Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 03:22 AM EDT

PDB ID	:	7JTQ
Title	:	Human Complement Factor B Inhibited by a Slow Off-Rate Modified Aptamer of 31 Bases
Authors	:	Xu, X.; Geisbrecht, B.V.
Deposited on	:	2020-08-18
Resolution	:	3.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

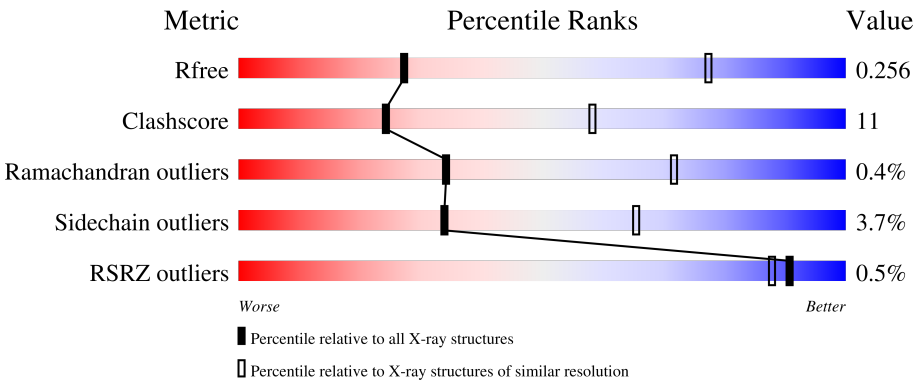
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	764	% 72% 18% • 8%
1	C	764	71% 19% • 8%
2	B	32	6% 50% 41% •
2	D	32	6% 62% 28% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12610 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 Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	703	5549	3494	963	1059	33	0	0	0
1	C	703	5549	3494	963	1059	33	0	0	0

- Molecule 2 is a DNA chain called DNA (32-MER).

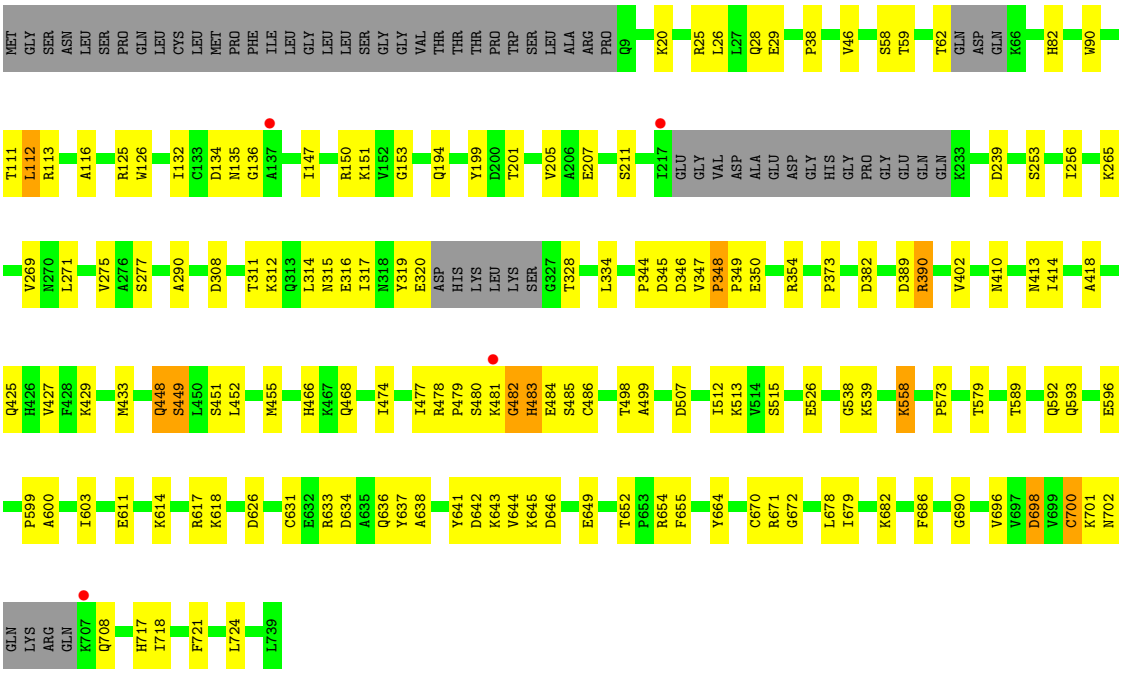
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	31	756	392	133	200	31	0	0	0
2	D	31	756	392	133	200	31	0	0	0

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.

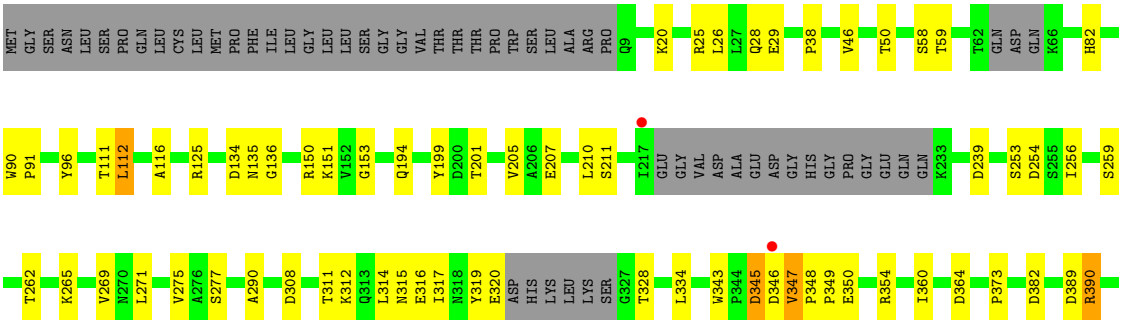
• Molecule 1: Complement factor B

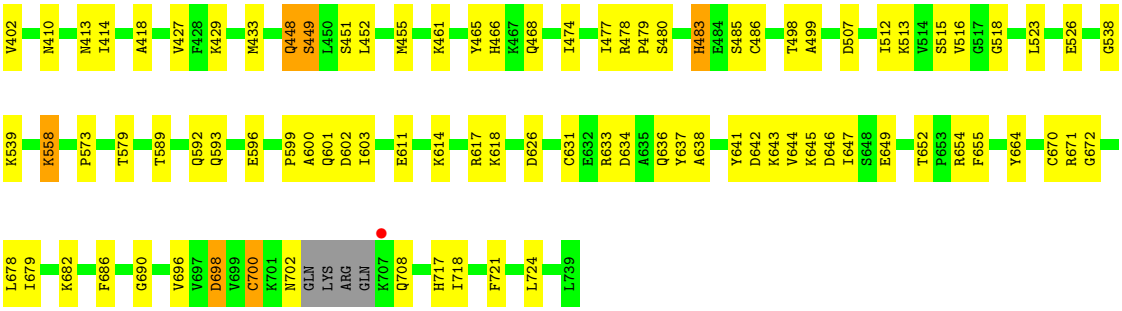
Chain A:



• Molecule 1: Complement factor B

Chain C:



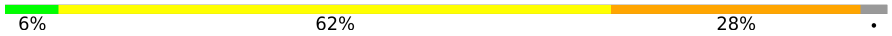


- Molecule 2: DNA (32-MER)

Chain B:

- Molecule 2: DNA (32-MER)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.04Å 145.75Å 87.06Å 90.00° 109.62° 90.00°	Depositor
Resolution (Å)	42.88 – 3.50 42.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (42.88-3.50) 96.6 (42.88-3.50)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.48Å)	Xtriage
Refinement program	PHENIX v1.17	Depositor
R, R_{free}	0.227 , 0.257 0.226 , 0.256	Depositor DCC
R_{free} test set	1998 reflections (8.01%)	wwPDB-VP
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.349 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12610	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMG, 85Y

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	0.47	5/5673 (0.1%)	0.52	3/7678 (0.0%)
1	C	0.43	2/5673 (0.0%)	0.50	0/7678
2	B	1.54	1/358 (0.3%)	1.30	1/544 (0.2%)
2	D	0.92	0/358	0.86	0/544
All	All	0.53	8/12062 (0.1%)	0.57	4/16444 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	LYS	C-N	10.68	1.52	1.33
1	C	479	PRO	N-CD	-9.37	1.34	1.47
1	A	479	PRO	N-CD	-9.36	1.34	1.47
1	A	348	PRO	N-CD	7.92	1.58	1.47
1	A	482	GLY	C-N	6.15	1.48	1.34
2	B	7	DG	C3'-O3'	-5.58	1.36	1.44
1	A	28	GLN	C-N	-5.53	1.21	1.34
1	C	28	GLN	C-N	-5.52	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	481	LYS	C-N-CA	-8.72	103.98	122.30
1	A	481	LYS	O-C-N	7.39	135.77	123.20
1	A	481	LYS	CA-C-N	-6.83	102.53	116.20
2	B	5	OMG	P-O3'-C3'	5.07	125.79	119.70

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	5549	0	5419	103	0
1	C	5549	0	5419	118	0
2	B	756	0	283	38	0
2	D	756	0	283	33	0
All	All	12610	0	11404	259	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 11.

