



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 6LVR / pdb_00006lvr
Title : Crystal structure of the PPR domain of Arabidopsis thaliana protein-only RNase P 1 (PRORP1) in complex with tRNA
Authors : Teramoto, T.; Hall, T.M.T.
Deposited on : 2020-02-04
Resolution : 2.85 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

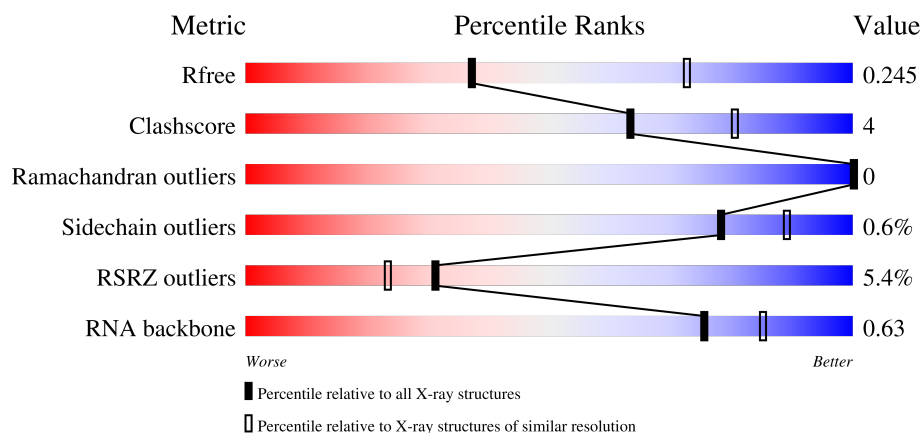
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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	208	79% 13% 7%
1	C	208	85% 8% 7%
2	B	76	13% 62% 24% 9% 5%
2	D	76	12% 54% 33% 7% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6226 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 Proteinaceous RNase P 1, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	194	Total	C	N	O	S	0	0	0
			1532	962	267	292	11			
1	A	193	Total	C	N	O	S	0	0	0
			1523	957	265	290	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	83	SER	-	expression tag	UNP Q66GI4
C	146	SER	GLU	See sequence details	UNP Q66GI4
C	?	-	ALA	See sequence details	UNP Q66GI4
C	?	-	THR	See sequence details	UNP Q66GI4
C	?	-	GLU	See sequence details	UNP Q66GI4
C	?	-	SER	See sequence details	UNP Q66GI4
C	153	SER	PRO	See sequence details	UNP Q66GI4
C	266	ASN	TYR	engineered mutation	UNP Q66GI4
C	284	GLN	PHE	engineered mutation	UNP Q66GI4
C	291	GLN	PHE	engineered mutation	UNP Q66GI4
A	83	SER	-	expression tag	UNP Q66GI4
A	146	SER	GLU	See sequence details	UNP Q66GI4
A	?	-	ALA	See sequence details	UNP Q66GI4
A	?	-	THR	See sequence details	UNP Q66GI4
A	?	-	GLU	See sequence details	UNP Q66GI4
A	?	-	SER	See sequence details	UNP Q66GI4
A	153	SER	PRO	See sequence details	UNP Q66GI4
A	266	ASN	TYR	engineered mutation	UNP Q66GI4
A	284	GLN	PHE	engineered mutation	UNP Q66GI4
A	291	GLN	PHE	engineered mutation	UNP Q66GI4

- Molecule 2 is a RNA chain called yeast phenylalanine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	72	Total 1568	C 708	N 278	O 510	P 72	0	0	0
2	B	72	Total 1568	C 708	N 278	O 510	P 72	0	0	0

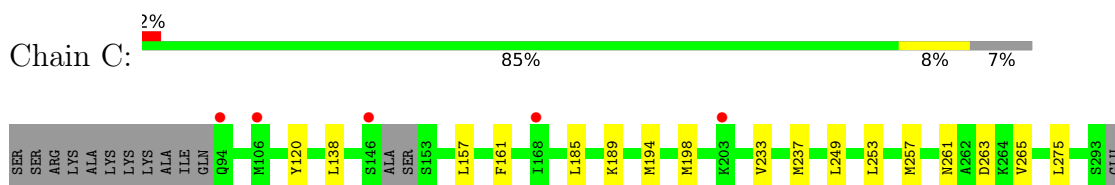
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	8	Total 8	O 8	0	0
3	A	18	Total 18	O 18	0	0
3	D	5	Total 5	O 5	0	0
3	B	4	Total 4	O 4	0	0

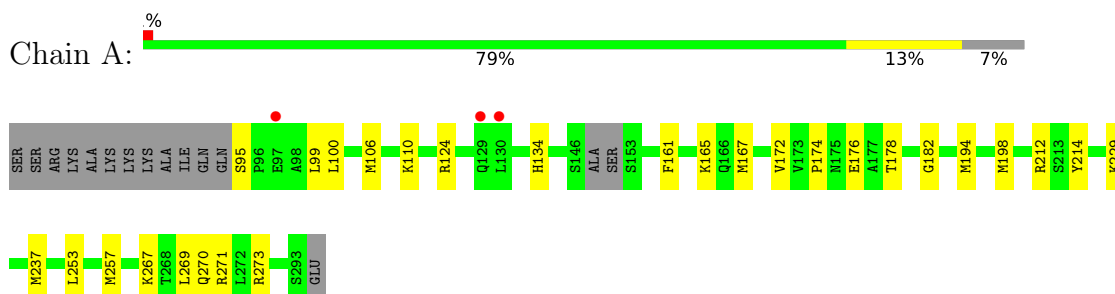
3 Residue-property plots

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.

