



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:46 pm BST

PDB ID : 3QHR
Title : Structure of a pCDK2/CyclinA transition-state mimic
Authors : Young, M.A.; Jacobsen, D.M.; Bao, Z.Q.
Deposited on : 2011-01-26
Resolution : 2.17 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

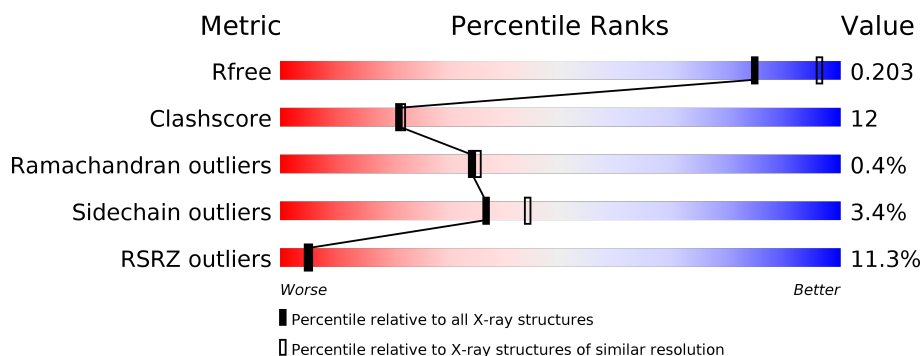
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	298	<div> <div>14%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	C	298	<div> <div>8%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	B	261	<div> <div>9%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	D	261	<div> <div>10%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
3	J	10	<div> <div>70%</div> <div>20%</div> <div>80%</div> </div>
3	K	10	<div> <div>20%</div> <div>90%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	10	
3	M	10	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	A	303	-	-	X	-
8	GOL	A	305	-	-	X	-
8	GOL	C	302	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10077 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	298	Total	C	N	O	P	S	0	0	0
			2396	1555	407	425	1	8			
1	C	298	Total	C	N	O	P	S	0	0	0
			2396	1555	407	425	1	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	HIS	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	HIS	-	EXPRESSION TAG	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S		0	0	0
			2099	1357	341	391	10				
2	D	261	Total	C	N	O	S		0	0	0
			2099	1357	341	391	10				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	SER	-	EXPRESSION TAG	UNP P51943
D	172	SER	-	EXPRESSION TAG	UNP P51943

- Molecule 3 is a protein called CDK2 substrate peptide: PKTPKKAKKL.

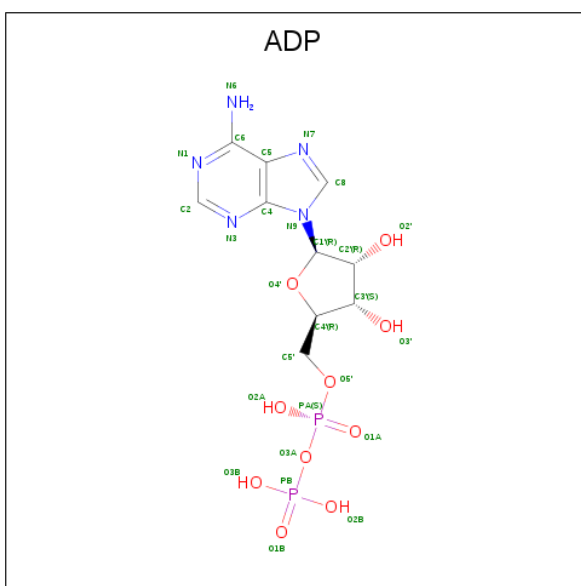
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	10	Total	C	N	O	0	0	0
			79	53	15	11			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	10	Total	C	N	O	0	0	0
			79	53	15	11			
3	L	10	Total	C	N	O	48	0	0
			79	53	15	11			
3	M	10	Total	C	N	O	48	0	0
			79	53	15	11			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

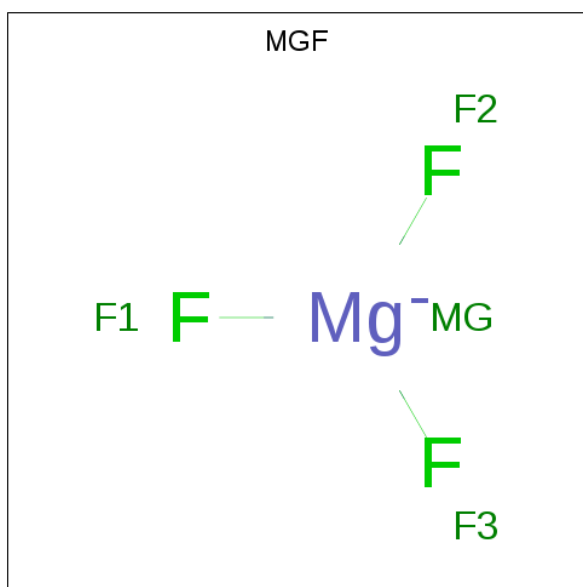


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula: F_3Mg).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	K	1	Total	C	O	0	0
			6	3	3		

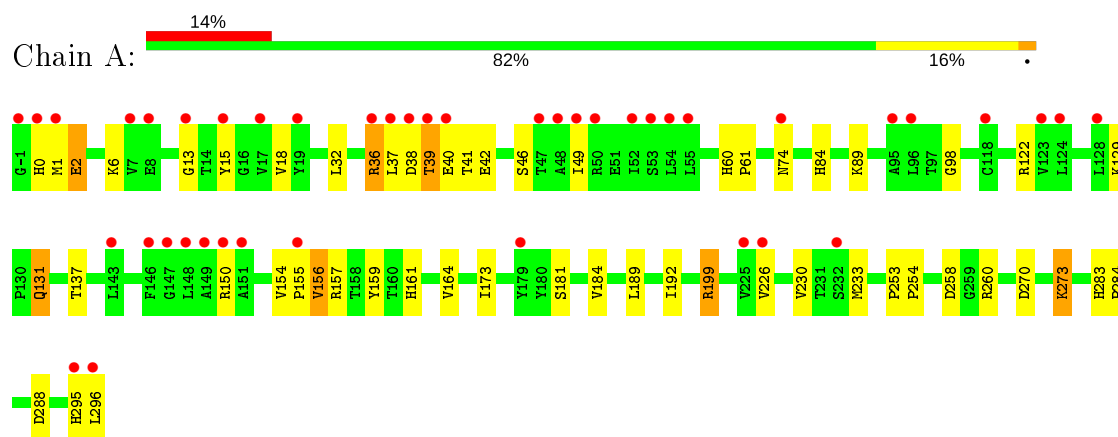
- Molecule 9 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	146	Total	O		0	0
			146	146			
9	B	156	Total	O		0	0
			156	156			
9	C	183	Total	O		0	0
			183	183			
9	D	104	Total	O		0	0
			104	104			
9	J	1	Total	O		0	0
			1	1			
9	K	5	Total	O		0	0
			5	5			
9	L	4	Total	O		0	0
			4	4			
9	M	2	Total	O		0	0
			2	2			

