W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 09:48 am GMT

PDB ID	:	3AGV
Title	:	Crystal structure of a human IgG-aptamer complex
Authors	:	Nomura, Y.; Sugiyama, S.; Sakamoto, T.; Miyakawa, S.; Adachi, H.; Takano, K.; Murakami, S.; Inoue, T.; Mori, Y.; Nakamura, Y.; Matsumura, H.
Deposited on	:	2010-04-08
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

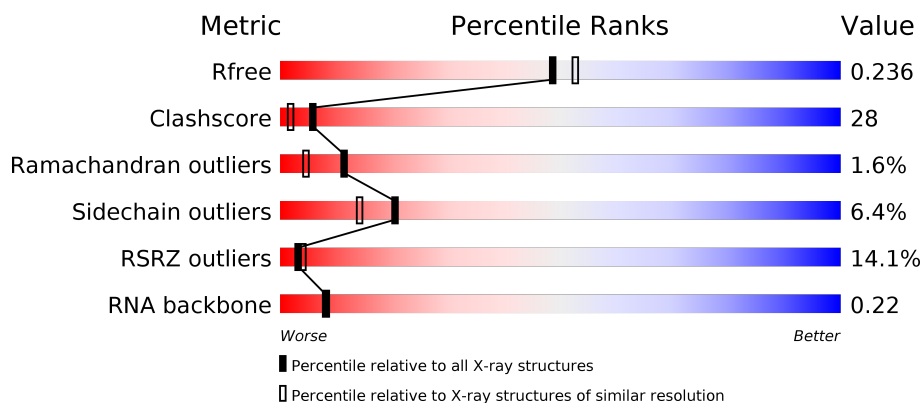|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		28
Ramachandran outliers		1.6%
Sidechain outliers		6.4%
RSRZ outliers		14.1%
RNA backbone		0.22

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)
RNA backbone	2435	1001 (2.70-1.62)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	211	15% / 46% 31% 7% 16%
1	B	211	10% / 72% 24% ··
2	S	24	4% / 13% 54% 8% · 21%
2	U	24	13% / 21% 58% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLA	A	7	-	-	-	X
4	NDG	B	2	-	-	X	-
4	GAL	B	7	-	-	X	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4413 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total 1433	C 916	N 240	O 271	S 6	0	0	0
1	B	208	Total 1664	C 1059	N 280	O 319	S 6	0	0	0

- Molecule 2 is a RNA chain called 5'-R(*GP*GP*AP*GP*GP*(UFT)P*GP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*GP*AP*AP*A*GP*GP*AP*AP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*A)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	S	19	Total 401	C 181	F 9	N 74	O 120	P 17	0	0	0
2	U	24	Total 515	C 231	F 9	N 99	O 153	P 23	0	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total 48	C 26	N 1	O 21	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	8	Total 97	C 54	N 3	O 40	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	S	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	U	1	Total 1	Ca 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	88	Total 88	O 88	0	0
6	B	126	Total 126	O 126	0	0
6	S	14	Total 14	O 14	0	0
6	U	25	Total 25	O 25	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
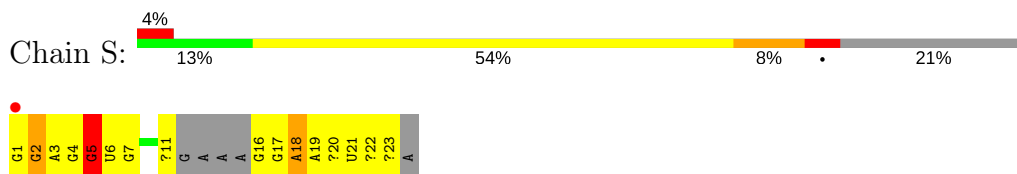
- Molecule 1: Ig gamma-1 chain C region
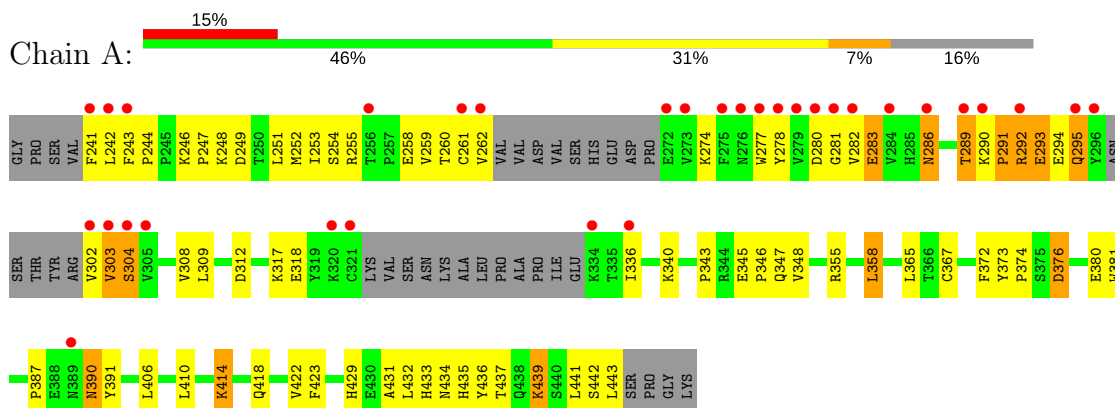
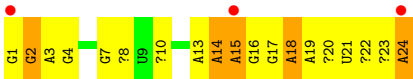- Molecule 1: Ig gamma-1 chain C region
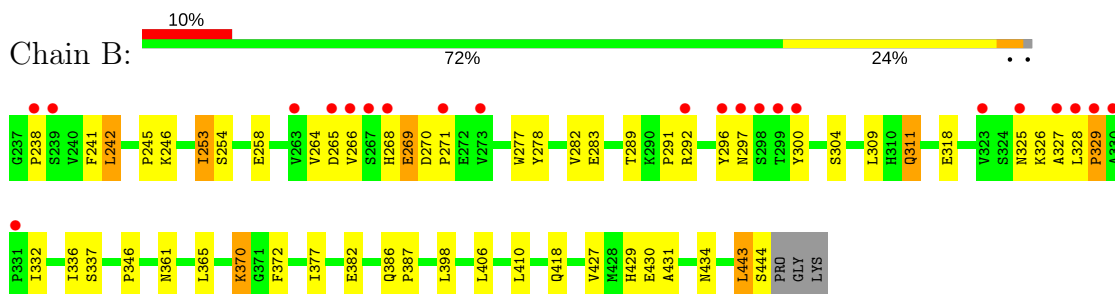
- Molecule 2: 5'-R(*GP*GP*AP*GP*GP*(UFT)P*GP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*GP *AP*AP*A*GP*GP*AP*AP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*A)-3'