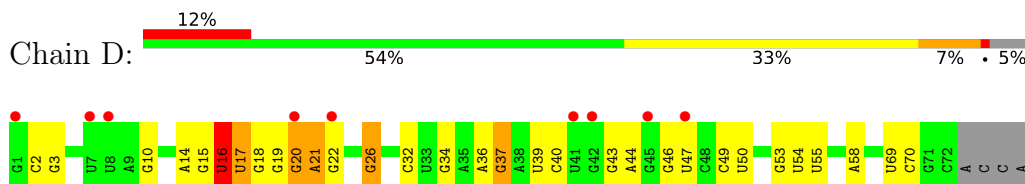
- Molecule 1: Proteinaceous RNase P 1, chloroplastic/mitochondrial



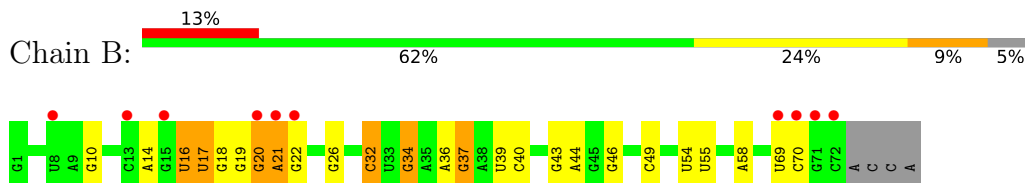
- Molecule 1: Proteinaceous RNase P 1, chloroplastic/mitochondrial



- Molecule 2: yeast phenylalanine tRNA



- Molecule 2: yeast phenylalanine tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.48Å 131.70Å 155.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 2.85 49.31 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.31-2.85) 99.8 (49.31-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.235 , 0.255 0.226 , 0.245	Depositor DCC
R_{free} test set	2087 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 118.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6226	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: H2U, 5MU, OMG, PSU, OMC, YYG, 7MG, M2G, 2MG, 5MC, 1MA

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	0.13	0/1546	0.33	0/2078
1	C	0.15	0/1555	0.30	0/2090
2	B	0.06	0/1393	0.17	0/2169
2	D	0.07	0/1393	0.18	0/2169
All	All	0.11	0/5887	0.26	0/8506

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1523	0	1535	19	0
1	C	1532	0	1543	10	0
2	B	1568	0	815	6	0
2	D	1568	0	815	8	0
3	A	18	0	0	0	0
3	B	4	0	0	0	0
3	C	8	0	0	0	0
3	D	5	0	0	0	0
All	All	6226	0	4708	43	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 4.

All (43) 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)
2:B:36:A:H2'	2:B:37:YYG:H8	1.70	0.71
2:D:36:A:H2'	2:D:37:YYG:H8	1.73	0.70
1:C:249:LEU:HD11	1:C:275:LEU:HD12	1.76	0.68
1:A:124:ARG:HH21	1:A:124:ARG:HG3	1.67	0.59
1:A:100:LEU:HD22	1:A:134:HIS:HD2	1.69	0.57
1:C:157:LEU:HD11	1:C:189:LYS:HG2	1.90	0.54
2:D:20:G:H4'	2:D:21:A:OP2	2.09	0.53
2:D:47:U:O2'	2:D:50:U:OP1	2.27	0.52
1:A:194:MET:O	1:A:198:MET:HG2	2.11	0.51
1:C:263:ASP:OD1	1:C:263:ASP:N	2.40	0.50
1:A:167:MET:HE1	1:A:178:THR:HG21	1.94	0.49
2:B:69:U:H2'	2:B:70:C:C6	2.47	0.49
1:A:161:PHE:O	1:A:165:LYS:HG3	2.13	0.49
1:A:214:TYR:CD2	1:A:237:MET:HG3	2.48	0.49
1:A:176:GLU:OE2	1:A:212:ARG:NH2	2.37	0.48
2:D:43:G:H2'	2:D:44:A:C8	2.48	0.48
1:A:106:MET:O	1:A:110:LYS:HG3	2.15	0.47
1:C:120:TYR:HB2	1:C:138:LEU:HD21	1.95	0.47
2:D:69:U:H2'	2:D:70:C:C6	2.50	0.47
1:A:253:LEU:O	1:A:257:MET:HG3	2.15	0.46
1:A:161:PHE:CZ	1:A:194:MET:HE3	2.50	0.45
2:B:34:OMG:H1'	2:B:34:OMG:HM23	1.70	0.45
1:C:161:PHE:CE1	1:C:185:LEU:HB3	2.52	0.45
1:C:233:VAL:O	1:C:237:MET:HG3	2.17	0.45
1:C:194:MET:O	1:C:198:MET:HG2	2.17	0.44
1:A:161:PHE:HB3	1:A:165:LYS:HE3	1.98	0.44
2:D:15:G:H5''	2:D:16:H2U:OP2	2.17	0.44
1:C:253:LEU:O	1:C:257:MET:HG3	2.18	0.43
1:C:198:MET:HE3	1:C:198:MET:HB3	1.81	0.43
1:A:182:GLY:HA3	1:A:198:MET:HE2	2.01	0.43
1:A:270:GLN:HA	1:A:273:ARG:HE	1.83	0.43
2:B:20:G:H3'	2:B:21:A:C5'	2.49	0.42
2:D:26:M2G:HM12	2:D:44:A:C2	2.53	0.42
1:A:174:PRO:HB3	1:A:178:THR:HG21	2.02	0.42
2:B:43:G:H2'	2:B:44:A:C8	2.55	0.42
1:A:267:LYS:O	1:A:271:ARG:HG3	2.20	0.41
1:A:95:SER:O	1:A:99:LEU:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ASN:O	1:C:265:VAL:HG23	2.20	0.41
1:A:100:LEU:HD22	1:A:134:HIS:CD2	2.53	0.40
2:D:2:C:H2'	2:D:3:G:C8	2.56	0.40
1:A:229:LYS:HD3	1:A:229:LYS:HA	1.87	0.40
2:B:32:OMC:HM23	2:B:32:OMC:H1'	1.92	0.40
1:A:124:ARG:HG3	1:A:124:ARG:NH2	2.36	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	189/208 (91%)	185 (98%)	4 (2%)	0	100	100
1	C	190/208 (91%)	186 (98%)	4 (2%)	0	100	100
All	All	379/416 (91%)	371 (98%)	8 (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	167/179 (93%)	165 (99%)	2 (1%)	63	80
1	C	168/179 (94%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	335/358 (94%)	333 (99%)	2 (1%)	78	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	71/76 (93%)	8 (11%)	1 (1%)
2	D	71/76 (93%)	9 (12%)	2 (2%)
All	All	142/152 (93%)	17 (11%)	3 (2%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	14	A
2	D	16	H2U
2	D	17	H2U
2	D	18	G
2	D	19	G
2	D	20	G
2	D	21	A
2	D	22	G
2	D	53	G
2	B	14	A
2	B	16	H2U
2	B	17	H2U
2	B	18	G
2	B	19	G
2	B	20	G
2	B	21	A
2	B	22	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	16	H2U
2	D	20	G
2	B	17	H2U