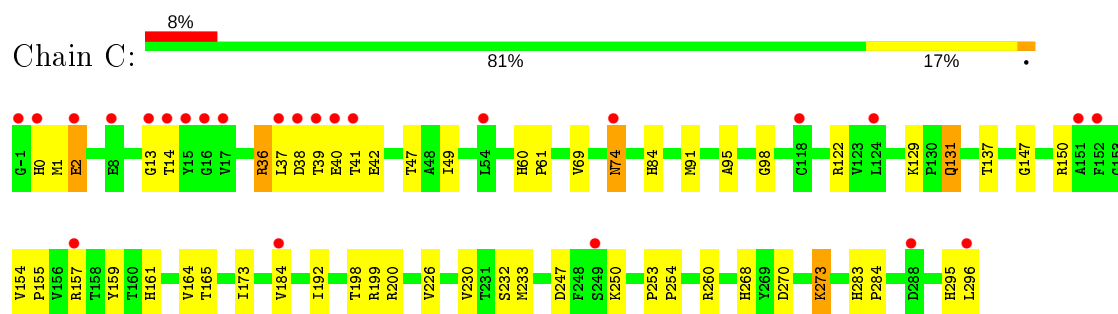
3 Residue-property plots [i](#)

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

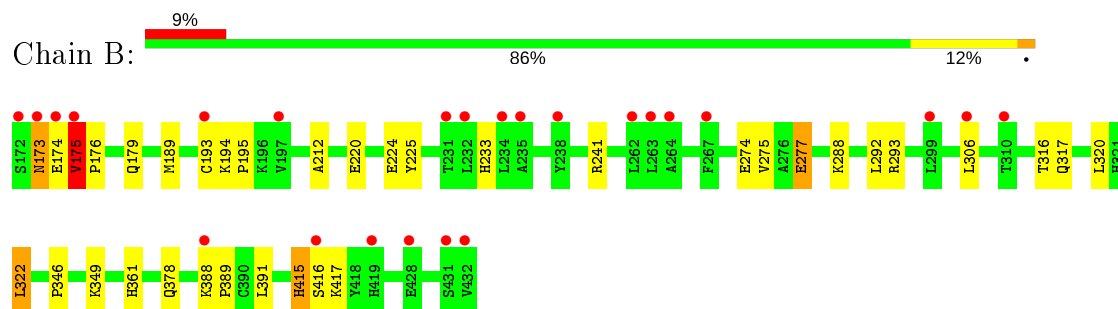
- Molecule 1: Cell division protein kinase 2



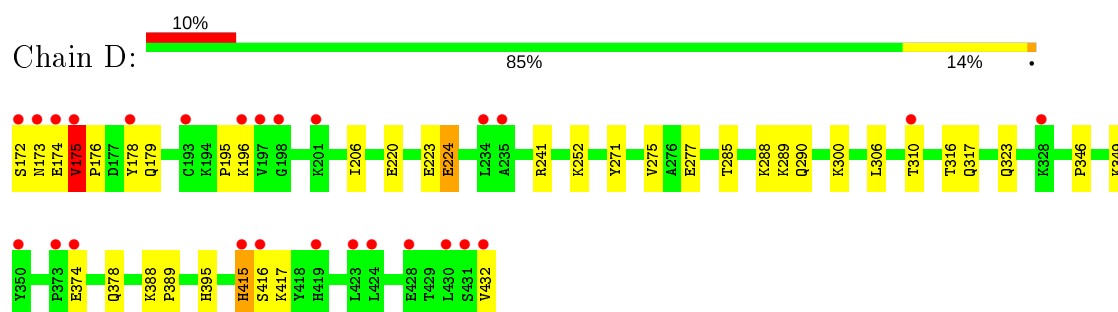
- Molecule 1: Cell division protein kinase 2



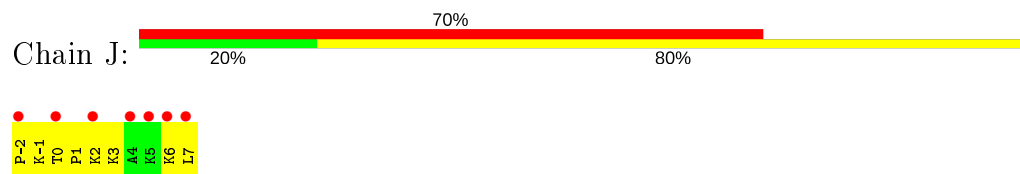
- Molecule 2: Cyclin-A2



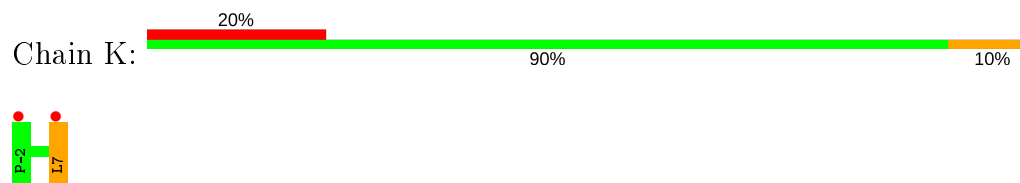
- Molecule 2: Cyclin-A2



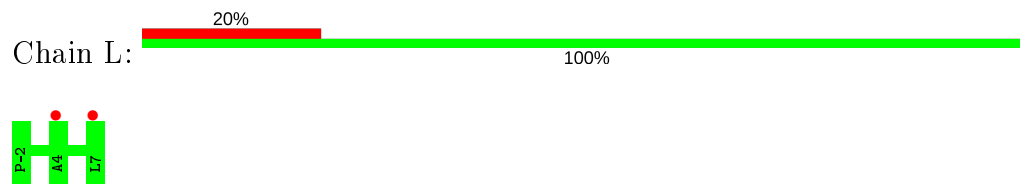
- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



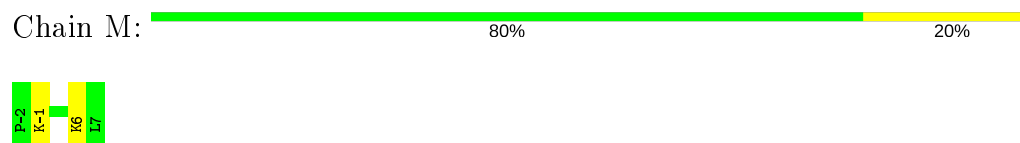
- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.69Å 163.91Å 73.28Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	37.80 – 2.17 37.80 – 2.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.80-2.17) 99.9 (37.80-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.179 , 0.210 0.172 , 0.203	Depositor DCC
R_{free} test set	4193 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10077	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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, MG, MGF, ADP, CL, TPO

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	0.49	0/2447	0.56	0/3320
1	C	0.51	0/2447	0.56	0/3320
2	B	0.50	0/2149	0.54	0/2921
2	D	0.45	0/2149	0.54	0/2921
3	J	0.88	0/80	0.98	0/103
3	K	1.27	0/80	0.98	0/103
3	L	0.92	0/80	0.94	0/103
3	M	1.19	0/80	0.91	0/103
All	All	0.52	0/9512	0.57	0/12894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2396	0	2435	66	0
1	C	2396	0	2435	73	0
2	B	2099	0	2110	52	0
2	D	2099	0	2110	49	0
3	J	79	0	104	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	79	0	104	4	0
3	L	79	0	104	0	0
3	M	79	0	104	1	0
4	A	27	0	12	2	0
4	C	27	0	12	2	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
7	A	1	0	0	1	0
7	C	1	0	0	1	0
8	A	24	0	32	10	0
8	B	30	0	40	4	0
8	C	12	0	16	7	0
8	D	30	0	40	4	0
8	K	6	0	8	0	0
9	A	146	0	0	9	0
9	B	156	0	0	8	0
9	C	183	0	0	11	0
9	D	104	0	0	3	0
9	J	1	0	0	5	0
9	K	5	0	0	0	0
9	L	4	0	0	0	0
9	M	2	0	0	0	0
All	All	10077	0	9666	229	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 12.

