



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2021 – 10:31 AM EST

PDB ID : 6VRD
Title : Crystal structure of RNase H/RNA/PS-ASO complex at an atomic level
Authors : Cho, Y.J.; Butler, D.
Deposited on : 2020-02-07
Resolution : 1.30 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 : 2.16
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) : 2.16

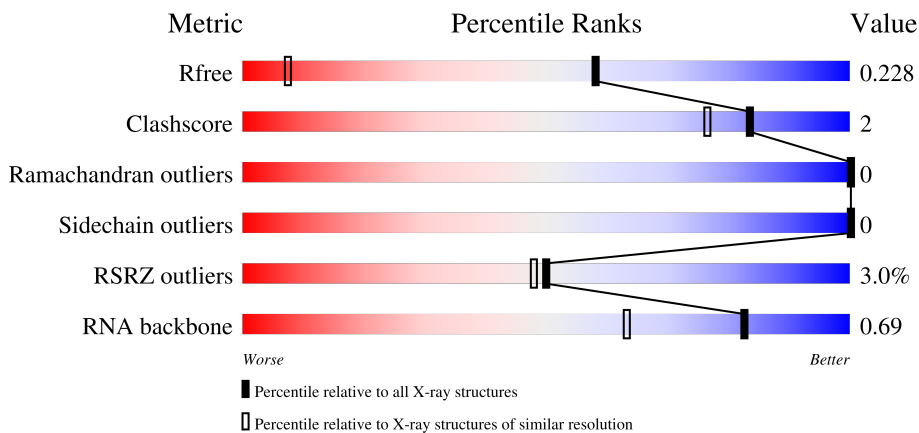
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)
RNA backbone	3102	1000 (2.34-0.62)

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	294	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div></div> <div>49%</div> </div> </div>
2	B	20	<div> <div>80%</div> <div>20%</div> </div>
3	C	20	<div> <div>80%</div> <div>20%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2513 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 Ribonuclease H1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	12	0
			1274	790	247	231	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP O60930
A	-6	HIS	-	expression tag	UNP O60930
A	-5	HIS	-	expression tag	UNP O60930
A	-4	HIS	-	expression tag	UNP O60930
A	-3	HIS	-	expression tag	UNP O60930
A	-2	HIS	-	expression tag	UNP O60930
A	-1	HIS	-	expression tag	UNP O60930
A	0	HIS	-	expression tag	UNP O60930
A	210	ASN	ASP	engineered mutation	UNP O60930

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*GP*GP*CP*GP*AP*GP*UP*GP*GP*GP*UP*GP*AP*GP*UP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			439	195	86	139	19			

- Molecule 3 is a RNA chain called RNA (5'-R(*(OMC)P*(N7X)P*(T39)P*(C5L)P*(A2M))-D(P*(SC)P*(PST)P*(SC)P*(AS)P*(SC)P*(SC)P*(SC)P*(AS)P*(SC)P*(PST))-R(P*(6O)O)P*(RFJ)P*(6OO)P*(6OO)P*(6NW))-3').

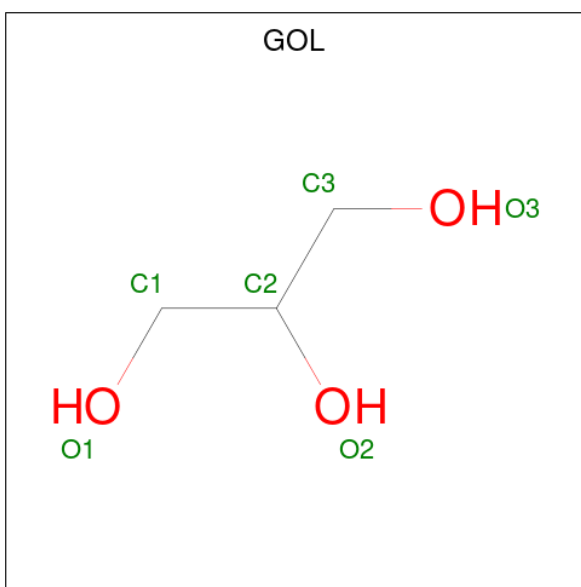
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	P	S	0	0
			422	206	67	114	19	16		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	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		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		

