Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 04:21 PM EDT

PDB ID	:	4XWT
Title	:	Crystal structure of RNase J complexed with UMP
Authors	:	Lu, M.; Zhang, H.; Xu, Q.; Hua, Y.; Zhao, Y.
Deposited on	:	2015-01-29
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

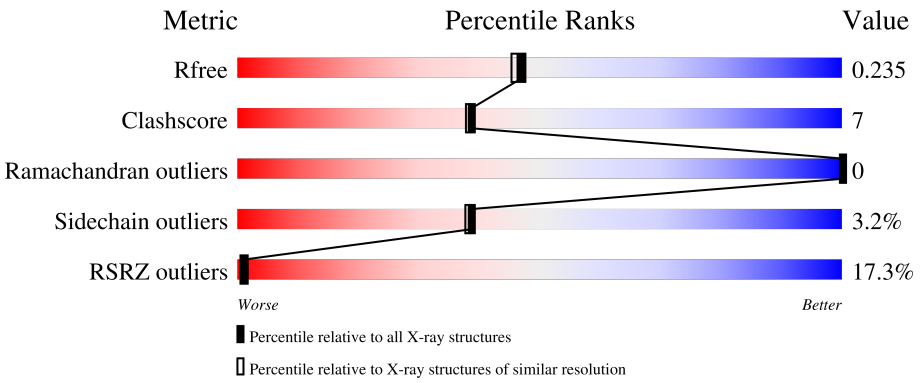
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	559	16% 83% 13% • •
1	B	559	18% 82% 14% • •

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
5	U5P	A	606	-	-	X	X
5	U5P	B	604	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8735 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 DR2417.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4206	2664	756	773	13	0	4	0
1	B	543	4147	2629	740	764	14	0	4	0

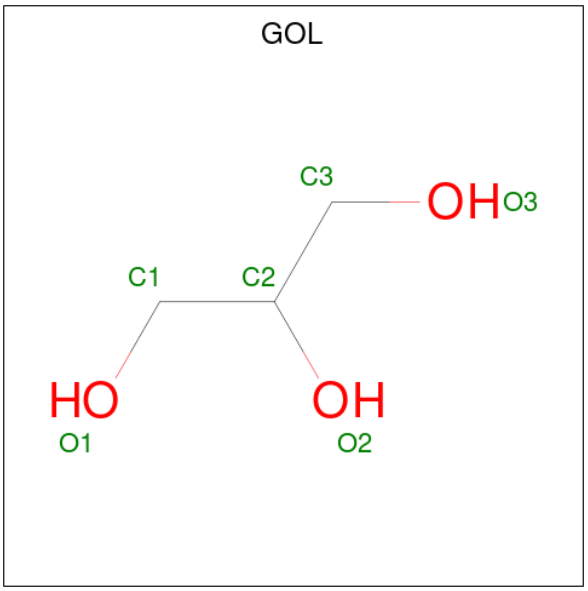
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

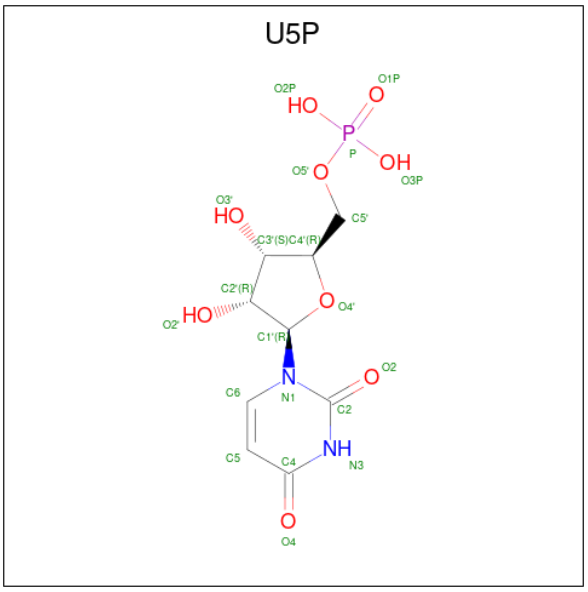
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	21	9	2	9	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	21	9	2	9	1	0	0

- Molecule 6 is water.

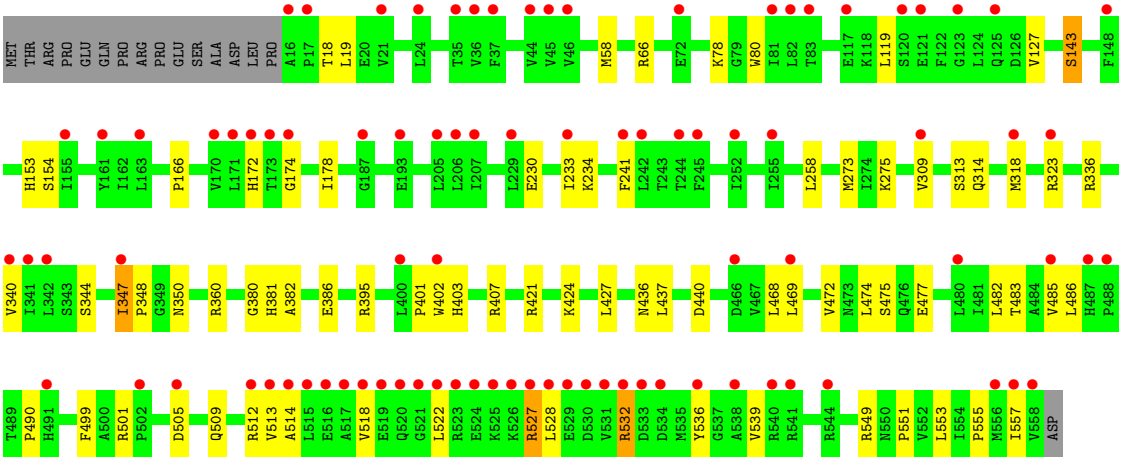
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	168	168	168	0	0
			Total	O		
6	B	154	154	154	0	0