All (229) 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:37:LEU:O	1:A:40:GLU:HB2	1.45	1.16
2:B:175:VAL:H	2:B:176:PRO:HD3	1.09	1.15
1:A:161:HIS:H	8:A:303:GOL:H12	1.12	1.14
1:C:37:LEU:O	1:C:40:GLU:HB2	1.50	1.10
1:C:41:THR:HG22	2:D:288:LYS:HE3	1.32	1.06
1:A:36:ARG:N	1:A:36:ARG:HD3	1.69	1.06
1:C:41:THR:CG2	2:D:288:LYS:HE3	1.84	1.05
1:A:154:VAL:O	2:B:316:THR:HG22	1.58	1.03
1:A:38:ASP:O	1:A:39:THR:HG23	1.59	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:H	1:A:36:ARG:CD	1.69	1.02
1:C:36:ARG:N	1:C:36:ARG:HD3	1.69	1.01
1:C:36:ARG:CD	1:C:36:ARG:H	1.69	1.00
1:A:36:ARG:H	1:A:36:ARG:HD3	0.83	0.99
1:C:41:THR:HG22	2:D:288:LYS:CE	1.92	0.98
2:D:175:VAL:H	2:D:176:PRO:HD3	1.30	0.95
1:C:36:ARG:HD3	1:C:36:ARG:H	0.83	0.95
2:B:175:VAL:N	2:B:176:PRO:CD	2.30	0.94
2:B:175:VAL:N	2:B:176:PRO:HD3	1.80	0.94
1:A:41:THR:HG22	2:B:288:LYS:CE	1.98	0.94
1:C:38:ASP:O	1:C:39:THR:HG23	1.69	0.91
1:A:41:THR:HG22	2:B:288:LYS:HE3	1.52	0.90
3:K:7:LEU:O	3:K:7:LEU:HD12	1.72	0.89
1:A:38:ASP:C	1:A:39:THR:HG23	1.88	0.89
2:D:175:VAL:H	2:D:176:PRO:CD	1.85	0.89
1:C:154:VAL:O	2:D:316:THR:HG22	1.72	0.88
2:D:174:GLU:OE1	2:D:174:GLU:HA	1.73	0.87
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.56	0.86
1:C:38:ASP:C	1:C:39:THR:HG23	1.96	0.86
2:B:175:VAL:H	2:B:176:PRO:CD	1.85	0.86
1:A:37:LEU:C	1:A:40:GLU:HB2	1.97	0.84
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.60	0.83
1:C:41:THR:CG2	2:D:288:LYS:CE	2.52	0.83
8:B:16:GOL:H31	9:B:483:HOH:O	1.80	0.82
3:J:6:LYS:O	3:J:7:LEU:CB	2.29	0.81
2:D:175:VAL:N	2:D:176:PRO:CD	2.42	0.81
2:D:175:VAL:O	2:D:175:VAL:CG2	2.30	0.80
1:A:154:VAL:HG11	2:B:179:GLN:OE1	1.83	0.79
3:K:7:LEU:O	3:K:7:LEU:CD1	2.30	0.79
1:C:37:LEU:O	1:C:40:GLU:CB	2.30	0.78
3:K:7:LEU:O	3:K:7:LEU:CG	2.30	0.78
1:A:38:ASP:O	1:A:39:THR:CG2	2.30	0.78
1:A:154:VAL:O	2:B:316:THR:CG2	2.31	0.77
2:B:293:ARG:HH22	1:C:2:GLU:HG2	1.51	0.76
3:J:-1:LYS:HD3	9:J:655:HOH:O	1.85	0.76
1:A:0:HIS:ND1	1:A:1:MET:HG2	2.01	0.75
1:A:37:LEU:O	1:A:40:GLU:CB	2.30	0.75
2:B:378:GLN:HG2	9:B:481:HOH:O	1.85	0.75
1:C:98:GLY:HA3	1:C:199:ARG:NH1	2.00	0.75
1:A:41:THR:HG22	2:B:288:LYS:NZ	2.00	0.75
1:C:161:HIS:HD2	9:C:380:HOH:O	1.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:0:HIS:ND1	1:C:1:MET:HG2	2.02	0.75
1:A:181:SER:HB3	9:A:342:HOH:O	1.87	0.74
1:C:154:VAL:CG2	2:D:317:GLN:HG2	2.18	0.73
2:D:196:LYS:HE3	9:D:626:HOH:O	1.88	0.73
2:B:415:HIS:ND1	2:B:416:SER:N	2.37	0.72
3:K:7:LEU:HG	3:K:7:LEU:O	1.87	0.72
2:D:415:HIS:ND1	2:D:416:SER:N	2.38	0.72
1:C:41:THR:HG23	2:D:288:LYS:NZ	2.05	0.71
9:A:509:HOH:O	2:B:193:CYS:SG	2.47	0.71
1:A:41:THR:CG2	2:B:288:LYS:NZ	2.54	0.71
3:J:6:LYS:O	3:J:7:LEU:HB2	1.92	0.70
2:B:173:ASN:OD1	2:B:173:ASN:C	2.30	0.69
8:A:303:GOL:H2	9:A:559:HOH:O	1.92	0.69
1:C:38:ASP:O	1:C:39:THR:CG2	2.39	0.69
1:A:260:ARG:HD3	9:A:569:HOH:O	1.91	0.69
2:B:220:GLU:O	2:B:224:GLU:HG2	1.93	0.69
1:C:260:ARG:HD3	9:C:395:HOH:O	1.93	0.68
1:A:161:HIS:N	8:A:303:GOL:H12	1.97	0.67
2:B:175:VAL:HG23	2:B:175:VAL:O	1.92	0.67
2:D:220:GLU:O	2:D:224:GLU:HG2	1.95	0.67
8:A:304:GOL:H31	8:A:305:GOL:H31	1.77	0.67
1:C:230:VAL:O	1:C:233:MET:HG3	1.95	0.66
1:C:154:VAL:HG23	2:D:317:GLN:HG2	1.76	0.66
1:A:157:ARG:HB3	1:A:159:TYR:CE1	2.31	0.65
1:C:69:VAL:HG23	8:C:303:GOL:H31	1.79	0.65
1:A:38:ASP:O	1:A:39:THR:CB	2.46	0.64
2:B:173:ASN:OD1	2:B:174:GLU:N	2.31	0.64
2:D:175:VAL:N	2:D:176:PRO:HD3	2.05	0.63
8:A:305:GOL:H11	2:D:300:LYS:NZ	2.14	0.63
1:C:38:ASP:C	1:C:39:THR:CG2	2.67	0.63
1:A:288:ASP:OD1	8:A:302:GOL:H12	2.00	0.62
1:A:36:ARG:NH2	9:A:370:HOH:O	2.32	0.62
3:J:0:THR:HG23	3:J:1:PRO:HD2	1.82	0.62
2:D:220:GLU:O	2:D:224:GLU:CG	2.48	0.61
2:D:388:LYS:HB2	2:D:389:PRO:HD3	1.82	0.61
2:D:395:HIS:ND1	9:D:589:HOH:O	2.31	0.61