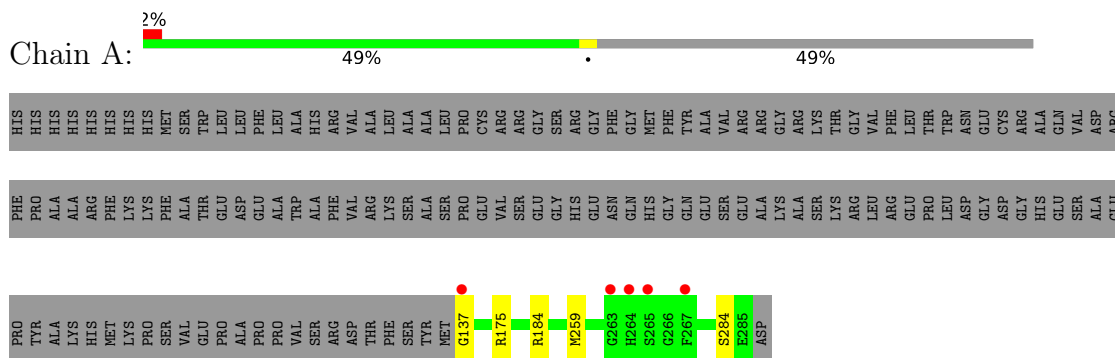
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	176	Total	O	0	0
			176	176		
7	B	82	Total	O	0	0
			82	82		
7	C	92	Total	O	0	0
			92	92		

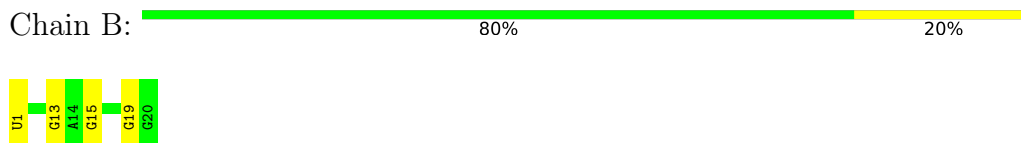
3 Residue-property plots

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.

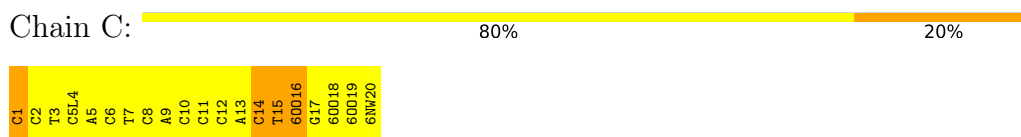
- Molecule 1: Ribonuclease H1



- Molecule 2: RNA (5'-R(*UP*GP*GP*CP*GP*AP*GP*UP*GP*GP*GP*UP*GP*AP*GP*UP*GP*AP*GP*G)-3')



● Molecule 3: RNA (5'-R*(OMC)P*(N7X)P*(T39)P*(C5L)P*(A2M))-D(P*(SC)P*(PST)P*(SC)P*(AS)P*(SC)P*(SC)P*(SC)P*(AS)P*(SC)P*(PST))-R(P*(6OO)P*(RFJ)P*(6OO)P*(6OO)P*(6NW))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.76Å 53.03Å 106.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.13 – 1.30 35.13 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.13-1.30) 99.8 (35.13-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.190 , 0.229 0.189 , 0.228	Depositor DCC
R_{free} test set	3320 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2513	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, GOL, PEG, 6OO, N7X, 6NW, AS, SO4, T39, SC, RFJ, C5L, A2M, PST

