



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:57 PM BST

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

<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 : 2.13.1
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) : 2.13.1

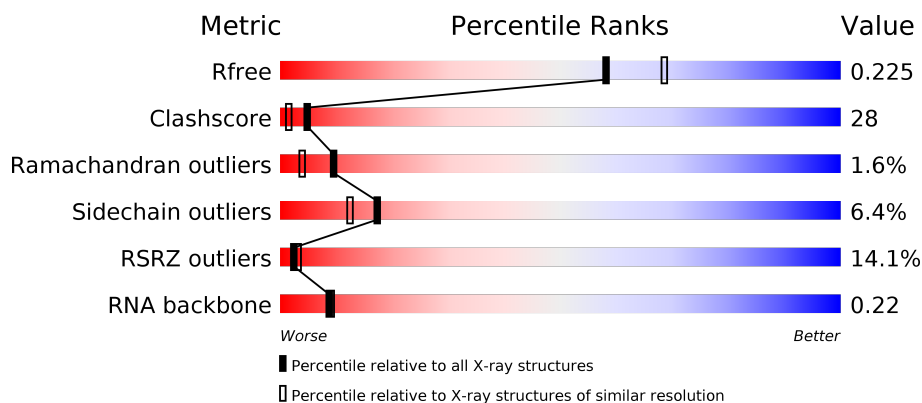
1 Overall quality at a glance

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.




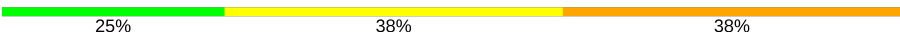
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)
RNA backbone	3102	1060 (2.60-1.72)

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 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	211	<div> <div>15%</div> <div>46%</div> <div>31%</div> <div>7%</div> <div>16%</div> </div>
1	B	211	<div> <div>10%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
2	S	24	<div> <div>4%</div> <div>42%</div> <div>33%</div> <div>•</div> <div>21%</div> </div>
2	U	24	<div> <div>13%</div> <div>8%</div> <div>38%</div> <div>54%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	4	
4	D	8	

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
4	GAL	D	6	-	-	X	-

2 Entry composition [i](#)

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	C	N	O	S	0	0	0
			1433	916	240	271	6			
1	B	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			

- 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'.

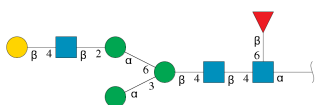
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	S	19	Total	C	F	N	O	P	0	0	0
			401	181	9	74	120	17			
2	U	24	Total	C	F	N	O	P	0	0	0
			515	231	9	99	153	23			

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



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

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



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

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

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

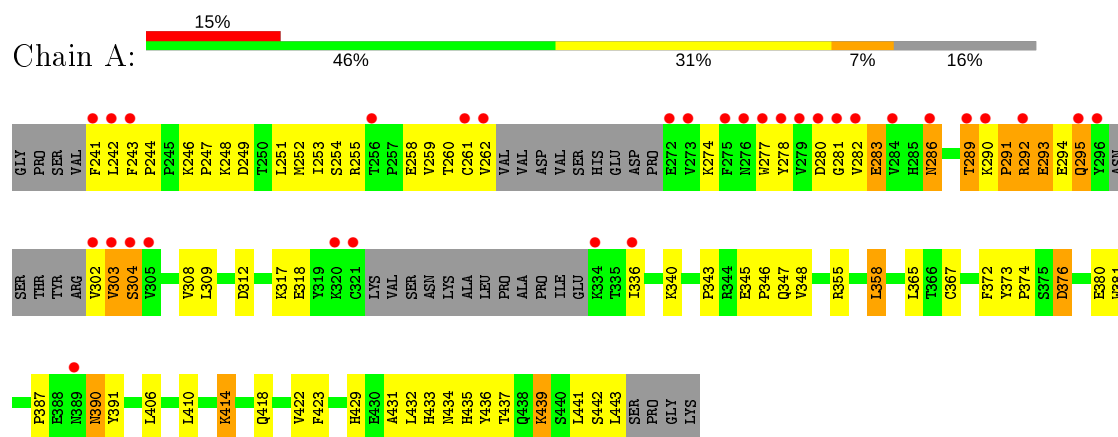
- Molecule 6 is water.

