



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:50 pm BST

PDB ID : 4XWW
Title : Crystal structure of RNase J complexed with RNA
Authors : Lu, M.; Zhang, H.; Xu, Q.; Hua, Y.; Zhao, Y.
Deposited on : 2015-01-29
Resolution : 1.70 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
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

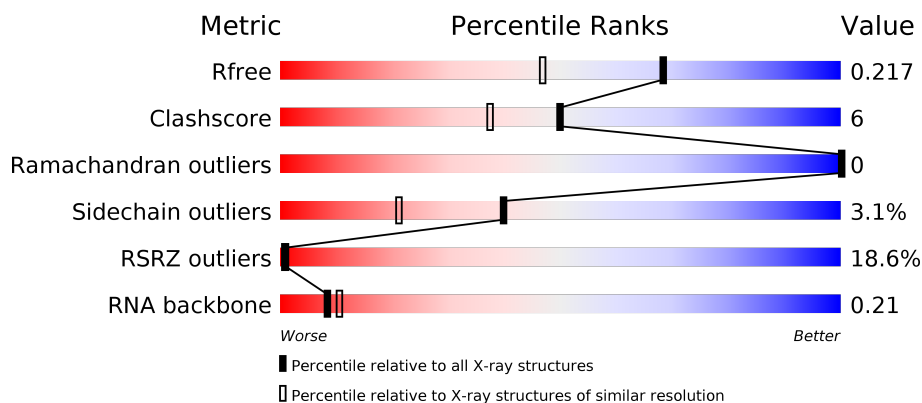
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)
RNA backbone	3102	1007 (2.38-1.02)

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	559	<div> <div>18%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	559	<div> <div>18%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
2	D	7	<div> <div>14%</div> <div> <div>29%</div> <div>29%</div> <div>43%</div> </div> </div>
2	E	7	<div> <div>14%</div> <div> <div>29%</div> <div>43%</div> <div>29%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9366 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	545	Total	C	N	O	S	0	3	0
			4203	2663	754	773	13			
1	B	543	Total	C	N	O	S	0	4	0
			4144	2628	740	762	14			

- Molecule 2 is a RNA chain called RNA (5'-D(UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	P	0	0	1
			121	54	12	49	6			
2	E	7	Total	C	N	O	P	0	0	1
			121	54	12	49	6			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

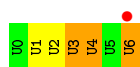
- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



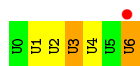
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	404	Total	O	0	0
			404	404		
6	B	339	Total	O	0	0
			339	339		
6	D	9	Total	O	0	0
			9	9		
6	E	7	Total	O	0	0
			7	7		



- Molecule 2: RNA (5'-D(UP*UP*UP*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.12Å 87.86Å 249.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 1.70 29.59 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (29.59-1.70) 96.6 (29.59-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.195 , 0.217 0.196 , 0.217	Depositor DCC
R_{free} test set	7892 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9366	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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, ZN, MN

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	0.37	0/4289	0.54	1/5832 (0.0%)
1	B	0.34	0/4230	0.53	0/5758
2	D	0.31	0/132	0.66	0/203
2	E	0.33	0/132	0.96	0/203
All	All	0.36	0/8783	0.55	1/11996 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	PRO	N-CA-CB	5.98	110.48	103.30

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	4203	0	4197	49	0
1	B	4144	0	4096	42	0
2	D	121	0	61	12	0
2	E	121	0	61	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	16	2	0
6	A	404	0	0	2	0
6	B	339	0	0	4	0
6	D	9	0	0	0	0
6	E	7	0	0	0	0
All	All	9366	0	8431	99	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 6.