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

28 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
2	1MA	B	58	2	21,25,26	2.87	6 (28%)	30,37,40	2.38	9 (30%)
2	YYG	B	37	2	38,42,43	2.19	14 (36%)	45,62,65	3.09	14 (31%)
2	5MC	B	40	2	19,22,23	3.90	8 (42%)	26,32,35	0.97	2 (7%)
2	M2G	B	26	2	24,27,28	2.61	8 (33%)	33,40,43	1.88	9 (27%)
2	7MG	D	46	2	23,26,27	3.64	11 (47%)	27,39,42	2.19	9 (33%)
2	H2U	D	16	2	18,21,22	1.02	2 (11%)	19,30,33	0.95	0
2	2MG	B	10	2	23,26,27	3.17	8 (34%)	33,38,41	2.16	10 (30%)
2	2MG	D	10	2	23,26,27	3.17	8 (34%)	33,38,41	2.15	10 (30%)
2	M2G	D	26	2	24,27,28	2.61	8 (33%)	33,40,43	1.87	9 (27%)
2	5MC	D	40	2	19,22,23	3.91	8 (42%)	26,32,35	0.97	2 (7%)
2	H2U	B	16	2	18,21,22	0.97	2 (11%)	19,30,33	0.99	1 (5%)
2	5MU	D	54	2	19,22,23	5.00	7 (36%)	27,32,35	3.60	9 (33%)
2	5MU	B	54	2	19,22,23	5.00	7 (36%)	27,32,35	3.63	9 (33%)
2	5MC	D	49	2	19,22,23	3.91	8 (42%)	26,32,35	1.00	1 (3%)
2	OMG	B	34	2	23,26,27	2.80	8 (34%)	32,38,41	2.87	10 (31%)
2	YYG	D	37	2	38,42,43	2.19	14 (36%)	45,62,65	3.10	14 (31%)
2	OMC	B	32	2	19,22,23	3.04	8 (42%)	25,31,34	0.72	0
2	7MG	B	46	2	23,26,27	3.63	11 (47%)	27,39,42	2.18	9 (33%)
2	PSU	B	55	2	18,21,22	4.21	5 (27%)	21,30,33	1.97	5 (23%)
2	OMG	D	34	2	23,26,27	2.80	8 (34%)	32,38,41	2.85	9 (28%)
2	PSU	D	55	2	18,21,22	4.20	5 (27%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	B	39	2	18,21,22	4.21	6 (33%)	21,30,33	1.97	5 (23%)
2	OMC	D	32	2	19,22,23	3.05	8 (42%)	25,31,34	0.72	0
2	H2U	D	17	2	18,21,22	0.91	2 (11%)	19,30,33	0.92	1 (5%)
2	5MC	B	49	2	19,22,23	3.91	8 (42%)	26,32,35	1.01	1 (3%)
2	H2U	B	17	2	18,21,22	0.94	1 (5%)	19,30,33	1.32	2 (10%)
2	PSU	D	39	2	18,21,22	4.19	6 (33%)	21,30,33	1.95	5 (23%)
2	1MA	D	58	2	21,25,26	2.87	6 (28%)	30,37,40	2.39	9 (30%)

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
2	1MA	B	58	2	-	0/7/25/26	0/3/3/3
2	YYG	B	37	2	-	9/24/42/43	0/4/4/4
2	5MC	B	40	2	-	0/7/25/26	0/2/2/2
2	M2G	B	26	2	-	0/11/29/30	0/3/3/3
2	7MG	D	46	2	-	2/7/37/38	0/3/3/3
2	H2U	D	16	2	-	3/7/38/39	0/2/2/2
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
2	2MG	D	10	2	-	0/9/27/28	0/3/3/3
2	M2G	D	26	2	-	0/11/29/30	0/3/3/3
2	5MC	D	40	2	-	0/7/25/26	0/2/2/2
2	H2U	B	16	2	-	7/7/38/39	0/2/2/2
2	5MU	D	54	2	-	0/7/25/26	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	5MC	D	49	2	-	0/7/25/26	0/2/2/2
2	OMG	B	34	2	-	1/9/27/28	0/3/3/3
2	YYG	D	37	2	-	8/24/42/43	0/4/4/4
2	OMC	B	32	2	-	0/9/27/28	0/2/2/2
2	7MG	B	46	2	-	1/7/37/38	0/3/3/3
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	OMG	D	34	2	-	1/9/27/28	0/3/3/3
2	PSU	D	55	2	-	0/7/25/26	0/2/2/2
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	OMC	D	32	2	-	0/9/27/28	0/2/2/2
2	H2U	D	17	2	-	3/7/38/39	0/2/2/2
2	5MC	B	49	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H2U	B	17	2	-	7/7/38/39	0/2/2/2
2	PSU	D	39	2	-	0/7/25/26	0/2/2/2
2	1MA	D	58	2	-	0/7/25/26	0/3/3/3