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

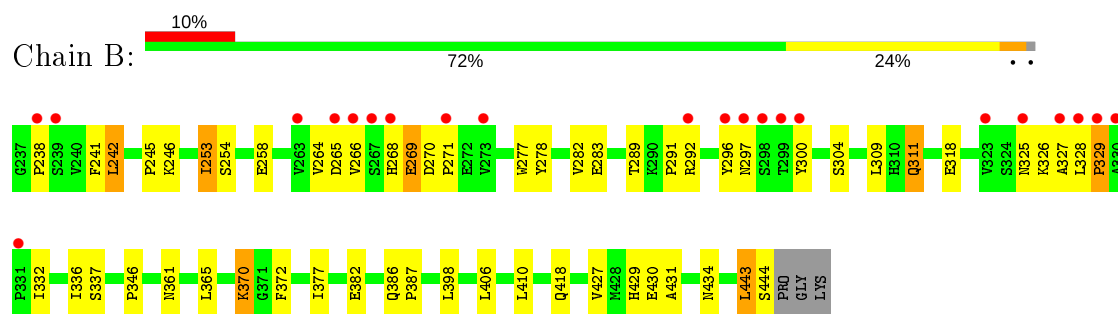
3 Residue-property plots

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.

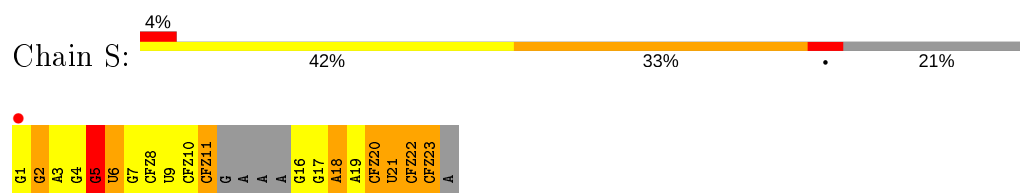
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region

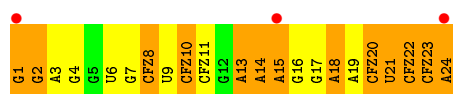


- Molecule 2: 5'-R(*GP*GP*AP*GP*GP*(UFT)P*GP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*GP*AP*AP*A*GP*GP*AP*AP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*A)-3'

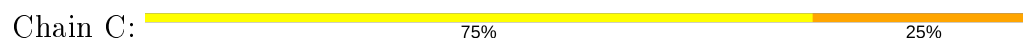


- Molecule 2: 5'-R(*GP*GP*AP*GP*GP*(UFT)P*GP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*GP*AP*AP*A*GP*GP*AP*AP*(CFZ)P*(UFT)P*(CFZ)P*(CFZ)P*A)-3'

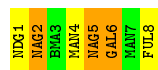
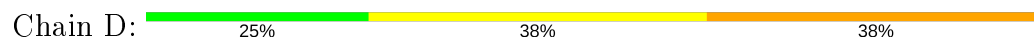