3 Residue-property plots (i)

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

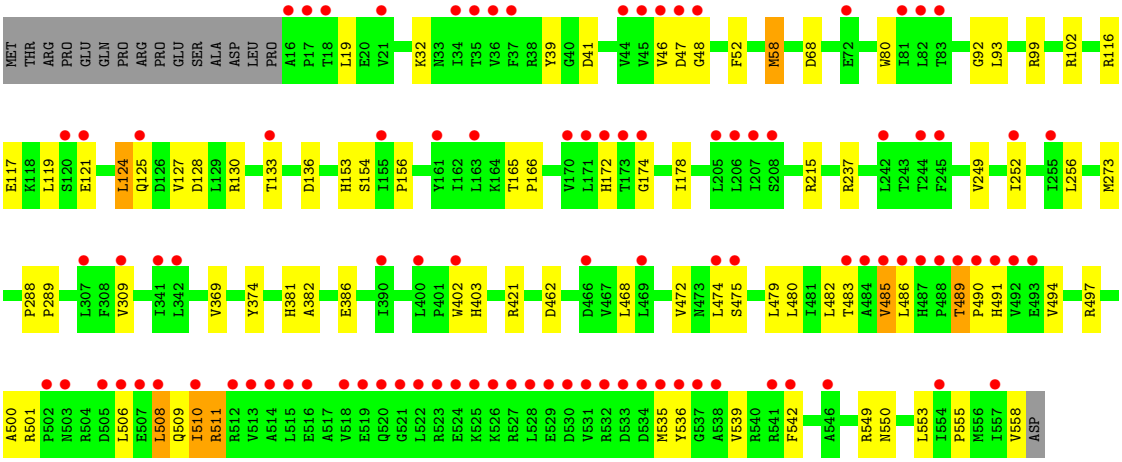
- Molecule 1: DR2417

Chain A:



- Molecule 1: DR2417

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.59Å 87.76Å 253.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.47 – 2.00 29.47 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.47-2.00) 97.5 (29.47-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.200 , 0.235 0.202 , 0.235	Depositor DCC
R_{free} test set	4898 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8735	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ZN, MN, U5P

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	0.39	0/4292	0.54	0/5836
1	B	0.37	0/4233	0.52	0/5762
All	All	0.38	0/8525	0.53	0/11598

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	4206	0	4207	70	0
1	B	4147	0	4098	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	16	2	0
5	A	21	0	11	8	0
5	B	21	0	11	1	0
6	A	168	0	0	4	0
6	B	154	0	0	5	0
All	All	8735	0	8343	125	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 7.

