



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2024 – 02:07 PM EDT

PDB ID : 8SWB  
Title : RNase H complex with streopure ASO and RNA  
Authors : Cho, Y.-J.; Iwamoto, N.  
Deposited on : 2023-05-18  
Resolution : 2.00 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

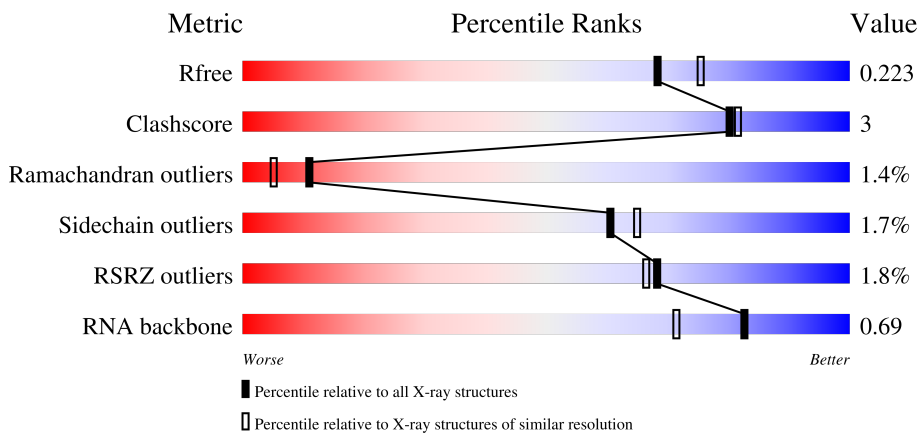
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)
RNA backbone	3102	1079 (2.50-1.50)

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  $\geq 3$ , 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	149	
2	B	20	
3	D	20	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2226 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
			Total	C	N	O	S			
1	A	149	1237	767	239	225	6	0	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ASN	ASP	conflict	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
			Total	C	N	O	P			
2	B	20	439	195	86	139	19	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
3	D	20	422	206	67	115	19	15	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

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



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

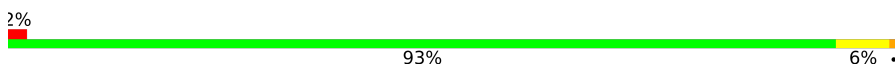
- Molecule 7 is water.

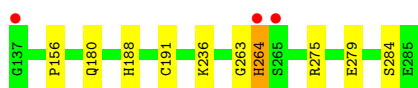
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	53	Total O 53 53	0	0
7	B	29	Total O 29 29	0	0
7	D	28	Total O 28 28	0	0

### 3 Residue-property plots [i](#)


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

Chain A: 




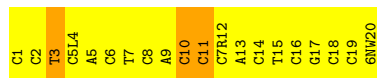
- Molecule 2: RNA (5'-R(\*UP\*GP\*GP\*CP\*GP\*AP\*GP\*UP\*GP\*GP\*GP\*UP\*GP\*AP\*GP\*UP\*GP\*AP\*GP\*G)-3')

Chain B: 



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

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.55Å 52.94Å 106.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.62 – 2.00 47.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.62-2.00) 99.7 (47.36-2.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.184 , 0.224 0.182 , 0.223	Depositor DCC
$R_{free}$ test set	916 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtrriage
Anisotropy	0.396	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OKQ, AS, N7X, PO4, C5L, C7R, T39, RFJ, 6NW, SC, OMC, PST, PEG, GOL, A2M

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	0.33	0/1264	0.54	0/1706
2	B	0.47	0/493	0.93	0/771
3	D	0.96	0/23	1.38	1/33 (3.0%)
All	All	0.39	0/1780	0.70	1/2510 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	9	DA	O4'-C1'-N9	6.21	112.35	108.00

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	1237	0	1201	5	0
2	B	439	0	218	1	0
3	D	422	0	163	3	0
4	A	6	0	8	0	0
5	A	5	0	0	0	0
6	D	7	0	10	1	0
7	A	53	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	29	0	0	0	0
7	D	28	0	0	0	0
All	All	2226	0	1600	9	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 3.