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	5MU	C2-N1	11.58	1.56	1.38
2	D	54	5MU	C2-N1	11.55	1.56	1.38
2	D	54	5MU	C4-C5	10.73	1.62	1.44
2	B	54	5MU	C4-C5	10.67	1.62	1.44
2	B	55	PSU	C6-C5	10.52	1.46	1.35
2	B	39	PSU	C6-C5	10.48	1.46	1.35
2	D	39	PSU	C6-C5	10.48	1.46	1.35
2	D	55	PSU	C6-C5	10.45	1.46	1.35
2	B	54	5MU	C6-N1	10.30	1.55	1.38
2	D	54	5MU	C6-N1	10.29	1.55	1.38
2	B	55	PSU	C2-N1	10.27	1.50	1.36
2	D	55	PSU	C2-N1	10.27	1.50	1.36
2	B	39	PSU	C2-N1	10.26	1.50	1.36
2	D	39	PSU	C2-N1	10.16	1.49	1.36
2	B	49	5MC	C6-C5	9.30	1.49	1.34
2	D	49	5MC	C6-C5	9.27	1.49	1.34
2	D	40	5MC	C6-C5	9.27	1.49	1.34
2	B	40	5MC	C6-C5	9.24	1.49	1.34
2	B	46	7MG	C8-N9	8.83	1.51	1.45
2	D	46	7MG	C8-N9	8.81	1.51	1.45
2	B	58	1MA	C2-N3	8.79	1.46	1.30
2	D	58	1MA	C2-N3	8.77	1.46	1.30
2	D	54	5MU	C4-N3	-8.10	1.23	1.38
2	B	54	5MU	C4-N3	-8.01	1.23	1.38
2	B	10	2MG	C2-N3	7.72	1.46	1.32
2	D	10	2MG	C2-N3	7.72	1.46	1.32
2	D	10	2MG	C4-N3	7.52	1.51	1.34
2	B	10	2MG	C4-N3	7.51	1.51	1.34
2	B	39	PSU	C2-N3	7.22	1.49	1.37
2	D	55	PSU	C2-N3	7.22	1.49	1.37
2	D	39	PSU	C2-N3	7.21	1.49	1.37
2	B	55	PSU	C2-N3	7.18	1.49	1.37
2	D	46	7MG	C5-N7	7.15	1.44	1.35
2	B	46	7MG	C5-N7	7.11	1.44	1.35
2	D	34	OMG	C4-N3	6.94	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	40	5MC	C4-N3	6.93	1.45	1.34
2	B	34	OMG	C4-N3	6.92	1.50	1.34
2	D	49	5MC	C4-N3	6.90	1.45	1.34
2	B	40	5MC	C4-N3	6.89	1.45	1.34
2	D	58	1MA	C4-N3	6.87	1.49	1.35
2	B	58	1MA	C4-N3	6.86	1.49	1.35
2	B	49	5MC	C4-N3	6.84	1.45	1.34
2	D	49	5MC	C5-C4	6.71	1.49	1.44
2	B	40	5MC	C5-C4	6.67	1.49	1.44
2	B	26	M2G	C4-N3	6.63	1.49	1.34
2	D	40	5MC	C5-C4	6.62	1.49	1.44
2	B	49	5MC	C5-C4	6.62	1.49	1.44
2	D	26	M2G	C4-N3	6.60	1.49	1.34
2	D	32	OMC	C2-N3	6.52	1.49	1.36
2	B	34	OMG	C2-N2	6.51	1.49	1.34
2	B	32	OMC	C2-N3	6.51	1.49	1.36
2	D	34	OMG	C2-N2	6.49	1.49	1.34
2	B	54	5MU	C6-C5	6.42	1.45	1.34
2	D	34	OMG	C2-N3	6.40	1.48	1.33
2	D	40	5MC	C2-N3	6.39	1.49	1.36
2	B	49	5MC	C2-N3	6.38	1.49	1.36
2	B	34	OMG	C2-N3	6.38	1.48	1.33
2	B	40	5MC	C2-N3	6.37	1.49	1.36
2	D	49	5MC	C2-N3	6.37	1.49	1.36
2	D	37	YYG	C2-N3	6.36	1.49	1.38
2	B	37	YYG	C2-N3	6.34	1.49	1.38
2	D	54	5MU	C6-C5	6.29	1.44	1.34
2	B	10	2MG	C2-N2	6.24	1.46	1.33
2	D	10	2MG	C2-N2	6.21	1.46	1.33
2	D	26	M2G	C2-N2	6.21	1.46	1.35
2	B	26	M2G	C2-N2	6.20	1.46	1.35
2	B	32	OMC	C6-C5	6.02	1.49	1.35
2	D	32	OMC	C6-C5	5.98	1.48	1.35
2	D	26	M2G	C2-N3	5.92	1.46	1.32
2	D	46	7MG	C2-N3	5.92	1.47	1.33
2	B	26	M2G	C2-N3	5.91	1.46	1.32
2	B	46	7MG	C2-N3	5.90	1.47	1.33
2	B	46	7MG	C4-N3	5.85	1.47	1.34
2	D	46	7MG	C4-N3	5.83	1.47	1.34
2	D	32	OMC	C4-N3	5.48	1.45	1.34
2	B	32	OMC	C4-N3	5.46	1.45	1.34
2	D	46	7MG	C4-N9	5.42	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	7MG	C4-N9	5.38	1.44	1.37
2	B	55	PSU	C6-N1	5.26	1.44	1.36
2	D	32	OMC	C2-N1	5.25	1.51	1.40
2	D	55	PSU	C6-N1	5.22	1.44	1.36
2	B	39	PSU	C6-N1	5.22	1.44	1.36
2	B	32	OMC	C2-N1	5.16	1.50	1.40
2	D	39	PSU	C6-N1	5.16	1.44	1.36
2	B	10	2MG	C2-N1	4.96	1.44	1.36
2	D	10	2MG	C2-N1	4.92	1.44	1.36
2	D	40	5MC	C6-N1	4.83	1.46	1.38
2	D	10	2MG	O6-C6	-4.82	1.14	1.23
2	D	49	5MC	C6-N1	4.82	1.46	1.38
2	B	49	5MC	C6-N1	4.81	1.46	1.38
2	B	40	5MC	C6-N1	4.78	1.46	1.38
2	B	10	2MG	O6-C6	-4.75	1.14	1.23
2	D	37	YYG	C4-N3	4.72	1.47	1.38
2	B	37	YYG	C4-N3	4.71	1.47	1.38
2	B	46	7MG	C2-N2	4.69	1.45	1.34
2	D	46	7MG	C2-N2	4.68	1.45	1.34
2	B	49	5MC	C2-N1	4.62	1.49	1.40
2	D	49	5MC	C2-N1	4.54	1.49	1.40
2	B	40	5MC	C2-N1	4.49	1.49	1.40
2	D	40	5MC	C2-N1	4.47	1.49	1.40
2	D	40	5MC	C4-N4	4.44	1.45	1.34