- Molecule 2: 5'-R(*GP*GP*AP*GP*GP*(UFT)P*GP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*GP *AP*AP*A*GP*GP*AP*AP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*A)-3'

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.59Å 107.24Å 79.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.37 – 2.15 65.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.1 (30.37-2.15) 97.2 (65.93-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.70 (at 2.14Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.277 0.239 , 0.236	Depositor DCC
R_{free} test set	1940 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4413	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, GLA, CA, NDG, GAL, CFZ, FUL, UFT, MAN

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	0.35	0/1470	0.59	0/1995
1	B	0.36	0/1710	0.59	0/2330
2	S	0.28	0/249	0.68	1/388 (0.3%)
2	U	0.24	0/377	0.73	0/585
All	All	0.34	0/3806	0.61	1/5298 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	5	G	C2'-C3'-O3'	5.50	122.50	113.70

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	1433	0	1401	80	0
1	B	1664	0	1631	54	0
2	S	401	0	201	27	2
2	U	515	0	254	44	2
3	A	48	0	42	7	0
4	B	97	0	84	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1	0	0	0	0
5	U	1	0	0	0	0
6	A	88	0	0	6	0
6	B	126	0	0	8	0
6	S	14	0	0	0	0
6	U	25	0	0	2	0
All	All	4413	0	3613	217	2

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 28.