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:D:10:SC:HN42	6:D:201:PEG:H11	1.71	0.55
1:A:264:HIS:O	1:A:264:HIS:ND1	2.40	0.54
1:A:275:ARG:O	1:A:279:GLU:HG3	2.09	0.53
2:B:12:U:H2'	2:B:13:G:O4'	2.14	0.47
1:A:156:PRO:HG2	1:A:180:GLN:HB2	1.97	0.47
1:A:264:HIS:O	1:A:264:HIS:CG	2.68	0.46
3:D:3:T39:HCA1	3:D:3:T39:H1'	1.68	0.45
3:D:10:SC:H2'	3:D:11:SC:H6	2.00	0.43
1:A:188[B]:HIS:HA	1:A:191:CYS:HB2	2.01	0.43

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	155/149 (104%)	146 (94%)	7 (4%)	2 (1%)	<b>12</b> <b>6</b>

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	GLY

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Mol	Chain	Res	Type
1	A	264	HIS

### 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	128/120 (107%)	126 (98%)	2 (2%)	62 67

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

Mol	Chain	Res	Type
1	A	236	LYS
1	A	284	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	19/20 (95%)	2 (10%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	13	G
2	B	19	G

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

19 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	D	14	3,2	17,20,21	2.52	5 (29%)	24,28,31	1.70	5 (20%)
3	C7R	D	12	3,2	17,20,21	0.66	1 (5%)	24,28,31	0.87	0
3	RFJ	D	17	3,2	18,26,27	2.87	6 (33%)	19,38,41	1.45	3 (15%)
3	6NW	D	20	3,2	18,25,26	1.27	2 (11%)	18,36,39	1.82	2 (11%)
3	OMC	D	1	3,2	19,19,23	1.55	3 (15%)	26,27,34	1.13	2 (7%)
3	SC	D	10	3,2	17,20,21	2.22	6 (35%)	24,28,31	1.45	4 (16%)
3	SC	D	8	3,2	17,20,21	2.61	5 (29%)	24,28,31	1.31	3 (12%)
3	OKQ	D	19	3,2	19,22,23	2.31	7 (36%)	26,31,34	1.50	3 (11%)
3	AS	D	13	3,2	18,23,24	1.33	2 (11%)	17,33,36	1.27	2 (11%)
3	PST	D	15	3,2,1	18,21,22	2.42	7 (38%)	26,30,33	1.92	4 (15%)
3	T39	D	3	3,2	23,26,27	1.56	4 (17%)	32,36,39	2.04	4 (12%)
3	N7X	D	2	3,2	22,26,27	1.62	6 (27%)	30,36,39	1.71	4 (13%)
3	SC	D	11	3,2	17,20,21	2.51	4 (23%)	24,28,31	1.51	6 (25%)
3	C5L	D	4	3,2	22,26,27	0.99	2 (9%)	30,36,39	3.57	4 (13%)
3	PST	D	7	3,2	18,21,22	2.25	8 (44%)	26,30,33	1.88	4 (15%)
3	OKQ	D	18	3,2	19,22,23	2.40	7 (36%)	26,31,34	1.55	6 (23%)
3	SC	D	6	3,2	17,20,21	2.66	5 (29%)	24,28,31	1.35	5 (20%)
3	A2M	D	5	3,2	18,25,26	2.01	3 (16%)	18,36,39	2.64	7 (38%)
3	OKQ	D	16	3,2	19,22,23	2.31	6 (31%)	26,31,34	1.53	4 (15%)