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.81	0.61
2:D:175:VAL:O	2:D:175:VAL:HG23	1.98	0.61
2:D:175:VAL:O	2:D:175:VAL:HG22	2.02	0.60
1:C:36:ARG:NH2	9:C:480:HOH:O	2.34	0.60
1:A:230:VAL:O	1:A:233:MET:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:C	1:A:39:THR:CG2	2.59	0.59
2:B:415:HIS:HB2	9:B:562:HOH:O	2.02	0.59
1:C:154:VAL:O	1:C:154:VAL:HG23	2.01	0.58
2:B:388:LYS:HB2	2:B:389:PRO:HD3	1.84	0.58
1:C:98:GLY:CA	1:C:199:ARG:NH1	2.67	0.58
1:C:38:ASP:O	1:C:39:THR:CB	2.51	0.58
2:D:172:SER:O	2:D:173:ASN:OD1	2.22	0.57
2:B:322:LEU:HD23	9:B:494:HOH:O	2.03	0.57
1:A:98:GLY:HA2	1:A:199:ARG:HD3	1.87	0.56
3:J:6:LYS:O	3:J:7:LEU:HB3	2.03	0.56
1:C:41:THR:CG2	2:D:288:LYS:NZ	2.68	0.56
2:B:388:LYS:NZ	2:B:388:LYS:HB3	2.20	0.56
2:D:223:GLU:HA	2:D:223:GLU:OE1	2.05	0.56
2:B:293:ARG:NH2	1:C:2:GLU:HG2	2.19	0.56
1:A:38:ASP:C	1:A:40:GLU:H	2.09	0.56
1:C:154:VAL:O	2:D:316:THR:CG2	2.49	0.55
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.06	0.55
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.88	0.55
2:D:388:LYS:NZ	2:D:388:LYS:HB3	2.21	0.55
1:A:154:VAL:CG1	2:B:179:GLN:OE1	2.53	0.55
8:A:305:GOL:H11	2:D:300:LYS:HZ2	1.71	0.54
1:C:1:MET:HG3	1:C:2:GLU:N	2.23	0.54
1:C:37:LEU:HB2	1:C:74:ASN:O	2.08	0.54
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.89	0.54
1:C:295:HIS:CE1	9:C:643:HOH:O	2.60	0.54
2:D:175:VAL:N	2:D:176:PRO:HD2	2.22	0.54
2:D:310:THR:HA	8:D:5:GOL:H12	1.89	0.54
9:C:358:HOH:O	3:J:-2:PRO:HD2	2.07	0.54
1:A:295:HIS:HD2	9:A:624:HOH:O	1.91	0.54
1:A:13:GLY:HA3	4:A:297:ADP:O1B	2.07	0.54
1:C:137:THR:HG22	1:C:296:LEU:HD12	1.90	0.54
3:J:-1:LYS:CG	9:J:655:HOH:O	2.54	0.54
1:A:270:ASP:OD2	1:A:273:LYS:HE2	2.09	0.53
1:A:154:VAL:HG13	2:B:175:VAL:HG21	1.90	0.53
2:D:285:THR:OG1	3:M:6:LYS:HB2	2.09	0.52
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.25	0.52
2:B:317:GLN:NE2	9:B:471:HOH:O	2.42	0.52
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.90	0.52
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.25	0.52
1:A:41:THR:CG2	2:B:288:LYS:HZ2	2.23	0.51
1:A:270:ASP:HB3	1:A:273:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:2:GLU:N	2.24	0.51
2:D:206:ILE:O	8:D:7:GOL:H32	2.10	0.51
1:A:41:THR:CG2	2:B:288:LYS:HE3	2.35	0.51
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.93	0.50
8:A:304:GOL:H31	8:A:305:GOL:C3	2.40	0.50
2:B:189:MET:CG	9:B:590:HOH:O	2.59	0.50
1:C:95:ALA:O	1:C:199:ARG:HD2	2.11	0.50
1:A:156:VAL:HG22	1:A:159:TYR:HE2	1.76	0.50
1:A:15:TYR:CD2	9:A:333:HOH:O	2.53	0.50
1:A:6:LYS:NZ	9:A:503:HOH:O	2.41	0.50
1:C:198:THR:O	1:C:199:ARG:HB2	2.11	0.50
1:C:98:GLY:CA	1:C:199:ARG:HH11	2.25	0.50
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.94	0.50
1:C:270:ASP:HB3	1:C:273:LYS:HE3	1.93	0.49
2:D:252:LYS:HE3	8:D:13:GOL:H32	1.94	0.49
1:A:258:ASP:OD2	8:A:302:GOL:H32	2.12	0.49
1:A:38:ASP:O	1:A:39:THR:OG1	2.30	0.49
1:A:42:GLU:OE2	2:B:274:GLU:HB2	2.12	0.49
1:C:14:THR:HG23	3:J:2:LYS:NZ	2.27	0.49
1:C:200:ARG:CA	8:C:302:GOL:O1	2.61	0.49
1:A:156:VAL:HG22	1:A:159:TYR:CE2	2.47	0.49
1:A:38:ASP:C	1:A:40:GLU:N	2.64	0.49
1:C:270:ASP:OD2	1:C:273:LYS:HE2	2.12	0.49
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.94	0.49
3:J:-1:LYS:HB3	9:J:655:HOH:O	2.13	0.48
1:C:37:LEU:C	1:C:40:GLU:HB2	2.30	0.48
2:D:346:PRO:O	2:D:349:LYS:HG2	2.12	0.48
1:A:131:GLN:HB3	7:A:301:CL:CL	2.50	0.48
3:J:0:THR:CG2	3:J:1:PRO:HD2	2.44	0.48
2:B:212:ALA:HB2	8:B:6:GOL:H32	1.95	0.48
1:C:157:ARG:HB2	1:C:159:TYR:CE1	2.48	0.48
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.49	0.48
1:C:154:VAL:CG2	1:C:154:VAL:O	2.62	0.47
1:A:41:THR:HG23	2:B:288:LYS:NZ	2.27	0.47
1:C:268:HIS:CD2	9:C:582:HOH:O	2.66	0.47
2:B:175:VAL:N	2:B:176:PRO:HD2	2.25	0.47
2:B:225:TYR:OH	2:B:277:GLU:HG2	2.14	0.47