All (125) 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:347:ILE:HD13	1:A:348:PRO:CD	1.80	1.12
1:A:347:ILE:HD13	1:A:348:PRO:N	1.68	1.06
1:A:347:ILE:HD13	1:A:348:PRO:HD2	1.41	1.03
1:A:347:ILE:HG22	1:A:350:ASN:ND2	1.74	1.01
1:A:347:ILE:CG2	1:A:350:ASN:ND2	2.31	0.93
1:A:347:ILE:HG22	1:A:350:ASN:HD22	1.31	0.93
5:A:606:U5P:H6	5:A:606:U5P:O5'	1.78	0.83
1:A:347:ILE:CD1	1:A:348:PRO:HD2	2.09	0.83
1:A:347:ILE:HG12	5:A:606:U5P:O2'	1.83	0.78
1:B:102:ARG:NH1	1:B:125:GLN:O	2.17	0.78
1:A:475:SER:OG	1:B:58[A]:MET:SD	2.43	0.75
1:A:499:PHE:O	1:A:549:ARG:NH2	2.20	0.74
4:A:605:GOL:HO3	4:A:605:GOL:HO1	1.35	0.72
1:B:52:PHE:O	6:B:778:HOH:O	2.07	0.71
1:A:475:SER:OG	1:B:58[B]:MET:SD	2.48	0.71
1:B:381:HIS:HD2	5:B:604:U5P:H4'	1.59	0.68
1:A:275:LYS:NZ	6:A:761:HOH:O	2.07	0.67
1:A:501:ARG:HH21	1:B:462:ASP:HA	1.59	0.67
1:B:119:LEU:HD13	1:B:127:VAL:HG21	1.78	0.65
1:A:424:LYS:NZ	1:A:440:ASP:OD1	2.29	0.65
1:A:347:ILE:HG12	5:A:606:U5P:HO2'	1.63	0.63
1:B:494:VAL:HG21	1:B:510:ILE:HD11	1.81	0.62
1:A:532:ARG:CZ	1:A:557:ILE:HG22	2.28	0.62
1:A:536:TYR:HB2	1:A:555:PRO:HG3	1.83	0.60
1:A:474:LEU:HD13	1:B:474:LEU:HD22	1.84	0.59
1:A:58:MET:SD	1:B:475:SER:OG	2.61	0.58
1:A:557:ILE:HG12	1:A:557:ILE:O	2.03	0.58
1:B:485:VAL:HG13	1:B:558:VAL:HB	1.86	0.57
1:A:347:ILE:HD13	1:A:347:ILE:C	2.25	0.56
1:A:395:ARG:HH21	1:A:421:ARG:HD3	1.70	0.56
1:B:41:ASP:OD2	6:B:840:HOH:O	2.18	0.54
1:A:347:ILE:CD1	1:A:348:PRO:N	2.58	0.54
1:A:532:ARG:NE	1:A:557:ILE:HG22	2.22	0.54
1:A:234:LYS:NZ	6:A:818:HOH:O	2.42	0.53
1:B:117:GLU:O	1:B:121:GLU:HG2	2.09	0.53
1:B:128:ASP:OD2	1:B:130:ARG:NH2	2.41	0.53
1:B:485:VAL:HG22	1:B:558:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:SD	1:A:309:VAL:HG12	2.50	0.52
1:B:32:LYS:HD2	6:B:746:HOH:O	2.09	0.51
1:A:485:VAL:O	1:A:490:PRO:HA	2.10	0.51
1:B:482:LEU:CD1	1:B:539:VAL:HG21	2.41	0.51
1:B:480:LEU:HB2	1:B:553:LEU:HD23	1.93	0.51
1:A:477:GLU:HB3	1:A:551:PRO:HA	1.92	0.50
1:A:323:ARG:NE	6:A:798:HOH:O	2.41	0.50
1:B:48:GLY:HA3	1:B:93:LEU:CD2	2.40	0.50
1:A:380:GLY:H	5:A:606:U5P:P	2.34	0.50
1:A:381:HIS:CD2	5:A:606:U5P:H5'2	2.46	0.50
1:B:506:LEU:O	1:B:510:ILE:HG23	2.12	0.50
1:A:505:ASP:OD1	1:A:509:GLN:NE2	2.35	0.49
1:A:360:ARG:NE	6:A:783:HOH:O	2.44	0.49
1:A:527:ARG:HH21	1:A:528:LEU:HD12	1.78	0.49
1:A:474:LEU:HB3	1:B:474:LEU:HB3	1.94	0.49
1:B:482:LEU:HD13	1:B:539:VAL:HG21	1.95	0.49
1:A:512:ARG:HG3	1:A:513:VAL:N	2.28	0.49
1:A:153:HIS:CG	1:A:154:SER:H	2.31	0.48
1:B:509:GLN:HB3	1:B:542:PHE:CZ	2.48	0.48
1:B:402:TRP:CG	1:B:403:HIS:N	2.81	0.48
1:B:119:LEU:HD22	1:B:124:LEU:HD13	1.95	0.48
1:B:46:VAL:O	1:B:47:ASP:HB2	2.13	0.48
1:B:273:MET:SD	1:B:309:VAL:HG12	2.53	0.48
1:B:369:VAL:HG13	1:B:374:TYR:CG	2.49	0.48
1:A:468:LEU:O	1:A:472:VAL:HG23	2.13	0.48
1:B:482:LEU:HB3	1:B:535:MET:HE2	1.96	0.48
1:A:518:VAL:O	1:A:522:LEU:HG	2.14	0.47
1:A:241:PHE:HB2	1:A:340:VAL:HG22	1.96	0.47
1:B:39:TYR:CE2	1:B:166:PRO:HG2	2.49	0.47
1:B:32:LYS:O	1:B:32:LYS:HG3	2.14	0.47