All (217) 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:S:22:CFZ:H2'	2:S:23:CFZ:H5'	1.26	1.17
1:B:270:ASP:HB2	1:B:326:LYS:HE2	1.37	1.06
1:A:260:THR:HG22	1:A:262:VAL:HG23	1.46	0.96
1:B:311:GLN:HE21	1:B:311:GLN:H	1.18	0.90
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.51	0.89
1:A:347:GLN:HG3	6:A:101:HOH:O	1.74	0.87
2:S:22:CFZ:C2'	2:S:23:CFZ:H5'	2.05	0.86
1:A:303:VAL:HG12	1:A:304:SER:H	1.41	0.85
1:A:260:THR:CG2	1:A:262:VAL:HG23	2.06	0.84
2:S:17:G:H2'	2:S:18:A:H5"	1.61	0.83
1:B:246:LYS:HD3	4:B:7:GAL:H5	1.59	0.81
3:A:4:MAN:O4	3:A:5:MAN:H5	1.80	0.81
4:B:2:NDG:H6C1	4:B:3:NAG:H82	1.61	0.81
2:S:2:G:H5'	2:S:3:A:OP2	1.81	0.80
2:U:2:G:H2'	2:U:3:A:H8	1.46	0.79
2:S:17:G:C2'	2:S:18:A:H5"	2.14	0.77
1:B:418:GLN:HA	1:B:443:LEU:HD12	1.68	0.75
1:B:238:PRO:HG3	1:B:266:VAL:HA	1.68	0.74
1:A:248:LYS:HD3	1:A:252:MET:HE3	1.70	0.74
1:B:398:LEU:HA	6:B:186:HOH:O	1.88	0.72
2:U:15:A:H2'	2:U:16:G:H5'	1.72	0.71
1:B:328:LEU:HD21	1:B:332:ILE:HG13	1.72	0.71
4:B:6:NAG:H4	4:B:7:GAL:O2	1.90	0.71
1:A:258:GLU:O	3:A:7:GLA:H62	1.92	0.70
1:B:429:HIS:CD2	1:B:431:ALA:H	2.09	0.70
1:A:309:LEU:HB2	1:A:312:ASP:OD2	1.92	0.69
1:B:297:ASN:ND2	4:B:2:NDG:H1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLN:NE2	1:B:311:GLN:H	1.88	0.69
4:B:7:GAL:H62	6:B:157:HOH:O	1.91	0.69
1:B:398:LEU:HD12	6:B:186:HOH:O	1.92	0.68
1:B:265:ASP:OD2	4:B:2:NDG:H8C1	1.92	0.68
1:A:422:VAL:HG22	1:A:442:SER:HB3	1.76	0.67
2:U:22:CFZ:F2'	2:U:23:CFZ:H5'A	1.83	0.67
1:B:382:GLU:HG3	6:B:231:HOH:O	1.94	0.67
2:S:4:G:H2'	2:S:5:G:H5'	1.76	0.67
1:A:436:TYR:O	6:A:216:HOH:O	2.14	0.66
1:B:270:ASP:OD1	1:B:326:LYS:HG2	1.97	0.65
2:S:1:G:H2'	2:S:2:G:O4'	1.96	0.65
1:A:290:LYS:HB3	1:A:291:PRO:CD	2.25	0.65
1:A:312:ASP:HB3	1:A:317:LYS:HD2	1.77	0.65
1:B:292:ARG:HB2	1:B:300:TYR:HD2	1.62	0.65
2:U:17:G:C2'	2:U:18:A:H5"	2.27	0.65
2:U:14:A:H2'	2:U:15:A:C5'	2.26	0.65
2:U:1:G:H2'	2:U:1:G:N3	2.11	0.65
2:U:15:A:C2'	2:U:16:G:H5'	2.27	0.65
2:U:14:A:H2'	2:U:15:A:H5"	1.78	0.64
2:U:18:A:H5'	2:U:18:A:H8	1.62	0.64
1:B:297:ASN:HD22	4:B:2:NDG:H1	1.63	0.63
1:B:246:LYS:NZ	4:B:6:NAG:O3	2.27	0.63
1:A:262:VAL:O	1:A:262:VAL:HG12	1.99	0.62
1:A:292:ARG:HD3	1:A:292:ARG:N	2.15	0.62
1:B:245:PRO:HA	4:B:7:GAL:H62	1.81	0.62
2:U:15:A:N3	2:U:15:A:H5'	2.15	0.62
2:U:18:A:H2'	2:U:19:A:H5'	1.83	0.61
1:A:290:LYS:HB3	1:A:291:PRO:HD2	1.82	0.61
2:S:18:A:H2'	2:S:19:A:H5'	1.83	0.61
2:U:17:G:H2'	2:U:18:A:H5"	1.82	0.61
1:A:243:PHE:HE1	1:A:262:VAL:HB	1.65	0.60
1:B:268:HIS:O	1:B:271:PRO:HD3	2.02	0.60
2:S:5:G:H2'	2:S:6:UFT:H5'A	1.82	0.60
1:A:406:LEU:C	1:A:406:LEU:HD12	2.22	0.60
1:A:303:VAL:HG12	1:A:304:SER:N	2.14	0.59
1:A:262:VAL:HG21	3:A:6:NDG:O6	2.02	0.58
1:B:429:HIS:HD2	1:B:431:ALA:H	1.51	0.58
2:U:2:G:O2'	2:U:3:A:H5'	2.03	0.58
2:S:18:A:H2'	2:S:19:A:C5'	2.33	0.58
2:U:22:CFZ:C2'	2:U:23:CFZ:H5'A	2.33	0.58
3:A:7:GLA:H3	6:A:450:HOH:O	2.02	0.57