1:C:232:SER:HB2	9:C:647:HOH:O	2.13	0.47
9:C:457:HOH:O	3:J:3:LYS:HE3	2.14	0.47
1:C:38:ASP:O	1:C:39:THR:OG1	2.30	0.47
1:C:199:ARG:O	8:C:302:GOL:H12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:HIS:CE1	2:B:417:LYS:H	2.32	0.46
2:D:289:LYS:HE3	9:D:606:HOH:O	2.15	0.46
1:A:161:HIS:HB2	8:A:303:GOL:H31	1.98	0.46
1:C:199:ARG:C	8:C:302:GOL:O1	2.55	0.46
2:B:275:VAL:HG21	2:B:292:LEU:HD21	1.98	0.46
8:B:1:GOL:H12	9:B:452:HOH:O	2.15	0.46
1:A:41:THR:HG23	2:B:288:LYS:HZ2	1.81	0.45
2:D:172:SER:C	2:D:173:ASN:OD1	2.54	0.45
2:D:415:HIS:CE1	2:D:417:LYS:H	2.34	0.45
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.52	0.45
1:C:91:MET:HB3	8:C:302:GOL:H31	1.99	0.45
3:J:-1:LYS:CB	9:J:655:HOH:O	2.65	0.45
1:A:84:HIS:ND1	1:A:296:LEU:HD13	2.32	0.45
1:C:147:GLY:HA3	9:C:551:HOH:O	2.16	0.45
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.99	0.45
2:B:233:HIS:ND1	8:B:1:GOL:O1	2.50	0.44
2:B:179:GLN:HE22	2:B:320:LEU:HD12	1.82	0.44
1:C:129:LYS:HE3	1:C:131:GLN:HG2	2.00	0.44
2:D:290:GLN:HE22	8:D:13:GOL:C3	2.30	0.44
1:A:157:ARG:HB3	1:A:159:TYR:HE1	1.82	0.44
1:C:41:THR:O	2:D:288:LYS:HE2	2.18	0.44
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.99	0.44
1:C:47:THR:HG23	9:C:604:HOH:O	2.17	0.44
1:A:18:VAL:HA	1:A:32:LEU:O	2.19	0.43
1:C:199:ARG:O	8:C:302:GOL:C1	2.66	0.43
2:D:220:GLU:O	2:D:224:GLU:HG3	2.18	0.43
1:A:41:THR:CG2	2:B:288:LYS:CE	2.85	0.43
2:B:179:GLN:HE22	2:B:320:LEU:CD1	2.30	0.43
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.78	0.43
1:C:13:GLY:HA3	4:C:297:ADP:O1B	2.18	0.43
3:J:-1:LYS:CD	9:J:655:HOH:O	2.51	0.43
1:C:273:LYS:HB2	1:C:273:LYS:HE3	1.88	0.43
2:D:174:GLU:OE1	2:D:174:GLU:CA	2.50	0.43
2:B:194:LYS:HD2	2:B:195:PRO:HD2	2.00	0.42
1:C:131:GLN:HB3	7:C:301:CL:CL	2.57	0.42
1:C:173:ILE:HD11	1:C:184:VAL:HG11	2.01	0.42
2:D:271:TYR:CD1	3:J:6:LYS:HB2	2.55	0.42
2:B:346:PRO:O	2:B:349:LYS:HG2	2.19	0.42
1:C:268:HIS:HD2	9:C:582:HOH:O	2.01	0.42
1:C:84:HIS:ND1	1:C:296:LEU:HD13	2.35	0.42
2:D:374:GLU:O	2:D:378:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.81	0.42
2:B:189:MET:HG3	9:B:590:HOH:O	2.17	0.42
1:C:129:LYS:HD3	1:C:165:THR:OG1	2.20	0.41
2:D:195:PRO:HG3	2:D:241:ARG:HG3	2.01	0.41
1:C:42:GLU:OE1	2:D:275:VAL:HG23	2.20	0.41
1:A:173:ILE:HD11	1:A:184:VAL:HG11	2.01	0.41
4:A:297:ADP:O5'	4:A:297:ADP:H8	2.04	0.41
1:A:273:LYS:HE3	1:A:273:LYS:HB2	1.89	0.41
1:C:247:ASP:O	1:C:250:LYS:HB3	2.21	0.41
1:A:89:LYS:HE3	9:A:366:HOH:O	2.20	0.41
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.56	0.41
2:B:195:PRO:HG3	2:B:241:ARG:HG3	2.03	0.40
4:C:297:ADP:O5'	4:C:297:ADP:H8	2.04	0.40
1:C:98:GLY:HA2	1:C:199:ARG:HH11	1.85	0.40
1:C:200:ARG:HA	8:C:302:GOL:O1	2.21	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	295/298 (99%)	286 (97%)	8 (3%)	1 (0%)	41	43
1	C	295/298 (99%)	283 (96%)	11 (4%)	1 (0%)	41	43
2	B	259/261 (99%)	253 (98%)	5 (2%)	1 (0%)	34	35
2	D	259/261 (99%)	255 (98%)	3 (1%)	1 (0%)	34	35
3	J	8/10 (80%)	8 (100%)	0	0	100	100
3	K	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	L	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	M	8/10 (80%)	7 (88%)	1 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1140/1158 (98%)	1106 (97%)	30 (3%)	4 (0%)	34	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL
2	D	175	VAL
2	B	175	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	261/261 (100%)	249 (95%)	12 (5%)	27	31
1	C	261/261 (100%)	253 (97%)	8 (3%)	40	48
2	B	234/234 (100%)	229 (98%)	5 (2%)	53	64
2	D	234/234 (100%)	226 (97%)	8 (3%)	37	44
3	J	9/9 (100%)	9 (100%)	0	100	100
3	K	9/9 (100%)	8 (89%)	1 (11%)	6	4
3	L	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	8 (89%)	1 (11%)	6	4
All	All	1026/1026 (100%)	991 (97%)	35 (3%)	37	44