- Molecule 3: alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose



- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose



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
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.14Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.277 0.238 , 0.225	Depositor DCC
R_{free} test set	1944 reflections (5.03%)	wwPDB-VP
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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: 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(°)	Ideal(°)
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 [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	1433	0	1401	80	0
1	B	1664	0	1631	52	0
2	S	401	0	201	27	2
2	U	515	0	254	44	2
3	C	48	0	41	7	0
4	D	97	0	81	17	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	3609	215	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 (215) 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:D:6:GAL:H5	1.59	0.81
3:C:1:MAN:O4	3:C:2:MAN:H5	1.80	0.81
4:D:1:NDG:H6C1	4:D:2: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:D:5:NAG:H4	4:D:6:GAL:O2	1.90	0.71
1:A:258:GLU:O	3:C:4: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:311:GLN:NE2	1:B:311:GLN:H	1.88	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:157:HOH:O	4:D:6:GAL:H62	1.91	0.69
1:B:398:LEU:HD12	6:B:186:HOH:O	1.92	0.68
1:B:265:ASP:OD2	4:D:1: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:246:LYS:NZ	4:D:5: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:D:6: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:B:429:HIS:HD2	1:B:431:ALA:H	1.51	0.58
1:A:262:VAL:HG21	3:C:3:NDG:O6	2.02	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
6:A:450:HOH:O	3:C:4:GLA:H3	2.02	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:2: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:D:1: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
6:B:157:HOH:O	4:D:6:GAL:C6	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
2:U:20:CFZ:O5'	2:U:20:CFZ:H6	2.12	0.50
1:A:246:LYS:HE3	3:C:4:GLA:O2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD13	1:B:336:ILE:HG22	1.93	0.49
1:A:258:GLU:O	3:C:4: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:D:1:NDG:C6	4:D:2: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:D:4:MAN:O5	4:D:5: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: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:D:5:NAG:C4	4:D:6:GAL:O2	2.63	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:B:17:HOH:O	4:D:6:GAL:H4	2.17	0.44
1:B:326:LYS:C	1:B:328:LEU:H	2.20	0.44
3:C:1:MAN:HO4	3:C:2: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
1:B:297:ASN:ND2	4:D:1:NDG:C1	2.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C8	2:U:18:A:H5'	2.51	0.41
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.92	0.41
4:D:1:NDG:O6	4:D:8:FUL:H63	2.21	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:D:6: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%)	4	1
1	B	206/211 (98%)	198 (96%)	7 (3%)	1 (0%)	29	22
All	All	375/422 (89%)	350 (93%)	19 (5%)	6 (2%)	9	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%)	12	7
1	B	194/196 (99%)	184 (95%)	10 (5%)	23	19
All	All	360/392 (92%)	337 (94%)	23 (6%)	17	12

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
1	A	295	GLN

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Mol	Chain	Res	Type
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	15/24 (62%)	6 (40%)	2 (13%)
All	All	23/48 (47%)	10 (43%)	2 (8%)