All (259) 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)
1:A:478:ARG:NH1	1:A:507:ASP:OD2	1.75	1.19
1:C:478:ARG:NH1	1:C:507:ASP:OD2	1.75	1.18
1:C:477:ILE:HD13	1:C:483:HIS:ND1	1.68	1.08
1:C:347:VAL:HB	1:C:348:PRO:HD3	1.37	1.04
1:C:50:THR:HB	2:D:22:85Y:C27	1.87	1.04
1:A:626:ASP:OD2	1:C:626:ASP:OD2	1.76	1.01
1:C:477:ILE:CD1	1:C:483:HIS:ND1	2.31	0.93
1:A:347:VAL:HB	1:A:348:PRO:HD3	1.48	0.92
1:C:50:THR:HB	2:D:22:85Y:C28	2.08	0.82
1:C:477:ILE:CD1	1:C:483:HIS:CE1	2.63	0.81
1:A:29:GLU:OE2	1:C:643:LYS:C	2.21	0.79
1:A:636:GLN:NE2	1:C:29:GLU:HA	1.98	0.79
1:A:347:VAL:HB	1:A:348:PRO:CD	2.13	0.78
1:A:29:GLU:HA	1:C:636:GLN:NE2	1.98	0.78
1:A:643:LYS:C	1:C:29:GLU:OE2	2.21	0.78
2:B:17:DA:H2"	2:B:18:OMG:OP1	1.85	0.77
2:B:13:DA:H1'	2:B:14:DA:H5'	1.68	0.76
1:C:111:THR:OG1	1:C:134:ASP:O	2.02	0.76
1:A:111:THR:OG1	1:A:134:ASP:O	2.02	0.75
1:A:29:GLU:HA	1:C:636:GLN:HE22	1.52	0.74
1:C:478:ARG:HD3	1:C:507:ASP:OD1	1.88	0.73
1:C:485:SER:O	1:C:672:GLY:HA2	1.88	0.73
1:A:485:SER:O	1:A:672:GLY:HA2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:DA:H2"	2:B:9:DA:H5'	1.70	0.72
1:A:600:ALA:HB3	1:C:600:ALA:HB3	1.72	0.71
1:C:345:ASP:O	1:C:346:ASP:OD1	2.08	0.71
1:A:478:ARG:HD3	1:A:507:ASP:OD1	1.88	0.71
1:A:636:GLN:HE22	1:C:29:GLU:HA	1.54	0.70
1:C:347:VAL:HB	1:C:348:PRO:CD	2.20	0.70
2:D:17:DA:H2"	2:D:18:OMG:OP1	1.92	0.69
1:C:389:ASP:OD1	1:C:390:ARG:N	2.27	0.67
1:A:389:ASP:OD1	1:A:390:ARG:N	2.27	0.67
1:A:600:ALA:CB	1:C:600:ALA:HB3	2.25	0.66
2:B:12:DG:N2	2:B:21:DG:H21	1.91	0.66
1:A:600:ALA:HB3	1:C:600:ALA:CB	2.25	0.65
1:C:347:VAL:CB	1:C:348:PRO:HD3	2.19	0.65
2:D:12:DG:N2	2:D:21:DG:H21	1.95	0.64
2:B:15:DG:H2'	2:B:16:85Y:C6	2.27	0.64
1:A:418:ALA:CB	1:A:427:VAL:HG22	2.28	0.63
1:C:418:ALA:CB	1:C:427:VAL:HG22	2.29	0.63
1:A:290:ALA:O	1:A:328:THR:HA	1.99	0.63
1:A:478:ARG:HG3	1:A:478:ARG:O	1.99	0.62
2:B:3:OMC:N4	2:B:29:OMG:HN1	1.96	0.62
1:C:478:ARG:O	1:C:478:ARG:HG3	1.99	0.62
1:C:290:ALA:O	1:C:328:THR:HA	1.99	0.62
1:A:350:GLU:OE2	1:A:354:ARG:NH2	2.33	0.61
1:C:350:GLU:OE2	1:C:354:ARG:NH2	2.33	0.61
2:B:19:OMG:HN22	2:B:26:DC:N4	1.98	0.61
1:C:82:HIS:CE1	1:C:150:ARG:HD3	2.36	0.61
1:C:579:THR:OG1	1:C:593:GLN:NE2	2.33	0.61
1:A:82:HIS:CE1	1:A:150:ARG:HD3	2.36	0.60
2:D:15:DG:H2'	2:D:16:85Y:C6	2.31	0.60
1:A:579:THR:OG1	1:A:593:GLN:NE2	2.33	0.59
1:A:410:ASN:ND2	1:A:413:ASN:OD1	2.35	0.59
1:C:468:GLN:HE21	1:C:617:ARG:HE	1.50	0.59
1:A:468:GLN:HE21	1:A:617:ARG:HE	1.50	0.59
1:C:410:ASN:ND2	1:C:413:ASN:OD1	2.36	0.58
1:C:526:GLU:HG3	1:C:558:LYS:HG3	1.85	0.58
1:A:452:LEU:HD23	1:A:455:MET:HG3	1.86	0.58
1:C:596:GLU:O	1:C:682:LYS:NZ	2.37	0.58
1:C:452:LEU:HD23	1:C:455:MET:HG3	1.86	0.57
1:C:256:ILE:HG12	1:C:433:MET:HE1	1.87	0.57
2:D:19:OMG:H4'	2:D:19:OMG:OP1	2.05	0.57
2:B:18:OMG:OP1	2:B:18:OMG:H4'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLU:HG3	1:A:558:LYS:HG3	1.85	0.57
1:A:599:PRO:HD2	1:A:603:ILE:HG12	1.85	0.57
1:C:599:PRO:HD2	1:C:603:ILE:HG12	1.85	0.56
1:A:596:GLU:O	1:A:682:LYS:NZ	2.37	0.56
1:A:670:CYS:HA	1:A:700:CYS:HB2	1.88	0.56
1:A:312:LYS:O	1:A:316:GLU:HG3	2.06	0.56
2:B:15:DG:H2"	2:B:16:85Y:O5'	2.06	0.56
1:C:670:CYS:HA	1:C:700:CYS:HB2	1.88	0.55
2:D:3:OMC:H6	2:D:3:OMC:H5'	1.71	0.55
2:B:9:DA:H61	2:B:13:DA:H2	1.55	0.55
1:A:644:VAL:N	1:C:29:GLU:OE2	2.40	0.55
1:A:29:GLU:OE2	1:C:644:VAL:N	2.39	0.55
2:B:19:OMG:H4'	2:B:19:OMG:OP1	2.07	0.55
1:C:253:SER:OG	1:C:328:THR:OG1	2.25	0.55
1:C:312:LYS:O	1:C:316:GLU:HG3	2.06	0.54
2:D:19:OMG:HN22	2:D:26:DC:N4	2.05	0.54
2:B:8:DA:H2"	2:B:9:DA:C5'	2.38	0.54
1:C:638:ALA:HB2	1:C:696:VAL:HA	1.90	0.54
1:A:253:SER:OG	1:A:328:THR:OG1	2.25	0.54
2:B:6:DA:H2"	2:B:7:DG:O5'	2.08	0.54
1:A:256:ILE:HG12	1:A:433:MET:HE1	1.89	0.54
1:A:347:VAL:CB	1:A:348:PRO:HD3	2.31	0.54
2:D:8:DA:H2"	2:D:9:DA:H5'	1.89	0.53
1:A:345:ASP:O	1:A:346:ASP:OD1	2.26	0.53
1:A:498:THR:OG1	1:A:499:ALA:N	2.42	0.53
2:B:11:DA:H2"	2:B:12:DG:H5'	1.91	0.53
1:A:112:LEU:HD21	1:A:116:ALA:HB2	1.90	0.53
1:A:646:ASP:HB3	1:A:649:GLU:HG3	1.90	0.53
1:C:343:TRP:CD1	1:C:349:PRO:HD3	2.43	0.53
1:A:38:PRO:HG3	1:A:664:TYR:HB3	1.91	0.53
1:A:638:ALA:HB2	1:A:696:VAL:HA	1.90	0.53
1:C:112:LEU:HD21	1:C:116:ALA:HB2	1.90	0.53
1:C:418:ALA:HB3	1:C:427:VAL:HG22	1.90	0.52
1:A:418:ALA:HB3	1:A:427:VAL:HG22	1.90	0.52
1:C:477:ILE:HD12	1:C:483:HIS:CE1	2.44	0.52
1:A:26:LEU:HD12	1:C:633:ARG:CD	2.39	0.52
1:A:135:ASN:OD1	1:A:136:GLY:N	2.42	0.52
2:B:3:OMC:H6	2:B:3:OMC:H5'	1.75	0.52
1:C:135:ASN:OD1	1:C:136:GLY:N	2.42	0.52
2:B:12:DG:H21	2:B:21:DG:H21	1.58	0.52
1:C:498:THR:OG1	1:C:499:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:DA:H2"	2:B:10:85Y:O5'	2.10	0.52
1:C:477:ILE:HD13	1:C:483:HIS:CE1	2.33	0.52
2:B:10:85Y:O4	2:B:10:85Y:N22	2.42	0.51
1:A:589:THR:N	1:A:592:GLN:OE1	2.34	0.51
1:A:642:ASP:O	1:C:29:GLU:OE1	2.29	0.51
1:C:38:PRO:HG3	1:C:664:TYR:HB3	1.91	0.51
1:A:59:THR:HG23	2:B:11:DA:OP1	2.11	0.51
1:C:646:ASP:HB3	1:C:649:GLU:HG3	1.90	0.51
1:A:347:VAL:CB	1:A:348:PRO:CD	2.83	0.51
1:A:265:LYS:HE3	1:A:317:ILE:HG12	1.93	0.51
1:C:265:LYS:HE3	1:C:317:ILE:HG12	1.93	0.50
1:A:207:GLU:O	1:A:211:SER:OG	2.30	0.50
1:C:465:TYR:CD2	1:C:518:GLY:HA3	2.46	0.50
1:C:46:VAL:HB	2:D:23:DA:N6	2.27	0.50
1:C:151:LYS:NZ	1:C:153:GLY:O	2.44	0.50
1:C:448:GLN:HB2	1:C:452:LEU:HD22	1.95	0.49
2:D:3:OMC:N4	2:D:29:OMG:HN1	2.10	0.49
2:B:19:OMG:N2	2:B:26:DC:N4	2.60	0.49
1:C:134:ASP:OD1	1:C:135:ASN:N	2.46	0.49
2:D:13:DA:N6	2:D:19:OMG:HN1	2.10	0.49
1:A:311:THR:O	1:A:315:ASN:ND2	2.46	0.49
1:A:151:LYS:NZ	1:A:153:GLY:O	2.43	0.48
1:A:334:LEU:HD12	1:A:373:PRO:HB2	1.95	0.48
1:A:477:ILE:HD13	1:A:483:HIS:ND1	2.28	0.48
1:A:26:LEU:HD12	1:C:633:ARG:HD2	1.96	0.48
1:C:46:VAL:HB	2:D:23:DA:C6	2.48	0.48
2:D:9:DA:H61	2:D:13:DA:H2	1.60	0.48