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	D	14	3,2	-	0/7/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C7R	D	12	3,2	-	1/6/21/22	0/2/2/2
3	RFJ	D	17	3,2	-	2/5/27/28	0/3/3/3
3	6NW	D	20	3,2	-	0/4/27/28	0/3/3/3
3	OMC	D	1	3,2	-	1/8/24/28	0/2/2/2
3	SC	D	10	3,2	-	0/7/21/22	0/2/2/2
3	SC	D	8	3,2	-	0/7/21/22	0/2/2/2
3	OKQ	D	19	3,2	-	0/8/27/28	0/2/2/2
3	AS	D	13	3,2	-	0/3/21/22	0/3/3/3
3	PST	D	15	3,2,1	-	0/7/21/22	0/2/2/2
3	T39	D	3	3,2	-	3/12/30/31	0/2/2/2
3	N7X	D	2	3,2	-	2/12/30/31	0/2/2/2
3	SC	D	11	3,2	-	0/7/21/22	0/2/2/2
3	C5L	D	4	3,2	-	2/12/30/31	0/2/2/2
3	PST	D	7	3,2	-	0/7/21/22	0/2/2/2
3	OKQ	D	18	3,2	-	0/8/27/28	0/2/2/2
3	SC	D	6	3,2	-	0/7/21/22	0/2/2/2
3	A2M	D	5	3,2	-	1/5/27/28	0/3/3/3
3	OKQ	D	16	3,2	-	1/8/27/28	0/2/2/2

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	17	RFJ	O6-C6	8.23	1.40	1.23
3	D	6	SC	C2-N3	7.19	1.50	1.36
3	D	11	SC	C2-N3	6.99	1.50	1.36
3	D	8	SC	C4-N4	6.40	1.49	1.33
3	D	14	SC	C2-N3	6.31	1.49	1.36
3	D	5	A2M	O5'-C5'	-6.31	1.29	1.44
3	D	8	SC	C2-N3	6.26	1.49	1.36
3	D	14	SC	C4-N4	6.21	1.48	1.33
3	D	11	SC	C4-N4	5.92	1.47	1.33
3	D	6	SC	C4-N4	5.89	1.47	1.33
3	D	15	PST	C1'-N1	5.60	1.62	1.48
3	D	10	SC	C4-N4	5.27	1.46	1.33
3	D	18	OKQ	C4-N4	5.24	1.46	1.33
3	D	19	OKQ	C4-N4	5.16	1.46	1.33
3	D	7	PST	C1'-N1	4.93	1.60	1.48
3	D	16	OKQ	C4-N4	4.77	1.45	1.33
3	D	19	OKQ	C1'-N1	4.66	1.61	1.47
3	D	18	OKQ	O3'-C3'	4.61	1.53	1.43
3	D	17	RFJ	C2-N2	4.56	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	16	OKQ	O3'-C3'	4.44	1.53	1.43
3	D	2	N7X	O5'-C5'	-4.38	1.34	1.44
3	D	16	OKQ	C2-N3	4.30	1.45	1.36
3	D	16	OKQ	C1'-N1	4.30	1.60	1.47
3	D	10	SC	C2-N3	4.24	1.44	1.36
3	D	17	RFJ	O4'-C1'	4.22	1.47	1.41
3	D	18	OKQ	C1'-N1	4.18	1.59	1.47
3	D	19	OKQ	C2-N3	4.10	1.44	1.36
3	D	15	PST	C6-N1	4.01	1.44	1.38
3	D	17	RFJ	C8-N7	3.96	1.41	1.35
3	D	18	OKQ	C2-N3	3.95	1.44	1.36
3	D	7	PST	C2-N3	3.91	1.44	1.38
3	D	15	PST	C2-N3	3.85	1.44	1.38