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:2:G:H2'	2:U:3:A:C8	2.35	0.57
2:U:22:CFZ:H6	2:U:22:CFZ:O5'	2.05	0.57
1:A:348:VAL:O	1:A:439:LYS:HD2	2.05	0.57
2:S:5:G:O2'	2:S:6:UFT:OP1	2.18	0.56
1:B:253:ILE:HD13	1:B:254:SER:N	2.20	0.56
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.71	0.56
1:A:290:LYS:HB2	1:A:303:VAL:HG11	1.87	0.55
1:A:286:ASN:H	1:A:286:ASN:ND2	2.04	0.55
1:A:355:ARG:HA	1:A:358:LEU:HD22	1.88	0.55
1:A:346:PRO:HD2	1:A:432:LEU:CD2	2.37	0.55
1:B:292:ARG:HB2	1:B:300:TYR:CD2	2.41	0.55
1:A:241:PHE:HB2	1:A:243:PHE:CE1	2.41	0.55
1:A:422:VAL:HG22	1:A:442:SER:CB	2.36	0.55
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.40	0.55
1:A:293:GLU:N	1:A:293:GLU:CD	2.60	0.54
2:S:2:G:H3'	2:S:3:A:C8	2.41	0.54
1:B:253:ILE:HD13	1:B:253:ILE:C	2.28	0.54
1:B:241:PHE:CE2	4:B:3:NAG:H4	2.43	0.54
2:U:13:A:H2'	2:U:14:A:O4'	2.08	0.54
2:S:4:G:C2'	2:S:5:G:H5'	2.37	0.54
2:S:17:G:H2'	2:S:18:A:C5'	2.33	0.54
2:S:5:G:C2'	2:S:6:UFT:H5'A	2.38	0.54
1:B:297:ASN:HD22	4:B:2:NDG:C1	2.21	0.54
1:B:361:ASN:ND2	6:B:179:HOH:O	2.41	0.53
2:U:24:A:N3	2:U:24:A:OP1	2.41	0.53
2:U:24:A:N3	2:U:24:A:P	2.82	0.53
1:A:436:TYR:CD1	1:A:437:THR:N	2.77	0.52
1:A:346:PRO:HG3	1:A:372:PHE:HB3	1.92	0.52
2:S:16:G:N2	2:S:17:G:H1'	2.24	0.52
1:A:289:THR:HA	1:A:304:SER:HA	1.91	0.51
1:A:290:LYS:O	1:A:291:PRO:O	2.28	0.51
1:A:247:PRO:HG3	1:A:376:ASP:OD2	2.10	0.51
1:A:429:HIS:CD2	1:A:431:ALA:H	2.28	0.51
1:A:248:LYS:HG3	6:A:160:HOH:O	2.10	0.51
4:B:7:GAL:C6	6:B:157:HOH:O	2.53	0.50
2:S:6:UFT:O4	2:S:17:G:H3'	2.11	0.50
2:U:14:A:C2'	2:U:15:A:H5"	2.40	0.50
1:B:291:PRO:HA	6:B:222:HOH:O	2.10	0.50
2:S:2:G:H3'	2:S:3:A:H8	1.76	0.50
2:U:1:G:H2'	2:U:2:G:O5'	2.12	0.50
2:U:24:A:H3'	2:U:24:A:OP1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:20:CFZ:O5'	2:U:20:CFZ:H6	2.12	0.50
1:A:246:LYS:HE3	3:A:7:GLA:O2	2.12	0.49
1:B:242:LEU:HD13	1:B:336:ILE:HG22	1.93	0.49
1:A:258:GLU:O	3:A:7:GLA:C6	2.59	0.49
2:U:14:A:H2'	2:U:15:A:H5'	1.94	0.49
1:A:247:PRO:O	1:A:251:LEU:HG	2.13	0.49
1:B:346:PRO:CB	1:B:372:PHE:HB3	2.33	0.49
4:B:2:NDG:C6	4:B:3:NAG:H82	2.38	0.48
1:A:387:PRO:HG2	6:A:170:HOH:O	2.13	0.48
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.96	0.48
1:B:430:GLU:HG3	1:B:431:ALA:N	2.28	0.48
1:A:260:THR:CG2	1:A:262:VAL:CG2	2.85	0.48
1:A:260:THR:HG21	1:A:262:VAL:HG23	1.95	0.48
1:B:238:PRO:CG	1:B:266:VAL:HA	2.41	0.48
1:A:390:ASN:ND2	6:A:131:HOH:O	2.46	0.47
1:B:238:PRO:HA	1:B:265:ASP:HB2	1.96	0.47
2:S:18:A:C2'	2:S:19:A:H5'	2.42	0.47
1:A:346:PRO:HD2	1:A:432:LEU:HD21	1.96	0.47
4:B:5:MAN:O5	4:B:6:NAG:H82	2.15	0.47
1:B:406:LEU:C	1:B:406:LEU:HD12	2.34	0.47
2:S:11:CFZ:N4	2:S:16:G:O6	2.48	0.47
1:B:277:TRP:O	1:B:283:GLU:HA	2.14	0.47
1:B:325:ASN:O	1:B:328:LEU:HB3	2.15	0.47
2:U:24:A:N3	2:U:24:A:OP2	2.47	0.47
1:A:243:PHE:CE1	1:A:262:VAL:HB	2.47	0.47
2:U:15:A:H2'	2:U:16:G:C5'	2.42	0.47
2:U:15:A:N3	2:U:15:A:H3'	2.31	0.46
1:A:303:VAL:O	1:A:304:SER:HB3	2.16	0.46
2:U:22:CFZ:H2'	2:U:23:CFZ:C5'	2.45	0.46
1:A:302:VAL:HG22	1:A:303:VAL:HG23	1.96	0.46
2:U:13:A:C2	2:U:14:A:H1'	2.51	0.46
2:U:18:A:C2'	2:U:19:A:H5'	2.43	0.46
1:A:292:ARG:CD	1:A:292:ARG:N	2.77	0.46
