



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:05 pm GMT

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

<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

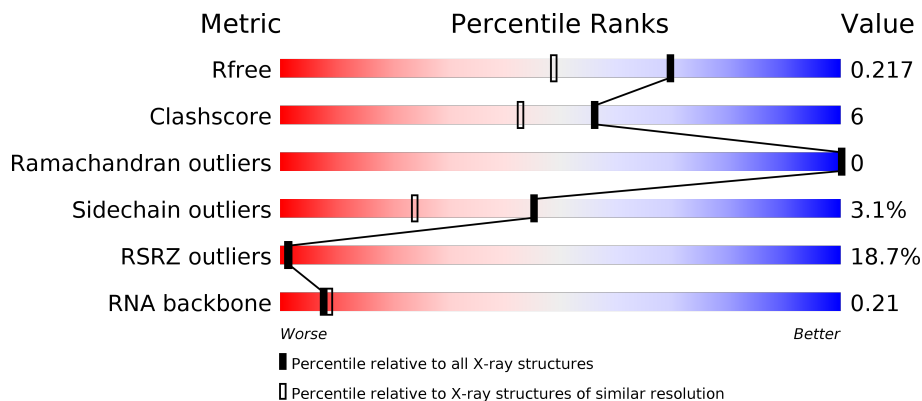
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)
RNA backbone	2435	1042 (2.60-0.88)

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>18%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	559	<div> <div>19%</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 [i](#)

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		

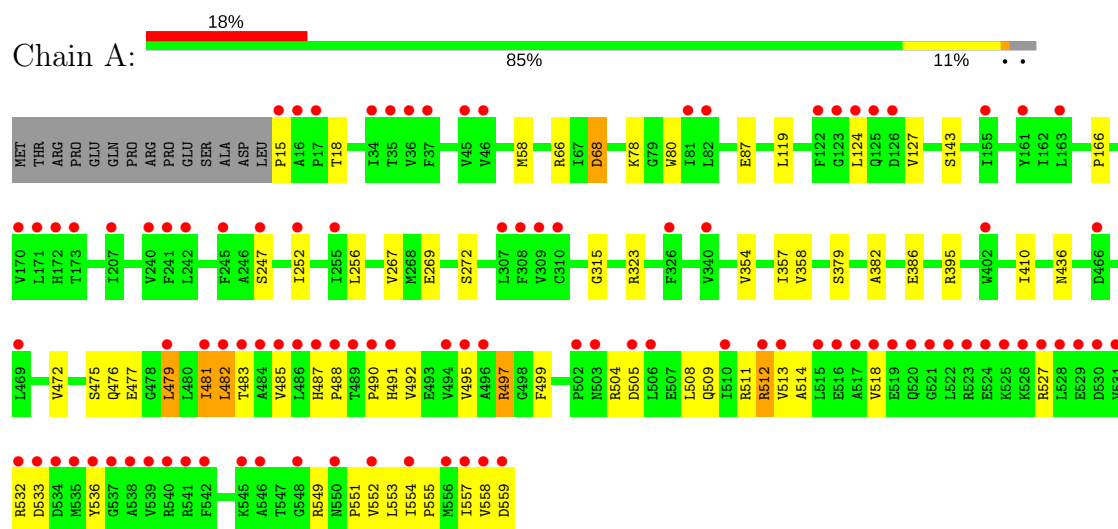
- Molecule 6 is water.