1:A:482:GLY:O	1:A:484:GLU:N	2.46	0.48
1:A:134:ASP:OD1	1:A:135:ASN:N	2.46	0.48
1:A:448:GLN:HB2	1:A:452:LEU:HD22	1.95	0.48
1:C:311:THR:O	1:C:315:ASN:ND2	2.46	0.48
1:C:334:LEU:HD12	1:C:373:PRO:HB2	1.95	0.48
1:C:589:THR:N	1:C:592:GLN:OE1	2.34	0.48
1:A:308:ASP:O	1:A:312:LYS:HG3	2.14	0.48
1:C:207:GLU:O	1:C:211:SER:OG	2.30	0.47
1:A:671:ARG:HE	1:A:698:ASP:CG	2.18	0.47
1:C:671:ARG:HE	1:C:698:ASP:CG	2.18	0.47
1:C:638:ALA:O	1:C:641:TYR:HB2	2.15	0.47
1:A:474:ILE:N	1:A:486:CYS:O	2.34	0.47
1:C:308:ASP:O	1:C:312:LYS:HG3	2.14	0.47
1:C:652:THR:H	1:C:655:PHE:HD2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:HA	1:A:320:GLU:HA	1.60	0.47
1:A:633:ARG:CD	1:C:26:LEU:HD12	2.44	0.47
1:A:652:THR:H	1:A:655:PHE:HD2	1.61	0.47
1:C:474:ILE:N	1:C:486:CYS:O	2.34	0.47
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.82	0.46
1:A:638:ALA:O	1:A:641:TYR:HB2	2.15	0.46
1:C:347:VAL:CB	1:C:348:PRO:CD	2.86	0.46
1:A:29:GLU:OE1	1:C:642:ASP:O	2.33	0.46
2:B:3:OMC:H5'	2:B:3:OMC:C6	2.50	0.46
1:C:516:VAL:HG22	1:C:523:LEU:HD11	1.97	0.46
1:A:46:VAL:HB	2:B:23:DA:C6	2.51	0.46
2:B:13:DA:C6	2:B:14:DA:C2	3.04	0.46
1:C:319:TYR:HA	1:C:320:GLU:HA	1.60	0.45
2:D:20:DA:H2"	2:D:21:DG:OP1	2.16	0.45
1:C:346:ASP:HA	1:C:347:VAL:HA	1.62	0.45
1:A:29:GLU:OE1	1:C:643:LYS:HA	2.17	0.45
2:B:5:OMG:H5"	2:B:6:DA:H5'	1.98	0.45
2:D:2:OMG:H1'	2:D:2:OMG:HM23	1.74	0.45
2:D:8:DA:H2"	2:D:9:DA:C5'	2.47	0.45
1:C:91:PRO:O	1:C:96:TYR:OH	2.30	0.45
2:D:18:OMG:HM22	2:D:18:OMG:H8	1.81	0.45
1:A:478:ARG:HH11	1:A:507:ASP:CG	2.09	0.44
1:A:633:ARG:HD2	1:C:26:LEU:HD12	1.99	0.44
2:B:12:DG:N2	2:B:21:DG:N2	2.64	0.44
1:C:343:TRP:CD1	1:C:343:TRP:O	2.70	0.44
1:C:611:GLU:O	1:C:614:LYS:HB2	2.17	0.44
1:A:46:VAL:HB	2:B:23:DA:N6	2.33	0.44
1:A:643:LYS:HA	1:C:29:GLU:OE1	2.17	0.44
2:B:19:OMG:H1'	2:B:19:OMG:HM23	1.59	0.44
1:A:611:GLU:O	1:A:614:LYS:HB2	2.17	0.44
2:D:18:OMG:OP1	2:D:18:OMG:H4'	2.18	0.44
1:C:259:SER:O	1:C:262:THR:OG1	2.28	0.44
1:A:637:TYR:O	1:A:637:TYR:CD2	2.70	0.44
1:A:634:ASP:O	1:A:696:VAL:HG21	2.18	0.43
2:B:30:OMC:H1'	2:B:30:OMC:HM23	1.63	0.43
1:C:618:LYS:HA	1:C:618:LYS:HD3	1.69	0.43
2:D:15:DG:H2"	2:D:16:85Y:O5'	2.17	0.43
1:C:271:LEU:O	1:C:275:VAL:HG23	2.18	0.43
1:A:643:LYS:CA	1:C:29:GLU:OE2	2.66	0.43
1:A:265:LYS:O	1:A:269:VAL:HG23	2.18	0.43
1:C:265:LYS:O	1:C:269:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:ARG:HE	1:C:390:ARG:HB3	1.62	0.43
1:C:634:ASP:O	1:C:696:VAL:HG21	2.18	0.43
1:C:637:TYR:O	1:C:637:TYR:CD2	2.70	0.43
1:A:701:LYS:HE2	1:A:701:LYS:HB2	1.89	0.43
2:B:27:85Y:N22	2:B:27:85Y:O4	2.52	0.43
1:C:199:TYR:CE1	1:C:429:LYS:HE2	2.54	0.43
1:C:478:ARG:HH11	1:C:507:ASP:CG	2.09	0.43
1:A:26:LEU:HD12	1:C:633:ARG:HD3	2.00	0.43
2:B:1:OMC:H4'	2:B:2:OMG:OP1	2.17	0.43
1:C:50:THR:HB	2:D:22:85Y:C33	2.44	0.43
1:A:314:LEU:C	1:A:316:GLU:H	2.23	0.43
2:D:8:DA:C6	2:D:9:DA:C2	3.06	0.43
1:A:199:TYR:CE1	1:A:429:LYS:HE2	2.53	0.43
1:A:402:VAL:HG11	1:A:414:ILE:HB	2.01	0.43
1:C:59:THR:HG23	2:D:11:DA:OP1	2.19	0.43
2:D:13:DA:C6	2:D:14:DA:C2	3.06	0.43
1:C:449:SER:OG	1:C:451:SER:N	2.49	0.42
1:A:690:GLY:HA2	1:A:718:ILE:O	2.20	0.42
1:C:402:VAL:HG11	1:C:414:ILE:HB	2.01	0.42
1:A:29:GLU:CA	1:C:636:GLN:NE2	2.77	0.42
2:B:8:DA:C6	2:B:9:DA:C2	3.07	0.42
1:C:647:ILE:HD12	1:C:647:ILE:HA	1.87	0.42
1:C:679:ILE:HG21	1:C:686:PHE:HB3	2.01	0.42
2:D:11:DA:H2"	2:D:12:DG:H5'	2.01	0.42
2:D:13:DA:N3	2:D:13:DA:H2'	2.33	0.42
2:D:29:OMG:HM23	2:D:29:OMG:H1'	1.78	0.42
1:A:679:ILE:HG21	1:A:686:PHE:HB3	2.01	0.42
2:B:9:DA:N1	2:B:13:DA:N1	2.66	0.42
1:C:589:THR:H	1:C:589:THR:HG1	1.64	0.42
1:A:271:LEU:O	1:A:275:VAL:HG23	2.18	0.42
1:A:390:ARG:HE	1:A:390:ARG:HB3	1.62	0.42
1:A:425:GLN:NE2	1:A:427:VAL:O	2.49	0.42
1:C:201:THR:O	1:C:205:VAL:HG23	2.20	0.42
1:C:678:LEU:HD22	1:C:717:HIS:CG	2.55	0.42
1:A:125:ARG:NH2	1:A:194:GLN:OE1	2.53	0.42
1:A:678:LEU:HD22	1:A:717:HIS:CG	2.55	0.42
1:C:512:ILE:O	1:C:513:LYS:HD3	2.20	0.42
1:C:125:ARG:NH2	1:C:194:GLN:OE1	2.53	0.41
2:D:11:DA:H5"	2:D:12:DG:C6	2.55	0.41
2:D:9:DA:H2"	2:D:10:85Y:O5'	2.21	0.41
1:A:346:ASP:HA	1:A:347:VAL:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ILE:O	1:A:513:LYS:HD3	2.20	0.41
1:C:271:LEU:HD21	1:C:360:ILE:HD13	2.02	0.41
1:C:314:LEU:C	1:C:316:GLU:H	2.23	0.41
1:C:690:GLY:HA2	1:C:718:ILE:O	2.19	0.41
1:C:573:PRO:HB3	1:C:721:PHE:CZ	2.55	0.41
1:C:724:LEU:HA	1:C:724:LEU:HD23	1.88	0.41
2:B:4:85Y:C32	2:B:18:OMG:HM22	2.50	0.41
1:C:538:GLY:HA3	1:C:539:LYS:C	2.41	0.41
2:D:21:DG:H2"	2:D:25:DG:O6	2.20	0.41
2:B:8:DA:C2'	2:B:9:DA:H5'	2.44	0.41
1:C:601:GLN:HB3	1:C:602:ASP:H	1.72	0.41
1:A:449:SER:OG	1:A:451:SER:N	2.49	0.41
1:A:573:PRO:HB3	1:A:721:PHE:CZ	2.55	0.41
1:A:724:LEU:HD23	1:A:724:LEU:HA	1.88	0.41
1:A:62:THR:C	2:B:10:85Y:C28	2.89	0.41
1:A:113:ARG:HG2	1:A:132:ILE:HB	2.03	0.41
1:A:618:LYS:HA	1:A:618:LYS:HD3	1.69	0.41
2:B:2:OMG:HM23	2:B:2:OMG:H1'	1.75	0.41
1:C:254:ASP:HB3	1:C:364:ASP:OD2	2.21	0.41
1:C:461:LYS:HE3	1:C:461:LYS:HB3	1.84	0.41
2:D:18:OMG:HM22	2:D:18:OMG:C8	2.56	0.41
2:D:19:OMG:HM23	2:D:19:OMG:H1'	1.89	0.41
2:D:5:OMG:C4	2:D:5:OMG:HM23	2.56	0.41
1:A:201:THR:O	1:A:205:VAL:HG23	2.20	0.40
2:B:13:DA:H2'	2:B:13:DA:N3	2.36	0.40
1:C:253:SER:HB3	1:C:290:ALA:HA	2.02	0.40
2:B:19:OMG:N2	2:B:26:DC:C4	2.88	0.40
1:C:269:VAL:HG22	1:C:311:THR:HG23	2.02	0.40
1:A:126:TRP:NE1	1:A:147:ILE:HG21	2.36	0.40
1:A:253:SER:HB3	1:A:290:ALA:HA	2.02	0.40
1:A:538:GLY:HA3	1:A:539:LYS:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	693/764 (91%)	643 (93%)	47 (7%)	3 (0%)	34	72
1	C	693/764 (91%)	646 (93%)	45 (6%)	2 (0%)	41	75
All	All	1386/1528 (91%)	1289 (93%)	92 (7%)	5 (0%)	34	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	PRO
1	A	483	HIS
1	C	483	HIS
1	C	347	VAL
1	A	349	PRO