1:B:153:HIS:CG	1:B:154:SER:H	2.33	0.47
1:A:19:LEU:HB3	1:A:437:LEU:HB3	1.97	0.47
1:A:395:ARG:NH2	1:A:421:ARG:HH11	2.13	0.47
1:A:501:ARG:NH2	1:B:462:ASP:HA	2.28	0.46
1:A:514:ALA:O	1:A:518:VAL:HG23	2.16	0.46
1:A:18:THR:OG1	1:A:436:ASN:ND2	2.48	0.46
1:B:468:LEU:O	1:B:472:VAL:HG23	2.16	0.45
1:A:407:ARG:HH22	4:A:605:GOL:H2	1.80	0.45
1:A:172:HIS:CD2	1:A:174:GLY:H	2.34	0.45
1:B:536:TYR:HB2	1:B:555:PRO:HG3	1.98	0.45
1:B:536:TYR:HD2	1:B:555:PRO:HD3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:O	1:A:166:PRO:HD3	2.17	0.45
5:A:606:U5P:H6	5:A:606:U5P:P	2.57	0.45
1:B:58[A]:MET:HE3	1:B:472:VAL:HA	1.98	0.45
1:B:536:TYR:CE2	1:B:553:LEU:HB2	2.51	0.44
1:A:78:LYS:HA	1:A:78:LYS:HD3	1.88	0.44
1:A:119:LEU:HD13	1:A:127:VAL:HG21	1.98	0.44
1:B:156:PRO:HD3	1:B:249:VAL:HB	1.99	0.44
1:A:58:MET:HE1	1:A:472:VAL:HA	1.98	0.44
1:A:178:ILE:HB	1:A:386:GLU:HG2	1.99	0.43
1:B:494:VAL:CG2	1:B:510:ILE:HD11	2.48	0.43
1:B:19:LEU:HD22	1:B:165:THR:HG21	2.01	0.43
1:A:382:ALA:HB1	1:A:386:GLU:HB2	2.01	0.43
1:B:133:THR:HG22	1:B:136:ASP:OD2	2.19	0.43
1:A:401:PRO:HD2	1:A:427:LEU:O	2.19	0.43
1:A:347:ILE:CD1	1:A:347:ILE:C	2.86	0.42
1:A:486:LEU:HD23	1:A:522:LEU:HD11	2.01	0.42
1:B:421:ARG:NH1	6:B:701:HOH:O	2.43	0.42
1:A:313:SER:HB2	1:A:344[B]:SER:OG	2.20	0.42
1:A:381:HIS:NE2	5:A:606:U5P:H5'2	2.34	0.42
1:A:395:ARG:HH21	1:A:421:ARG:HH11	1.68	0.42
1:A:402:TRP:CG	1:A:403:HIS:N	2.87	0.42
1:A:482:LEU:HD13	1:A:539:VAL:HG21	2.01	0.42
1:B:58[B]:MET:HE3	1:B:472:VAL:HA	2.00	0.42
1:A:509:GLN:O	1:A:512:ARG:HG2	2.20	0.42
1:B:48:GLY:HA3	1:B:93:LEU:HD23	2.01	0.42
1:A:230:GLU:HA	1:A:258:LEU:HD13	2.02	0.41
1:B:501:ARG:NH2	6:B:771:HOH:O	2.53	0.41
1:A:381:HIS:CD2	5:A:606:U5P:C5'	3.03	0.41
1:B:382:ALA:HB1	1:B:386:GLU:HB2	2.01	0.41
1:B:178:ILE:HB	1:B:386:GLU:HG2	2.02	0.41
1:B:508:LEU:HA	1:B:508:LEU:HD22	1.84	0.41
1:B:510:ILE:HG13	1:B:511:ARG:N	2.35	0.41
1:B:535:MET:O	1:B:539:VAL:HG23	2.21	0.41
1:B:494:VAL:HG23	1:B:511:ARG:HH21	1.86	0.41
1:A:233:ILE:HD12	1:A:258:LEU:HD11	2.03	0.41
1:A:313:SER:HB2	1:A:344[A]:SER:OG	2.21	0.41
1:B:500:ALA:HB2	1:B:549:ARG:NH2	2.35	0.41
1:A:557:ILE:O	1:A:557:ILE:HG23	2.21	0.41
1:B:288:PRO:HA	1:B:289:PRO:HD2	1.98	0.41
1:A:527:ARG:HA	1:A:527:ARG:HD2	1.71	0.41
1:B:48:GLY:O	1:B:92:GLY:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ILE:O	1:B:256:LEU:HG	2.21	0.41
1:B:489:THR:HG22	1:B:490:PRO:HD2	2.02	0.41
1:A:314:GLN:OE1	1:A:347:ILE:HG22	2.22	0.40
1:B:479:LEU:N	1:B:497:ARG:O	2.49	0.40
1:A:528:LEU:H	1:A:528:LEU:HG	1.71	0.40
1:B:172:HIS:CD2	1:B:174:GLY:H	2.39	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	545/559 (98%)	535 (98%)	10 (2%)	0	100	100
1	B	545/559 (98%)	538 (99%)	7 (1%)	0	100	100
All	All	1090/1118 (98%)	1073 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	446/467 (96%)	435 (98%)	11 (2%)	47	49
1	B	432/467 (92%)	414 (96%)	18 (4%)	30	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	878/934 (94%)	849 (97%)	29 (3%)	39 37