All (99) 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:558:VAL:HG13	1:A:559:ASP:OXT	1.53	1.06
1:B:224:GLU:OE2	1:B:375:ARG:NH1	2.13	0.82
1:A:499:PHE:O	1:A:549:ARG:NH2	2.16	0.78
1:A:558:VAL:CG1	1:A:559:ASP:OXT	2.30	0.77
1:A:315:GLY:HA2	1:A:357:ILE:HD12	1.66	0.77
1:B:102:ARG:NH1	1:B:125:GLN:O	2.18	0.77
1:B:518:VAL:O	1:B:522:LEU:N	2.19	0.75
1:A:358:VAL:HG21	5:A:605:GOL:H12	1.69	0.75
1:B:480:LEU:HB2	1:B:553:LEU:HD23	1.67	0.74
1:A:558:VAL:HA	1:A:559:ASP:C	2.06	0.74
1:A:479:LEU:HD21	1:A:497:ARG:HB2	1.68	0.74
1:A:481:ILE:HG23	1:A:495:VAL:HB	1.71	0.71
1:A:558:VAL:HA	1:A:559:ASP:OXT	1.91	0.71
1:B:315:GLY:HA2	1:B:357:ILE:HD12	1.73	0.70
2:D:3:U:O2'	2:D:4:U:OP1	2.11	0.69
1:B:379:SER:OG	2:E:1:U:OP2	2.03	0.68
2:D:3:U:H6	2:D:3:U:H5'	1.58	0.68
1:B:268:MET:HG3	1:B:273:MET:HG3	1.77	0.66
1:B:509:GLN:HB3	1:B:542:PHE:CZ	2.33	0.64
1:A:477:GLU:HB3	1:A:551:PRO:HA	1.78	0.64
1:A:558:VAL:CA	1:A:559:ASP:OXT	2.47	0.62
1:A:323:ARG:CZ	2:D:6:U:H3'	2.29	0.62
1:B:494:VAL:HG21	1:B:510:ILE:HD11	1.81	0.62
1:A:504:ARG:O	1:A:508:LEU:HG	2.01	0.60
1:B:536:TYR:HD2	1:B:555:PRO:HG3	1.67	0.59
1:B:119:LEU:HD13	1:B:127:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:TYR:HB2	1:A:555:PRO:HG3	1.85	0.57
2:E:1:U:O2	2:E:1:U:H2'	2.05	0.57
1:A:87:GLU:HG3	2:D:3:U:H5'	1.85	0.56
2:E:6:U:H5'	2:E:6:U:C6	2.40	0.56
1:B:268:MET:HG3	1:B:273:MET:CG	2.35	0.56
2:E:6:U:H2'	2:E:6:U:O2	2.06	0.56
1:B:117:GLU:O	1:B:121:GLU:HG2	2.06	0.55
1:A:481:ILE:HD12	1:A:554:ILE:HG22	1.88	0.55
2:D:3:U:HO2'	2:D:4:U:P	2.30	0.54
2:D:2:U:O2'	2:D:3:U:H5''	2.06	0.54
1:A:557:ILE:HG22	1:A:557:ILE:O	2.08	0.53
1:A:18:THR:OG1	1:A:436:ASN:ND2	2.41	0.53
1:B:234:LYS:NZ	6:B:1024:HOH:O	2.28	0.51
1:B:322:GLY:O	1:B:326:PHE:HD1	1.93	0.51
1:B:503:ASN:HB3	1:B:506:LEU:HB3	1.93	0.50
1:A:382:ALA:HB1	1:A:386:GLU:HB2	1.93	0.50
1:A:505:ASP:OD1	1:A:509:GLN:NE2	2.45	0.50
1:B:479:LEU:HD12	1:B:552:VAL:O	2.11	0.50
2:E:3:U:C5'	2:E:3:U:H6	2.24	0.49
1:A:536:TYR:CE2	1:A:553:LEU:HB2	2.47	0.49
1:A:379:SER:OG	2:D:1:U:OP2	2.23	0.49
1:A:323:ARG:NE	2:D:6:U:H3'	2.28	0.49
1:A:66:ARG:NH2	1:A:68:ASP:OD2	2.46	0.48
1:A:410:ILE:HD12	1:B:362:TYR:HB3	1.94	0.48
1:B:500:ALA:HB2	1:B:549:ARG:NH2	2.28	0.48
1:B:506:LEU:O	1:B:510:ILE:HG23	2.14	0.48
1:A:482:LEU:O	1:A:555:PRO:HA	2.14	0.47
1:A:476:GLN:HG3	6:A:1036:HOH:O	2.14	0.47
1:A:481:ILE:HD12	1:A:554:ILE:O	2.15	0.47
1:A:532:ARG:HG2	1:A:533:ASP:N	2.29	0.47