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	0.61	0/1301	0.76	2/1754 (0.1%)
2	B	1.16	0/493	1.71	7/771 (0.9%)
All	All	0.80	0/1794	1.14	9/2525 (0.4%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ARG	NE-CZ-NH1	8.08	124.34	120.30
2	B	15	G	N7-C8-N9	-7.78	109.21	113.10
2	B	13	G	C4-C5-N7	-7.53	107.79	110.80
2	B	1	U	N3-C4-O4	6.54	123.98	119.40
2	B	15	G	C8-N9-C4	6.42	108.97	106.40
1	A	259	MET	CG-SD-CE	6.04	109.87	100.20
2	B	19	G	N1-C6-O6	-5.50	116.60	119.90
2	B	13	G	C5-N7-C8	5.23	106.91	104.30
2	B	13	G	N9-C4-C5	5.12	107.45	105.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1274	0	1240	3	0
2	B	439	0	218	0	0
3	C	422	0	175	4	0
4	A	10	0	0	1	0
4	C	5	0	0	0	0
5	A	6	0	8	2	0
6	C	7	0	10	1	0
7	A	176	0	0	2	1
7	B	82	0	0	0	0
7	C	92	0	0	1	0
All	All	2513	0	1651	9	1

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 2.

All (9) 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)
3:C:15:PST:C1'	3:C:15:PST:O4'	1.64	1.13
1:A:284:SER:HA	5:A:303:GOL:H11	1.59	0.82
4:A:301:SO4:O1	7:A:401:HOH:O	2.05	0.73
1:A:137:GLY:O	7:A:402:HOH:O	2.19	0.51
6:C:201:PEG:H32	7:C:340:HOH:O	2.10	0.50
3:C:15:PST:H2''	3:C:16:6OO:C6	2.43	0.49
3:C:14:SC:H6	3:C:14:SC:H5'	1.97	0.46
3:C:1:OMC:CM2	3:C:1:OMC:O3'	2.65	0.44
1:A:175:ARG:HH12	5:A:303:GOL:H12	1.84	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:458:HOH:O	7:A:520:HOH:O[4_455]	2.08	0.12

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	159/294 (54%)	154 (97%)	5 (3%)	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	132/239 (55%)	132 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	19/20 (95%)	0	0
3	C	1/20 (5%)	0	0
All	All	20/40 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

20 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
3	SC	C	11	3,2	15,20,21	3.07	7 (46%)	17,28,31	1.41	2 (11%)
3	T39	C	3	3,2	18,26,27	1.66	3 (16%)	20,36,39	1.61	2 (10%)
3	C5L	C	4	3,2	18,26,27	1.42	3 (16%)	23,36,39	1.18	1 (4%)
3	SC	C	10	3,2	15,20,21	3.08	6 (40%)	17,28,31	1.20	2 (11%)
3	OMC	C	1	3,2	15,19,23	1.61	2 (13%)	17,27,34	2.32	4 (23%)
3	AS	C	13	3,2	18,23,24	2.97	7 (38%)	17,33,36	1.85	4 (23%)
3	SC	C	14	3,2	15,20,21	3.59	9 (60%)	17,28,31	1.95	4 (23%)
3	6NW	C	20	3,2	18,25,26	3.67	8 (44%)	18,36,39	1.50	2 (11%)
3	SC	C	6	3,2	15,20,21	2.79	7 (46%)	17,28,31	1.38	3 (17%)
3	PST	C	15	3,2	15,21,22	4.07	7 (46%)	16,30,33	2.07	2 (12%)
3	RFJ	C	17	3,2	18,26,27	4.37	8 (44%)	20,38,41	2.23	5 (25%)
3	6OO	C	18	3,2	15,22,23	4.41	9 (60%)	17,31,34	1.20	2 (11%)
3	6OO	C	16	3,2	15,22,23	4.73	8 (53%)	17,31,34	1.84	4 (23%)
3	A2M	C	5	3,2	18,25,26	1.15	2 (11%)	18,36,39	1.82	2 (11%)
3	PST	C	7	3,2	15,21,22	3.35	7 (46%)	16,30,33	2.31	2 (12%)
3	SC	C	12	3,2	15,20,21	2.71	8 (53%)	17,28,31	1.30	2 (11%)
3	6OO	C	19	3,2	15,22,23	4.22	8 (53%)	17,31,34	1.49	4 (23%)
3	N7X	C	2	3,2	18,26,27	3.64	8 (44%)	23,36,39	1.60	4 (17%)
3	AS	C	9	3,2	18,23,24	2.26	6 (33%)	17,33,36	1.29	2 (11%)
3	SC	C	8	3,2	15,20,21	2.67	8 (53%)	17,28,31	1.31	1 (5%)