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		

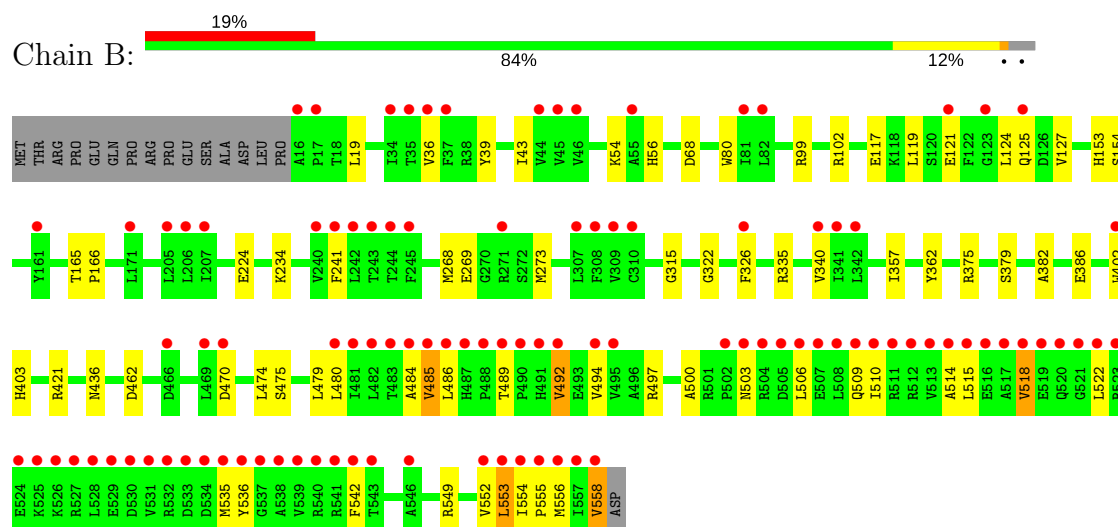
3 Residue-property plots

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.

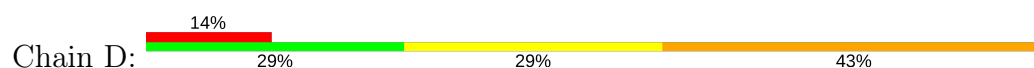
• Molecule 1: DR2417

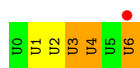


• Molecule 1: DR2417

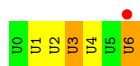


• Molecule 2: RNA (5'-D(UP*UP*UP*UP*UP*UP*U)-3')





- 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	Depositor
R, R_{free}	0.195 , 0.217 0.195 , 0.217	Depositor DCC
R_{free} test set	7888 reflections (5.02%)	DCC
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	53	33
1	B	431/467 (92%)	415 (96%)	16 (4%)	39	17
All	All	875/934 (94%)	848 (97%)	27 (3%)	45	24

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

Continued on next page...

Continued from previous page...

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%)	0
2	E	5/7 (71%)	4 (80%)	0
All	All	10/14 (71%)	7 (70%)	0

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

There are no RNA pucker outliers to report.

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	0.29	0	5,5,5	0.63	0
5	GOL	A	605	-	5,5,5	0.32	0	5,5,5	0.66	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	-	-	0/4/4/4	0/0/0/0
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	104 (19%)  	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%)	0.98	206 (18%)  	15, 31, 84, 115	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	VAL	14.2
1	B	522	LEU	13.3
1	B	518	VAL	13.0
1	B	490	PRO	12.7
1	B	531	VAL	12.2
1	B	489	THR	11.8
1	B	486	LEU	11.4
1	B	508	LEU	10.9
1	B	484	ALA	10.4
1	A	558	VAL	10.3
1	B	483	THR	10.0
1	B	527	ARG	9.9
1	B	528	LEU	9.7
1	B	523	ARG	9.7
1	B	558	VAL	9.6
1	B	525	LYS	9.4
1	A	486	LEU	9.4
1	A	531	VAL	9.3
1	B	536	TYR	8.9
1	B	514	ALA	8.8
1	B	538	ALA	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	15	PRO	8.8
1	B	526	LYS	8.7
1	B	521	GLY	8.7
1	B	510	ILE	8.5
1	A	522	LEU	8.4
1	A	525	LYS	8.4
1	B	529	GLU	8.3
1	A	559	ASP	8.2
1	B	524	GLU	8.0
1	B	557	ILE	7.9
1	A	527	ARG	7.8
1	B	534	ASP	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	16	ALA	7.3
1	A	490	PRO	7.3
1	B	488	PRO	7.3
1	B	556	MET	7.3
1	A	523	ARG	7.2
1	A	529	GLU	7.2
1	A	557	ILE	7.1
1	A	530	ASP	7.1
1	B	487	HIS	7.0
1	B	533	ASP	6.8
1	A	536	TYR	6.4
1	A	521	GLY	6.3
1	A	526	LYS	6.2
1	B	506	LEU	6.2
1	A	524	GLU	6.1
1	A	518	VAL	6.1
1	B	519	GLU	6.0
1	A	513	VAL	6.0
1	B	515	LEU	6.0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	487	HIS	5.4
1	A	517	ALA	5.4
1	B	520	GLN	5.3
1	A	512	ARG	5.1
1	A	538	ALA	5.1
1	B	516	GLU	5.0
1	A	488	PRO	5.0
1	B	504	ARG	4.9
1	B	207	ILE	4.8
1	B	494	VAL	4.7
2	E	6	U	4.7
1	B	539	VAL	4.7
1	B	495	VAL	4.5
2	D	6	U	4.5
1	B	125	GLN	4.5
1	B	552	VAL	4.5
1	A	515	LEU	4.5
1	B	17	PRO	4.4
1	A	510	ILE	4.4
1	A	534	ASP	4.3
1	A	552	VAL	4.2
1	A	483	THR	4.2
1	B	505	ASP	4.2
1	A	482	LEU	4.2
1	A	506	LEU	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	A	494	VAL	4.0
1	B	532	ARG	3.9
1	B	540	ARG	3.9
1	B	535	MET	3.8
1	A	541	ARG	3.8
1	B	469	LEU	3.6
1	B	509	GLN	3.6
1	B	309	VAL	3.6
1	A	207	ILE	3.6
1	B	46	VAL	3.5