1:B:421:ARG:NH2	6:B:923:HOH:O	2.39	0.47
1:A:558:VAL:CB	1:A:559:ASP:OXT	2.63	0.46
1:B:269:GLU:OE1	6:B:880:HOH:O	2.20	0.46
1:B:515:LEU:O	1:B:518:VAL:HG23	2.16	0.46
1:A:247:SER:OG	2:D:3:U:OP1	2.20	0.46
1:A:485:VAL:HB	1:A:491:HIS:CE1	2.51	0.45
1:B:382:ALA:HB1	1:B:386:GLU:HB2	1.97	0.45
1:A:119:LEU:HD13	1:A:127:VAL:HG21	1.98	0.45
1:A:512:ARG:HG3	1:A:513:VAL:N	2.30	0.45
1:A:514:ALA:O	1:A:518:VAL:HG23	2.17	0.45
1:A:354:VAL:HG12	5:A:605:GOL:H11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG12	1:A:269:GLU:HG2	1.99	0.45
1:B:462:ASP:N	1:B:462:ASP:OD1	2.49	0.45
1:B:485:VAL:HG13	1:B:558:VAL:HG23	1.99	0.45
1:A:143:SER:O	1:A:166:PRO:HD3	2.16	0.44
1:B:494:VAL:HG11	1:B:510:ILE:HD11	1.98	0.44
1:B:54:LYS:HB2	1:B:56:HIS:CE1	2.52	0.44
2:D:3:U:H6	2:D:3:U:C5'	2.27	0.44
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.82	0.44
1:B:19:LEU:HD22	1:B:165:THR:HG21	1.99	0.44
1:A:58:MET:HE1	1:A:472:VAL:HA	2.00	0.43
1:A:492:VAL:O	1:A:511:ARG:HD3	2.18	0.43
1:B:241:PHE:HB2	1:B:340:VAL:HG22	1.99	0.43
1:B:514:ALA:O	1:B:518:VAL:HG22	2.19	0.43
1:A:78:LYS:HD3	1:A:78:LYS:HA	1.84	0.42
1:A:87:GLU:HG3	2:D:3:U:C5'	2.49	0.42
1:B:39:TYR:CE1	1:B:166:PRO:HG2	2.54	0.42
1:B:402:TRP:CG	1:B:403:HIS:N	2.86	0.42
1:A:487:HIS:HA	1:A:488:PRO:C	2.39	0.42
1:B:554:ILE:O	1:B:554:ILE:HG13	2.20	0.42
1:B:515:LEU:HA	1:B:518:VAL:CG2	2.49	0.42
1:A:395:ARG:NH2	6:A:704:HOH:O	2.52	0.42
1:B:484:ALA:HB2	1:B:492:VAL:HG13	2.01	0.42
1:B:497:ARG:HA	1:B:497:ARG:HD3	1.88	0.42
1:B:536:TYR:HE2	1:B:553:LEU:O	2.03	0.42
1:B:335[A]:ARG:NH1	6:B:702:HOH:O	2.45	0.41
1:A:485:VAL:O	1:A:490:PRO:HA	2.20	0.41
1:A:479:LEU:CD2	1:A:497:ARG:HB2	2.43	0.41
2:D:3:U:O2'	2:D:4:U:P	2.79	0.41
1:B:153:HIS:CG	1:B:154:SER:H	2.38	0.41
1:A:475:SER:HB3	1:B:475:SER:HB3	2.03	0.41
1:B:36:VAL:HG13	1:B:43:ILE:HG23	2.03	0.40
1:A:252:ILE:O	1:A:256:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	546/559 (98%)	536 (98%)	10 (2%)	0	100	100
1	B	545/559 (98%)	536 (98%)	9 (2%)	0	100	100
All	All	1091/1118 (98%)	1072 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	444/467 (95%)	433 (98%)	11 (2%)	47	29
1	B	431/467 (92%)	415 (96%)	16 (4%)	34	15
All	All	875/934 (94%)	848 (97%)	27 (3%)	40	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	80	TRP
1	A	272	SER
1	A	479	LEU
1	A	481	ILE
1	A	482	LEU
1	A	483	THR
1	A	497	ARG
1	A	512	ARG
1	A	527	ARG
1	A	552	VAL
1	B	68	ASP
1	B	80	TRP
1	B	99	ARG