2	D	49	5MC	C4-N4	4.43	1.45	1.34
2	B	40	5MC	C4-N4	4.43	1.45	1.34
2	B	49	5MC	C4-N4	4.41	1.45	1.34
2	B	37	YYG	C21-N20	4.35	1.45	1.34
2	D	37	YYG	C21-N20	4.35	1.45	1.34
2	B	58	1MA	C2-N1	4.21	1.44	1.35
2	D	32	OMC	C4-N4	4.21	1.44	1.33
2	D	58	1MA	C2-N1	4.19	1.44	1.35
2	B	32	OMC	C4-N4	4.18	1.44	1.33
2	B	46	7MG	C2-N1	3.94	1.47	1.37
2	D	46	7MG	C2-N1	3.93	1.47	1.37
2	D	58	1MA	C5-C6	3.86	1.54	1.43
2	B	58	1MA	C5-C6	3.82	1.53	1.43
2	D	46	7MG	C5-C6	3.74	1.52	1.43
2	B	46	7MG	C5-C6	3.72	1.52	1.43
2	D	37	YYG	O23-C21	3.62	1.40	1.34
2	B	37	YYG	O23-C21	3.61	1.40	1.34
2	D	26	M2G	C2-N1	3.49	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	M2G	C2-N1	3.47	1.44	1.36
2	D	39	PSU	C4-N3	3.35	1.45	1.38
2	B	39	PSU	C4-N3	3.32	1.45	1.38
2	D	55	PSU	C4-N3	3.29	1.45	1.38
2	B	46	7MG	C6-N1	3.29	1.45	1.38
2	D	34	OMG	O6-C6	-3.27	1.17	1.23
2	B	34	OMG	O6-C6	-3.27	1.17	1.23
2	D	46	7MG	C6-N1	3.24	1.44	1.38
2	B	55	PSU	C4-N3	3.22	1.44	1.38
2	B	32	OMC	C6-N1	3.17	1.45	1.38
2	D	32	OMC	C6-N1	3.15	1.45	1.38
2	D	37	YYG	C12-N1	-3.12	1.33	1.40
2	B	37	YYG	C12-N1	-3.07	1.33	1.40
2	D	34	OMG	C6-N1	2.95	1.44	1.38
2	B	34	OMG	C6-N1	2.93	1.44	1.38
2	D	10	2MG	C6-N1	2.93	1.44	1.38
2	B	10	2MG	C6-N1	2.89	1.44	1.38
2	B	34	OMG	C5-C6	2.88	1.55	1.44
2	D	34	OMG	C5-C6	2.87	1.55	1.44
2	B	37	YYG	O18-C16	2.86	1.40	1.33
2	D	16	H2U	C2-N3	-2.86	1.33	1.38
2	B	37	YYG	C5-C6	2.83	1.52	1.45
2	D	37	YYG	O18-C16	2.83	1.40	1.33
2	D	37	YYG	C5-C6	2.81	1.52	1.45
2	B	32	OMC	C5-C4	2.80	1.49	1.42
2	B	34	OMG	C2-N1	2.79	1.44	1.37
2	D	34	OMG	C2-N1	2.79	1.44	1.37
2	D	32	OMC	C5-C4	2.78	1.49	1.42
2	B	54	5MU	O4-C4	-2.71	1.18	1.23
2	B	26	M2G	C5-N7	-2.71	1.33	1.39
2	B	10	2MG	C5-C6	2.69	1.54	1.44
2	D	10	2MG	C5-C6	2.69	1.54	1.44
2	D	26	M2G	C5-N7	-2.68	1.33	1.39
2	D	54	5MU	O4-C4	-2.67	1.18	1.23
2	B	26	M2G	C5-C6	2.67	1.54	1.44
2	D	26	M2G	C5-C6	2.67	1.54	1.44
2	B	37	YYG	C13-C12	2.63	1.53	1.50
2	D	37	YYG	C13-C12	2.62	1.53	1.50
2	D	58	1MA	C5-N7	-2.61	1.33	1.39
2	B	10	2MG	C5-N7	-2.60	1.33	1.39
2	D	34	OMG	C5-N7	-2.59	1.33	1.39
2	D	16	H2U	C4-N3	-2.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	YYG	C11-N2	-2.58	1.32	1.38
2	D	37	YYG	C11-N2	-2.57	1.32	1.38
2	D	10	2MG	C5-N7	-2.57	1.33	1.39
2	B	58	1MA	C5-N7	-2.57	1.33	1.39
2	B	16	H2U	C2-N3	-2.57	1.33	1.38
2	D	37	YYG	C5-N7	-2.57	1.33	1.39
2	D	49	5MC	O2-C2	-2.56	1.18	1.23
2	D	40	5MC	O2-C2	-2.56	1.18	1.23
2	B	37	YYG	C5-N7	-2.56	1.33	1.39
2	D	26	M2G	O6-C6	-2.56	1.18	1.23
2	B	40	5MC	O2-C2	-2.56	1.19	1.23
2	B	34	OMG	C5-N7	-2.56	1.33	1.39
2	B	26	M2G	O6-C6	-2.55	1.18	1.23
2	B	49	5MC	O2-C2	-2.52	1.19	1.23
2	B	16	H2U	C4-N3	-2.48	1.33	1.37
2	D	46	7MG	O6-C6	-2.48	1.18	1.23
2	B	46	7MG	O6-C6	-2.45	1.18	1.23
2	D	37	YYG	C6-N1	2.44	1.47	1.42
2	D	26	M2G	C6-N1	2.43	1.43	1.38
2	B	37	YYG	C6-N1	2.42	1.47	1.42
2	B	17	H2U	C2-N3	-2.41	1.33	1.38
2	B	26	M2G	C6-N1	2.39	1.43	1.38
2	D	17	H2U	C2-N3	-2.34	1.33	1.38
2	D	17	H2U	C4-N3	-2.32	1.33	1.37
2	B	37	YYG	O18-C19	-2.27	1.40	1.45
2	D	37	YYG	O18-C19	-2.25	1.40	1.45
2	B	58	1MA	C4-N9	-2.25	1.32	1.38
2	D	32	OMC	O2-C2	-2.24	1.19	1.23
2	D	54	5MU	O2-C2	-2.20	1.19	1.23
2	B	37	YYG	O23-C24	-2.20	1.40	1.45
2	B	54	5MU	O2-C2	-2.19	1.19	1.23
2	B	32	OMC	O2-C2	-2.19	1.19	1.23
2	D	37	YYG	O23-C24	-2.17	1.40	1.45
2	D	58	1MA	C4-N9	-2.16	1.32	1.38
2	B	39	PSU	C4-C5	2.10	1.50	1.44
2	D	46	7MG	C5-C4	2.10	1.44	1.37
2	B	46	7MG	C5-C4	2.08	1.44	1.37
2	D	37	YYG	O6-C6	-2.08	1.18	1.23
2	D	39	PSU	C4-C5	2.07	1.50	1.44
2	B	37	YYG	O6-C6	-2.03	1.18	1.23