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	537	GLY	2.6
1	A	163	LEU	2.6
1	B	81	ILE	2.6
1	B	205	LEU	2.6
1	A	535	MET	2.6
1	B	503	ASN	2.6
1	B	402	TRP	2.6
1	B	37	PHE	2.6
1	A	45	VAL	2.5
1	A	540	ARG	2.5
1	B	244	THR	2.5
1	B	340	VAL	2.5
1	A	171	LEU	2.5
1	A	505	ASP	2.5
1	A	545	LYS	2.5
1	B	481	ILE	2.5
1	A	326	PHE	2.5
1	A	554	ILE	2.4
1	A	161	TYR	2.4
1	A	550	ASN	2.4
1	A	307	LEU	2.4
1	A	496	ALA	2.4
1	B	121	GLU	2.4
1	A	516	GLU	2.4
1	B	206	LEU	2.3
1	B	342	LEU	2.3
1	B	326	PHE	2.3
1	A	479	LEU	2.3
1	B	171	LEU	2.3
1	B	245	PHE	2.3
1	A	36	VAL	2.3
1	A	240	VAL	2.3
1	A	308	PHE	2.3
1	A	466	ASP	2.3
1	A	548	GLY	2.3
1	A	537	GLY	2.2
1	A	340	VAL	2.2
1	B	341	ILE	2.2
1	B	123	GLY	2.2
1	A	124	LEU	2.2
1	A	481	ILE	2.2
1	A	123	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	2.1
1	B	307	LEU	2.1
1	B	243	THR	2.1
1	A	255	ILE	2.1
1	A	484	ALA	2.1
1	B	240	VAL	2.1
1	B	513	VAL	2.1
1	B	308	PHE	2.1
1	B	553	LEU	2.1
1	A	34	ILE	2.1
1	A	173	THR	2.1
1	A	122	PHE	2.0
1	A	247	SER	2.0
1	A	172	HIS	2.0
1	A	35	THR	2.0
1	B	36	VAL	2.0
1	B	470	ASP	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	GOL	A	604	6/6	0.87	0.13	1.00	25,34,40,40	0
5	GOL	A	605	6/6	0.94	0.10	0.42	24,33,39,43	0
4	MN	A	603	1/1	0.76	0.11	0.16	78,78,78,78	0
4	MN	B	603	1/1	0.72	0.09	-1.39	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	601	1/1	1.00	0.08	-2.97	21,21,21,21	0
3	ZN	B	602	1/1	0.98	0.08	-3.11	23,23,23,23	0
3	ZN	B	601	1/1	0.99	0.04	-4.90	35,35,35,35	0
3	ZN	A	602	1/1	0.99	0.04	-6.32	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.