



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 AM UTC

PDB ID : 4XWW / pdb_00004xww
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

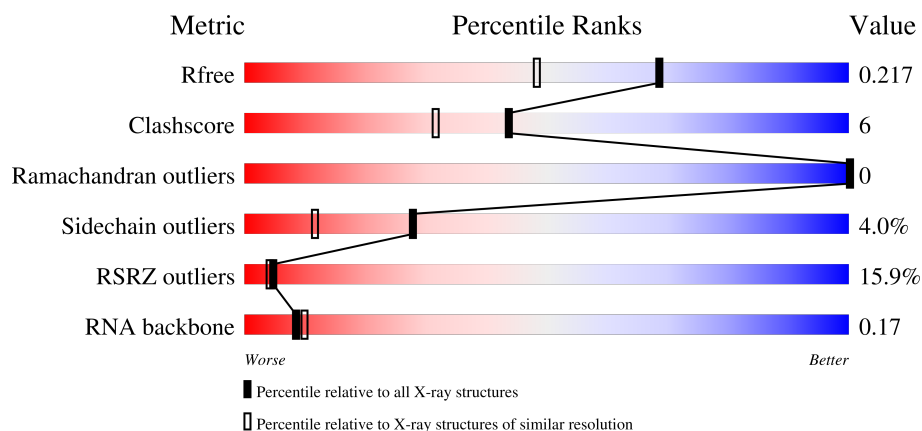
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)
RNA backbone	3983	1094 (2.20-1.20)

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 $\leq 5\%$. 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	15% 84% 12% ..
1	B	559	16% 83% 13% ..
2	D	7	29% 29% 29% 43%
2	E	7	29% 29% 43% 29%

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is GLYCEROL (CCD ID: 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		

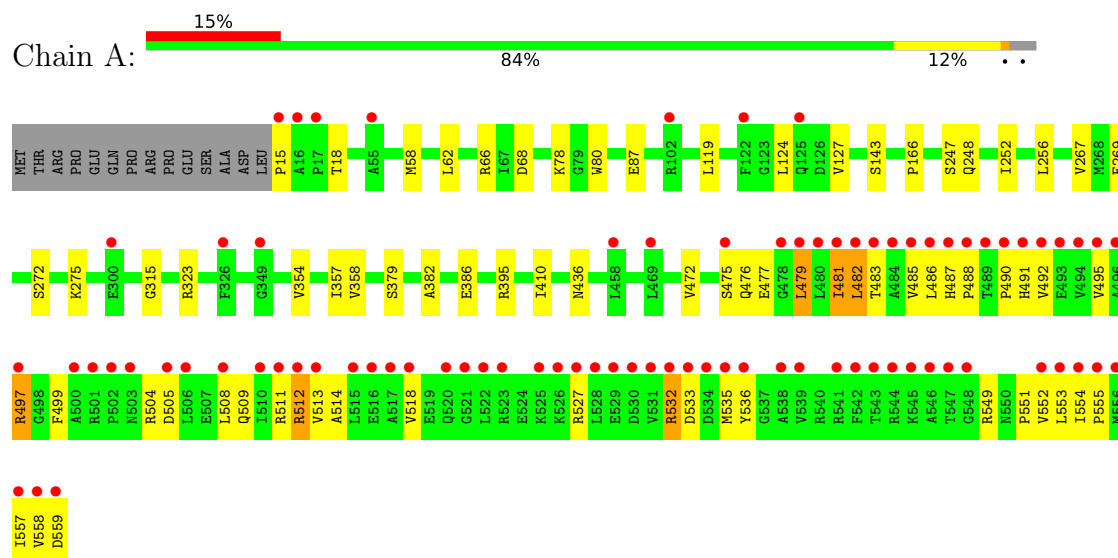
- Molecule 6 is water.