3	D	3	T39	C2-N3	3.81	1.44	1.38
3	D	6	SC	C5-C4	3.74	1.51	1.42
3	D	3	T39	C4-C5	3.65	1.50	1.44
3	D	10	SC	C5-C4	3.62	1.51	1.42
3	D	19	OKQ	O3'-C3'	3.47	1.51	1.43
3	D	7	PST	C4-N3	3.43	1.45	1.38
3	D	8	SC	C5-C4	3.31	1.50	1.42
3	D	18	OKQ	C2-N1	3.30	1.47	1.40
3	D	1	OMC	C2-N3	3.28	1.43	1.36
3	D	15	PST	C4-N3	3.27	1.44	1.38
3	D	7	PST	C4-C5	3.25	1.50	1.44
3	D	1	OMC	C2-N1	3.25	1.47	1.40
3	D	10	SC	C6-C5	3.25	1.42	1.35
3	D	3	T39	C2-N1	3.18	1.43	1.38
3	D	14	SC	C5-C4	3.14	1.50	1.42
3	D	3	T39	O4-C4	-3.09	1.17	1.23
3	D	11	SC	C5-C4	3.03	1.49	1.42
3	D	15	PST	C6-C5	3.02	1.39	1.34
3	D	14	SC	C6-C5	2.99	1.42	1.35
3	D	16	OKQ	C2-N1	2.89	1.46	1.40
3	D	4	C5L	C6-C5	2.86	1.39	1.34
3	D	19	OKQ	C2-N1	2.82	1.46	1.40
3	D	17	RFJ	C5-C4	2.75	1.50	1.43
3	D	2	N7X	C6-C5	2.74	1.39	1.34
3	D	7	PST	C6-N1	2.67	1.42	1.38
3	D	15	PST	C4-C5	2.65	1.49	1.44
3	D	7	PST	C5M-C5	2.63	1.57	1.50
3	D	15	PST	C5M-C5	2.59	1.57	1.50
3	D	12	C7R	C2-N3	2.59	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	19	OKQ	C6-C5	2.54	1.40	1.35
3	D	18	OKQ	C6-C5	2.50	1.40	1.35
3	D	5	A2M	C2-N1	2.46	1.38	1.33
3	D	2	N7X	C1'-N1	2.44	1.54	1.47
3	D	1	OMC	C4-N4	2.43	1.39	1.33
3	D	5	A2M	C2-N3	2.42	1.36	1.32
3	D	11	SC	C6-C5	2.42	1.40	1.35
3	D	16	OKQ	C6-C5	2.39	1.40	1.35
3	D	13	AS	O4'-C1'	-2.38	1.37	1.42
3	D	20	6NW	C2-N3	2.37	1.35	1.32
3	D	8	SC	C6-C5	2.34	1.40	1.35
3	D	14	SC	C6-N1	2.22	1.43	1.38
3	D	6	SC	C6-C5	2.22	1.40	1.35
3	D	18	OKQ	C5-C4	2.19	1.47	1.42
3	D	4	C5L	C2-N3	2.19	1.40	1.36
3	D	6	SC	C6-N1	2.18	1.43	1.38
3	D	2	N7X	C2'-C1'	2.18	1.58	1.53
3	D	10	SC	C2-N1	2.17	1.44	1.40
3	D	8	SC	C6-N1	2.17	1.43	1.38
3	D	19	OKQ	C5-C4	2.16	1.47	1.42
3	D	10	SC	C6-N1	2.10	1.43	1.38
3	D	7	PST	C6-C5	2.08	1.38	1.34
3	D	7	PST	O4'-C1'	-2.08	1.37	1.42
3	D	13	AS	C5'-C4'	2.08	1.58	1.51
3	D	2	N7X	C4-N4	2.06	1.39	1.34
3	D	20	6NW	C2-N1	2.04	1.37	1.33
3	D	2	N7X	C2-N3	2.02	1.40	1.36
3	D	17	RFJ	C4-N3	2.02	1.42	1.37