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	80	TRP
1	A	143	SER
1	A	318	MET
1	A	336	ARG
1	A	347	ILE
1	A	469	LEU
1	A	483	THR
1	A	527	ARG
1	A	532	ARG
1	A	553	LEU
1	B	58[A]	MET
1	B	58[B]	MET
1	B	68	ASP
1	B	80	TRP
1	B	99	ARG
1	B	116	ARG
1	B	124	LEU
1	B	215	ARG
1	B	237	ARG
1	B	483	THR
1	B	485	VAL
1	B	486	LEU
1	B	489	THR
1	B	491	HIS
1	B	508	LEU
1	B	510	ILE
1	B	511	ARG
1	B	550	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	GOL	A	605	-	5,5,5	0.25	0	5,5,5	0.26	0
4	GOL	A	604	-	5,5,5	0.25	0	5,5,5	0.28	0
5	U5P	B	604	-	22,22,22	1.18	3 (13%)	33,33,33	1.55	4 (12%)
5	U5P	A	606	-	22,22,22	1.16	3 (13%)	33,33,33	1.65	5 (15%)

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	GOL	A	605	-	-	0/4/4/4	-
4	GOL	A	604	-	-	0/4/4/4	-
5	U5P	B	604	-	-	6/10/26/26	0/2/2/2
5	U5P	A	606	-	-	0/10/26/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	U5P	C4-N3	-2.57	1.34	1.38
5	B	604	U5P	C4-N3	-2.45	1.34	1.38
5	B	604	U5P	C2-N3	-2.19	1.34	1.38
5	A	606	U5P	C2-N3	-2.16	1.34	1.38
5	A	606	U5P	C5-C4	-2.05	1.39	1.43
5	B	604	U5P	C5-C4	-2.01	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	606	U5P	C4-N3-C2	-4.42	120.75	126.58
5	A	606	U5P	N3-C2-N1	4.06	120.28	114.89
5	B	604	U5P	C4-N3-C2	-4.04	121.25	126.58
5	B	604	U5P	N3-C2-N1	3.91	120.08	114.89
5	A	606	U5P	C5-C4-N3	3.76	120.47	114.84
5	B	604	U5P	C5-C4-N3	3.28	119.75	114.84
5	A	606	U5P	O4-C4-C5	-2.94	119.99	125.16
5	B	604	U5P	O4-C4-C5	-2.83	120.19	125.16
5	A	606	U5P	O5'-P-O1P	-2.33	99.95	106.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	604	U5P	C5'-O5'-P-O2P
5	B	604	U5P	C5'-O5'-P-O3P
5	B	604	U5P	C5'-O5'-P-O1P
5	B	604	U5P	C4'-C5'-O5'-P
5	B	604	U5P	C2'-C1'-N1-C2
5	B	604	U5P	C2'-C1'-N1-C6

There are no ring outliers.

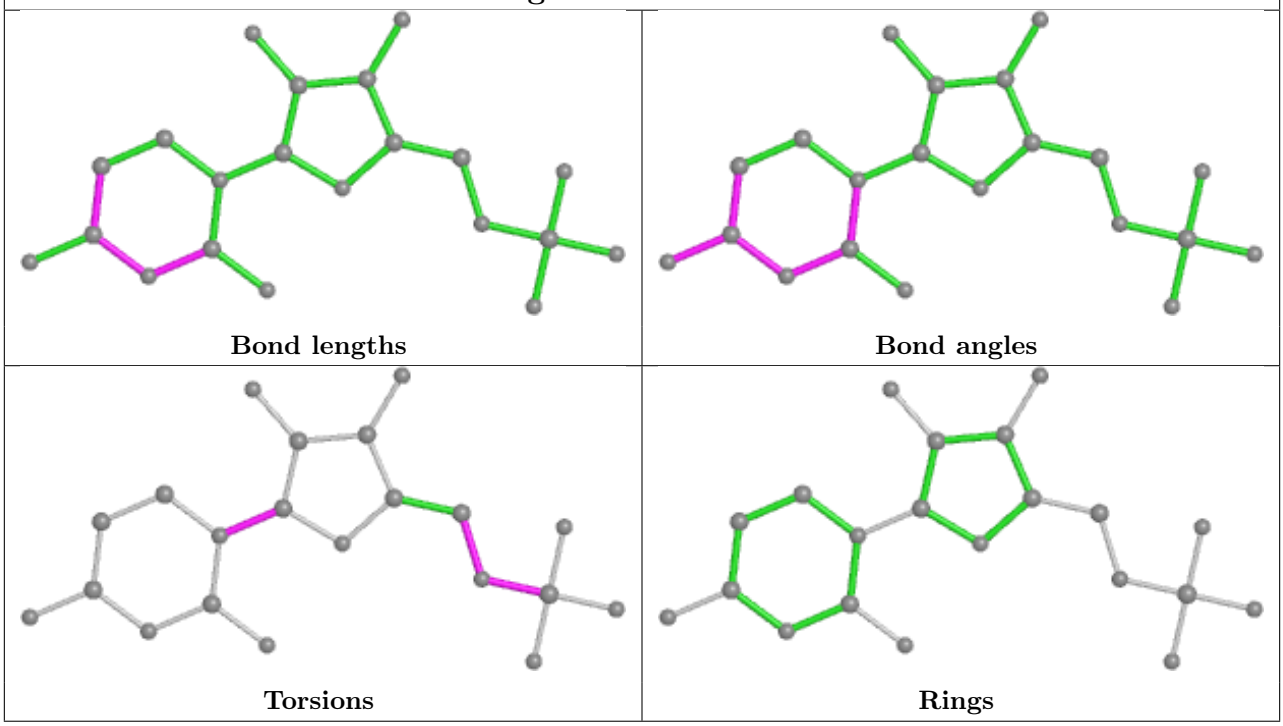
3 monomers are involved in 11 short contacts:

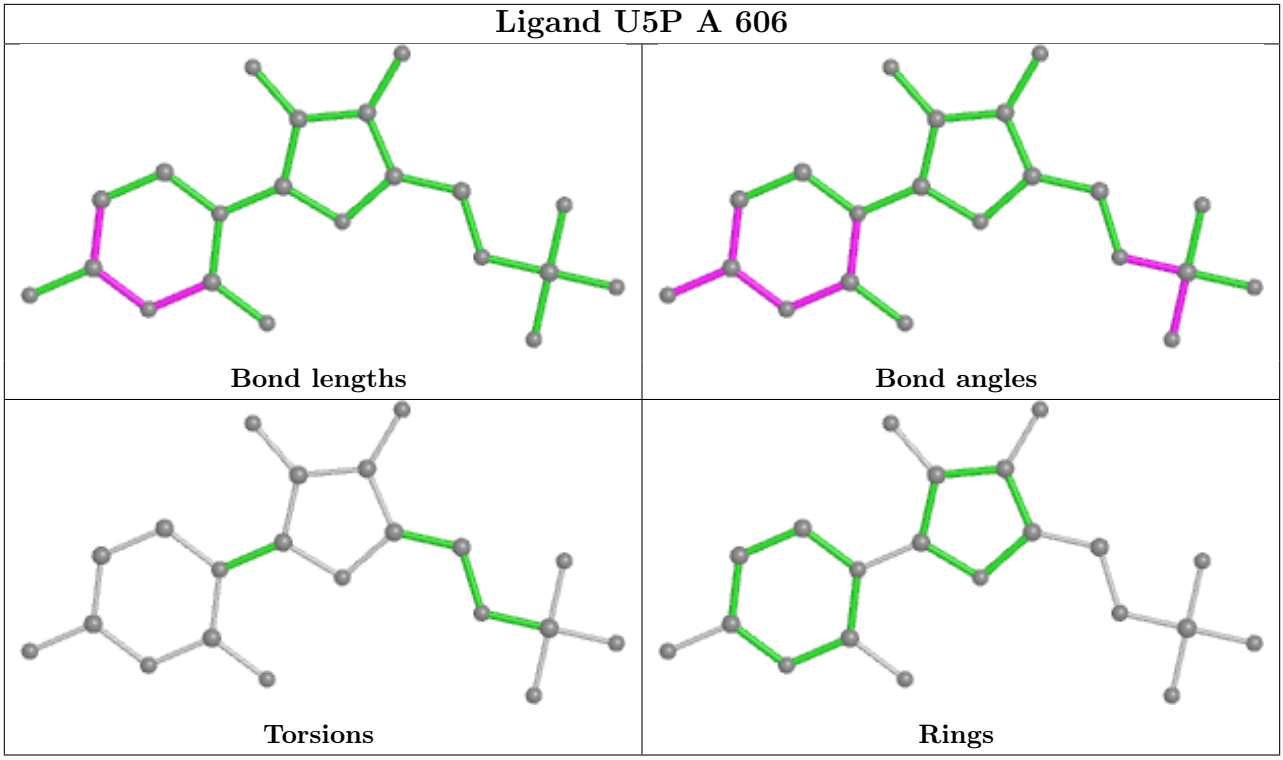
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	GOL	2	0
5	B	604	U5P	1	0
5	A	606	U5P	8	0

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 then 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.