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	36	ARG
1	A	39	THR
1	A	46	SER
1	A	74	ASN
1	A	122	ARG

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Mol	Chain	Res	Type
1	A	131	GLN
1	A	150	ARG
1	A	156	VAL
1	A	199	ARG
1	A	226	VAL
1	A	273	LYS
2	B	173	ASN
2	B	175	VAL
2	B	277	GLU
2	B	322	LEU
2	B	415	HIS
1	C	2	GLU
1	C	36	ARG
1	C	74	ASN
1	C	122	ARG
1	C	131	GLN
1	C	150	ARG
1	C	226	VAL
1	C	273	LYS
2	D	175	VAL
2	D	178	TYR
2	D	179	GLN
2	D	224	GLU
2	D	277	GLU
2	D	323	GLN
2	D	415	HIS
2	D	432	VAL
3	K	7	LEU
3	M	-1	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
2	B	296	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.05	0	10,14,16	1.59	1 (10%)
1	TPO	A	160	1	8,10,11	1.08	0	10,14,16	1.52	1 (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
1	TPO	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	P-OG1-CB	-4.39	109.96	123.21
1	A	160	TPO	P-OG1-CB	-3.97	111.20	123.21

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 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
8	GOL	D	2	-	5,5,5	0.33	0	5,5,5	0.52	0
8	GOL	A	304	-	5,5,5	0.42	0	5,5,5	0.82	0
8	GOL	D	13	-	5,5,5	0.38	0	5,5,5	0.54	0
4	ADP	C	297	5,6	24,29,29	0.99	1 (4%)	29,45,45	1.27	4 (13%)
8	GOL	C	303	-	5,5,5	0.53	0	5,5,5	0.79	0
8	GOL	B	1	-	5,5,5	0.65	0	5,5,5	0.94	0
6	MGF	A	300	3,4	0,3,3	0.00	-	-		
8	GOL	K	12	-	5,5,5	0.18	0	5,5,5	0.59	0
8	GOL	B	8	-	5,5,5	0.53	0	5,5,5	0.77	0
8	GOL	D	15	-	5,5,5	0.30	0	5,5,5	0.56	0
8	GOL	B	16	-	5,5,5	0.78	0	5,5,5	0.49	0
8	GOL	D	5	-	5,5,5	0.60	0	5,5,5	0.68	0
8	GOL	A	302	-	5,5,5	0.36	0	5,5,5	0.56	0
8	GOL	C	302	-	5,5,5	0.44	0	5,5,5	0.70	0
8	GOL	A	305	-	5,5,5	0.31	0	5,5,5	0.59	0
8	GOL	B	6	-	5,5,5	0.57	0	5,5,5	0.41	0
8	GOL	D	7	-	5,5,5	0.50	0	5,5,5	0.47	0
6	MGF	C	300	3,4	0,3,3	0.00	-	-		
8	GOL	B	3	-	5,5,5	0.43	0	5,5,5	0.42	0
8	GOL	A	303	-	5,5,5	0.41	0	5,5,5	0.43	0
4	ADP	A	297	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.25	3 (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
4	ADP	C	297	5,6	-	2/12/32/32	0/3/3/3
8	GOL	A	304	-	-	0/4/4/4	-
8	GOL	D	13	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	D	2	-	-	4/4/4/4	-
8	GOL	C	303	-	-	2/4/4/4	-
8	GOL	B	1	-	-	2/4/4/4	-
8	GOL	K	12	-	-	1/4/4/4	-
8	GOL	B	8	-	-	4/4/4/4	-
8	GOL	D	15	-	-	2/4/4/4	-
8	GOL	B	16	-	-	4/4/4/4	-
8	GOL	D	5	-	-	4/4/4/4	-
8	GOL	A	302	-	-	2/4/4/4	-
8	GOL	C	302	-	-	3/4/4/4	-
8	GOL	A	305	-	-	0/4/4/4	-
8	GOL	B	6	-	-	2/4/4/4	-
8	GOL	D	7	-	-	2/4/4/4	-
8	GOL	B	3	-	-	2/4/4/4	-
8	GOL	A	303	-	-	2/4/4/4	-
4	ADP	A	297	5,6	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	297	ADP	C5-C4	2.42	1.47	1.40
4	C	297	ADP	C5-C4	2.39	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	297	ADP	N3-C2-N1	-3.55	123.12	128.68
4	C	297	ADP	N3-C2-N1	-3.22	123.64	128.68
4	C	297	ADP	C3'-C2'-C1'	2.78	105.16	100.98
4	A	297	ADP	C3'-C2'-C1'	2.58	104.86	100.98
4	C	297	ADP	C4-C5-N7	-2.45	106.85	109.40
4	C	297	ADP	O3B-PB-O2B	2.20	116.04	107.64
4	A	297	ADP	C4-C5-N7	-2.15	107.16	109.40

There are no chirality outliers.

All (40) torsion outliers are listed below:

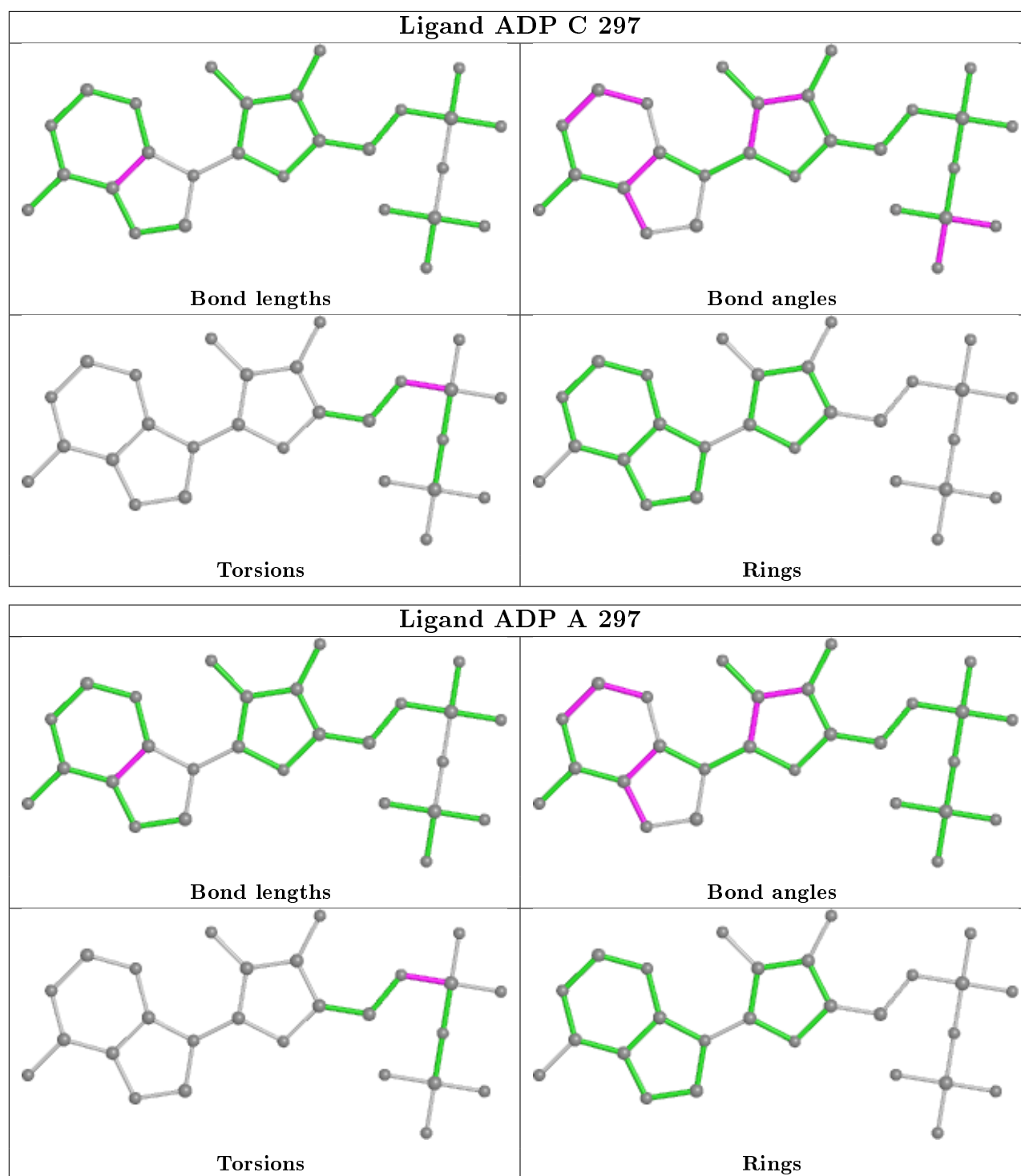
Mol	Chain	Res	Type	Atoms
8	D	2	GOL	O1-C1-C2-C3
8	D	5	GOL	O1-C1-C2-C3
8	A	302	GOL	O1-C1-C2-C3
8	C	302	GOL	O1-C1-C2-C3
4	C	297	ADP	C5'-O5'-PA-O1A
8	B	16	GOL	O1-C1-C2-C3
8	D	7	GOL	O1-C1-C2-C3
8	B	1	GOL	O1-C1-C2-C3
8	C	303	GOL	O1-C1-C2-C3
8	B	8	GOL	O1-C1-C2-C3
8	B	3	GOL	O1-C1-C2-C3
8	B	6	GOL	O1-C1-C2-O2
8	B	6	GOL	O1-C1-C2-C3
4	A	297	ADP	C5'-O5'-PA-O1A
8	B	3	GOL	O1-C1-C2-O2
8	D	2	GOL	C1-C2-C3-O3
8	D	5	GOL	C1-C2-C3-O3
8	C	302	GOL	C1-C2-C3-O3
8	B	16	GOL	C1-C2-C3-O3
8	D	15	GOL	C1-C2-C3-O3
8	B	8	GOL	C1-C2-C3-O3
8	A	303	GOL	C1-C2-C3-O3
8	D	2	GOL	O1-C1-C2-O2
8	D	5	GOL	O1-C1-C2-O2
8	D	5	GOL	O2-C2-C3-O3
8	A	302	GOL	O1-C1-C2-O2
8	C	302	GOL	O1-C1-C2-O2
8	D	7	GOL	O1-C1-C2-O2
8	C	303	GOL	O1-C1-C2-O2
8	B	8	GOL	O1-C1-C2-O2
8	B	16	GOL	O1-C1-C2-O2
8	B	1	GOL	O1-C1-C2-O2
8	A	303	GOL	O2-C2-C3-O3
8	D	2	GOL	O2-C2-C3-O3
8	D	15	GOL	O2-C2-C3-O3
8	B	8	GOL	O2-C2-C3-O3
4	C	297	ADP	C5'-O5'-PA-O3A
4	A	297	ADP	C5'-O5'-PA-O3A
8	B	16	GOL	O2-C2-C3-O3
8	K	12	GOL	O2-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	304	GOL	2	0
8	D	13	GOL	2	0
4	C	297	ADP	2	0
8	C	303	GOL	1	0
8	B	1	GOL	2	0
8	B	16	GOL	1	0
8	D	5	GOL	1	0
8	A	302	GOL	2	0
8	C	302	GOL	6	0
8	A	305	GOL	4	0
8	B	6	GOL	1	0
8	D	7	GOL	1	0
8	A	303	GOL	4	0
4	A	297	ADP	2	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	297/298 (99%)	0.63	43 (14%) 2 2	25, 45, 106, 163	0
1	C	297/298 (99%)	0.46	25 (8%) 11 11	25, 45, 106, 163	0
2	B	261/261 (100%)	0.48	24 (9%) 9 9	24, 43, 95, 163	0
2	D	261/261 (100%)	0.56	26 (9%) 7 7	27, 48, 96, 163	0
3	J	10/10 (100%)	2.67	7 (70%) 0 0	72, 92, 119, 132	0
3	K	10/10 (100%)	1.17	2 (20%) 1 1	71, 93, 113, 140	0
3	L	4/10 (40%)	2.26	2 (50%) 0 0	65, 71, 75, 82	0
3	M	4/10 (40%)	1.10	0 100 100	64, 72, 78, 83	0
All	All	1144/1158 (98%)	0.57	129 (11%) 5 5	24, 46, 106, 163	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	173	ASN	9.9
1	A	38	ASP	9.9
2	D	173	ASN	9.1
2	B	431	SER	8.6
2	D	172	SER	8.6
2	D	174	GLU	8.0
1	C	38	ASP	7.3
1	C	39	THR	7.2
2	D	175	VAL	6.9
1	A	39	THR	6.9
3	J	7	LEU	6.5
2	B	432	VAL	6.1
2	D	193	CYS	6.0
2	B	193	CYS	5.7
2	D	197	VAL	5.3
3	K	7	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	174	GLU	5.2
1	A	0	HIS	5.0
2	B	172	SER	4.8
2	D	432	VAL	4.8
1	C	14	THR	4.6
1	A	295	HIS	4.3
1	C	-1	GLY	4.3
1	C	0	HIS	4.2
2	B	175	VAL	4.2
1	A	40	GLU	4.1
2	D	431	SER	4.1
1	A	-1	GLY	4.1
1	A	8	GLU	3.9
2	D	196	LYS	3.8
2	B	306	LEU	3.8
1	C	13	GLY	3.8
1	C	296	LEU	3.7
3	L	4	ALA	3.7
1	A	74	ASN	3.6
1	C	17	VAL	3.6
1	A	17	VAL	3.6
2	D	428	GLU	3.6
3	J	-2	PRO	3.5
1	C	15	TYR	3.4
1	C	249	SER	3.4
2	B	263	LEU	3.4
1	A	13	GLY	3.4
1	A	149	ALA	3.4
2	D	423	LEU	3.3
1	A	225	VAL	3.3
3	K	-2	PRO	3.3
2	D	419	HIS	3.2
1	C	16	GLY	3.2
3	J	4	ALA	3.2
1	A	124	LEU	3.1
2	D	416	SER	3.1
1	A	296	LEU	3.0
3	J	0	THR	3.0
1	C	40	GLU	3.0
1	A	49	ILE	3.0
2	D	374	GLU	3.0
1	A	128	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	2.9
3	L	7	LEU	2.9
2	D	415	HIS	2.9
1	A	52	ILE	2.9
1	C	74	ASN	2.9
1	A	47	THR	2.9
1	A	151	ALA	2.8
1	A	54	LEU	2.8
1	C	288	ASP	2.8
1	A	143	LEU	2.8
1	A	48	ALA	2.8
1	A	1	MET	2.8
1	C	152	PHE	2.8
2	B	234	LEU	2.7
1	A	232	SER	2.7
1	A	148	LEU	2.7
1	C	37	LEU	2.7
2	B	419	HIS	2.7
2	D	235	ALA	2.7
3	J	2	LYS	2.7
2	D	424	LEU	2.7
1	A	50	ARG	2.7
2	B	267	PHE	2.7
1	A	96	LEU	2.7
1	A	37	LEU	2.6
1	C	8	GLU	2.6
1	C	151	ALA	2.6
2	D	328	LYS	2.6
1	A	147	GLY	2.6
1	C	124	LEU	2.6
3	J	5	LYS	2.5
1	A	53	SER	2.4
2	B	262	LEU	2.4
2	D	430	LEU	2.3
2	B	264	ALA	2.3
1	A	15	TYR	2.3
2	B	388	LYS	2.3
1	A	150	ARG	2.3
2	D	201	LYS	2.3
2	B	299	LEU	2.3
2	D	234	LEU	2.3
1	A	118	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	428	GLU	2.3
1	A	95	ALA	2.2
1	A	7	VAL	2.2
1	A	55	LEU	2.2
2	B	416	SER	2.2
3	J	6	LYS	2.2
2	B	310	THR	2.2
2	D	310	THR	2.2
1	A	19	TYR	2.2
1	A	146	PHE	2.2
1	A	179	TYR	2.2
1	A	226	VAL	2.2
2	B	232	LEU	2.1
1	C	184	VAL	2.1
1	C	157	ARG	2.1
1	C	41	THR	2.1
1	A	155	PRO	2.1
2	D	373	PRO	2.1
2	D	198	GLY	2.1
1	C	118	CYS	2.1
2	D	178	TYR	2.1
2	D	350	TYR	2.1
1	A	36	ARG	2.0
2	B	231	THR	2.0
2	B	235	ALA	2.0
2	B	197	VAL	2.0
2	B	238	TYR	2.0
1	C	2	GLU	2.0
1	C	54	LEU	2.0