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	YYG	C10-C11-N2	-12.41	94.42	119.32
2	D	37	YYG	C10-C11-N2	-12.35	94.55	119.32
2	B	54	5MU	C5-C4-N3	11.86	125.63	115.32
2	D	54	5MU	C5-C4-N3	11.77	125.56	115.32
2	B	54	5MU	C5-C6-N1	-9.60	112.88	123.31
2	D	54	5MU	C5-C6-N1	-9.52	112.97	123.31
2	B	34	OMG	C1'-N9-C8	-9.14	100.77	126.73
2	D	34	OMG	C1'-N9-C8	-9.02	101.10	126.73
2	B	34	OMG	C1'-N9-C4	8.40	151.30	126.49
2	D	34	OMG	C1'-N9-C4	8.31	151.04	126.49
2	B	37	YYG	C1'-N9-C8	-7.55	105.28	126.73
2	D	37	YYG	C1'-N9-C8	-7.52	105.38	126.73
2	B	37	YYG	C5-C4-N3	-7.24	118.12	123.99
2	D	37	YYG	C5-C4-N3	-7.14	118.20	123.99
2	B	58	1MA	C1'-N9-C8	-6.63	107.89	126.73
2	D	58	1MA	C1'-N9-C8	-6.63	107.91	126.73
2	B	10	2MG	C2-N3-C4	6.60	120.26	112.00
2	D	10	2MG	C2-N3-C4	6.59	120.24	112.00
2	D	37	YYG	O23-C21-N20	5.53	120.08	110.77
2	B	37	YYG	O23-C21-N20	5.50	120.02	110.77
2	B	10	2MG	C5-C4-N3	-5.45	119.72	128.39
2	D	10	2MG	C5-C4-N3	-5.43	119.74	128.39
2	D	58	1MA	C1'-N9-C4	5.29	142.12	126.49
2	B	58	1MA	C1'-N9-C4	5.27	142.05	126.49
2	B	34	OMG	C5-C4-N3	-5.24	120.05	128.39
2	B	58	1MA	N1-C2-N3	-5.24	119.77	126.00
2	D	58	1MA	N1-C2-N3	-5.24	119.78	126.00
2	D	34	OMG	C5-C4-N3	-5.21	120.10	128.39
2	B	26	M2G	C5-C4-N3	-5.01	120.41	128.39
2	D	26	M2G	C5-C4-N3	-4.97	120.47	128.39
2	D	46	7MG	C5-C6-N1	4.96	119.67	110.94
2	B	46	7MG	C5-C6-N1	4.96	119.67	110.94
2	B	54	5MU	O4-C4-C5	-4.94	119.27	124.92
2	D	54	5MU	O4-C4-C5	-4.88	119.33	124.92
2	B	54	5MU	C4-N3-C2	-4.80	121.05	127.34
2	D	55	PSU	C4-N3-C2	-4.75	119.83	126.37
2	B	55	PSU	C4-N3-C2	-4.72	119.86	126.37
2	D	54	5MU	C4-N3-C2	-4.72	121.15	127.34
2	D	37	YYG	N3-C2-N2	4.70	133.11	126.62
2	B	39	PSU	C4-N3-C2	-4.70	119.90	126.37
2	D	39	PSU	C4-N3-C2	-4.68	119.92	126.37
2	B	37	YYG	N3-C2-N2	4.65	133.04	126.62
2	B	54	5MU	N3-C2-N1	4.61	120.89	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	7MG	C2-N3-C4	4.60	120.23	112.30
2	D	46	7MG	C2-N3-C4	4.60	120.23	112.30
2	B	34	OMG	C2-N3-C4	4.58	120.19	112.30
2	D	54	5MU	N3-C2-N1	4.57	120.84	114.89
2	D	34	OMG	C2-N3-C4	4.56	120.16	112.30
2	D	37	YYG	C11-C12-N1	4.42	108.42	105.31
2	B	39	PSU	N1-C2-N3	4.41	119.82	115.17
2	D	39	PSU	N1-C2-N3	4.39	119.80	115.17
2	B	55	PSU	N1-C2-N3	4.35	119.76	115.17
2	B	37	YYG	C11-C12-N1	4.33	108.36	105.31
2	D	55	PSU	N1-C2-N3	4.28	119.68	115.17
2	D	46	7MG	C5-C4-N3	-4.22	120.21	128.13
2	D	58	1MA	C5-C4-N3	-4.21	121.08	127.27
2	D	26	M2G	C2-N3-C4	4.20	120.28	112.51
2	B	10	2MG	C2-N1-C6	-4.20	119.47	124.55
2	B	46	7MG	C5-C4-N3	-4.19	120.26	128.13
2	B	58	1MA	C5-C4-N3	-4.16	121.14	127.27
2	D	10	2MG	C2-N1-C6	-4.16	119.52	124.55
2	B	26	M2G	C2-N3-C4	4.14	120.16	112.51
2	D	54	5MU	C5M-C5-C4	3.98	123.03	118.78
2	B	54	5MU	C5M-C5-C4	3.94	122.99	118.78
2	D	54	5MU	C5M-C5-C6	-3.92	117.55	122.85
2	B	54	5MU	C5M-C5-C6	-3.90	117.57	122.85
2	D	46	7MG	C4-C5-N7	3.88	109.96	105.38
2	B	46	7MG	C4-C5-N7	3.87	109.95	105.38
2	B	26	M2G	C1'-N9-C8	-3.86	115.77	126.73
2	D	58	1MA	N9-C8-N7	-3.85	106.26	113.40
2	B	58	1MA	N9-C8-N7	-3.85	106.26	113.40
2	D	58	1MA	C2-N3-C4	3.73	119.85	112.53
2	B	58	1MA	C2-N3-C4	3.70	119.79	112.53
2	D	37	YYG	N1-C2-N2	-3.62	108.84	114.03
2	D	26	M2G	C1'-N9-C8	-3.62	116.46	126.73
2	B	37	YYG	N1-C2-N2	-3.59	108.89	114.03
2	D	37	YYG	O18-C16-C15	3.35	120.02	111.49
2	B	37	YYG	O18-C16-C15	3.34	120.00	111.49
2	D	10	2MG	N9-C4-N3	3.32	132.58	125.95
2	B	10	2MG	N9-C4-N3	3.29	132.53	125.95
2	D	10	2MG	N1-C2-N2	3.28	119.91	116.56
2	B	55	PSU	C6-N1-C2	-3.26	119.66	122.69
2	B	10	2MG	N1-C2-N2	3.26	119.89	116.56
2	D	39	PSU	C6-N1-C2	-3.24	119.69	122.69