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

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	U	1	G
2	U	13	A

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

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	U	11	2	15,21,22	0.80	0	17,30,33	1.17	2 (11%)
2	CFZ	U	10	2	15,21,22	0.81	0	17,30,33	1.17	2 (11%)
2	CFZ	S	11	2	15,21,22	0.80	0	17,30,33	1.18	2 (11%)
2	CFZ	S	8	2	15,21,22	0.78	0	17,30,33	1.14	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CFZ	U	20	2	15,21,22	0.79	0	17,30,33	1.24	2 (11%)
2	CFZ	S	22	2	15,21,22	0.78	0	17,30,33	1.17	2 (11%)
2	UFT	S	6	2	14,21,22	1.11	1 (7%)	14,30,33	1.42	2 (14%)
2	CFZ	U	23	2	15,21,22	0.83	0	17,30,33	1.18	1 (5%)
2	UFT	U	21	2	14,21,22	1.13	1 (7%)	14,30,33	1.33	2 (14%)
2	UFT	S	21	2	14,21,22	1.14	1 (7%)	14,30,33	1.31	1 (7%)
2	UFT	U	9	2	14,21,22	1.11	1 (7%)	14,30,33	1.32	1 (7%)
2	CFZ	S	23	2	15,21,22	0.72	0	17,30,33	1.19	2 (11%)
2	UFT	S	9	2	14,21,22	1.18	1 (7%)	14,30,33	1.31	2 (14%)
2	UFT	U	6	2	14,21,22	1.20	2 (14%)	14,30,33	1.50	3 (21%)
2	CFZ	U	22	2	15,21,22	0.82	0	17,30,33	1.18	1 (5%)
2	CFZ	S	10	2	15,21,22	0.87	0	17,30,33	1.21	1 (5%)
2	CFZ	U	8	2	15,21,22	0.82	0	17,30,33	1.16	2 (11%)
2	CFZ	S	20	2	15,21,22	0.77	0	17,30,33	1.16	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
2	CFZ	U	11	2	-	0/5/25/26	0/2/2/2
2	CFZ	U	10	2	-	0/5/25/26	0/2/2/2
2	CFZ	S	11	2	-	0/5/25/26	0/2/2/2
2	CFZ	S	8	2	-	0/5/25/26	0/2/2/2
2	CFZ	U	20	2	-	0/5/25/26	0/2/2/2
2	CFZ	S	22	2	-	0/5/25/26	0/2/2/2
2	UFT	S	6	2	-	3/5/25/26	0/2/2/2
2	CFZ	U	23	2	-	0/5/25/26	0/2/2/2
2	UFT	U	21	2	-	0/5/25/26	0/2/2/2
2	UFT	S	21	2	-	0/5/25/26	0/2/2/2
2	UFT	U	9	2	-	0/5/25/26	0/2/2/2
2	CFZ	S	23	2	-	1/5/25/26	0/2/2/2
2	UFT	S	9	2	-	0/5/25/26	0/2/2/2
2	UFT	U	6	2	-	3/5/25/26	0/2/2/2
2	CFZ	U	22	2	-	0/5/25/26	0/2/2/2
2	CFZ	S	10	2	-	0/5/25/26	0/2/2/2
2	CFZ	U	8	2	-	0/5/25/26	0/2/2/2
2	CFZ	S	20	2	-	0/5/25/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	6	UFT	C4-N3	3.35	1.38	1.33
2	S	9	UFT	C4-N3	3.23	1.38	1.33
2	S	21	UFT	C4-N3	3.07	1.38	1.33
2	U	9	UFT	C4-N3	3.07	1.38	1.33
2	S	6	UFT	C4-N3	3.03	1.38	1.33
2	U	21	UFT	C4-N3	2.97	1.38	1.33
2	U	6	UFT	C6-N1	2.14	1.38	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	6	UFT	C5-C4-N3	-3.96	114.59	123.31
2	S	9	UFT	C5-C4-N3	-3.96	114.60	123.31
2	U	9	UFT	C5-C4-N3	-3.96	114.61	123.31
2	U	21	UFT	C5-C4-N3	-3.93	114.66	123.31
2	S	6	UFT	C5-C4-N3	-3.92	114.67	123.31
2	S	21	UFT	C5-C4-N3	-3.92	114.69	123.31
2	S	8	CFZ	C2-N3-C4	3.67	120.06	116.34
2	U	20	CFZ	C2-N3-C4	3.62	120.01	116.34
2	U	8	CFZ	C2-N3-C4	3.62	120.01	116.34
2	S	10	CFZ	C2-N3-C4	3.60	120.00	116.34
2	S	11	CFZ	C2-N3-C4	3.55	119.94	116.34
2	S	20	CFZ	C2-N3-C4	3.55	119.94	116.34
2	U	11	CFZ	C2-N3-C4	3.54	119.93	116.34
2	U	10	CFZ	C2-N3-C4	3.54	119.93	116.34
2	U	22	CFZ	C2-N3-C4	3.53	119.92	116.34
2	S	23	CFZ	C2-N3-C4	3.52	119.91	116.34
2	U	23	CFZ	C2-N3-C4	3.47	119.86	116.34
2	S	22	CFZ	C2-N3-C4	3.44	119.83	116.34
2	S	6	UFT	O4'-C1'-C2'	2.47	108.34	105.79
2	U	20	CFZ	F2'-C2'-C1'	2.36	114.00	109.08
2	S	23	CFZ	F2'-C2'-C1'	2.32	113.91	109.08
2	U	6	UFT	O4'-C1'-C2'	2.28	108.14	105.79
2	U	6	UFT	F2'-C2'-C1'	2.23	113.73	109.08
2	S	22	CFZ	F2'-C2'-C1'	2.21	113.68	109.08
2	U	8	CFZ	F2'-C2'-C1'	2.17	113.60	109.08
2	S	9	UFT	F2'-C2'-C1'	2.11	113.48	109.08
2	U	21	UFT	F2'-C2'-C1'	2.08	113.41	109.08
2	S	11	CFZ	F2'-C2'-C1'	2.08	113.40	109.08
2	U	11	CFZ	F2'-C2'-C1'	2.02	113.29	109.08
2	U	10	CFZ	F2'-C2'-C1'	2.02	113.28	109.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	6	UFT	C3'-C4'-C5'-O5'
2	S	6	UFT	O4'-C4'-C5'-O5'
2	U	6	UFT	C3'-C4'-C5'-O5'
2	S	6	UFT	C4'-C5'-O5'-P
2	U	6	UFT	O4'-C4'-C5'-O5'
2	U	6	UFT	C4'-C5'-O5'-P
2	S	23	CFZ	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	U	10	CFZ	1	0
2	S	11	CFZ	1	2
2	U	20	CFZ	2	0
2	S	22	CFZ	3	0
2	S	6	UFT	4	0
2	U	23	CFZ	5	0
2	U	21	UFT	1	0
2	S	21	UFT	1	0
2	S	23	CFZ	2	0
2	U	22	CFZ	6	0
2	U	8	CFZ	1	0
2	S	20	CFZ	1	0