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
3	SC	C	11	3,2	-	0/4/21/22	0/2/2/2
3	T39	C	3	3,2	-	2/10/30/31	0/2/2/2
3	C5L	C	4	3,2	-	0/10/30/31	0/2/2/2
3	SC	C	10	3,2	-	0/4/21/22	0/2/2/2
3	OMC	C	1	3,2	-	1/6/24/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AS	C	13	3,2	-	0/3/21/22	0/3/3/3
3	SC	C	14	3,2	-	0/4/21/22	0/2/2/2
3	6NW	C	20	3,2	-	0/4/27/28	0/3/3/3
3	SC	C	6	3,2	-	0/4/21/22	0/2/2/2
3	PST	C	15	3,2	-	0/4/21/22	0/2/2/2
3	RFJ	C	17	3,2	-	0/5/27/28	0/3/3/3
3	6OO	C	18	3,2	-	0/6/27/28	0/2/2/2
3	6OO	C	16	3,2	-	0/6/27/28	0/2/2/2
3	A2M	C	5	3,2	-	0/5/27/28	0/3/3/3
3	PST	C	7	3,2	-	0/4/21/22	0/2/2/2
3	SC	C	12	3,2	-	0/4/21/22	0/2/2/2
3	6OO	C	19	3,2	-	0/6/27/28	0/2/2/2
3	N7X	C	2	3,2	-	0/10/30/31	0/2/2/2
3	AS	C	9	3,2	-	0/3/21/22	0/3/3/3
3	SC	C	8	3,2	-	1/4/21/22	0/2/2/2