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	614/665 (92%)	592 (96%)	22 (4%)	35	66
1	C	614/665 (92%)	591 (96%)	23 (4%)	34	65
All	All	1228/1330 (92%)	1183 (96%)	45 (4%)	34	65

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	25	ARG
1	A	58	SER
1	A	90	TRP
1	A	112	LEU
1	A	239	ASP
1	A	277	SER
1	A	382	ASP

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Mol	Chain	Res	Type
1	A	390	ARG
1	A	448	GLN
1	A	449	SER
1	A	466	HIS
1	A	480	SER
1	A	515	SER
1	A	558	LYS
1	A	631	CYS
1	A	645	LYS
1	A	654	ARG
1	A	698	ASP
1	A	700	CYS
1	A	702	ASN
1	A	708	GLN
1	C	20	LYS
1	C	25	ARG
1	C	58	SER
1	C	90	TRP
1	C	112	LEU
1	C	239	ASP
1	C	277	SER
1	C	345	ASP
1	C	382	ASP
1	C	390	ARG
1	C	448	GLN
1	C	449	SER
1	C	466	HIS
1	C	480	SER
1	C	515	SER
1	C	558	LYS
1	C	631	CYS
1	C	645	LYS
1	C	654	ARG
1	C	698	ASP
1	C	700	CYS
1	C	702	ASN
1	C	708	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	GLN

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Mol	Chain	Res	Type
1	A	636	GLN
1	C	468	GLN
1	C	636	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

32 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	OMC	D	30	2	19,22,23	3.39	8 (42%)	26,31,34	0.65	0
2	85Y	B	24	2	33,36,37	4.51	15 (45%)	47,51,54	2.90	11 (23%)
2	85Y	D	22	2	33,36,37	4.50	14 (42%)	47,51,54	2.50	10 (21%)
2	85Y	D	28	2	33,36,37	4.72	14 (42%)	47,51,54	3.05	11 (23%)
2	85Y	D	24	2	33,36,37	4.61	15 (45%)	47,51,54	2.86	11 (23%)
2	OMC	B	3	2	19,22,23	3.19	8 (42%)	26,31,34	1.05	2 (7%)
2	OMC	B	1	2	19,22,23	3.57	8 (42%)	26,31,34	1.87	7 (26%)
2	OMG	D	18	2	18,26,27	2.76	7 (38%)	19,38,41	1.54	4 (21%)
2	85Y	B	4	2	33,36,37	4.70	14 (42%)	47,51,54	3.12	13 (27%)
2	85Y	D	10	2	33,36,37	4.49	14 (42%)	47,51,54	2.73	10 (21%)
2	85Y	B	16	2	33,36,37	4.54	16 (48%)	47,51,54	3.18	15 (31%)
2	OMG	B	29	2	18,26,27	2.67	7 (38%)	19,38,41	1.61	4 (21%)
2	OMG	D	19	2	18,26,27	2.37	7 (38%)	19,38,41	1.36	4 (21%)
2	OMC	D	3	2	19,22,23	3.29	8 (42%)	26,31,34	0.81	0
2	OMG	B	5	2	18,26,27	2.70	7 (38%)	19,38,41	1.90	4 (21%)
2	OMG	B	18	2	18,26,27	3.13	7 (38%)	19,38,41	1.97	7 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	85Y	B	27	2	33,36,37	4.81	14 (42%)	47,51,54	3.54	18 (38%)
2	OMC	D	1	2	19,22,23	3.48	8 (42%)	26,31,34	1.71	7 (26%)
2	85Y	D	16	2	33,36,37	4.63	15 (45%)	47,51,54	2.67	16 (34%)
2	OMG	B	19	2	18,26,27	2.19	7 (38%)	19,38,41	1.23	3 (15%)
2	OMG	B	31	2	18,26,27	3.01	6 (33%)	19,38,41	1.59	6 (31%)
2	OMG	D	2	2	18,26,27	2.62	8 (44%)	19,38,41	1.47	3 (15%)
2	85Y	B	22	2	33,36,37	4.53	15 (45%)	47,51,54	2.82	14 (29%)
2	OMG	D	29	2	18,26,27	2.60	8 (44%)	19,38,41	1.47	5 (26%)
2	OMC	B	30	2	19,22,23	3.51	8 (42%)	26,31,34	0.74	0
2	85Y	B	28	2	33,36,37	4.78	14 (42%)	47,51,54	3.50	15 (31%)
2	85Y	D	27	2	33,36,37	4.68	14 (42%)	47,51,54	3.12	14 (29%)
2	OMG	D	5	2	18,26,27	2.71	7 (38%)	19,38,41	1.70	4 (21%)
2	85Y	B	10	2	33,36,37	4.42	12 (36%)	47,51,54	3.38	18 (38%)
2	85Y	D	4	2	33,36,37	4.64	15 (45%)	47,51,54	2.96	11 (23%)
2	OMG	D	31	2	18,26,27	2.76	7 (38%)	19,38,41	1.50	5 (26%)
2	OMG	B	2	2	18,26,27	2.84	7 (38%)	19,38,41	1.57	4 (21%)

