



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:58 pm GMT

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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

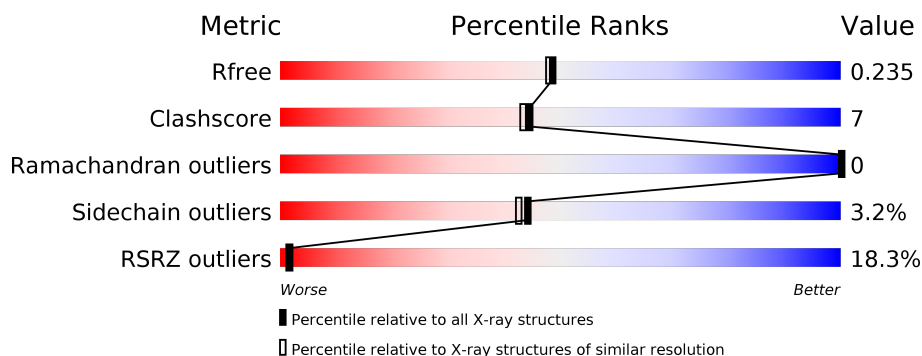
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	559	<div> <div>17%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	559	<div> <div>18%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>

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

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
1	A	543	Total	C	N	O	S	0	4	0
			4206	2664	756	773	13			
1	B	543	Total	C	N	O	S	0	4	0
			4147	2629	740	764	14			

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

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

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

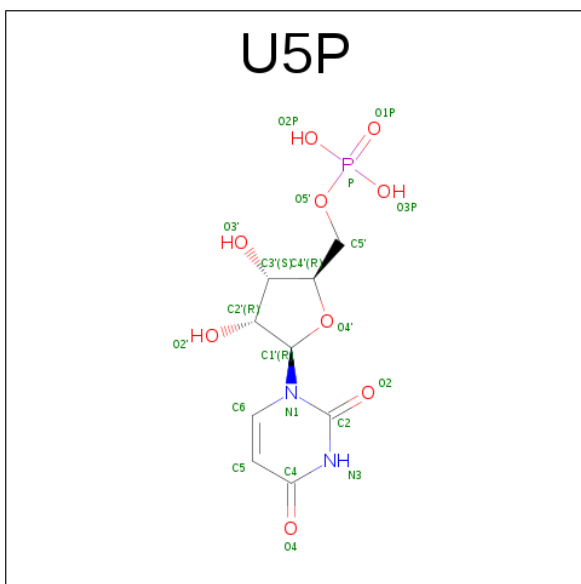
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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



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

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

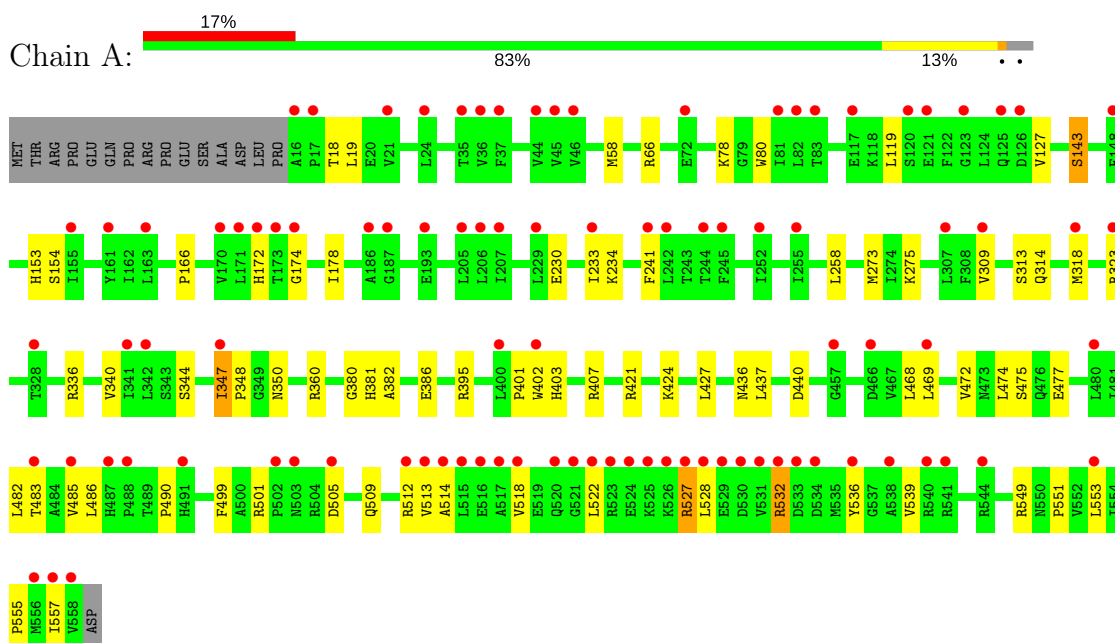
- Molecule 6 is water.