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	16	6OO	C3'-C2'	-12.19	1.25	1.52
3	C	20	6NW	C3'-C2'	-11.10	1.28	1.52
3	C	2	N7X	C3'-C2'	-11.02	1.28	1.52
3	C	18	6OO	C3'-C2'	-10.79	1.28	1.52
3	C	17	RFJ	C3'-C2'	-10.73	1.29	1.52
3	C	19	6OO	C3'-C2'	-10.73	1.29	1.52
3	C	15	PST	O4'-C1'	10.06	1.64	1.42
3	C	7	PST	O4'-C1'	8.29	1.60	1.42
3	C	17	RFJ	O4'-C1'	8.09	1.52	1.41
3	C	16	6OO	O4'-C1'	7.99	1.52	1.41
3	C	20	6NW	O4'-C1'	-7.95	1.30	1.41
3	C	14	SC	O4'-C1'	7.12	1.58	1.42
3	C	2	N7X	O4'-C1'	-6.89	1.31	1.41
3	C	17	RFJ	O4'-C4'	-6.75	1.29	1.45
3	C	18	6OO	O4'-C1'	6.73	1.50	1.41
3	C	19	6OO	O4'-C1'	6.72	1.50	1.41
3	C	15	PST	O4'-C4'	-6.71	1.30	1.45
3	C	14	SC	C3'-C4'	-6.51	1.35	1.53
3	C	18	6OO	O4'-C4'	-6.51	1.30	1.45
3	C	16	6OO	O4'-C4'	-6.43	1.30	1.45
3	C	11	SC	O4'-C1'	6.42	1.56	1.42
3	C	13	AS	O4'-C1'	6.41	1.56	1.42
3	C	15	PST	C2'-C1'	-6.33	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6	SC	O4'-C1'	6.32	1.56	1.42
3	C	12	SC	O4'-C4'	6.28	1.59	1.45
3	C	10	SC	O4'-C1'	6.22	1.56	1.42
3	C	19	6OO	O4'-C4'	-6.09	1.31	1.45
3	C	17	RFJ	O6-C6	5.86	1.39	1.24
3	C	13	AS	O4'-C4'	-5.85	1.31	1.45
3	C	8	SC	O4'-C1'	5.64	1.55	1.42
3	C	14	SC	C2'-C1'	-5.61	1.36	1.52
3	C	13	AS	C2'-C3'	-5.52	1.38	1.52
3	C	3	T39	O4-C4	5.44	1.38	1.24
3	C	10	SC	C2'-C1'	-5.37	1.37	1.52
3	C	17	RFJ	C2-N2	5.27	1.44	1.33
3	C	15	PST	C5M-C5	5.26	1.61	1.51
3	C	11	SC	C2'-C1'	-5.25	1.37	1.52
3	C	10	SC	C3'-C4'	-5.24	1.38	1.53
3	C	16	6OO	C3'-C4'	5.19	1.66	1.53
3	C	18	6OO	C3'-C4'	5.00	1.65	1.53
3	C	12	SC	C3'-C4'	-4.90	1.39	1.53
3	C	18	6OO	O2'-C2'	4.80	1.54	1.42
3	C	17	RFJ	C3'-C4'	4.80	1.65	1.53
3	C	8	SC	C2'-C1'	-4.77	1.39	1.52
3	C	7	PST	O4'-C4'	-4.74	1.34	1.45
3	C	19	6OO	C3'-C4'	4.73	1.65	1.53
3	C	6	SC	C2'-C1'	-4.55	1.39	1.52
3	C	7	PST	C5M-C5	4.54	1.59	1.51
3	C	7	PST	C2'-C1'	-4.48	1.39	1.52
3	C	9	AS	C3'-C4'	-4.45	1.40	1.53
3	C	16	6OO	O2'-C2'	4.29	1.53	1.42
3	C	11	SC	C3'-C4'	-4.29	1.41	1.53
3	C	19	6OO	O2'-C2'	4.27	1.53	1.42
3	C	9	AS	C2'-C1'	-4.15	1.40	1.52
3	C	19	6OO	C4-N4	4.13	1.47	1.35
3	C	1	OMC	C4-N4	4.11	1.47	1.35
3	C	6	SC	C3'-C4'	-4.07	1.41	1.53
3	C	4	C5L	C4-N4	4.00	1.44	1.34
3	C	2	N7X	C4-N4	3.97	1.44	1.34
3	C	12	SC	O4'-C1'	-3.95	1.33	1.42
3	C	1	OMC	C6-N1	-3.84	1.31	1.35
3	C	13	AS	C1'-N9	-3.83	1.38	1.49
3	C	11	SC	C2'-C3'	3.80	1.62	1.52
3	C	20	6NW	C5'-C4'	-3.76	1.39	1.51
3	C	14	SC	C2'-C3'	3.67	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	14	SC	O5'-C5'	-3.65	1.35	1.44
3	C	16	6OO	C4-N4	3.65	1.45	1.35
3	C	17	RFJ	O2'-C2'	3.62	1.51	1.42
3	C	10	SC	C2'-C3'	3.61	1.62	1.52