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	OMC	D	30	2	-	4/9/27/28	0/2/2/2
2	85Y	B	24	2	-	1/16/30/31	0/4/4/4
2	85Y	D	22	2	-	4/16/30/31	0/4/4/4
2	85Y	D	28	2	-	7/16/30/31	0/4/4/4
2	85Y	D	24	2	-	1/16/30/31	0/4/4/4
2	OMC	B	3	2	-	2/9/27/28	0/2/2/2
2	OMC	B	1	2	-	5/9/27/28	0/2/2/2
2	OMG	D	18	2	-	4/5/27/28	0/3/3/3
2	85Y	B	4	2	-	2/16/30/31	0/4/4/4
2	85Y	D	10	2	-	3/16/30/31	0/4/4/4
2	85Y	B	16	2	-	3/16/30/31	0/4/4/4
2	OMG	B	29	2	-	2/5/27/28	0/3/3/3
2	OMG	D	19	2	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	D	3	2	-	0/9/27/28	0/2/2/2
2	OMG	B	5	2	-	3/5/27/28	0/3/3/3
2	OMG	B	18	2	-	4/5/27/28	0/3/3/3
2	85Y	B	27	2	-	2/16/30/31	0/4/4/4
2	OMC	D	1	2	-	5/9/27/28	0/2/2/2
2	85Y	D	16	2	-	0/16/30/31	0/4/4/4
2	OMG	B	19	2	-	4/5/27/28	0/3/3/3
2	OMG	B	31	2	-	3/5/27/28	0/3/3/3
2	OMG	D	2	2	-	3/5/27/28	0/3/3/3
2	85Y	B	22	2	-	6/16/30/31	0/4/4/4
2	OMG	D	29	2	-	3/5/27/28	0/3/3/3
2	OMC	B	30	2	-	4/9/27/28	0/2/2/2
2	85Y	B	28	2	-	7/16/30/31	0/4/4/4
2	85Y	D	27	2	-	2/16/30/31	0/4/4/4
2	OMG	D	5	2	-	2/5/27/28	0/3/3/3
2	85Y	B	10	2	-	7/16/30/31	0/4/4/4
2	85Y	D	4	2	-	2/16/30/31	0/4/4/4
2	OMG	D	31	2	-	3/5/27/28	0/3/3/3
2	OMG	B	2	2	-	2/5/27/28	0/3/3/3