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

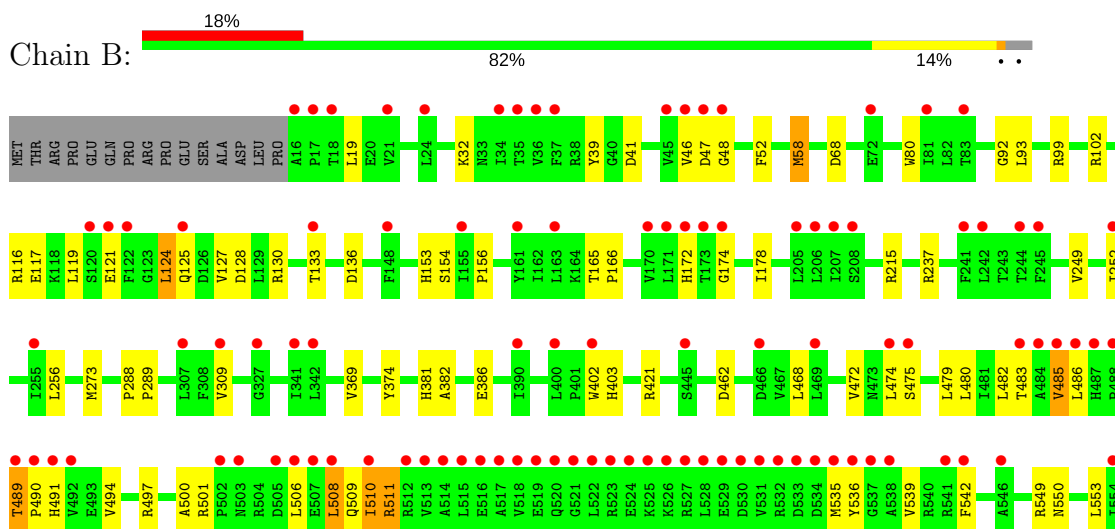
3 Residue-property plots [i](#)

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: DR2417



• Molecule 1: DR2417





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.200 , 0.235 0.200 , 0.235	Depositor DCC
R_{free} test set	4902 reflections (4.99%)	DCC
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	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	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.*

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: 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

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:HO1	4:A:605:GOL:HO3	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:557:ILE:HG12	1:A:557:ILE:O	2.03	0.58
1:A:58:MET:SD	1:B:475:SER:OG	2.61	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:273:MET:SD	1:B:309:VAL:HG12	2.53	0.48
1:B:46:VAL:O	1:B:47:ASP:HB2	2.13	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:395:ARG:NH2	1:A:421:ARG:HH11	2.13	0.47
1:A:19:LEU:HB3	1:A:437:LEU:HB3	1.97	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:HD3	1:A:78:LYS:HA	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:402:TRP:CG	1:A:403:HIS:N	2.87	0.42
1:A:395:ARG:HH21	1:A:421:ARG:HH11	1.68	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:HD22	1:B:508:LEU:HA	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:HG23	1:A:557:ILE:O	2.21	0.41
1:B:288:PRO:HA	1:B:289:PRO:HD2	1.98	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLY:O	1:B:92:GLY:N	2.49	0.41
1:A:527:ARG:HA	1:A:527:ARG:HD2	1.71	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%)	53	54
1	B	432/467 (92%)	414 (96%)	18 (4%)	34	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	878/934 (94%)	849 (97%)	29 (3%)	44	41

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	604	-	5,5,5	0.20	0	5,5,5	0.26	0
4	GOL	A	605	-	5,5,5	0.21	0	5,5,5	0.24	0
5	U5P	A	606	-	18,22,22	0.82	1 (5%)	22,33,33	1.93	2 (9%)
5	U5P	B	604	-	18,22,22	0.87	1 (5%)	22,33,33	2.03	2 (9%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	U5P	C2-N3	-2.07	1.34	1.38
5	A	606	U5P	C2-N3	-2.04	1.34	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	U5P	O5'-P-O1P	-2.33	99.95	106.47
5	B	604	U5P	O4'-C1'-N1	2.31	112.70	108.08
5	A	606	U5P	C4-N3-C2	7.71	120.75	114.13
5	B	604	U5P	C4-N3-C2	8.29	121.25	114.13

There are no chirality outliers.