3	C	18	6OO	C4-N4	3.55	1.45	1.35
3	C	9	AS	O4'-C4'	3.54	1.52	1.45
3	C	8	SC	C2'-C3'	3.47	1.62	1.52
3	C	14	SC	O4'-C4'	3.46	1.52	1.45
3	C	10	SC	O4'-C4'	3.46	1.52	1.45
3	C	5	A2M	C6-N6	3.45	1.46	1.34
3	C	16	6OO	O3'-C3'	3.43	1.51	1.43
3	C	20	6NW	O4'-C4'	3.41	1.52	1.45
3	C	9	AS	C2'-C3'	3.38	1.61	1.52
3	C	2	N7X	O4'-C4'	3.33	1.52	1.45
3	C	14	SC	C2-N3	-3.31	1.31	1.38
3	C	17	RFJ	O3'-C3'	3.29	1.50	1.43
3	C	13	AS	C3'-C4'	3.29	1.62	1.53
3	C	6	SC	C2'-C3'	3.28	1.61	1.52
3	C	11	SC	C2-N3	-3.25	1.31	1.38
3	C	2	N7X	O2'-C2'	3.14	1.48	1.43
3	C	18	6OO	C6-N1	3.13	1.39	1.35
3	C	2	N7X	C5'-C4'	-3.12	1.41	1.51
3	C	11	SC	O4'-C4'	3.10	1.51	1.45
3	C	8	SC	C3'-C4'	-3.06	1.44	1.53
3	C	8	SC	C4-N4	3.02	1.44	1.35
3	C	14	SC	C4-N4	2.97	1.43	1.35
3	C	10	SC	C2-N3	-2.96	1.32	1.38
3	C	6	SC	C4-N4	2.87	1.43	1.35
3	C	20	6NW	C3'-C4'	2.84	1.60	1.53
3	C	13	AS	C6-N6	2.82	1.44	1.34
3	C	6	SC	C2-N3	-2.81	1.32	1.38
3	C	9	AS	O4'-C1'	2.78	1.48	1.42
3	C	11	SC	C4-N4	2.77	1.43	1.35
3	C	6	SC	O4'-C4'	2.75	1.51	1.45
3	C	7	PST	C3'-C4'	2.74	1.60	1.53
3	C	12	SC	C2-N3	-2.74	1.32	1.38
3	C	20	6NW	C6-N6	2.70	1.43	1.34
3	C	15	PST	O3'-C3'	-2.64	1.37	1.43
3	C	9	AS	C6-N6	2.62	1.43	1.34
3	C	18	6OO	O3'-C3'	2.59	1.49	1.43
3	C	7	PST	C4-N3	2.52	1.37	1.33
3	C	18	6OO	C2-N3	-2.51	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	16	6OO	C2-N3	-2.48	1.33	1.38
3	C	4	C5L	C7-C5	2.45	1.55	1.51
3	C	13	AS	O5'-C5'	-2.45	1.38	1.44
3	C	12	SC	C4-N4	2.39	1.42	1.35
3	C	8	SC	O3'-C3'	2.39	1.48	1.43
3	C	12	SC	C4-N3	-2.38	1.31	1.35
3	C	2	N7X	O3'-C3'	2.37	1.48	1.43
3	C	12	SC	C2'-C1'	2.33	1.58	1.52
3	C	19	6OO	C2-N3	-2.30	1.33	1.38
3	C	12	SC	O3'-C3'	2.28	1.48	1.43
3	C	15	PST	C3'-C4'	2.27	1.59	1.53
3	C	8	SC	C1'-N1	-2.25	1.42	1.49
3	C	19	6OO	O3'-C3'	2.24	1.48	1.43
3	C	3	T39	C7-C5	2.23	1.55	1.51
3	C	20	6NW	O2'-C2'	2.20	1.48	1.42
3	C	2	N7X	C7-C5	2.19	1.55	1.51
3	C	8	SC	O4'-C4'	2.13	1.49	1.45
3	C	7	PST	C5'-C4'	2.12	1.58	1.51
3	C	15	PST	C5'-C4'	2.12	1.58	1.51
3	C	20	6NW	O3'-C3'	2.10	1.47	1.43
3	C	14	SC	C4-N3	-2.09	1.32	1.35
3	C	5	A2M	O4'-C1'	2.02	1.43	1.41
3	C	4	C5L	C2-N3	-2.02	1.34	1.38
3	C	3	T39	C2-N3	-2.02	1.34	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	PST	C4-N3-C2	7.58	121.54	115.14
3	C	15	PST	C4-N3-C2	6.62	120.73	115.14
3	C	17	RFJ	C5-C6-N1	-6.06	115.14	123.43
3	C	5	A2M	N3-C2-N1	-5.99	119.31	128.68
3	C	1	OMC	C2-N3-C4	5.70	122.12	116.34
3	C	3	T39	C4-N3-C2	5.08	119.43	115.14
3	C	13	AS	N3-C2-N1	-4.90	121.01	128.68
3	C	17	RFJ	C6-N1-C2	4.69	123.38	115.93
3	C	1	OMC	N4-C4-N3	4.50	123.60	116.49