2:S:18:A:H8	2:S:18:A:H5'	1.81	0.46
1:A:348:VAL:CG1	1:A:439:LYS:HG3	2.45	0.46
2:S:5:G:H5'	2:S:5:G:H8	1.80	0.46
1:A:262:VAL:O	1:A:262:VAL:CG1	2.63	0.45
1:B:297:ASN:HB2	4:B:2:NDG:H1	1.98	0.45
1:B:311:GLN:N	1:B:311:GLN:HE21	1.99	0.45
2:U:14:A:C2'	2:U:15:A:C5'	2.95	0.45
4:B:6:NAG:C4	4:B:7:GAL:O2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.52	0.45
1:A:286:ASN:N	1:A:286:ASN:HD22	2.14	0.45
1:A:374:PRO:O	1:A:429:HIS:HE1	1.99	0.45
1:A:358:LEU:O	1:A:414:LYS:HE3	2.16	0.45
1:B:325:ASN:OD1	1:B:327:ALA:HB3	2.17	0.45
1:A:241:PHE:HB2	1:A:243:PHE:CZ	2.52	0.44
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.52	0.44
1:B:328:LEU:HD12	1:B:329:PRO:HD2	2.00	0.44
4:B:7:GAL:H4	6:B:17:HOH:O	2.17	0.44
1:B:326:LYS:C	1:B:328:LEU:H	2.20	0.44
3:A:4:MAN:HO4	3:A:5:MAN:H5	1.80	0.44
2:U:1:G:N2	2:U:2:G:O4'	2.50	0.44
1:A:253:ILE:HG13	1:A:254:SER:N	2.32	0.44
2:U:10:CFZ:H5	6:U:117:HOH:O	2.16	0.44
1:B:269:GLU:OE2	1:B:326:LYS:HE3	2.17	0.44
1:B:238:PRO:HA	1:B:265:ASP:CB	2.47	0.44
1:A:286:ASN:N	1:A:286:ASN:ND2	2.64	0.43
2:U:21:UFT:H2'	2:U:22:CFZ:C6	2.48	0.43
1:B:318:GLU:HA	1:B:337:SER:HB3	1.99	0.43
2:U:1:G:C2'	2:U:2:G:O5'	2.64	0.43
1:A:242:LEU:O	1:A:336:ILE:HD12	2.19	0.43
1:A:433:HIS:O	1:A:434:ASN:HB2	2.17	0.43
1:B:370:LYS:HB2	1:B:370:LYS:HE2	1.71	0.43
1:A:280:ASP:OD1	1:A:318:GLU:HG2	2.18	0.43
1:A:365:LEU:HD12	1:A:410:LEU:HD23	2.00	0.43
1:A:260:THR:HG22	1:A:262:VAL:CG2	2.33	0.43
2:U:17:G:H2'	2:U:18:A:C5'	2.47	0.43
1:A:293:GLU:O	1:A:294:GLU:HG3	2.19	0.43
1:B:289:THR:HA	1:B:304:SER:HA	2.00	0.43
1:A:345:GLU:HA	1:A:346:PRO:HD3	1.81	0.43
1:A:249:ASP:OD2	1:A:255:ARG:HD3	2.18	0.42
1:A:277:TRP:O	1:A:283:GLU:HA	2.18	0.42
2:U:13:A:O2'	2:U:14:A:P	2.77	0.42
1:A:259:VAL:HG23	1:A:308:VAL:HG11	2.00	0.42
1:A:278:TYR:HB3	1:A:281:GLY:O	2.20	0.42
2:S:4:G:C3'	2:S:5:G:H5'	2.49	0.42
1:B:268:HIS:N	1:B:268:HIS:CD2	2.85	0.42
2:U:4:G:N2	2:U:20:CFZ:O2	2.52	0.42
1:A:355:ARG:O	1:A:358:LEU:HB2	2.20	0.42
1:A:406:LEU:CD1	1:A:406:LEU:C	2.88	0.42
2:U:8:CFZ:H5	6:U:82:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TYR:HA	1:B:282:VAL:O	2.19	0.41
2:U:22:CFZ:C2'	2:U:23:CFZ:C5'	2.97	0.41
1:A:293:GLU:OE1	1:A:302:VAL:CG1	2.68	0.41
1:A:343:PRO:HA	1:A:373:TYR:O	2.20	0.41
2:U:1:G:HO2'	2:U:2:G:P	2.42	0.41
1:B:377:ILE:HD11	1:B:427:VAL:CG1	2.51	0.41
1:A:259:VAL:HG12	1:A:260:THR:N	2.36	0.41
1:B:238:PRO:HB3	1:B:264:VAL:O	2.21	0.41
2:S:17:G:C2'	2:S:18:A:C5'	2.95	0.41
2:U:18:A:H5'	2:U:18:A:C8	2.51	0.41
4:B:1:FUL:H63	4:B:2:NDG:O6	2.21	0.41
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.92	0.41
2:U:2:G:C6	2:U:23:CFZ:N4	2.89	0.41
1:A:418:GLN:HA	1:A:443:LEU:HD22	2.03	0.41
2:U:13:A:HO2'	2:U:14:A:P	2.43	0.41
1:A:259:VAL:HG23	1:A:308:VAL:CG1	2.51	0.40
1:A:380:GLU:HG2	1:A:391:TYR:OH	2.21	0.40
1:B:365:LEU:HD12	1:B:410:LEU:HD23	2.03	0.40
1:A:244:PRO:HD3	1:A:336:ILE:HD11	2.02	0.40
1:A:423:PHE:O	1:A:441:LEU:N	2.54	0.40
2:S:21:UFT:H2'	2:S:22:CFZ:H6	2.02	0.40
1:A:429:HIS:O	1:A:435:HIS:HA	2.22	0.40
2:S:20:CFZ:H6	2:S:20:CFZ:O5'	2.21	0.40
2:S:2:G:H2'	2:S:2:G:N3	2.36	0.40
1:A:365:LEU:HB2	1:A:410:LEU:HB3	2.03	0.40
1:B:258:GLU:O	4:B:7:GAL:O6	2.25	0.40