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		

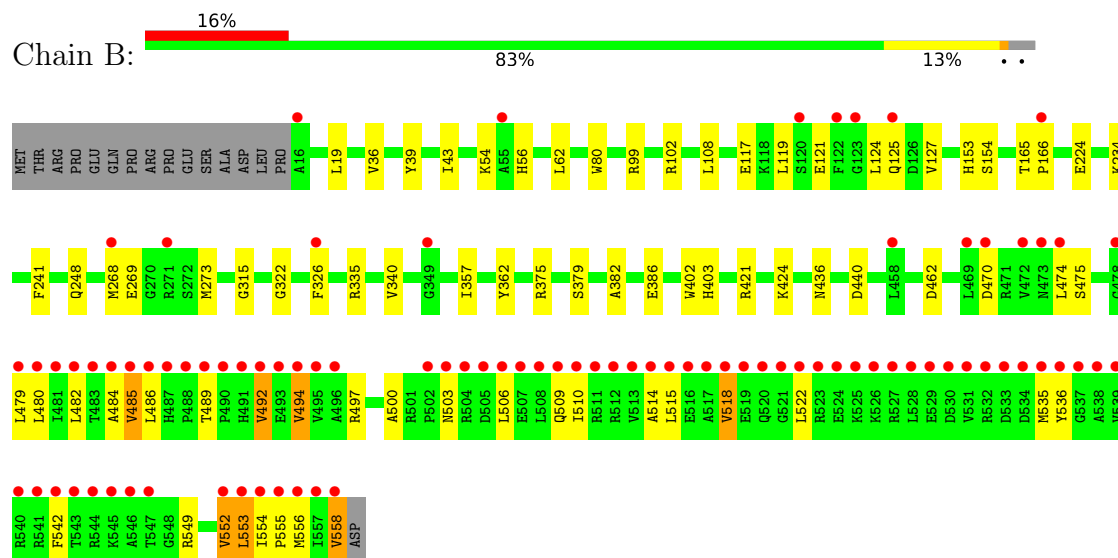
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

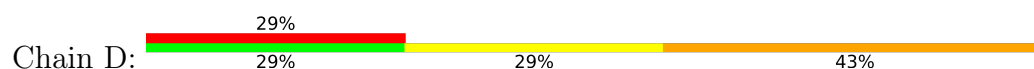
• Molecule 1: DR2417

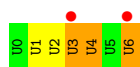


• Molecule 1: DR2417

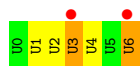


• Molecule 2: RNA (5'-D(UP*UP*UP*UP*UP*UP*U)-3')





- 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 (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 (4.85%)	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)	0.36 , 47.6	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	0.48	0/4289	0.78	1/5832 (0.0%)
1	B	0.46	0/4230	0.77	1/5758 (0.0%)
2	D	0.33	0/132	0.52	0/203
2	E	0.33	0/132	0.75	0/203
All	All	0.47	0/8783	0.77	2/11996 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	PRO	N-CA-CB	6.80	110.48	103.00
1	B	494	VAL	N-CA-C	6.07	117.03	108.17

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	51	0
1	B	4144	0	4096	43	0
2	D	121	0	61	13	0
2	E	121	0	61	5	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	16	3	0
6	A	404	0	0	3	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	104	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 (104) 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:558:VAL:HA	1:A:559:ASP:C	2.06	0.78
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:479:LEU:HD21	1:A:497:ARG:HB2	1.68	0.74
1:A:58:MET:HE1	1:A:472:VAL:HA	1.69	0.73
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
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
5:A:604:GOL:O2	6:A:1063:HOH:O	2.13	0.66
1:B:234:LYS:NZ	6:B:1024:HOH:O	2.28	0.65
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:B:379:SER:OG	2:E:1:U:OP2	2.03	0.63
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:536:TYR:HB2	1:A:555:PRO:HG3	1.85	0.57
2:E:1:U:H2'	2:E:1:U:O2	2.05	0.57
1:A:87:GLU:HG3	2:D:3:U:H5'	1.85	0.56
2:E:6:U:C6	2:E:6:U:H5'	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: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: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:379:SER:OG	2:D:1:U:OP2	2.23	0.49
1:A:536:TYR:CE2	1:A:553:LEU:HB2	2.47	0.49
1:B:424:LYS:NZ	1:B:440:ASP:OD1	2.45	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
2:D:6:U:O2	2:D:6:U:O2'	2.28	0.47
2:D:3:U:HO2'	2:D:4:U:P	2.37	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:487:HIS:HA	1:A:488:PRO:C	2.39	0.47
1:A:532:ARG:HG2	1:A:533:ASP:N	2.29	0.47
1:A:535:MET:HE2	1:A:557:ILE:CD1	2.44	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:A:247:SER:OG	2:D:3:U:OP1	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:O	1:B:518:VAL:HG23	2.16	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:354:VAL:HG12	5:A:605:GOL:H11	1.99	0.45
1:A:514:ALA:O	1:A:518:VAL:HG23	2.17	0.45
1:A:267:VAL:HG12	1:A:269:GLU:HG2	1.99	0.45
1:B:462:ASP:OD1	1:B:462:ASP:N	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:HD23	1:A:124:LEU:HA	1.82	0.44
1:B:19:LEU:HD22	1:B:165:THR:HG21	1.99	0.44
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: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:HD3	1:B:497:ARG:HA	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:558:VAL:CA	1:A:559:ASP:C	2.86	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%)	429 (97%)	15 (3%)	32	16
1	B	431/467 (92%)	411 (95%)	20 (5%)	24	9
All	All	875/934 (94%)	840 (96%)	35 (4%)	28	12