3	C	20	6NW	N3-C2-N1	-4.22	122.08	128.68
3	C	4	C5L	C5-C6-N1	-4.14	117.74	122.19
3	C	2	N7X	C5-C6-N1	-4.11	117.77	122.19
3	C	15	PST	C5-C6-N1	-4.05	117.83	122.19
3	C	16	6OO	C2-N3-C4	4.03	120.42	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	SC	O5'-C5'-C4'	-3.84	95.92	108.99
3	C	14	SC	C2-N3-C4	3.78	120.17	116.34
3	C	1	OMC	CM2-O2'-C2'	3.75	124.37	114.52
3	C	2	N7X	C2-N3-C4	3.73	120.53	116.02
3	C	1	OMC	C5-C4-N3	-3.70	117.45	121.72
3	C	13	AS	C2-N1-C6	3.68	125.05	118.75
3	C	3	T39	C5-C6-N1	-3.66	118.25	122.19
3	C	9	AS	N3-C2-N1	-3.53	123.15	128.68
3	C	10	SC	C2-N3-C4	3.51	119.90	116.34
3	C	16	6OO	O2'-C2'-C1'	-3.40	102.35	109.09
3	C	5	A2M	C2-N1-C6	3.29	124.39	118.75
3	C	16	6OO	N4-C4-N3	3.22	121.58	116.49
3	C	6	SC	C2-N3-C4	3.11	119.50	116.34
3	C	8	SC	C2-N3-C4	3.06	119.45	116.34
3	C	7	PST	C5-C6-N1	-3.04	118.92	122.19
3	C	2	N7X	O4'-C4'-C3'	-2.94	99.29	105.11
3	C	18	6OO	O2'-C2'-C1'	-2.84	103.47	109.09
3	C	2	N7X	O2'-C2'-C1'	-2.74	103.85	109.04
3	C	18	6OO	O3'-C3'-C2'	2.73	118.93	111.17
3	C	20	6NW	C2-N1-C6	2.70	123.37	118.75
3	C	17	RFJ	O5'-C5'-C4'	-2.48	100.57	108.99
3	C	16	6OO	O4'-C1'-C2'	-2.46	102.33	106.59
3	C	6	SC	N4-C4-N3	2.42	120.32	116.49
3	C	11	SC	C5-C6-N1	-2.34	115.46	120.68
3	C	17	RFJ	N2-C2-N3	-2.27	114.09	117.79
3	C	19	6OO	C5-C6-N1	-2.24	115.69	120.68
3	C	10	SC	C4'-O4'-C1'	-2.20	104.13	109.45
3	C	17	RFJ	N2-C2-N1	2.18	120.65	117.25
3	C	13	AS	O4'-C1'-C2'	-2.17	102.14	106.25
3	C	14	SC	O3'-C3'-C4'	-2.17	101.81	110.10
3	C	12	SC	O4'-C4'-C3'	-2.12	100.73	105.67
3	C	13	AS	C5-C6-N1	-2.10	115.59	120.35
3	C	12	SC	C5-C4-N4	-2.07	117.54	121.14
3	C	14	SC	C5-C4-N3	-2.07	119.33	121.72
3	C	19	6OO	O4'-C1'-C2'	-2.07	103.00	106.59
3	C	19	6OO	C2-N3-C4	2.06	118.43	116.34
3	C	11	SC	C5-C4-N4	-2.06	117.56	121.14
3	C	6	SC	C6-N1-C2	-2.05	117.95	121.20
3	C	9	AS	C4'-O4'-C1'	-2.02	104.58	109.45
3	C	19	6OO	O3'-C3'-C4'	-2.01	105.25	111.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	OMC	C3'-C2'-O2'-CM2
3	C	8	SC	O4'-C1'-N1-C6
3	C	3	T39	O2'-CA'-CB'-OC'
3	C	3	T39	CA'-CB'-OC'-CD'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	OMC	1	0
3	C	14	SC	1	0
3	C	15	PST	2	0
3	C	16	6OO	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands 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	$\# Z > 2$
4	SO4	C	202	-	4,4,4	0.12	0	6,6,6	0.51	0
4	SO4	A	301	-	4,4,4	0.12	0	6,6,6	0.23	0
4	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.37	0
5	GOL	A	303	-	5,5,5	0.87	0	5,5,5	1.06	0
6	PEG	C	201	-	6,6,6	0.77	0	5,5,5	1.90	1 (20%)