5.5 Carbohydrates ⓘ

12 monosaccharides 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	C	1	3	12,12,12	0.54	0	17,17,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	C	2	3	11,11,12	0.69	0	15,15,17	0.67	0
3	NDG	C	3	3	14,14,15	0.59	0	17,19,21	0.93	2 (11%)
3	GLA	C	4	3	11,11,12	0.67	0	15,15,17	0.72	0
4	NDG	D	1	4	15,15,15	0.55	0	21,21,21	0.64	0
4	NAG	D	2	4	14,14,15	0.56	0	17,19,21	0.78	1 (5%)
4	BMA	D	3	4	11,11,12	0.50	0	15,15,17	0.57	0
4	MAN	D	4	4	11,11,12	0.43	0	15,15,17	0.59	0
4	NAG	D	5	4	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
4	GAL	D	6	4	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
4	MAN	D	7	4	11,11,12	0.55	0	15,15,17	0.46	0
4	FUL	D	8	4	10,10,11	0.62	0	14,14,16	0.67	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	C	1	3	-	2/2/22/22	0/1/1/1
3	MAN	C	2	3	-	0/2/19/22	0/1/1/1
3	NDG	C	3	3	-	3/6/23/26	0/1/1/1
3	GLA	C	4	3	-	2/2/19/22	0/1/1/1
4	NDG	D	1	4	-	2/6/26/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	NAG	D	5	4	-	4/6/23/26	0/1/1/1
4	GAL	D	6	4	-	2/2/19/22	0/1/1/1
4	MAN	D	7	4	-	2/2/19/22	0/1/1/1
4	FUL	D	8	4	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6	GAL	C1-O5-C5	3.19	116.51	112.19
3	C	3	NDG	C1-O5-C5	2.67	115.81	112.19
3	C	3	NDG	C2-N2-C7	-2.10	119.91	122.90
4	D	2	NAG	C2-N2-C7	-2.06	119.97	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	NDG	C8-C7-N2-C2
3	C	3	NDG	O7-C7-N2-C2
4	D	1	NDG	C8-C7-N2-C2
4	D	1	NDG	O7-C7-N2-C2
4	D	5	NAG	C8-C7-N2-C2
4	D	5	NAG	O7-C7-N2-C2
4	D	6	GAL	O5-C5-C6-O6
3	C	1	MAN	C4-C5-C6-O6
4	D	7	MAN	O5-C5-C6-O6
3	C	4	GLA	C4-C5-C6-O6
4	D	7	MAN	C4-C5-C6-O6
3	C	4	GLA	O5-C5-C6-O6
4	D	6	GAL	C4-C5-C6-O6
3	C	1	MAN	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	3	NDG	O5-C5-C6-O6
4	D	5	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	5	NAG	O5-C5-C6-O6
4	D	2	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	MAN	2	0
4	D	5	NAG	4	0
4	D	4	MAN	1	0
3	C	3	NDG	1	0
3	C	4	GLA	4	0
4	D	2	NAG	3	0
4	D	6	GAL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NDG	6	0
3	C	2	MAN	2	0
4	D	8	FUL	1	0

5.6 Ligand geometry [i](#)

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 [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 ⓘ