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

Mol	Chain	Res	Type
1	A	62	LEU
1	A	80	TRP
1	A	248	GLN
1	A	272	SER
1	A	275	LYS
1	A	479	LEU
1	A	481	ILE
1	A	482	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	483	THR
1	A	486	LEU
1	A	497	ARG
1	A	512	ARG
1	A	527	ARG
1	A	532	ARG
1	A	552	VAL
1	B	62	LEU
1	B	80	TRP
1	B	99	ARG
1	B	108	LEU
1	B	124	LEU
1	B	248	GLN
1	B	436	ASN
1	B	470	ASP
1	B	474	LEU
1	B	482	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	552	VAL
1	B	553	LEU
1	B	556	MET
1	B	558	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	476	GLN
1	B	302	GLN
1	B	550	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	5/7 (71%)	3 (60%)	1 (20%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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 oligosaccharides 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	0.72	0
5	GOL	A	605	-	5,5,5	0.32	0	5,5,5	0.73	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	GOL	1	0
5	A	605	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	545/559 (97%)	0.63	82 (15%) 5 5	10, 29, 81, 109	3 (0%)
1	B	543/559 (97%)	0.87	89 (16%) 4 4	10, 34, 87, 115	4 (0%)
2	D	7/7 (100%)	1.43	2 (28%) 1 1	25, 45, 55, 66	0
2	E	7/7 (100%)	1.59	2 (28%) 1 1	28, 48, 55, 67	0
All	All	1102/1132 (97%)	0.76	175 (15%) 5 4	10, 31, 84, 115	7 (0%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	THR	9.9
1	B	485	VAL	8.1
1	A	558	VAL	7.9
1	B	490	PRO	7.8
1	B	515	LEU	7.5
1	A	531	VAL	7.4
1	A	485	VAL	7.2
1	B	557	ILE	7.1
1	B	523	ARG	6.7
1	B	534	ASP	6.6
1	A	534	ASP	6.4
1	B	552	VAL	6.3
1	B	528	LEU	6.1
1	B	558	VAL	6.0
1	B	536	TYR	6.0
1	B	486	LEU	6.0
1	B	538	ALA	5.9
1	B	484	ALA	5.8
1	B	531	VAL	5.8
1	B	542	PHE	5.7
1	A	487	HIS	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	524	GLU	5.6
1	B	529	GLU	5.5
1	B	487	HIS	5.5
1	B	521	GLY	5.5
1	A	483	THR	5.4
1	A	557	ILE	5.4
1	B	546	ALA	5.3
1	A	538	ALA	5.3
1	B	533	ASP	5.2
1	B	506	LEU	5.1
1	B	510	ILE	5.0
1	B	522	LEU	5.0
1	B	480	LEU	5.0
1	A	528	LEU	5.0
1	B	488	PRO	4.9
1	B	495	VAL	4.9
1	B	532	ARG	4.9
1	B	530	ASP	4.9
1	B	553	LEU	4.8
1	A	495	VAL	4.8
1	B	508	LEU	4.7
1	A	490	PRO	4.7
1	B	492	VAL	4.7
1	B	519	GLU	4.6
1	B	514	ALA	4.6
1	B	491	HIS	4.5
1	A	546	ALA	4.5
1	B	512	ARG	4.5
1	A	469	LEU	4.4
1	A	510	ILE	4.4
1	A	15	PRO	4.4
1	A	553	LEU	4.4
1	A	542	PHE	4.3
1	A	521	GLY	4.3
1	A	491	HIS	4.3
1	A	536	TYR	4.3
1	A	525	LYS	4.3
1	A	539	VAL	4.3
1	A	481	ILE	4.3
1	A	479	LEU	4.2
1	A	522	LEU	4.2