Ligand U5P B 604





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	543/559 (97%)	0.80	90 (16%) 1 1	28, 47, 94, 122	0
1	B	543/559 (97%)	1.01	98 (18%) 1 1	29, 49, 106, 136	0
All	All	1086/1118 (97%)	0.90	188 (17%) 1 1	28, 48, 100, 136	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	GLU	9.9
1	B	522	LEU	9.6
1	B	523	ARG	9.6
1	B	521	GLY	9.1
1	B	490	PRO	8.2
1	B	484	ALA	8.1
1	B	16	ALA	8.1
1	B	485	VAL	8.0
1	B	534	ASP	7.7
1	B	530	ASP	7.6
1	B	525	LYS	7.4
1	B	518	VAL	7.3
1	A	522	LEU	7.1
1	B	524	GLU	7.0
1	B	512	ARG	6.9
1	B	529	GLU	6.9
1	B	489	THR	6.8
1	A	528	LEU	6.8
1	B	533	ASP	6.7
1	B	486	LEU	6.7
1	B	487	HIS	6.6
1	B	528	LEU	6.6
1	B	520	GLN	6.2
1	B	538	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	524	GLU	6.0
1	A	523	ARG	5.9
1	B	531	VAL	5.9
1	A	16	ALA	5.8
1	A	525	LYS	5.7
1	B	514	ALA	5.6
1	B	508	LEU	5.5
1	A	521	GLY	5.5
1	A	207	ILE	5.3
1	A	530	ASP	5.1
1	A	531	VAL	5.1
1	A	520	GLN	5.1
1	A	37	PHE	5.1
1	B	527	ARG	5.0
1	B	526	LYS	4.9
1	B	491	HIS	4.9
1	B	120	SER	4.9
1	B	207	ILE	4.9
1	B	17	PRO	4.9
1	B	488	PRO	4.9
1	B	503	ASN	4.8
1	B	483	THR	4.8
1	A	526	LYS	4.8
1	B	515	LEU	4.7
1	B	536	TYR	4.6
1	A	534	ASP	4.5
1	B	37	PHE	4.5
1	A	527	ARG	4.5
1	A	517	ALA	4.4
1	B	513	VAL	4.4
1	B	171	LEU	4.3
1	A	21	VAL	4.1
1	A	81	ILE	4.1
1	B	557	ILE	4.0
1	A	163	LEU	4.0
1	A	161	TYR	4.0
1	B	161	TYR	4.0
1	A	538	ALA	4.0
1	A	532	ARG	3.9
1	A	533	ASP	3.9
1	B	532	ARG	3.9
1	A	485	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	558	VAL	3.8
1	A	170	VAL	3.8
1	A	125	GLN	3.7
1	B	400	LEU	3.7
1	B	546	ALA	3.6
1	B	81	ILE	3.6
1	A	400	LEU	3.6
1	A	516	GLU	3.6
1	A	402	TRP	3.6
1	A	46	VAL	3.5
1	A	255	ILE	3.5
1	A	242	LEU	3.5
1	B	163	LEU	3.5
1	B	172	HIS	3.5
1	A	206	LEU	3.5
1	B	309	VAL	3.4
1	B	255	ILE	3.4
1	B	537	GLY	3.4
1	A	35	THR	3.3
1	B	516	GLU	3.3
1	A	536	TYR	3.2
1	A	171	LEU	3.2
1	B	170	VAL	3.2
1	B	173	THR	3.2
1	A	514	ALA	3.2
1	B	242	LEU	3.2
1	A	513	VAL	3.1
1	B	510	ILE	3.1
1	A	541	ARG	3.1
1	B	121	GLU	3.1
1	B	46	VAL	3.1
1	B	244	THR	3.0
1	B	125	GLN	3.0
1	A	82	LEU	3.0
1	B	21	VAL	2.9
1	B	252	ILE	2.9
1	A	117	GLU	2.9
1	A	173	THR	2.9
1	B	34	ILE	2.9
1	B	402	TRP	2.9
1	A	229	LEU	2.9
1	B	342	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	491	HIS	2.9
1	A	309	VAL	2.8
1	B	245	PHE	2.8
1	A	529	GLU	2.8
1	A	518	VAL	2.8
1	A	544	ARG	2.8
1	A	72	GLU	2.8
1	A	45	VAL	2.8
1	A	512	ARG	2.8
1	A	205	LEU	2.8
1	B	206	LEU	2.8
1	B	35	THR	2.7
1	A	17	PRO	2.7
1	B	542	PHE	2.7
1	A	515	LEU	2.7
1	A	123	GLY	2.7
1	A	557	ILE	2.7
1	B	205	LEU	2.7
1	B	507	GLU	2.7
1	B	83	THR	2.7
1	B	307	LEU	2.7
1	B	466	ASP	2.7
1	A	488	PRO	2.7
1	A	172	HIS	2.6
1	B	506	LEU	2.6
1	A	44	VAL	2.6
1	B	45	VAL	2.6
1	A	252	ILE	2.6
1	B	48	GLY	2.6
1	A	174	GLY	2.6
1	B	493	GLU	2.6
1	B	492	VAL	2.5
1	A	480	LEU	2.5
1	B	535	MET	2.5
1	A	540	ARG	2.5
1	B	155	ILE	2.5
1	A	323	ARG	2.5
1	A	556	MET	2.5
1	A	155	ILE	2.4
1	A	24	LEU	2.4
1	B	541	ARG	2.4
1	A	244	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	341	ILE	2.4
1	A	519	GLU	2.3
1	B	474	LEU	2.3
1	A	487	HIS	2.3
1	B	133	THR	2.3
1	A	342	LEU	2.3
1	B	469	LEU	2.3
1	A	193	GLU	2.3
1	A	241	PHE	2.3
1	B	475	SER	2.3
1	A	341	ILE	2.2
1	A	121	GLU	2.2
1	B	44	VAL	2.2
1	A	233	ILE	2.2
1	B	390	ILE	2.2
1	A	469	LEU	2.2
1	A	120	SER	2.2
1	A	83	THR	2.2
1	A	347	ILE	2.2
1	B	554	ILE	2.2
1	A	318	MET	2.2
1	A	502	PRO	2.2
1	A	340	VAL	2.2
1	A	505	ASP	2.2
1	B	18	THR	2.2
1	B	47	ASP	2.2
1	B	82	LEU	2.1
1	B	72	GLU	2.1
1	A	245	PHE	2.1
1	B	208	SER	2.1
1	A	466	ASP	2.1
1	B	174	GLY	2.1
1	B	36	VAL	2.1
1	B	505	ASP	2.1
1	A	148	PHE	2.1
1	A	187	GLY	2.0
1	B	502	PRO	2.0
1	A	36	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