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	C5L	CA'-O2'-C2'	16.34	153.30	114.32
3	D	4	C5L	O2'-C2'-C3'	8.58	132.30	110.94
3	D	3	T39	C7-C5-C4	-7.13	110.92	118.77
3	D	5	A2M	CM'-O2'-C2'	7.02	132.94	114.52
3	D	20	6NW	CM'-O2'-C2'	6.14	130.63	114.52
3	D	7	PST	C4-N3-C2	-5.88	119.74	127.35
3	D	3	T39	C5-C4-N3	-5.70	110.44	115.31
3	D	15	PST	C4-N3-C2	-5.41	120.35	127.35
3	D	2	N7X	C12-O12-C1	5.16	145.03	112.96
3	D	15	PST	C5-C4-N3	5.09	119.66	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	T39	C6-C5-C4	5.07	122.27	118.03
3	D	7	PST	C5-C4-N3	4.80	119.41	115.31
3	D	5	A2M	O2'-C2'-C1'	4.64	118.29	109.09
3	D	14	SC	O4'-C1'-N1	4.45	115.81	107.86
3	D	2	N7X	C6-N1-C2	-4.20	115.06	120.87
3	D	5	A2M	O4'-C1'-C2'	-4.19	99.31	106.59
3	D	10	SC	C4-N3-C2	3.79	126.38	120.25
3	D	14	SC	C4-N3-C2	3.69	126.22	120.25
3	D	19	OKQ	C1'-N1-C6	3.44	128.33	120.84
3	D	5	A2M	C5-C6-N6	3.42	125.55	120.35
3	D	7	PST	N3-C2-N1	3.32	119.29	114.89
3	D	18	OKQ	C1'-N1-C6	3.31	128.06	120.84
3	D	15	PST	N3-C2-N1	3.28	119.25	114.89
3	D	8	SC	C4-N3-C2	3.21	125.44	120.25
3	D	11	SC	C4-N3-C2	3.20	125.42	120.25
3	D	6	SC	O4'-C1'-N1	3.11	113.43	107.86
3	D	10	SC	O4'-C1'-N1	3.11	113.42	107.86
3	D	17	RFJ	C5-C6-N1	3.05	119.34	113.95
3	D	13	AS	C5-C6-N6	3.00	124.91	120.35
3	D	16	OKQ	C2'-C1'-N1	2.99	120.03	114.22
3	D	3	T39	C7-C5-C6	2.97	126.81	122.85
3	D	19	OKQ	C2'-C1'-N1	2.93	119.92	114.22
3	D	14	SC	C1'-N1-C6	2.89	127.26	121.55
3	D	20	6NW	C5-C6-N6	2.86	124.70	120.35
3	D	17	RFJ	C2-N1-C6	-2.80	119.94	125.10
3	D	18	OKQ	O3'-C3'-C4'	2.76	119.03	111.05
3	D	5	A2M	O4'-C4'-C5'	2.76	118.45	109.37
3	D	4	C5L	O2'-CA'-CB'	-2.75	100.19	109.72
3	D	11	SC	C5-C4-N3	-2.73	116.68	121.33
3	D	6	SC	C4-N3-C2	2.73	124.66	120.25
3	D	16	OKQ	C1'-N1-C6	2.73	126.78	120.84
3	D	2	N7X	C3'-C2'-C1'	-2.69	97.84	102.89
3	D	1	OMC	C6-N1-C2	-2.62	115.95	120.49
3	D	15	PST	O4'-C4'-C3'	-2.61	99.59	105.67
3	D	16	OKQ	O4'-C1'-N1	-2.59	102.44	108.36
3	D	18	OKQ	C2'-C1'-N1	2.59	119.25	114.22
3	D	11	SC	C1'-N1-C6	2.58	126.65	121.55
3	D	4	C5L	O2'-C2'-C1'	-2.54	104.28	109.02
3	D	16	OKQ	O2'-C2'-C1'	2.53	114.02	109.08
3	D	14	SC	C1'-N1-C2	-2.52	113.31	117.74
3	D	17	RFJ	C8-N7-C5	2.50	107.75	102.99
3	D	13	AS	C2'-C1'-N9	2.49	120.01	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	SC	C1'-N1-C6	2.45	126.39	121.55
3	D	11	SC	C1'-N1-C2	-2.44	113.45	117.74
3	D	14	SC	C5-C4-N3	-2.44	117.17	121.33
3	D	8	SC	N4-C4-N3	2.39	122.17	117.97
3	D	6	SC	C5-C4-N3	-2.37	117.30	121.33
3	D	10	SC	C1'-N1-C2	-2.36	113.59	117.74
3	D	5	A2M	C2'-C3'-C4'	-2.32	96.96	101.99
3	D	5	A2M	C3'-C2'-C1'	-2.30	98.56	102.89
3	D	8	SC	C5-C4-N3	-2.29	117.43	121.33
3	D	2	N7X	C1'-N1-C6	2.29	124.93	121.12
3	D	6	SC	N4-C4-N3	2.28	121.97	117.97
3	D	11	SC	O4'-C1'-N1	2.21	111.82	107.86
3	D	18	OKQ	O4'-C4'-C3'	-2.20	100.76	105.11
3	D	11	SC	N4-C4-N3	2.15	121.74	117.97
3	D	7	PST	O2-C2-N3	-2.13	117.54	121.50
3	D	18	OKQ	C4-N3-C2	2.09	123.64	120.25
3	D	1	OMC	C4'-O4'-C1'	2.09	114.09	109.47
3	D	18	OKQ	O2'-C2'-C1'	2.09	113.15	109.08
3	D	6	SC	C1'-N1-C6	2.07	125.63	121.55
3	D	19	OKQ	C4-N3-C2	2.06	123.58	120.25