All (2) 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)
2:S:11:CFZ:O4'	2:U:24:A:O2'[4_556]	2.09	0.11
2:S:11:CFZ:O5'	2:U:24:A:O2'[4_556]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/211 (80%)	152 (90%)	12 (7%)	5 (3%)	5	1
1	B	206/211 (98%)	198 (96%)	7 (3%)	1 (0%)	32	25
All	All	375/422 (89%)	350 (93%)	19 (5%)	6 (2%)	11	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	PRO
1	A	303	VAL
1	A	282	VAL
1	A	295	GLN
1	A	304	SER
1	B	329	PRO

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	166/196 (85%)	153 (92%)	13 (8%)	15	9
1	B	194/196 (99%)	184 (95%)	10 (5%)	27	22
All	All	360/392 (92%)	337 (94%)	23 (6%)	20	14

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LYS
1	A	283	GLU
1	A	286	ASN
1	A	289	THR
1	A	292	ARG
1	A	293	GLU

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Mol	Chain	Res	Type
1	A	295	GLN
1	A	340	LYS
1	A	358	LEU
1	A	376	ASP
1	A	390	ASN
1	A	414	LYS
1	A	439	LYS
1	B	242	LEU
1	B	253	ILE
1	B	269	GLU
1	B	296	TYR
1	B	309	LEU
1	B	311	GLN
1	B	370	LYS
1	B	434	ASN
1	B	443	LEU
1	B	444	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	295	GLN
1	A	315	ASN
1	A	361	ASN
1	A	362	GLN
1	A	390	ASN
1	A	419	GLN
1	A	429	HIS
1	A	434	ASN
1	A	438	GLN
1	B	297	ASN
1	B	311	GLN
1	B	361	ASN
1	B	390	ASN
1	B	429	HIS
1	B	434	ASN
1	B	438	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S	8/24 (33%)	4 (50%)	0
2	U	14/24 (58%)	6 (42%)	0
All	All	22/48 (45%)	10 (45%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S	2	G
2	S	5	G
2	S	7	G
2	S	18	A
2	U	2	G
2	U	7	G
2	U	14	A
2	U	15	A
2	U	18	A
2	U	24	A

There are no RNA pucker outliers to report.

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

18 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	CFZ	S	10	2	15,21,22	0.94	0	18,30,33	0.80	0
2	CFZ	S	11	2	15,21,22	0.81	0	18,30,33	0.80	1 (5%)
2	CFZ	S	20	2	15,21,22	0.81	0	18,30,33	0.74	0
2	UFT	S	21	2	14,21,22	1.16	1 (7%)	17,30,33	3.79	2 (11%)
2	CFZ	S	22	2	15,21,22	0.80	0	18,30,33	0.79	1 (5%)
2	CFZ	S	23	2	15,21,22	0.75	0	18,30,33	0.80	1 (5%)
2	UFT	S	6	2	14,21,22	1.15	1 (7%)	17,30,33	3.81	3 (17%)
2	CFZ	S	8	2	15,21,22	0.83	0	18,30,33	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
2	UFT	S	9	2	14,21,22	1.20	1 (7%)	17,30,33	3.79	3 (17%)
2	CFZ	U	10	2	15,21,22	0.86	0	18,30,33	0.77	0
2	CFZ	U	11	2	15,21,22	0.86	0	18,30,33	0.78	0
2	CFZ	U	20	2	15,21,22	0.83	0	18,30,33	0.84	1 (5%)
2	UFT	U	21	2	14,21,22	1.15	1 (7%)	17,30,33	3.80	3 (17%)
2	CFZ	U	22	2	15,21,22	0.90	0	18,30,33	0.76	0
2	CFZ	U	23	2	15,21,22	0.84	0	18,30,33	0.95	0
2	UFT	U	6	2	14,21,22	1.21	1 (7%)	17,30,33	3.86	4 (23%)
2	CFZ	U	8	2	15,21,22	0.87	0	18,30,33	0.72	1 (5%)
2	UFT	U	9	2	14,21,22	1.11	1 (7%)	17,30,33	3.77	2 (11%)

