	B	2	ATP	PB-O3B	2.56	1.62	1.59
4	B	2	ATP	C4-N9	-2.51	1.32	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	ATP	C5-C4-N3	-5.70	118.87	126.72
4	B	2	ATP	C5-C4-N3	-5.60	119.01	126.72
4	A	1	ATP	N3-C2-N1	-4.92	121.13	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	ATP	N3-C4-N9	4.66	135.10	127.17
4	B	2	ATP	N3-C4-N9	4.43	134.71	127.17
4	A	1	ATP	C2'-C1'-N9	-4.40	104.28	114.63
4	A	1	ATP	C2-N3-C4	4.11	121.88	111.83
4	B	2	ATP	N3-C2-N1	-4.00	122.52	128.58
4	B	2	ATP	C2-N3-C4	3.92	121.41	111.83
4	B	2	ATP	C4-C5-N7	-3.03	107.12	110.58
4	A	1	ATP	O4'-C1'-N9	2.95	113.26	107.96
4	A	1	ATP	C2-N1-C6	2.89	123.48	118.73
4	B	2	ATP	C2'-C1'-N9	-2.67	108.34	114.63
4	B	2	ATP	C4-N9-C8	2.55	108.41	105.74
4	A	1	ATP	C4-C5-N7	-2.46	107.76	110.58
4	A	1	ATP	C4-N9-C8	2.46	108.32	105.74
4	B	2	ATP	C5-N7-C8	2.34	107.12	103.45
4	B	2	ATP	C2-N1-C6	2.16	122.28	118.73
4	B	2	ATP	N9-C8-N7	-2.03	111.06	113.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	ATP	C5'-O5'-PA-O1A
4	B	2	ATP	C5'-O5'-PA-O2A
4	B	2	ATP	C5'-O5'-PA-O3A
4	B	2	ATP	O4'-C4'-C5'-O5'
4	A	1	ATP	PB-O3B-PG-O1G
4	B	2	ATP	C3'-C4'-C5'-O5'
4	A	1	ATP	PB-O3B-PG-O2G
4	A	1	ATP	PB-O3B-PG-O3G
4	A	1	ATP	O4'-C1'-N9-C4