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Mol	Chain	Res	Type
1	B	124	LEU
1	B	436	ASN
1	B	470	ASP
1	B	474	LEU
1	B	485	VAL
1	B	486	LEU
1	B	489	THR
1	B	492	VAL
1	B	518	VAL
1	B	535	MET
1	B	553	LEU
1	B	556	MET
1	B	558	VAL

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	417	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	5/7 (71%)	3 (60%)	1 (20%)
2	E	5/7 (71%)	4 (80%)	1 (20%)
All	All	10/14 (71%)	7 (70%)	2 (20%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	3	U
2	D	4	U
2	D	6	U
2	E	2	U
2	E	3	U
2	E	4	U
2	E	6	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	3	U
2	E	3	U

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	604	-	5,5,5	0.31	0	5,5,5	0.67	0
5	GOL	A	605	-	5,5,5	0.32	0	5,5,5	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	604	-	-	4/4/4/4	-
5	GOL	A	605	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	GOL	C1-C2-C3-O3
5	A	605	GOL	O1-C1-C2-C3
5	A	605	GOL	O2-C2-C3-O3
5	A	604	GOL	O1-C1-C2-C3
5	A	605	GOL	C1-C2-C3-O3
5	A	604	GOL	O2-C2-C3-O3
5	A	605	GOL	O1-C1-C2-O2
5	A	604	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	GOL	2	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	545/559 (97%)	0.84	100 (18%)  	15, 29, 81, 109	0
1	B	543/559 (97%)	1.14	103 (18%)  	15, 34, 87, 115	0
2	D	7/7 (100%)	0.79	1 (14%)  	25, 45, 55, 66	0
2	E	7/7 (100%)	0.81	1 (14%)  	28, 48, 55, 67	0
All	All	1102/1132 (97%)	0.99	205 (18%)  	15, 31, 84, 115	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	VAL	14.2
1	B	522	LEU	13.4
1	B	518	VAL	12.9
1	B	490	PRO	12.8
1	B	531	VAL	12.3
1	B	489	THR	11.9
1	B	486	LEU	11.4
1	B	508	LEU	10.9
1	B	484	ALA	10.4
1	A	558	VAL	10.2
1	B	483	THR	9.9
1	B	527	ARG	9.9
1	B	558	VAL	9.8
1	B	528	LEU	9.8
1	B	523	ARG	9.6
1	A	486	LEU	9.5
1	B	525	LYS	9.4
1	A	531	VAL	9.3
1	B	536	TYR	8.9
1	B	514	ALA	8.8
1	A	15	PRO	8.8