There are no torsion outliers.

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	A	606	U5P	8	0
5	B	604	U5P	1	0

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	543/559 (97%)	0.86	96 (17%) 2 2	28, 47, 94, 122	0
1	B	543/559 (97%)	1.07	103 (18%) 1 1	29, 49, 106, 136	0
All	All	1086/1118 (97%)	0.97	199 (18%) 1 2	28, 48, 100, 136	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	ARG	10.3
1	B	519	GLU	9.2
1	B	522	LEU	8.9
1	B	521	GLY	8.8
1	B	484	ALA	8.8
1	B	530	ASP	8.7
1	B	490	PRO	8.6
1	B	534	ASP	8.3
1	B	529	GLU	8.3
1	B	518	VAL	8.3
1	B	16	ALA	8.3
1	B	525	LYS	7.9
1	B	524	GLU	7.8
1	B	528	LEU	7.8
1	B	533	ASP	7.5
1	A	16	ALA	7.2
1	A	528	LEU	7.2
1	B	487	HIS	7.1
1	B	485	VAL	7.1
1	A	522	LEU	6.9
1	B	538	ALA	6.9
1	B	512	ARG	6.8
1	B	486	LEU	6.8
1	A	524	GLU	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	514	ALA	6.6
1	B	520	GLN	6.4
1	A	525	LYS	6.3
1	B	489	THR	6.3
1	A	523	ARG	6.2
1	B	531	VAL	6.2
1	B	491	HIS	5.6
1	A	207	ILE	5.3
1	B	207	ILE	5.2
1	B	120	SER	5.1
1	A	521	GLY	5.1
1	A	520	GLN	5.0
1	A	530	ASP	4.9
1	A	527	ARG	4.9
1	B	536	TYR	4.9
1	B	508	LEU	4.9
1	A	531	VAL	4.9
1	B	17	PRO	4.9
1	A	37	PHE	4.9
1	A	534	ASP	4.9
1	B	503	ASN	4.9
1	B	488	PRO	4.8
1	B	527	ARG	4.8
1	A	517	ALA	4.7
1	B	37	PHE	4.7
1	A	526	LYS	4.7
1	A	533	ASP	4.6
1	A	558	VAL	4.5
1	B	513	VAL	4.5
1	B	526	LYS	4.5
1	B	171	LEU	4.4
1	A	538	ALA	4.3
1	B	483	THR	4.3
1	B	557	ILE	4.3
1	A	21	VAL	4.2
1	A	170	VAL	4.2
1	A	532	ARG	4.1
1	B	161	TYR	4.0
1	A	125	GLN	4.0
1	A	81	ILE	4.0
1	B	532	ARG	3.9
1	A	163	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	510	ILE	3.9
1	A	516	GLU	3.9
1	A	46	VAL	3.9
1	B	515	LEU	3.8
1	A	161	TYR	3.8
1	B	537	GLY	3.8
1	A	488	PRO	3.7
1	B	81	ILE	3.7
1	A	242	LEU	3.7
1	B	546	ALA	3.7
1	A	514	ALA	3.7
1	A	541	ARG	3.6
1	A	400	LEU	3.6
1	B	172	HIS	3.6
1	A	35	THR	3.6
1	A	123	GLY	3.5
1	A	255	ILE	3.5
1	B	400	LEU	3.5
1	A	206	LEU	3.5
1	B	46	VAL	3.5
1	B	121	GLU	3.4
1	A	402	TRP	3.4
1	B	255	ILE	3.4
1	B	173	THR	3.4
1	A	485	VAL	3.4
1	A	171	LEU	3.3
1	A	513	VAL	3.3
1	A	518	VAL	3.3
1	B	170	VAL	3.3
1	B	554	ILE	3.3
1	B	242	LEU	3.3
1	B	309	VAL	3.3
1	B	163	LEU	3.2
1	B	516	GLU	3.2
1	A	117	GLU	3.2
1	B	125	GLN	3.2
1	B	206	LEU	3.2
1	A	556	MET	3.2
1	B	556	MET	3.2