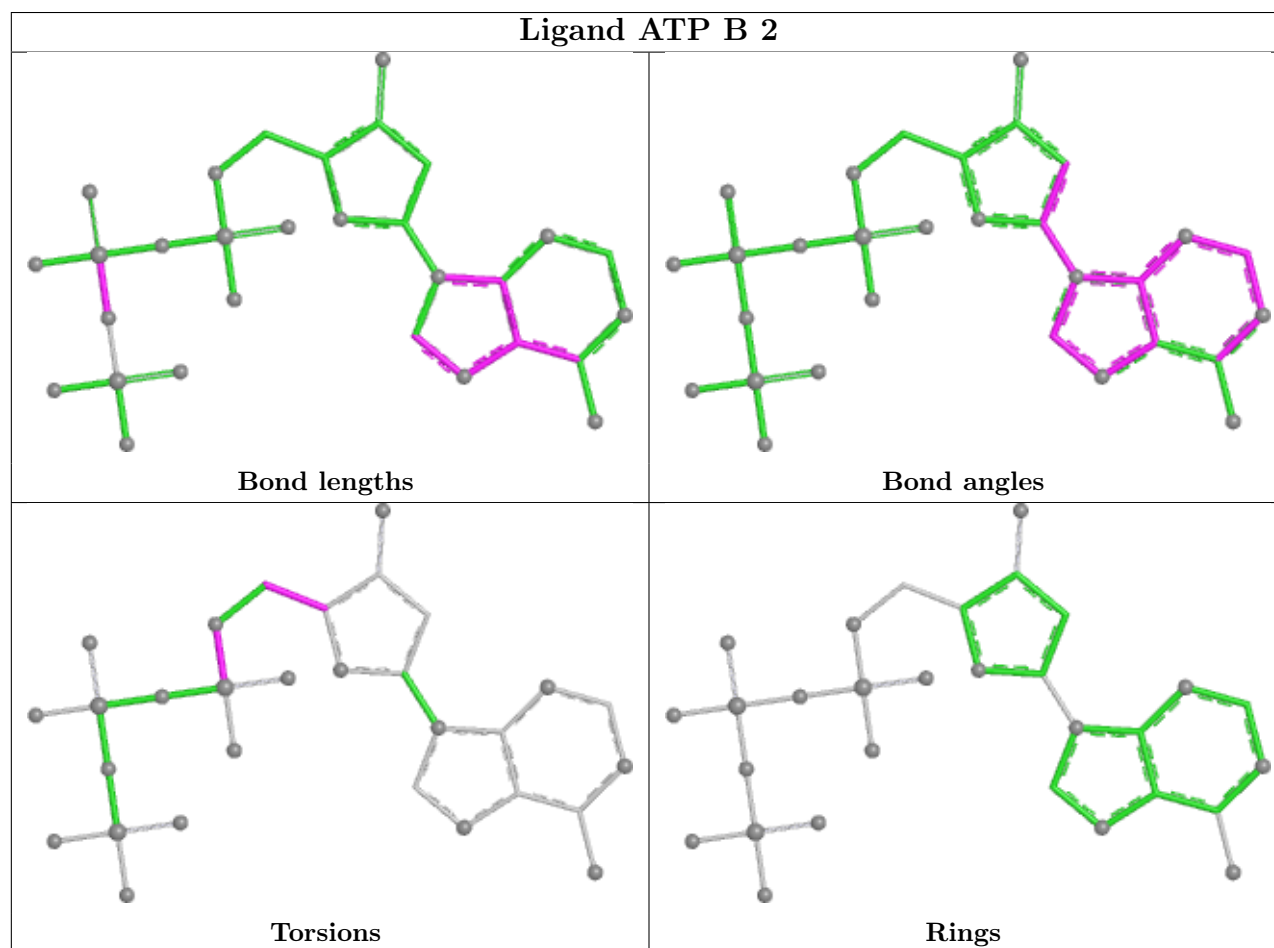
There are no ring outliers.