1	B	481	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	512	ARG	4.1
1	A	543	THR	4.1
1	B	518	VAL	4.1
1	B	543	THR	4.1
1	A	484	ALA	4.1
1	A	552	VAL	4.1
1	B	539	VAL	4.1
1	B	554	ILE	4.1
1	A	526	LYS	4.0
1	B	517	ALA	4.0
1	A	494	VAL	4.0
1	A	513	VAL	4.0
1	B	489	THR	4.0
1	B	55	ALA	4.0
1	B	513	VAL	4.0
1	A	529	GLU	3.9
1	A	554	ILE	3.9
1	A	508	LEU	3.8
1	A	496	ALA	3.8
1	B	494	VAL	3.7
1	A	505	ASP	3.7
1	A	520	GLN	3.7
1	B	505	ASP	3.7
1	A	492	VAL	3.7
1	A	527	ARG	3.7
1	A	515	LEU	3.7
1	A	488	PRO	3.6
1	A	517	ALA	3.6
1	A	16	ALA	3.6
1	B	527	ARG	3.5
1	A	518	VAL	3.5
1	A	530	ASP	3.5
1	B	526	LYS	3.4
1	A	482	LEU	3.4
1	A	559	ASP	3.4
1	B	511	ARG	3.4
1	B	493	GLU	3.4
1	B	516	GLU	3.4
1	A	502	PRO	3.3
1	B	525	LYS	3.3
1	B	556	MET	3.3
1	B	555	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	544	ARG	3.2
1	A	489	THR	3.2
1	B	496	ALA	3.2
1	A	102[A]	ARG	3.1
1	A	555	PRO	3.1
1	B	125	GLN	3.1
1	A	533	ASP	3.1
2	E	6	U	3.0
1	A	486	LEU	3.0
1	A	511	ARG	3.0
1	A	478	GLY	3.0
1	A	503	ASN	3.0
1	A	17	PRO	2.9
1	B	520	GLN	2.9
1	A	506	LEU	2.9
1	B	535	MET	2.8
1	B	470	ASP	2.8
1	A	125	GLN	2.8
1	A	535	MET	2.8
1	B	547	THR	2.8
1	A	349	GLY	2.8
1	A	548	GLY	2.7
1	A	326	PHE	2.7
1	B	482	LEU	2.7
1	A	556	MET	2.6
1	B	507	GLU	2.6
2	D	3	U	2.6
1	A	523	ARG	2.6
1	B	509	GLN	2.6
1	B	268	MET	2.6
1	B	473	ASN	2.6
1	B	469	LEU	2.5
1	A	547	THR	2.5
1	A	122	PHE	2.5
1	A	480	LEU	2.5
1	B	474	LEU	2.5
1	A	541	ARG	2.5
2	E	3	U	2.5
1	A	545	LYS	2.5
1	B	504	ARG	2.4
1	A	55	ALA	2.4
1	B	503	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	541	ARG	2.4
2	D	6	U	2.4
1	B	540	ARG	2.4
1	B	545	LYS	2.4
1	B	537	GLY	2.3
1	A	300	GLU	2.3
1	A	493	GLU	2.3
1	A	497	ARG	2.3
1	B	349	GLY	2.3
1	A	458	LEU	2.3
1	B	544	ARG	2.3
1	B	472	VAL	2.3
1	B	479	LEU	2.2
1	A	516	GLU	2.2
1	A	475	SER	2.2
1	B	16	ALA	2.2
1	B	123	GLY	2.2
1	B	166	PRO	2.2
1	B	120	SER	2.2
1	B	122	PHE	2.1
1	B	326	PHE	2.1
1	B	458	LEU	2.1
1	B	478	GLY	2.1
1	B	502	PRO	2.1
1	B	271	ARG	2.0
1	A	501	ARG	2.0
1	A	532	ARG	2.0
1	A	500	ALA	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 oligosaccharides 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
4	MN	A	603	1/1	0.73	0.21	78,78,78,78	0
4	MN	B	603	1/1	0.78	0.15	62,62,62,62	0
5	GOL	A	604	6/6	0.89	0.12	25,34,40,40	0
5	GOL	A	605	6/6	0.94	0.09	24,33,39,43	0
3	ZN	B	601	1/1	0.98	0.08	35,35,35,35	0
3	ZN	A	602	1/1	0.99	0.10	30,30,30,30	0
3	ZN	B	602	1/1	0.99	0.04	23,23,23,23	0
3	ZN	A	601	1/1	1.00	0.01	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.