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

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	0.94	0.16	32,47,65,75	4
1	TPO	A	160	11/12	0.95	0.14	32,45,62,73	4

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

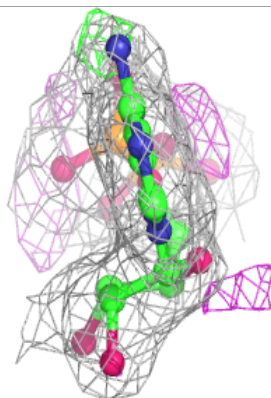
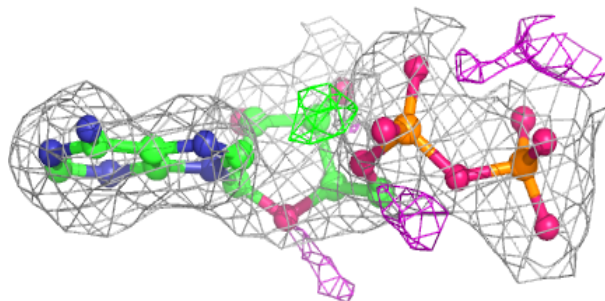
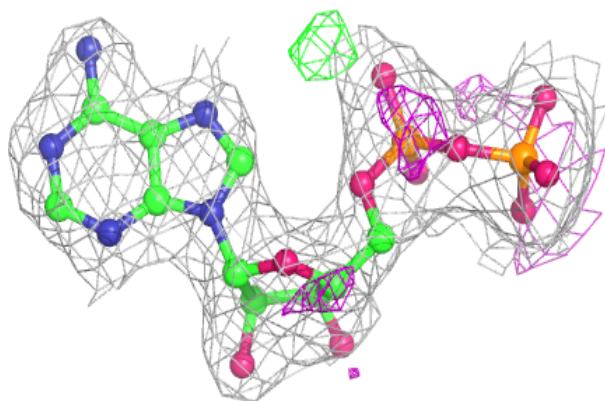
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	C	302	6/6	0.71	0.34	93,99,114,131	0
5	MG	C	298	1/1	0.77	0.08	71,71,71,71	0
8	GOL	D	7	6/6	0.81	0.35	78,85,94,99	0
8	GOL	A	305	6/6	0.81	0.15	78,83,87,91	0
8	GOL	D	2	6/6	0.82	0.16	81,92,100,109	0
8	GOL	C	303	6/6	0.88	0.21	78,87,101,105	0
5	MG	C	299	1/1	0.89	0.08	41,41,41,41	0
8	GOL	A	302	6/6	0.91	0.12	69,77,79,86	0
8	GOL	D	5	6/6	0.91	0.26	40,69,77,82	0
8	GOL	B	3	6/6	0.91	0.30	66,75,85,90	0
5	MG	A	298	1/1	0.91	0.04	58,58,58,58	0
8	GOL	B	6	6/6	0.92	0.15	58,80,93,98	0
8	GOL	D	15	6/6	0.93	0.18	64,70,77,85	0
4	ADP	C	297	27/27	0.93	0.15	45,60,78,106	0
8	GOL	K	12	6/6	0.93	0.19	65,77,85,96	0
8	GOL	B	1	6/6	0.93	0.18	27,63,71,81	0
8	GOL	B	8	6/6	0.94	0.22	71,72,84,84	0
6	MGF	A	300	4/4	0.94	0.13	56,67,80,97	0
8	GOL	A	303	6/6	0.94	0.13	56,76,86,92	0
4	ADP	A	297	27/27	0.94	0.13	53,60,73,104	0
8	GOL	D	13	6/6	0.95	0.18	71,81,89,89	0
8	GOL	A	304	6/6	0.95	0.15	37,62,73,79	0
7	CL	A	301	1/1	0.96	0.07	60,60,60,60	0
8	GOL	B	16	6/6	0.96	0.21	50,75,84,95	0
7	CL	C	301	1/1	0.97	0.09	60,60,60,60	0
6	MGF	C	300	4/4	0.97	0.22	61,64,70,171	0
5	MG	A	299	1/1	0.99	0.05	36,36,36,36	0

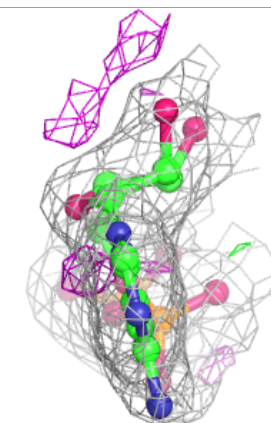
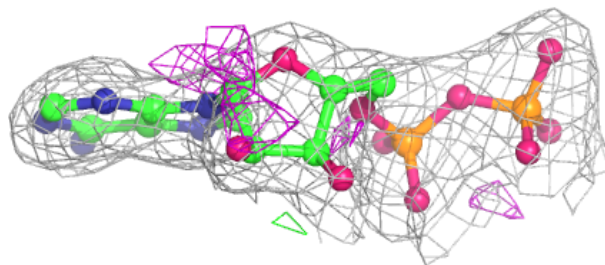
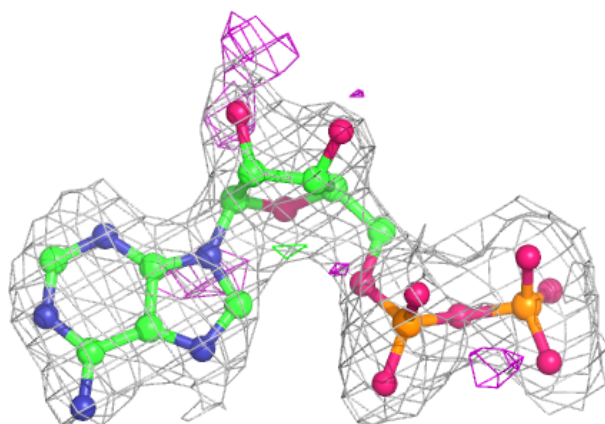
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 297:

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

**Electron density around ADP A 297:**

$2mF_o-DF_c$ (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.