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	303	-	-	2/4/4/4	-
6	PEG	C	201	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	201	PEG	O2-C3-C4	-3.50	94.70	110.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	GOL	C1-C2-C3-O3
5	A	303	GOL	O2-C2-C3-O3
6	C	201	PEG	O2-C3-C4-O4
6	C	201	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	SO4	1	0
5	A	303	GOL	2	0
6	C	201	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	149/294 (50%)	-0.07	5 (3%) 45 42	12, 18, 35, 72	1 (0%)
2	B	20/20 (100%)	-0.45	0 100 100	14, 23, 32, 33	0
3	C	0/20	-	-	-	-
All	All	169/334 (50%)	-0.11	5 (2%) 50 48	12, 19, 35, 72	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	HIS	6.2
1	A	265	SER	5.4
1	A	137	GLY	5.1
1	A	263	GLY	3.5
1	A	267	PHE	3.0

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
3	OMC	C	1	18/22	0.79	0.14	25,34,40,42	0
3	N7X	C	2	25/26	0.92	0.09	20,27,37,47	0
3	PST	C	15	20/21	0.94	0.07	21,26,31,34	0
3	RFJ	C	17	24/25	0.94	0.07	19,22,25,25	0
3	6OO	C	16	21/22	0.94	0.07	22,25,33,33	0
3	SC	C	14	19/20	0.94	0.09	18,24,31,37	0
3	SC	C	6	19/20	0.95	0.08	13,15,22,24	0
3	T39	C	3	25/26	0.96	0.07	18,23,32,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A2M	C	5	23/24	0.96	0.07	13,18,24,30	0
3	6OO	C	18	21/22	0.96	0.05	17,20,23,24	0
3	C5L	C	4	25/26	0.97	0.07	16,20,28,48	0
3	6NW	C	20	23/24	0.97	0.07	19,25,40,43	0
3	SC	C	12	19/20	0.97	0.06	13,15,19,21	0
3	6OO	C	19	21/22	0.97	0.06	17,19,21,23	0
3	AS	C	13	21/22	0.97	0.06	15,18,20,23	0
3	SC	C	8	19/20	0.97	0.06	11,13,18,19	0
3	SC	C	10	19/20	0.98	0.08	13,15,16,17	0
3	PST	C	7	20/21	0.98	0.04	13,14,17,19	0
3	AS	C	9	21/22	0.98	0.05	12,14,15,16	0
3	SC	C	11	19/20	0.98	0.07	13,15,19,19	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
5	GOL	A	303	6/6	0.82	0.10	40,46,47,53	0
6	PEG	C	201	7/7	0.88	0.12	22,27,36,39	0
4	SO4	C	202	5/5	0.95	0.21	34,34,44,57	0
4	SO4	A	302	5/5	0.95	0.22	38,44,54,61	0
4	SO4	A	301	5/5	0.98	0.10	25,37,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.