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	T39	C1'-C2'-O2'-CA'
3	D	1	OMC	O4'-C4'-C5'-O5'
3	D	17	RFJ	C3'-C4'-C5'-O5'
3	D	4	C5L	O2'-CA'-CB'-OC'
3	D	2	N7X	O2'-C-C1-O12
3	D	2	N7X	C-C1-O12-C12
3	D	4	C5L	CA'-CB'-OC'-CD'
3	D	5	A2M	C3'-C2'-O2'-CM'
3	D	3	T39	O2'-CA'-CB'-OC'
3	D	12	C7R	C3'-C4'-C5'-O5'
3	D	16	OKQ	O4'-C4'-C5'-O5'
3	D	17	RFJ	O4'-C4'-C5'-O5'
3	D	3	T39	CA'-CB'-OC'-CD'

There are no ring outliers.

3 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	10	SC	2	0
3	D	3	T39	1	0
3	D	11	SC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	GOL	A	301	-	5,5,5	1.08	0	5,5,5	0.84	0
6	PEG	D	201	-	6,6,6	0.08	0	5,5,5	0.15	0
5	PO4	A	302	-	4,4,4	0.86	0	6,6,6	0.41	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
4	GOL	A	301	-	-	2/4/4/4	-
6	PEG	D	201	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	201	PEG	O2-C3-C4-O4
4	A	301	GOL	O1-C1-C2-C3
6	D	201	PEG	O1-C1-C2-O2
4	A	301	GOL	O1-C1-C2-O2
6	D	201	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	149/149 (100%)	0.04	3 (2%) 65 63	25, 38, 65, 118	0
2	B	20/20 (100%)	-0.98	0 100 100	30, 45, 53, 54	0
3	D	1/20 (5%)	-0.44	0 100 100	32, 32, 32, 32	0
All	All	170/189 (89%)	-0.08	3 (1%) 68 66	25, 39, 62, 118	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	GLY	5.5
1	A	264	HIS	4.4
1	A	265	SER	2.5

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	OMC	D	1	18/22	0.88	0.15	41,50,56,64	0
3	N7X	D	2	25/26	0.94	0.11	40,49,55,75	0
3	RFJ	D	17	24/25	0.94	0.11	31,44,52,54	0
3	C5L	D	4	25/26	0.95	0.13	36,47,59,77	0
3	6NW	D	20	23/24	0.95	0.12	33,47,59,62	0
3	OKQ	D	16	21/22	0.96	0.10	37,42,53,62	0
3	T39	D	3	25/26	0.96	0.13	35,43,54,60	0
3	OKQ	D	19	21/22	0.96	0.11	29,37,43,50	0
3	PST	D	15	20/21	0.96	0.10	36,44,54,56	0
3	AS	D	13	21/22	0.97	0.11	28,36,40,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SC	D	14	19/20	0.97	0.10	33,40,52,53	0
3	A2M	D	5	23/24	0.97	0.10	28,34,49,50	0
3	SC	D	6	19/20	0.97	0.10	22,32,44,49	0
3	PST	D	7	20/21	0.97	0.10	27,31,37,39	0
3	OKQ	D	18	21/22	0.97	0.10	27,39,42,45	0
3	SC	D	11	19/20	0.97	0.11	31,35,39,43	0
3	C7R	D	12	19/20	0.97	0.12	27,33,40,54	0
3	SC	D	8	19/20	0.98	0.10	18,28,36,39	0
3	SC	D	10	19/20	0.98	0.11	26,29,36,39	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	301	6/6	0.75	0.20	55,62,73,75	0
6	PEG	D	201	7/7	0.93	0.13	48,55,57,62	0
5	PO4	A	302	5/5	0.97	0.07	53,56,58,62	0

### 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.