2	B	39	PSU	C6-N1-C2	-3.23	119.70	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	M2G	C1'-N9-C4	3.20	135.94	126.49
2	B	37	YYG	O23-C21-O22	-3.19	119.98	124.62
2	D	37	YYG	O23-C21-O22	-3.18	119.99	124.62
2	D	26	M2G	N9-C8-N7	-3.16	107.54	113.40
2	B	46	7MG	C5-C4-N9	3.12	110.33	106.33
2	D	46	7MG	C5-C4-N9	3.11	110.32	106.33
2	D	55	PSU	C6-N1-C2	-3.09	119.82	122.69
2	B	39	PSU	C6-C5-C4	3.09	120.26	118.17
2	B	26	M2G	N9-C8-N7	-3.08	107.69	113.40
2	D	40	5MC	C5-C6-N1	-3.06	119.99	123.31
2	D	55	PSU	C6-C5-C4	3.05	120.23	118.17
2	B	34	OMG	C2-N1-C6	-3.04	119.60	125.11
2	D	34	OMG	C2-N1-C6	-3.04	119.61	125.11
2	D	37	YYG	O22-C21-N20	-3.01	119.93	124.86
2	B	55	PSU	C6-C5-C4	3.01	120.20	118.17
2	D	39	PSU	C6-C5-C4	2.98	120.18	118.17
2	B	40	5MC	C5-C6-N1	-2.97	120.09	123.31
2	B	37	YYG	O22-C21-N20	-2.96	120.00	124.86
2	B	34	OMG	N9-C4-N3	2.96	131.87	125.95
2	D	26	M2G	C1'-N9-C4	2.95	135.21	126.49
2	D	34	OMG	N9-C4-N3	2.95	131.85	125.95
2	D	37	YYG	N9-C8-N7	-2.94	107.95	113.40
2	D	49	5MC	C5-C6-N1	-2.91	120.15	123.31
2	B	54	5MU	O2-C2-N1	-2.91	119.02	122.80
2	B	37	YYG	N9-C8-N7	-2.90	108.02	113.40
2	B	34	OMG	N9-C8-N7	-2.85	108.11	113.40
2	B	17	H2U	C5-C4-N3	2.85	119.72	116.69
2	D	34	OMG	N9-C8-N7	-2.81	108.18	113.40
2	D	46	7MG	O6-C6-C5	-2.81	120.73	127.62
2	B	46	7MG	O6-C6-C5	-2.79	120.78	127.62
2	B	49	5MC	C5-C6-N1	-2.79	120.29	123.31
2	B	17	H2U	C5-C6-N1	-2.78	103.10	111.52
2	D	46	7MG	C2-N1-C6	-2.78	120.08	125.11
2	B	46	7MG	C2-N1-C6	-2.76	120.10	125.11
2	B	26	M2G	N9-C4-N3	2.76	131.47	125.95
2	D	46	7MG	N9-C4-N3	2.74	129.47	125.46
2	D	10	2MG	N9-C8-N7	-2.72	108.35	113.40
2	B	10	2MG	N9-C8-N7	-2.72	108.35	113.40
2	B	46	7MG	N9-C4-N3	2.69	129.41	125.46
2	B	10	2MG	C5-C6-N1	2.68	120.07	113.25
2	B	39	PSU	O2-C2-N1	-2.67	120.03	122.79
2	D	26	M2G	C5-C6-N1	2.67	120.05	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	O4-C4-N3	-2.66	115.10	120.11
2	D	26	M2G	N9-C4-N3	2.66	131.28	125.95
2	D	54	5MU	O4-C4-N3	-2.66	115.11	120.11
2	D	34	OMG	C5-C6-N1	2.66	120.02	113.25
2	D	10	2MG	C5-C6-N1	2.66	120.02	113.25
2	B	34	OMG	C5-C6-N1	2.65	119.99	113.25
2	D	54	5MU	O2-C2-N1	-2.64	119.36	122.80
2	B	26	M2G	C5-C6-N1	2.63	119.94	113.25
2	D	39	PSU	O2-C2-N1	-2.56	120.15	122.79
2	B	10	2MG	O6-C6-C5	-2.53	119.85	126.53
2	D	10	2MG	O6-C6-C5	-2.51	119.92	126.53
2	D	34	OMG	O6-C6-C5	-2.50	119.93	126.53
2	B	55	PSU	O2-C2-N1	-2.49	120.22	122.79
2	D	58	1MA	C8-N7-C5	2.49	108.70	104.26
2	B	58	1MA	C8-N7-C5	2.49	108.70	104.26
2	B	37	YYG	C3-N3-C4	-2.49	118.29	123.11
2	D	26	M2G	O6-C6-C5	-2.47	120.00	126.53
2	B	34	OMG	O6-C6-C5	-2.47	120.01	126.53
2	D	37	YYG	C3-N3-C4	-2.46	118.34	123.11
2	B	26	M2G	O6-C6-C5	-2.46	120.04	126.53
2	D	46	7MG	N9-C8-N7	2.45	106.84	103.37
2	B	46	7MG	N9-C8-N7	2.41	106.79	103.37
2	D	55	PSU	O2-C2-N1	-2.37	120.34	122.79
2	D	26	M2G	C8-N7-C5	2.27	108.31	104.26
2	D	37	YYG	C8-N7-C5	2.24	108.26	104.26
2	B	16	H2U	O2-C2-N3	-2.24	117.36	121.49
2	B	37	YYG	N9-C4-N3	2.22	133.04	129.45
2	B	37	YYG	C8-N7-C5	2.21	108.19	104.26
2	D	37	YYG	N9-C4-N3	2.19	133.00	129.45
2	B	26	M2G	C8-N7-C5	2.18	108.15	104.26
2	B	58	1MA	C8-N9-C4	2.15	110.06	106.03
2	D	10	2MG	N1-C2-N3	-2.13	120.08	123.68
2	B	10	2MG	N1-C2-N3	-2.13	120.10	123.68
2	D	58	1MA	N9-C4-N3	2.12	131.73	126.90
2	B	58	1MA	N9-C4-N3	2.11	131.71	126.90
2	D	58	1MA	C8-N9-C4	2.11	109.97	106.03
2	D	40	5MC	CM5-C5-C6	-2.09	120.03	122.85
2	B	10	2MG	C8-N7-C5	2.08	107.96	104.26
2	D	10	2MG	C8-N7-C5	2.06	107.93	104.26
2	B	34	OMG	C8-N7-C5	2.04	107.90	104.26
2	B	40	5MC	CM5-C5-C6	-2.04	120.09	122.85
2	D	17	H2U	O4-C4-N3	2.00	123.39	120.30