1	B	244	THR	3.1
1	A	536	TYR	3.1
1	B	342	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	173	THR	3.0
1	A	72	GLU	3.0
1	B	506	LEU	3.0
1	A	512	ARG	2.9
1	B	492	VAL	2.9
1	A	515	LEU	2.8
1	A	491	HIS	2.8
1	B	252	ILE	2.8
1	A	529	GLU	2.8
1	B	466	ASP	2.8
1	B	402	TRP	2.8
1	B	245	PHE	2.8
1	A	45	VAL	2.8
1	B	21	VAL	2.8
1	A	309	VAL	2.7
1	A	172	HIS	2.7
1	B	35	THR	2.7
1	A	174	GLY	2.7
1	A	155	ILE	2.7
1	A	17	PRO	2.7
1	A	342	LEU	2.7
1	B	34	ILE	2.7
1	B	48	GLY	2.7
1	A	229	LEU	2.7
1	A	480	LEU	2.7
1	B	341	ILE	2.6
1	A	540	ARG	2.6
1	B	174	GLY	2.6
1	A	252	ILE	2.6
1	A	502	PRO	2.6
1	A	323	ARG	2.6
1	B	155	ILE	2.6
1	B	390	ILE	2.6
1	B	205	LEU	2.6
1	B	505	ASP	2.5
1	B	45	VAL	2.5
1	A	205	LEU	2.5
1	B	502	PRO	2.5
1	A	82	LEU	2.5
1	A	36	VAL	2.5
1	B	307	LEU	2.5
1	A	328	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	121	GLU	2.5
1	A	120	SER	2.5
1	A	557	ILE	2.5
1	B	542	PHE	2.5
1	A	466	ASP	2.5
1	A	148	PHE	2.4
1	A	544	ARG	2.4
1	A	187	GLY	2.4
1	A	44	VAL	2.4
1	A	241	PHE	2.4
1	A	244	THR	2.4
1	A	318	MET	2.3
1	B	517	ALA	2.3
1	A	457	GLY	2.3
1	A	24	LEU	2.3
1	A	347	ILE	2.3
1	B	72	GLU	2.3
1	B	241	PHE	2.3
1	A	186	ALA	2.3
1	B	133	THR	2.3
1	B	541	ARG	2.3
1	B	36	VAL	2.3
1	B	47	ASP	2.2
1	B	507	GLU	2.2
1	B	445	SER	2.2
1	B	83	THR	2.2
1	B	122	PHE	2.2
1	B	475	SER	2.2
1	A	233	ILE	2.2
1	B	148	PHE	2.2
1	B	535	MET	2.2
1	A	341	ILE	2.1
1	A	505	ASP	2.1
1	A	245	PHE	2.1
1	A	503	ASN	2.1
1	A	126	ASP	2.1
1	A	469	LEU	2.1
1	B	24	LEU	2.1
1	A	83	THR	2.1
1	A	483	THR	2.1
1	B	18	THR	2.1
1	A	487	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	469	LEU	2.1
1	B	474	LEU	2.1
1	A	193	GLU	2.0
1	B	208	SER	2.0
1	B	327	GLY	2.0
1	A	307	LEU	2.0
1	A	553	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	U5P	A	606	21/21	0.37	0.48	8.96	116,139,200,206	0
5	U5P	B	604	21/21	0.49	0.42	6.25	93,119,228,236	0
4	GOL	A	605	6/6	0.89	0.17	0.56	61,72,78,79	0
4	GOL	A	604	6/6	0.91	0.12	-0.19	40,58,62,64	0
2	ZN	B	601	1/1	0.99	0.12	-1.36	37,37,37,37	0
2	ZN	B	602	1/1	0.98	0.11	-1.54	34,34,34,34	0
3	MN	A	603	1/1	0.89	0.07	-1.60	49,49,49,49	0
2	ZN	A	602	1/1	0.99	0.10	-1.76	32,32,32,32	0
2	ZN	A	601	1/1	0.99	0.10	-1.85	36,36,36,36	0
3	MN	B	603	1/1	0.91	0.08	-3.74	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.