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Mol	Chain	Res	Type	RSRZ
1	B	538	ALA	8.8
1	B	526	LYS	8.7
1	B	510	ILE	8.6
1	B	521	GLY	8.6
1	A	522	LEU	8.4
1	A	525	LYS	8.4
1	B	529	GLU	8.4
1	A	559	ASP	8.3
1	B	524	GLU	8.0
1	B	534	ASP	7.8
1	B	557	ILE	7.8
1	A	527	ARG	7.8
1	B	492	VAL	7.6
1	A	16	ALA	7.5
1	A	528	LEU	7.5
1	B	491	HIS	7.4
1	B	517	ALA	7.4
1	A	485	VAL	7.4
1	B	488	PRO	7.4
1	B	16	ALA	7.4
1	A	490	PRO	7.3
1	A	529	GLU	7.2
1	A	523	ARG	7.2
1	B	556	MET	7.2
1	B	487	HIS	7.1
1	A	557	ILE	7.1
1	A	530	ASP	7.0
1	B	533	ASP	6.8
1	A	536	TYR	6.4
1	A	521	GLY	6.3
1	A	526	LYS	6.3
1	B	506	LEU	6.2
1	A	524	GLU	6.2
1	A	518	VAL	6.1
1	A	513	VAL	6.0
1	B	519	GLU	6.0
1	B	515	LEU	5.9
1	B	542	PHE	5.7
1	B	530	ASP	5.7
1	A	489	THR	5.6
1	A	533	ASP	5.5
1	A	520	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	487	HIS	5.4
1	B	520	GLN	5.3
1	A	517	ALA	5.3
1	A	538	ALA	5.1
1	A	512	ARG	5.1
1	A	488	PRO	5.0
1	B	516	GLU	4.9
1	B	504	ARG	4.9
1	B	207	ILE	4.8
1	B	494	VAL	4.8
2	E	6	U	4.7
1	B	539	VAL	4.7
2	D	6	U	4.6
1	B	125	GLN	4.5
1	B	495	VAL	4.5
1	B	552	VAL	4.5
1	B	17	PRO	4.5
1	A	515	LEU	4.4
1	A	510	ILE	4.4
1	A	552	VAL	4.3
1	A	534	ASP	4.3
1	A	482	LEU	4.2
1	A	506	LEU	4.2
1	B	505	ASP	4.2
1	A	483	THR	4.2
1	B	543	THR	4.2
1	B	55	ALA	4.1
1	A	125	GLN	4.1
1	A	309	VAL	4.1
1	A	17	PRO	4.1
1	A	469	LEU	4.0
1	B	512	ARG	4.0
1	B	540	ARG	4.0
1	A	494	VAL	3.9
1	B	532	ARG	3.9
1	A	541	ARG	3.9
1	B	535	MET	3.8
1	B	509	GLN	3.6
1	B	469	LEU	3.6
1	B	309	VAL	3.6
1	A	207	ILE	3.6
1	B	46	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	554	ILE	3.5
1	A	126	ASP	3.5
1	A	519	GLU	3.4
1	A	495	VAL	3.4
1	A	491	HIS	3.4
1	A	46	VAL	3.3
1	A	542	PHE	3.3
1	A	503	ASN	3.3
1	B	541	ARG	3.3
1	B	242	LEU	3.3
1	B	511	ARG	3.3
1	A	242	LEU	3.2
1	A	245	PHE	3.2
1	A	310[A]	CYS	3.2
1	A	502	PRO	3.1
1	B	466	ASP	3.1
1	B	241	PHE	3.1
1	A	539	VAL	3.1
1	B	555	PRO	3.1
1	A	37	PHE	3.1
1	B	44	VAL	3.1
1	A	402	TRP	3.1
1	B	546	ALA	3.0
1	A	170	VAL	3.0
1	A	252	ILE	3.0
1	B	82	LEU	3.0
1	B	507	GLU	2.9
1	A	241	PHE	2.9
1	A	532	ARG	2.9
1	B	161	TYR	2.9
1	B	271	ARG	2.9
1	A	155	ILE	2.9
1	B	480	LEU	2.9
1	A	81	ILE	2.9
1	B	482	LEU	2.8
1	B	502	PRO	2.8
1	A	546	ALA	2.8
1	A	556	MET	2.7
1	B	45	VAL	2.7
1	B	35	THR	2.7
1	B	310[A]	CYS	2.7
1	B	34	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	2.7
1	B	537	GLY	2.6
1	B	81	ILE	2.6
1	B	503	ASN	2.6
1	A	535	MET	2.6
1	B	205	LEU	2.6
1	B	402	TRP	2.6
1	A	540	ARG	2.6
1	A	45	VAL	2.6
1	B	37	PHE	2.5
1	A	171	LEU	2.5
1	B	244	THR	2.5
1	B	340	VAL	2.5
1	A	505	ASP	2.5
1	B	481	ILE	2.5
1	A	550	ASN	2.4
1	A	326	PHE	2.4
1	A	545	LYS	2.4
1	A	161	TYR	2.4
1	B	121	GLU	2.4
1	A	307	LEU	2.4
1	A	554	ILE	2.4
1	B	342	LEU	2.4
1	A	516	GLU	2.4
1	A	496	ALA	2.4
1	A	479	LEU	2.3
1	B	206	LEU	2.3
1	B	326	PHE	2.3
1	B	171	LEU	2.3
1	A	36	VAL	2.3
1	B	245	PHE	2.3
1	A	240	VAL	2.2
1	A	466	ASP	2.2
1	A	537	GLY	2.2
1	A	548	GLY	2.2
1	A	308	PHE	2.2
1	A	340	VAL	2.2
1	B	123	GLY	2.2
1	B	341	ILE	2.2
1	B	513	VAL	2.2
1	A	481	ILE	2.2
1	A	123	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	243	THR	2.2
1	A	82	LEU	2.1
1	A	124	LEU	2.1
1	B	307	LEU	2.1
1	A	255	ILE	2.1
1	B	308	PHE	2.1
1	B	240	VAL	2.1
1	A	484	ALA	2.1
1	A	34	ILE	2.1
1	A	173	THR	2.1
1	A	122	PHE	2.1
1	A	172	HIS	2.1
1	B	36	VAL	2.0
1	A	247	SER	2.0
1	B	553	LEU	2.0
1	A	35	THR	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. 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
4	MN	B	603	1/1	0.71	0.09	62,62,62,62	0
4	MN	A	603	1/1	0.76	0.11	78,78,78,78	0
5	GOL	A	604	6/6	0.87	0.13	25,34,40,40	0
5	GOL	A	605	6/6	0.94	0.10	24,33,39,43	0
3	ZN	B	602	1/1	0.98	0.08	23,23,23,23	0
3	ZN	B	601	1/1	0.99	0.04	35,35,35,35	0
3	ZN	A	602	1/1	0.99	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	601	1/1	1.00	0.08	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.