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	16	H2U	C4'-C5'-O5'-P
2	D	16	H2U	O4'-C1'-N1-C6
2	B	16	H2U	O4'-C1'-N1-C6
2	D	17	H2U	O4'-C4'-C5'-O5'
2	B	17	H2U	O4'-C1'-N1-C2
2	B	17	H2U	O4'-C1'-N1-C6
2	D	34	OMG	C1'-C2'-O2'-CM2
2	B	34	OMG	C1'-C2'-O2'-CM2
2	D	37	YYG	C15-C16-O18-C19
2	D	37	YYG	O22-C21-N20-C15
2	D	37	YYG	N20-C21-O23-C24
2	D	37	YYG	O22-C21-O23-C24
2	B	37	YYG	C15-C16-O18-C19
2	B	37	YYG	O22-C21-N20-C15
2	B	37	YYG	N20-C21-O23-C24
2	B	37	YYG	O22-C21-O23-C24
2	D	46	7MG	C2'-C1'-N9-C8
2	B	46	7MG	C2'-C1'-N9-C8
2	B	37	YYG	O17-C16-O18-C19
2	D	37	YYG	O17-C16-O18-C19
2	B	37	YYG	O23-C21-N20-C15
2	D	37	YYG	O23-C21-N20-C15
2	B	16	H2U	C3'-C4'-C5'-O5'
2	D	17	H2U	C3'-C4'-C5'-O5'
2	D	37	YYG	C12-C13-C14-C15
2	B	17	H2U	O4'-C4'-C5'-O5'
2	B	17	H2U	C3'-C4'-C5'-O5'
2	B	37	YYG	C13-C14-C15-N20
2	B	16	H2U	O4'-C4'-C5'-O5'
2	B	37	YYG	C12-C13-C14-C15
2	B	16	H2U	C2'-C1'-N1-C2
2	B	16	H2U	C4'-C5'-O5'-P
2	D	17	H2U	C4'-C5'-O5'-P
2	B	37	YYG	C13-C14-C15-C16
2	B	16	H2U	C2'-C1'-N1-C6
2	D	16	H2U	O4'-C1'-N1-C2
2	B	16	H2U	O4'-C1'-N1-C2
2	B	17	H2U	C2'-C1'-N1-C6
2	D	37	YYG	C13-C14-C15-N20
2	B	17	H2U	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	D	46	7MG	C2'-C1'-N9-C4
2	B	17	H2U	C2'-C1'-N1-C2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	37	YYG	1	0
2	D	16	H2U	1	0
2	D	26	M2G	1	0
2	B	34	OMG	1	0
2	D	37	YYG	1	0
2	B	32	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	193/208 (92%)	0.23	3 (1%) 70 64	50, 71, 109, 153	0
1	C	194/208 (93%)	0.42	5 (2%) 57 48	47, 73, 117, 150	0
2	B	58/76 (76%)	0.86	10 (17%) 4 3	59, 202, 325, 335	0
2	D	58/76 (76%)	0.98	9 (15%) 5 4	67, 192, 315, 333	0
All	All	503/568 (88%)	0.46	27 (5%) 31 23	47, 79, 248, 335	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	45	G	4.3
1	C	146	SER	4.2
1	C	168	ILE	4.2
2	D	47	U	3.5
2	B	21	A	3.5
2	B	72	C	3.3
1	C	94	GLN	3.2
1	C	203	LYS	3.1
2	B	20	G	3.1
2	B	71	G	2.9
2	B	22	G	2.8
1	A	130	LEU	2.7
2	D	8	U	2.5
2	D	42	G	2.5
1	A	97	GLU	2.5
2	D	22	G	2.4
2	B	8	U	2.4
2	D	20	G	2.4
2	B	70	C	2.3
1	A	129	GLN	2.3
2	B	13	C	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	1	G	2.3
2	B	15	G	2.3
2	D	7	U	2.2
1	C	106	MET	2.2
2	B	69	U	2.2
2	D	41	U	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	OMG	B	34	24/25	-0.00	0.23	319,342,350,351	0
2	OMG	D	34	24/25	0.15	0.21	303,329,336,339	0
2	H2U	D	17	20/21	0.43	0.14	143,194,225,226	0
2	PSU	B	39	20/21	0.45	0.11	306,323,337,341	0
2	OMC	D	32	21/22	0.50	0.17	309,323,328,337	0
2	YYG	B	37	39/40	0.52	0.17	313,336,361,363	0
2	PSU	D	39	20/21	0.56	0.15	275,287,298,299	0
2	YYG	D	37	39/40	0.56	0.17	298,338,343,347	0
2	H2U	B	16	20/21	0.57	0.19	168,239,264,267	0
2	5MC	B	40	21/22	0.60	0.14	293,311,331,334	0
2	OMC	B	32	21/22	0.62	0.12	286,306,321,327	0
2	H2U	D	16	20/21	0.66	0.18	173,209,227,237	0
2	H2U	B	17	20/21	0.72	0.17	137,203,228,230	0
2	5MC	D	40	21/22	0.76	0.18	249,267,287,291	0
2	M2G	B	26	25/26	0.77	0.14	202,253,263,278	0
2	M2G	D	26	25/26	0.79	0.14	180,204,223,232	0
2	2MG	D	10	24/25	0.84	0.15	168,192,209,215	0
2	2MG	B	10	24/25	0.86	0.12	176,229,245,257	0
2	7MG	D	46	24/25	0.86	0.19	145,169,222,227	0
2	7MG	B	46	24/25	0.90	0.14	132,171,216,224	0
2	5MC	B	49	21/22	0.95	0.14	123,145,171,173	0
2	1MA	B	58	23/24	0.95	0.11	68,83,102,137	0
2	5MU	D	54	21/22	0.96	0.11	52,65,96,109	0
2	5MC	D	49	21/22	0.96	0.09	104,115,144,162	0
2	PSU	D	55	20/21	0.97	0.08	45,63,85,86	0
2	PSU	B	55	20/21	0.97	0.09	48,59,86,106	0
2	1MA	D	58	23/24	0.97	0.09	64,73,106,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5MU	B	54	21/22	0.97	0.09	51,66,87,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.