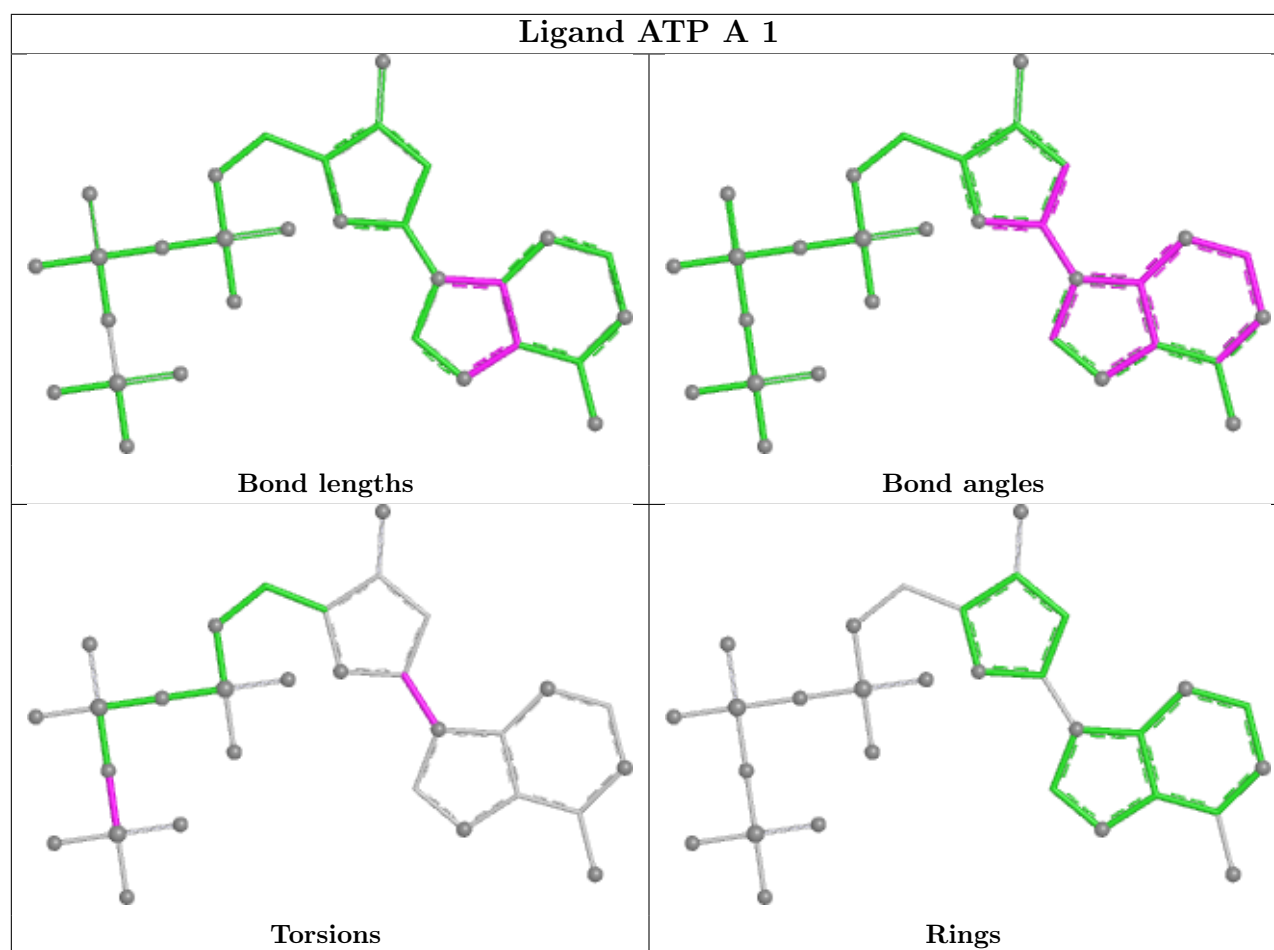
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	ATP	1	0
4	A	1	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	438/508 (86%)	-0.08	7 (1%) 70 51	21, 47, 75, 89	1 (0%)
1	B	437/508 (86%)	0.12	13 (2%) 52 33	33, 55, 84, 97	0
2	P	10/13 (76%)	0.41	1 (10%) 12 8	42, 63, 98, 116	0
2	Q	11/13 (84%)	0.11	1 (9%) 15 9	48, 59, 91, 102	0
3	T	14/18 (77%)	1.00	2 (14%) 6 5	43, 79, 129, 133	0
3	U	13/18 (72%)	0.42	0 100 100	49, 66, 100, 109	0
All	All	923/1078 (85%)	0.04	24 (2%) 57 37	21, 52, 81, 133	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	ASN	4.7
1	B	27	GLY	4.0
2	P	3	DG	3.8
3	T	16	DC	3.8
1	A	224	LYS	3.6
3	T	2	DC	3.5
1	B	26	ALA	3.4
1	B	217	ASP	3.1
1	B	222	PHE	2.7
1	A	28	MET	2.7
1	A	29	GLU	2.7
1	B	25	LYS	2.6
1	A	449	GLU	2.6
1	B	218	LYS	2.5
1	B	284	VAL	2.5
1	A	26	ALA	2.4
1	A	25	LYS	2.4
1	B	468	LYS	2.3
1	A	410	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	223	ILE	2.2
2	Q	2	DG	2.2
1	B	171	PHE	2.2
1	B	50	TYR	2.1
1	B	23	ASP	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
3	8OG	T	5	23/24	0.94	0.10	38,40,42,43	0
2	DOC	Q	13	18/19	0.96	0.10	51,54,56,57	0
2	DOC	P	13	18/19	0.97	0.08	38,39,44,44	0
3	8OG	U	5	23/24	0.97	0.07	39,42,46,47	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.