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	CFZ	S	10	2	-	0/3/25/26	0/2/2/2
2	CFZ	S	11	2	-	0/3/25/26	0/2/2/2
2	CFZ	S	20	2	-	0/3/25/26	0/2/2/2
2	UFT	S	21	2	-	0/3/25/26	0/2/2/2
2	CFZ	S	22	2	-	0/3/25/26	0/2/2/2
2	CFZ	S	23	2	-	0/3/25/26	0/2/2/2
2	UFT	S	6	2	-	0/3/25/26	0/2/2/2
2	CFZ	S	8	2	-	0/3/25/26	0/2/2/2
2	UFT	S	9	2	-	0/3/25/26	0/2/2/2
2	CFZ	U	10	2	-	0/3/25/26	0/2/2/2
2	CFZ	U	11	2	-	0/3/25/26	0/2/2/2
2	CFZ	U	20	2	-	0/3/25/26	0/2/2/2
2	UFT	U	21	2	-	0/3/25/26	0/2/2/2
2	CFZ	U	22	2	-	0/3/25/26	0/2/2/2
2	CFZ	U	23	2	-	0/3/25/26	0/2/2/2
2	UFT	U	6	2	-	0/3/25/26	0/2/2/2
2	CFZ	U	8	2	-	0/3/25/26	0/2/2/2
2	UFT	U	9	2	-	0/3/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	21	UFT	C4-N3	2.85	1.38	1.33
2	S	6	UFT	C4-N3	2.90	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	9	UFT	C4-N3	2.95	1.38	1.33
2	S	21	UFT	C4-N3	2.95	1.38	1.33
2	S	9	UFT	C4-N3	3.10	1.38	1.33
2	U	6	UFT	C4-N3	3.21	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	6	UFT	C5-C4-N3	-3.57	114.59	123.12
2	S	9	UFT	C5-C4-N3	-3.57	114.60	123.12
2	U	9	UFT	C5-C4-N3	-3.57	114.61	123.12
2	U	21	UFT	C5-C4-N3	-3.54	114.66	123.12
2	S	6	UFT	C5-C4-N3	-3.54	114.67	123.12
2	S	21	UFT	C5-C4-N3	-3.53	114.69	123.12
2	S	11	CFZ	F2'-C2'-C1'	2.02	113.40	109.28
2	U	21	UFT	F2'-C2'-C1'	2.02	113.41	109.28
2	S	9	UFT	F2'-C2'-C1'	2.05	113.48	109.28
2	U	8	CFZ	F2'-C2'-C1'	2.11	113.60	109.28
2	S	22	CFZ	F2'-C2'-C1'	2.15	113.68	109.28
2	U	6	UFT	F2'-C2'-C1'	2.17	113.73	109.28
2	S	23	CFZ	F2'-C2'-C1'	2.26	113.91	109.28
2	U	6	UFT	O4'-C1'-C2'	2.27	108.14	105.74
2	U	20	CFZ	F2'-C2'-C1'	2.31	114.00	109.28
2	S	6	UFT	O4'-C1'-C2'	2.46	108.34	105.74
2	U	9	UFT	C4-N3-C2	14.85	126.89	114.13
2	S	6	UFT	C4-N3-C2	14.91	126.94	114.13
2	S	21	UFT	C4-N3-C2	14.93	126.95	114.13
2	U	6	UFT	C4-N3-C2	14.95	126.97	114.13
2	S	9	UFT	C4-N3-C2	14.96	126.98	114.13
2	U	21	UFT	C4-N3-C2	14.98	127.00	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	11	CFZ	1	2
2	S	20	CFZ	1	0
2	S	21	UFT	1	0
2	S	22	CFZ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	23	CFZ	2	0
2	S	6	UFT	4	0
2	U	10	CFZ	1	0
2	U	20	CFZ	2	0
2	U	21	UFT	1	0
2	U	22	CFZ	6	0
2	U	23	CFZ	5	0
2	U	8	CFZ	1	0

5.5 Carbohydrates ⓘ

12 carbohydrates 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	MAN	A	4	3	12,12,12	0.54	0	17,17,17	0.51	0
3	MAN	A	5	3	11,11,12	0.69	0	13,15,17	0.72	0
3	NDG	A	6	3	14,14,15	0.59	0	15,19,21	0.99	2 (13%)
3	GLA	A	7	3	11,11,12	0.68	0	13,15,17	0.76	0
4	FUL	B	1	4	9,10,11	0.51	0	13,14,16	0.73	0
4	NDG	B	2	4	15,15,15	0.56	0	21,21,21	0.63	0
4	NAG	B	3	4	14,14,15	0.55	0	15,19,21	0.85	1 (6%)
4	BMA	B	4	4	11,11,12	0.51	0	13,15,17	0.61	0
4	MAN	B	5	4	11,11,12	0.42	0	13,15,17	0.63	0
4	NAG	B	6	4	14,14,15	0.46	0	15,19,21	0.80	0
4	GAL	B	7	4	11,11,12	0.58	0	13,15,17	1.13	1 (7%)
4	MAN	B	8	4	11,11,12	0.55	0	13,15,17	0.47	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
3	MAN	A	4	3	-	0/2/22/22	0/1/1/1
3	MAN	A	5	3	-	0/2/19/22	0/1/1/1
3	NDG	A	6	3	-	0/6/23/26	0/1/1/1
3	GLA	A	7	3	-	0/2/19/22	0/1/1/1
4	FUL	B	1	4	-	0/0/17/20	0/1/1/1
4	NDG	B	2	4	-	0/6/26/26	0/1/1/1
4	NAG	B	3	4	-	0/6/23/26	0/1/1/1
4	BMA	B	4	4	-	0/2/19/22	0/1/1/1
4	MAN	B	5	4	-	0/2/19/22	0/1/1/1
4	NAG	B	6	4	-	0/6/23/26	0/1/1/1
4	GAL	B	7	4	-	0/2/19/22	0/1/1/1
4	MAN	B	8	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	6	NDG	C2-N2-C7	-2.08	119.91	122.94
4	B	3	NAG	C2-N2-C7	-2.04	119.97	122.94
3	A	6	NDG	C1-O-C5	2.64	115.81	112.17
4	B	7	GAL	C1-O5-C5	3.15	116.51	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4	MAN	2	0
3	A	5	MAN	2	0
3	A	6	NDG	1	0
3	A	7	GLA	4	0
4	B	1	FUL	1	0
4	B	2	NDG	8	0
4	B	3	NAG	3	0
4	B	5	MAN	1	0
4	B	6	NAG	4	0
4	B	7	GAL	8	0