All (334) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	85Y	C2-N1	12.23	1.58	1.38
2	D	28	85Y	C6-N1	11.87	1.58	1.38
2	B	27	85Y	C6-N1	11.86	1.58	1.38
2	B	27	85Y	C5-C4	11.86	1.66	1.45
2	D	27	85Y	C6-N1	11.85	1.58	1.38
2	B	28	85Y	C6-N1	11.77	1.58	1.38
2	B	4	85Y	C6-N1	11.73	1.58	1.38
2	D	27	85Y	C5-C4	11.69	1.66	1.45
2	D	28	85Y	C5-C4	11.66	1.66	1.45
2	D	4	85Y	C6-N1	11.54	1.57	1.38
2	B	4	85Y	C5-C4	11.52	1.66	1.45
2	D	24	85Y	C6-N1	11.48	1.57	1.38
2	D	16	85Y	C2-N1	11.48	1.56	1.38
2	D	16	85Y	C6-N1	11.38	1.57	1.38
2	B	28	85Y	C5-C4	11.38	1.65	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	85Y	C5-C4	11.37	1.65	1.45
2	D	24	85Y	C5-C4	11.19	1.65	1.45
2	D	10	85Y	C2-N1	11.15	1.56	1.38
2	D	16	85Y	C5-C4	11.11	1.65	1.45
2	B	10	85Y	C2-N1	11.06	1.56	1.38
2	B	24	85Y	C5-C4	11.03	1.65	1.45
2	D	22	85Y	C5-C4	11.03	1.65	1.45
2	B	22	85Y	C6-N1	11.00	1.56	1.38
2	D	10	85Y	C6-N1	10.99	1.56	1.38
2	B	24	85Y	C6-N1	10.89	1.56	1.38
2	D	22	85Y	C6-N1	10.88	1.56	1.38
2	D	28	85Y	C2-N1	10.81	1.55	1.38
2	B	28	85Y	C2-N1	10.77	1.55	1.38
2	D	27	85Y	C2-N1	10.73	1.55	1.38
2	D	22	85Y	C2-N1	10.67	1.55	1.38
2	B	22	85Y	C5-C4	10.58	1.64	1.45
2	D	4	85Y	C2-N1	10.57	1.55	1.38
2	B	16	85Y	C6-N1	10.55	1.56	1.38
2	D	10	85Y	C5-C4	10.54	1.64	1.45
2	B	10	85Y	C6-N1	10.49	1.55	1.38
2	B	22	85Y	C2-N1	10.47	1.55	1.38
2	B	16	85Y	C5-C4	10.45	1.64	1.45
2	D	24	85Y	C2-N1	10.43	1.55	1.38
2	B	27	85Y	C2-N1	10.39	1.55	1.38
2	B	10	85Y	C5-C4	10.13	1.63	1.45
2	B	24	85Y	C2-N1	9.98	1.54	1.38
2	B	4	85Y	C2-N1	9.91	1.54	1.38
2	D	10	85Y	O4'-C1'	8.75	1.61	1.42
2	B	28	85Y	O4'-C1'	8.57	1.61	1.42
2	D	24	85Y	O4'-C1'	8.54	1.61	1.42
2	B	10	85Y	O4'-C1'	8.54	1.61	1.42
2	D	28	85Y	O4'-C1'	8.51	1.61	1.42
2	B	22	85Y	O4'-C1'	8.46	1.61	1.42
2	D	4	85Y	O4'-C1'	8.44	1.61	1.42
2	D	27	85Y	O4'-C1'	8.43	1.61	1.42
2	B	27	85Y	O4'-C1'	8.41	1.61	1.42
2	B	4	85Y	C2'-C1'	-8.40	1.28	1.52
2	D	16	85Y	O4'-C1'	8.38	1.61	1.42
2	B	24	85Y	O4'-C1'	8.37	1.61	1.42
2	D	22	85Y	O4'-C1'	8.36	1.61	1.42
2	B	16	85Y	O4'-C1'	8.28	1.60	1.42
2	B	4	85Y	O4'-C1'	8.16	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	85Y	C20-N22	8.13	1.47	1.33
2	D	4	85Y	C2'-C1'	-8.09	1.29	1.52
2	B	27	85Y	C20-N22	8.07	1.47	1.33
2	B	27	85Y	C2'-C1'	-8.07	1.29	1.52
2	D	24	85Y	C2'-C1'	-7.94	1.30	1.52
2	B	24	85Y	C2'-C1'	-7.88	1.30	1.52
2	D	22	85Y	C2'-C1'	-7.83	1.30	1.52
2	B	4	85Y	O4'-C4'	-7.80	1.27	1.45
2	D	27	85Y	C2'-C1'	-7.78	1.30	1.52
2	B	22	85Y	C20-N22	7.74	1.46	1.33
2	B	22	85Y	C2'-C1'	-7.74	1.30	1.52
2	D	16	85Y	C2'-C1'	-7.69	1.30	1.52
2	D	28	85Y	C2'-C1'	-7.64	1.31	1.52
2	B	28	85Y	C2'-C1'	-7.63	1.31	1.52
2	D	4	85Y	O4'-C4'	-7.55	1.28	1.45
2	B	16	85Y	C2'-C1'	-7.53	1.31	1.52
2	B	10	85Y	C2'-C1'	-7.41	1.31	1.52
2	B	10	85Y	O4'-C4'	-7.41	1.28	1.45
2	D	10	85Y	C2'-C1'	-7.39	1.31	1.52
2	D	10	85Y	O4'-C4'	-7.36	1.28	1.45
2	D	16	85Y	O4'-C4'	-7.25	1.28	1.45
2	B	27	85Y	O4'-C4'	-7.18	1.29	1.45
2	D	27	85Y	O4'-C4'	-7.13	1.29	1.45
2	B	1	OMC	C2-N3	7.12	1.50	1.36
2	D	28	85Y	O4'-C4'	-7.11	1.29	1.45
2	B	4	85Y	C20-N22	7.10	1.45	1.33
2	D	28	85Y	C20-N22	7.04	1.45	1.33
2	D	24	85Y	O4'-C4'	-7.03	1.29	1.45
2	B	16	85Y	O4'-C4'	-7.02	1.29	1.45
2	B	1	OMC	C4-N3	6.96	1.48	1.34
2	D	22	85Y	O4'-C4'	-6.90	1.29	1.45
2	B	30	OMC	C4-N3	6.88	1.48	1.34
2	B	24	85Y	O4'-C4'	-6.86	1.29	1.45
2	D	27	85Y	C20-N22	6.85	1.45	1.33
2	D	1	OMC	C2-N3	6.77	1.50	1.36
2	B	22	85Y	O4'-C4'	-6.71	1.30	1.45
2	B	28	85Y	O4'-C4'	-6.61	1.30	1.45
2	D	1	OMC	C4-N3	6.55	1.47	1.34
2	D	24	85Y	C20-N22	6.51	1.44	1.33
2	B	24	85Y	C20-N22	6.48	1.44	1.33
2	B	1	OMC	C6-C5	6.45	1.50	1.35
2	D	30	OMC	C4-N3	6.43	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	30	OMC	C2-N3	6.41	1.49	1.36
2	D	30	OMC	C2-N3	6.36	1.49	1.36
2	B	30	OMC	C6-C5	6.35	1.49	1.35
2	D	30	OMC	C6-C5	6.35	1.49	1.35
2	D	1	OMC	C6-C5	6.32	1.49	1.35
2	D	3	OMC	C4-N3	6.32	1.47	1.34
2	D	22	85Y	C20-N22	6.31	1.44	1.33
2	D	3	OMC	C2-N3	6.26	1.49	1.36
2	D	4	85Y	C20-N22	6.20	1.44	1.33
2	B	18	OMG	C2-N3	6.19	1.48	1.33
2	B	3	OMC	C4-N3	6.10	1.46	1.34
2	B	2	OMG	C2-N3	6.06	1.47	1.33
2	B	1	OMC	C4-N4	6.06	1.48	1.33
2	B	3	OMC	C2-N3	6.05	1.48	1.36
2	D	3	OMC	C6-C5	6.03	1.49	1.35
2	B	31	OMG	C4-N3	6.01	1.51	1.37
2	D	16	85Y	C20-N22	5.97	1.43	1.33
2	B	30	OMC	C4-N4	5.95	1.47	1.33
2	D	30	OMC	C4-N4	5.89	1.47	1.33
2	D	1	OMC	C4-N4	5.87	1.47	1.33
2	B	18	OMG	C2-N2	5.87	1.48	1.34
2	B	2	OMG	C4-N3	5.86	1.51	1.37
2	B	24	85Y	O2-C2	-5.79	1.12	1.23