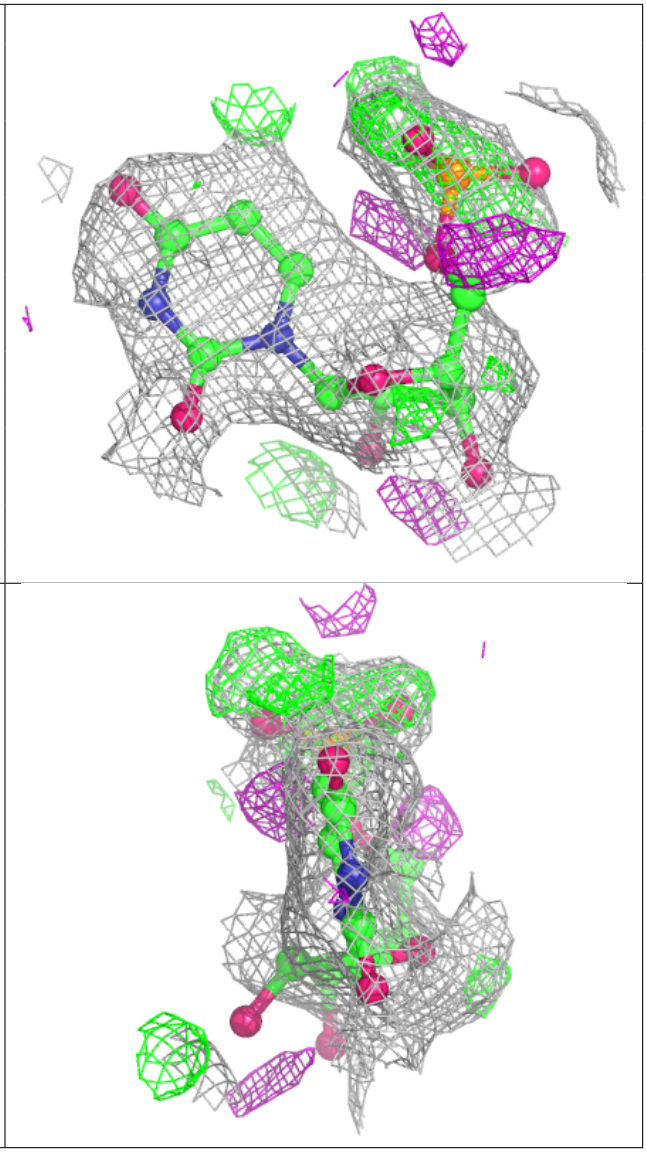
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	U5P	A	606	21/21	0.41	0.46	116,139,200,206	0
5	U5P	B	604	21/21	0.51	0.41	93,119,228,236	0
3	MN	A	603	1/1	0.89	0.07	49,49,49,49	0
4	GOL	A	605	6/6	0.89	0.18	61,72,78,79	0
3	MN	B	603	1/1	0.91	0.09	49,49,49,49	0
4	GOL	A	604	6/6	0.92	0.12	40,58,62,64	0
2	ZN	B	602	1/1	0.98	0.12	34,34,34,34	0
2	ZN	A	602	1/1	0.99	0.10	32,32,32,32	0
2	ZN	B	601	1/1	0.99	0.11	37,37,37,37	0
2	ZN	A	601	1/1	0.99	0.11	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.

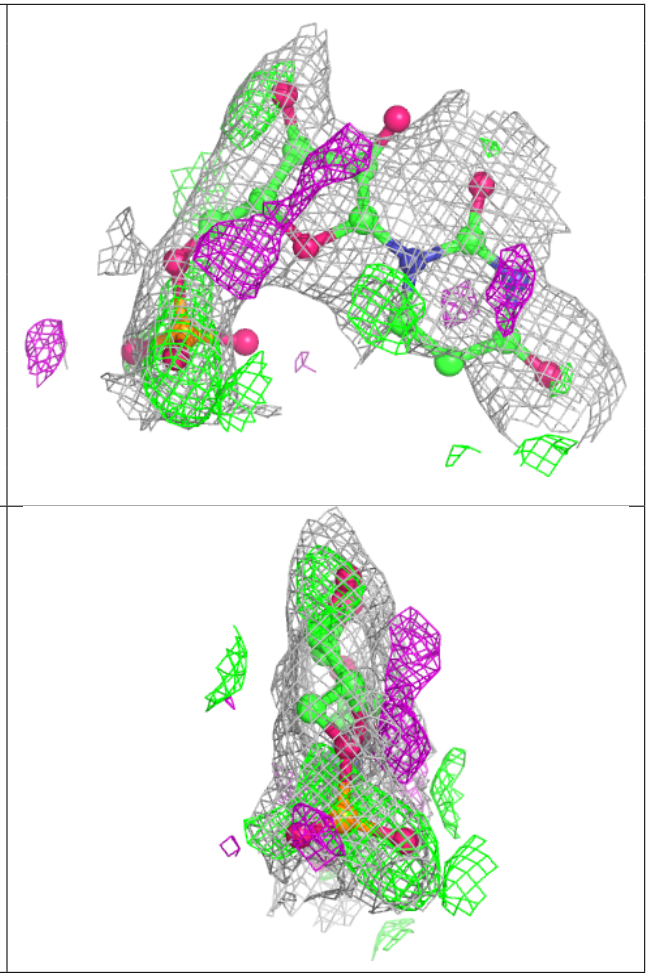
Electron density around U5P A 606:

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



Electron density around U5P B 604:

$2mF_o$-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.