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	177/211 (83%)	1.14	32 (18%)	1	2	21, 41, 96, 107	0
1	B	208/211 (98%)	0.77	22 (10%)	7	9	21, 38, 88, 100	0
2	S	10/24 (41%)	0.41	1 (10%)	8	11	48, 77, 98, 107	0
2	U	15/24 (62%)	0.60	3 (20%)	1	2	38, 79, 111, 117	0
All	All	410/470 (87%)	0.91	58 (14%)	3	4	21, 40, 94, 117	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PHE	10.7
1	B	296	TYR	8.9
1	A	278	TYR	7.9
1	A	302	VAL	7.5
1	A	303	VAL	6.6
1	A	289	THR	5.9
1	A	273	VAL	5.4
1	A	284	VAL	5.2
1	B	271	PRO	5.1
1	A	296	TYR	5.0
1	A	262	VAL	4.7
1	B	300	TYR	4.6
1	B	330	ALA	4.6
1	A	277	TRP	4.4
1	A	256	THR	4.4
1	B	239	SER	4.1
1	B	323	VAL	4.1
1	B	267	SER	4.0
1	A	286	ASN	4.0
1	B	299	THR	3.9
1	A	290	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	280	ASP	3.7
1	A	304	SER	3.6
1	B	328	LEU	3.6
1	B	331	PRO	3.5
1	A	305	VAL	3.4
1	B	297	ASN	3.4
1	B	265	ASP	3.4
1	B	298	SER	3.3
1	A	336	ILE	3.2
1	B	238	PRO	3.2
1	A	295	GLN	3.2
1	B	273	VAL	3.2
1	B	327	ALA	3.1
1	A	243	PHE	3.0
1	B	266	VAL	3.0
1	A	276	ASN	2.9
1	A	261	CYS	2.9
1	B	325	ASN	2.8
1	A	272	GLU	2.8
1	A	292	ARG	2.8
1	B	329	PRO	2.7
2	U	24	A	2.7
1	A	281	GLY	2.6
2	U	1	G	2.5
1	A	320	LYS	2.5
1	A	275	PHE	2.5
1	B	268	HIS	2.4
2	U	15	A	2.3
1	A	279	VAL	2.3
1	A	321	CYS	2.2
2	S	1	G	2.2
1	A	334	LYS	2.2
1	A	242	LEU	2.2
1	B	263	VAL	2.1
1	A	389	ASN	2.1
1	A	282	VAL	2.1
1	B	292	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CFZ	U	11	20/21	0.94	0.12	-	46,49,55,57	0
2	CFZ	U	10	20/21	0.92	0.14	-	44,46,49,49	0
2	CFZ	S	11	20/21	0.76	0.22	-	68,81,83,83	0
2	CFZ	S	8	20/21	0.95	0.13	-	35,42,52,52	0
2	CFZ	U	20	20/21	0.90	0.17	-	37,40,45,47	0
2	CFZ	S	22	20/21	0.87	0.22	-	65,84,87,88	0
2	UFT	S	6	20/21	0.89	0.22	-	62,66,68,71	0
2	CFZ	U	23	20/21	0.74	0.21	-	83,90,95,97	0
2	UFT	U	21	20/21	0.94	0.15	-	41,52,54,55	0
2	UFT	S	21	20/21	0.90	0.19	-	54,62,69,69	0
2	UFT	U	9	20/21	0.95	0.13	-	38,41,44,46	0
2	CFZ	S	23	20/21	0.65	0.25	-	89,91,95,95	0
2	UFT	S	9	20/21	0.92	0.12	-	43,48,53,56	0
2	UFT	U	6	20/21	0.88	0.16	-	48,52,61,62	0
2	CFZ	U	22	20/21	0.92	0.18	-	57,75,76,81	0
2	CFZ	S	10	20/21	0.85	0.14	-	53,57,63,68	0
2	CFZ	U	8	20/21	0.97	0.11	-	31,38,45,46	0
2	CFZ	S	20	20/21	0.92	0.17	-	51,53,54,57	0

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GAL	B	7	11/12	0.68	0.25	8.50	72,74,75,77	0
3	GLA	A	7	11/12	0.79	0.36	4.27	106,107,108,108	0
4	NAG	B	3	14/15	0.81	0.17	-0.44	74,80,83,84	0
4	NAG	B	6	14/15	0.86	0.12	-1.09	68,69,70,71	0
4	MAN	B	5	11/12	0.85	0.17	-	69,70,72,73	0
4	MAN	B	8	11/12	0.74	0.19	-	79,80,81,82	0
3	MAN	A	4	12/12	0.82	0.16	-	110,111,112,112	0
4	NDG	B	2	15/15	0.79	0.34	-	85,87,92,96	0
4	BMA	B	4	11/12	0.87	0.12	-	71,76,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NDG	A	6	14/15	0.86	0.23	-	107,108,109,109	0
4	FUL	B	1	10/11	0.87	0.39	-	99,101,101,102	0
3	MAN	A	5	11/12	0.82	0.17	-	110,111,112,112	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CA	U	25	1/1	0.97	0.15	-	56,56,56,56	0
5	CA	S	25	1/1	0.89	0.06	-	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.