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 1	21, 41, 96, 107	0
1	B	208/211 (98%)	0.77	22 (10%) 6 9	21, 38, 88, 100	0
2	S	10/24 (41%)	0.41	1 (10%) 7 11	48, 77, 98, 107	0
2	U	15/24 (62%)	0.60	3 (20%) 1 1	38, 79, 111, 117	0
All	All	410/470 (87%)	0.92	58 (14%) 2 3	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	5.3
1	B	271	PRO	5.1
1	A	296	TYR	5.0
1	A	262	VAL	4.7
1	B	300	TYR	4.7
1	B	330	ALA	4.6
1	A	277	TRP	4.5
1	A	256	THR	4.4
1	B	239	SER	4.1
1	B	267	SER	4.0
1	B	323	VAL	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	3.4
1	A	336	ILE	3.2
1	A	295	GLN	3.2
1	B	238	PRO	3.2
1	B	273	VAL	3.2
1	B	327	ALA	3.1
1	A	243	PHE	3.1
1	B	266	VAL	3.0
1	A	261	CYS	2.9
1	B	325	ASN	2.9
1	A	276	ASN	2.8
1	A	272	GLU	2.8
1	A	292	ARG	2.8
2	U	24	A	2.7
1	B	329	PRO	2.7
1	A	281	GLY	2.7
1	A	320	LYS	2.5
2	U	1	G	2.5
1	A	275	PHE	2.5
1	B	268	HIS	2.4
2	U	15	A	2.4
1	A	279	VAL	2.3
1	A	334	LYS	2.2
2	S	1	G	2.2
1	A	321	CYS	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. 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	CFZ	S	23	20/21	0.65	0.25	89,91,95,95	0
2	CFZ	U	23	20/21	0.74	0.21	83,90,95,97	0
2	CFZ	S	11	20/21	0.76	0.22	68,81,83,83	0
2	CFZ	S	10	20/21	0.85	0.14	53,57,63,68	0
2	CFZ	S	22	20/21	0.87	0.22	65,84,87,88	0
2	UFT	U	6	20/21	0.88	0.16	48,52,61,62	0
2	UFT	S	6	20/21	0.89	0.22	62,66,68,71	0
2	UFT	S	21	20/21	0.90	0.19	54,62,69,69	0
2	CFZ	U	20	20/21	0.90	0.17	37,40,45,47	0
2	CFZ	U	10	20/21	0.92	0.14	44,46,49,49	0
2	CFZ	U	22	20/21	0.92	0.18	57,75,76,81	0
2	UFT	S	9	20/21	0.92	0.12	43,48,53,56	0
2	CFZ	S	20	20/21	0.92	0.17	51,53,54,57	0
2	UFT	U	21	20/21	0.94	0.15	41,52,54,55	0
2	CFZ	U	11	20/21	0.95	0.12	46,49,55,57	0
2	CFZ	S	8	20/21	0.95	0.13	35,42,52,52	0
2	UFT	U	9	20/21	0.95	0.13	38,41,44,46	0
2	CFZ	U	8	20/21	0.97	0.11	31,38,45,46	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GAL	D	6	11/12	0.68	0.25	72,74,75,77	0
4	MAN	D	7	11/12	0.73	0.19	79,80,81,82	0
3	GLA	C	4	11/12	0.79	0.36	106,107,108,108	0
4	NDG	D	1	15/15	0.79	0.34	85,87,92,96	0
4	NAG	D	2	14/15	0.81	0.17	74,80,83,84	0
3	MAN	C	1	12/12	0.82	0.17	110,111,112,112	0
3	MAN	C	2	11/12	0.82	0.17	110,111,112,112	0
4	MAN	D	4	11/12	0.85	0.17	69,70,72,73	0
3	NDG	C	3	14/15	0.85	0.23	107,108,109,109	0
4	NAG	D	5	14/15	0.86	0.12	68,69,70,71	0
4	BMA	D	3	11/12	0.87	0.12	71,76,77,77	0
4	FUL	D	8	10/11	0.87	0.39	99,101,101,102	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

6.5 Other polymers [i](#)

There are no such residues in this entry.