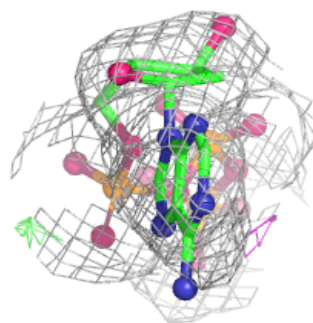
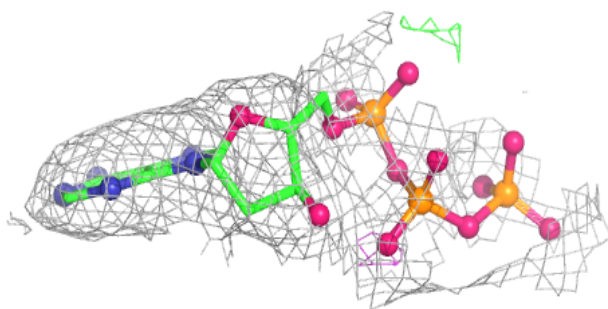
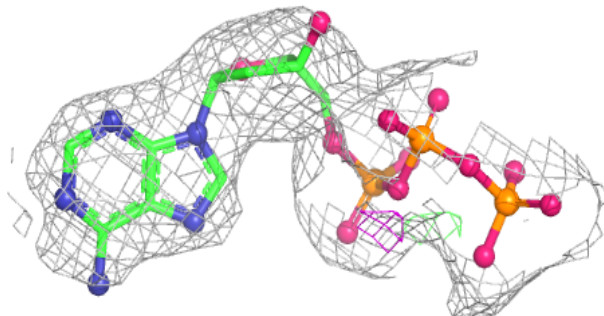
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	B	4	1/1	0.70	0.23	57,57,57,57	0
5	MG	A	3	1/1	0.90	0.10	41,41,41,41	0
4	ATP	B	2	30/31	0.96	0.08	49,55,59,60	0
4	ATP	A	1	30/31	0.98	0.05	29,33,35,35	0
5	MG	B	1	1/1	0.99	0.03	37,37,37,37	0
5	MG	A	2	1/1	1.00	0.02	26,26,26,26	0

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

orientation to approximate a three-dimensional view.

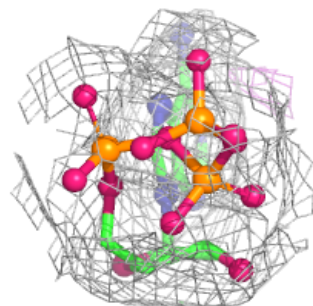
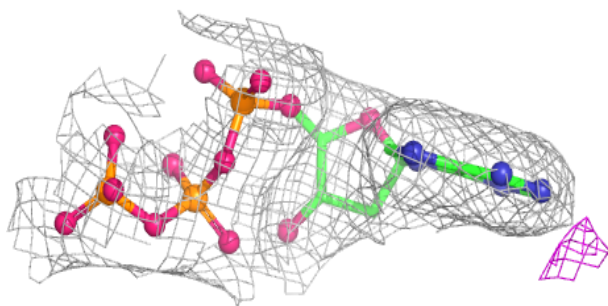
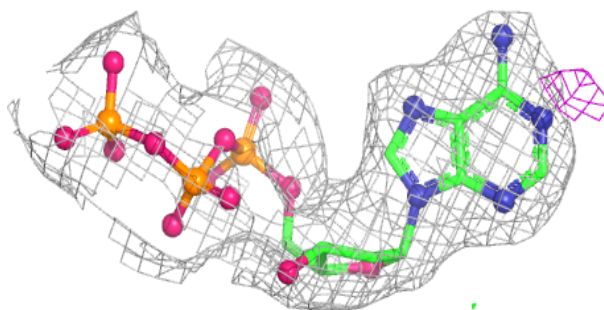
Electron density around ATP B 2:

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



Electron density around ATP A 1:

$2mF_o-DF_c$ (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.