2	B	16	85Y	C20-N22	5.79	1.43	1.33
2	D	3	OMC	C4-N4	5.78	1.47	1.33
2	B	27	85Y	O2-C2	-5.76	1.12	1.23
2	B	3	OMC	C4-N4	5.71	1.47	1.33
2	D	1	OMC	C2-N1	5.68	1.52	1.40
2	B	31	OMG	C2-N3	5.68	1.47	1.33
2	B	18	OMG	C4-N3	5.68	1.51	1.37
2	B	3	OMC	C2-N1	5.65	1.52	1.40
2	D	18	OMG	C2-N3	5.65	1.46	1.33
2	D	5	OMG	C2-N3	5.62	1.46	1.33
2	B	1	OMC	C2-N1	5.61	1.52	1.40
2	D	31	OMG	C2-N3	5.59	1.46	1.33
2	B	10	85Y	O2-C2	-5.57	1.12	1.23
2	B	31	OMG	C6-N1	5.56	1.46	1.37
2	D	2	OMG	C2-N3	5.55	1.46	1.33
2	B	5	OMG	C2-N3	5.55	1.46	1.33
2	B	30	OMC	C2-N1	5.51	1.51	1.40
2	B	29	OMG	C4-N3	5.48	1.50	1.37
2	B	29	OMG	C2-N3	5.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	24	85Y	O2-C2	-5.44	1.13	1.23
2	B	3	OMC	C6-C5	5.39	1.47	1.35
2	D	31	OMG	C4-N3	5.38	1.50	1.37
2	B	27	85Y	C4-N3	-5.31	1.29	1.38
2	B	5	OMG	C4-N3	5.30	1.50	1.37
2	D	29	OMG	C2-N3	5.26	1.46	1.33
2	D	19	OMG	C2-N3	5.25	1.45	1.33
2	D	10	85Y	O2-C2	-5.21	1.13	1.23
2	D	5	OMG	C4-N3	5.21	1.50	1.37
2	B	28	85Y	C4-N3	-5.20	1.29	1.38
2	B	4	85Y	O2-C2	-5.18	1.13	1.23
2	D	2	OMG	C4-N3	5.18	1.49	1.37
2	D	27	85Y	O2-C2	-5.18	1.13	1.23
2	D	28	85Y	O2-C2	-5.17	1.13	1.23
2	D	3	OMC	C2-N1	5.13	1.51	1.40
2	D	18	OMG	C2-N2	5.11	1.46	1.34
2	D	30	OMC	C2-N1	5.11	1.51	1.40
2	D	18	OMG	C4-N3	5.10	1.49	1.37
2	B	19	OMG	C2-N3	5.09	1.45	1.33
2	B	18	OMG	C5-C6	5.07	1.57	1.47
2	D	29	OMG	C4-N3	5.06	1.49	1.37
2	D	10	85Y	C20-N22	5.03	1.42	1.33
2	B	28	85Y	O2-C2	-5.01	1.13	1.23
2	B	31	OMG	C2-N2	4.99	1.46	1.34
2	D	4	85Y	O2-C2	-4.98	1.13	1.23
2	B	29	OMG	C2-N2	4.96	1.46	1.34
2	B	18	OMG	C6-N1	4.92	1.45	1.37
2	D	31	OMG	C2-N2	4.91	1.45	1.34
2	B	2	OMG	C2-N2	4.90	1.45	1.34
2	D	22	85Y	O2-C2	-4.87	1.14	1.23
2	B	10	85Y	C4-N3	-4.85	1.29	1.38
2	D	29	OMG	C2-N2	4.84	1.45	1.34
2	D	27	85Y	C4-N3	-4.81	1.29	1.38
2	B	30	OMC	C6-N1	4.72	1.49	1.38
2	D	5	OMG	C2-N2	4.72	1.45	1.34
2	B	28	85Y	C5-C20	4.67	1.64	1.49
2	D	2	OMG	C2-N2	4.62	1.45	1.34
2	D	16	85Y	O2-C2	-4.60	1.14	1.23
2	B	22	85Y	O2-C2	-4.58	1.14	1.23
2	B	27	85Y	C5-C20	4.55	1.64	1.49
2	D	31	OMG	C6-N1	4.52	1.44	1.37
2	B	16	85Y	O2-C2	-4.51	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	19	OMG	C4-N3	4.48	1.48	1.37
2	D	10	85Y	C4-N3	-4.47	1.30	1.38
2	D	28	85Y	C4-N3	-4.46	1.30	1.38
2	D	19	OMG	C2-N2	4.46	1.44	1.34
2	D	30	OMC	C6-N1	4.37	1.48	1.38
2	B	5	OMG	C2-N2	4.35	1.44	1.34
2	B	4	85Y	C4-N3	-4.28	1.30	1.38
2	D	18	OMG	C6-N1	4.27	1.44	1.37
2	B	1	OMC	C6-N1	4.23	1.48	1.38
2	B	31	OMG	C5-C6	4.16	1.55	1.47
2	D	28	85Y	C5-C20	4.16	1.62	1.49
2	D	5	OMG	C6-N1	4.15	1.44	1.37
2	B	2	OMG	C6-N1	4.13	1.44	1.37
2	D	4	85Y	C4-N3	-4.11	1.31	1.38
2	D	1	OMC	C6-N1	4.11	1.47	1.38
2	D	27	85Y	C5-C20	4.06	1.62	1.49
2	B	22	85Y	C4-N3	-4.05	1.31	1.38
2	B	19	OMG	C2-N2	4.05	1.43	1.34
2	B	10	85Y	O3'-C3'	-4.04	1.34	1.43
2	D	24	85Y	C4-N3	-4.04	1.31	1.38
2	B	2	OMG	C5-C6	4.02	1.55	1.47
2	B	16	85Y	O21-C20	-4.01	1.16	1.23
2	B	19	OMG	C4-N3	3.98	1.47	1.37
2	B	5	OMG	C6-N1	3.97	1.43	1.37
2	D	29	OMG	C6-N1	3.96	1.43	1.37
2	B	10	85Y	C20-N22	3.96	1.40	1.33
2	B	29	OMG	C6-N1	3.89	1.43	1.37
2	D	18	OMG	C5-C6	3.87	1.55	1.47
2	D	22	85Y	C4-N3	-3.87	1.31	1.38
2	D	16	85Y	C4-N3	-3.86	1.31	1.38
2	B	5	OMG	C5-C6	3.83	1.55	1.47
2	D	3	OMC	C6-N1	3.82	1.47	1.38
2	D	4	85Y	C5-C20	3.80	1.61	1.49
2	B	4	85Y	C5-C20	3.79	1.61	1.49
2	D	2	OMG	C6-N1	3.78	1.43	1.37
2	B	16	85Y	C4-N3	-3.77	1.31	1.38
2	B	22	85Y	C5-C20	3.76	1.61	1.49
2	B	10	85Y	O21-C20	-3.63	1.16	1.23
2	D	5	OMG	C5-C6	3.59	1.54	1.47
2	B	24	85Y	C4-N3	-3.52	1.32	1.38
2	B	31	OMG	C2-N1	3.51	1.46	1.37
2	D	4	85Y	O3'-C3'	-3.50	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	OMC	C6-N1	3.48	1.46	1.38
2	D	31	OMG	C5-C6	3.48	1.54	1.47
2	B	28	85Y	O4-C4	-3.46	1.17	1.23
2	D	24	85Y	C5-C20	3.45	1.60	1.49
2	D	2	OMG	C5-C6	3.45	1.54	1.47
2	D	22	85Y	C5-C20	3.44	1.60	1.49
2	B	4	85Y	O3'-C3'	-3.44	1.36	1.43
2	D	16	85Y	C5-C20	3.42	1.60	1.49
2	D	10	85Y	O3'-C3'	-3.41	1.36	1.43
2	B	18	OMG	C2-N1	3.40	1.46	1.37
2	B	22	85Y	O3'-C3'	-3.38	1.36	1.43
2	D	22	85Y	O3'-C3'	-3.30	1.36	1.43
2	D	16	85Y	O21-C20	-3.26	1.17	1.23
2	B	28	85Y	C23-N22	3.14	1.52	1.46
2	B	16	85Y	C2-N3	3.14	1.43	1.38
2	B	30	OMC	C5-C4	3.12	1.50	1.42
2	B	24	85Y	C23-N22	3.11	1.52	1.46
2	D	31	OMG	C2-N1	3.07	1.45	1.37
2	D	16	85Y	O3'-C3'	-3.07	1.36	1.43
2	D	19	OMG	C6-N1	3.07	1.42	1.37
2	D	10	85Y	O21-C20	-3.03	1.17	1.23
2	B	19	OMG	O6-C6	-3.03	1.17	1.23
2	B	24	85Y	C5-C20	3.02	1.59	1.49
2	D	18	OMG	C2-N1	3.02	1.45	1.37
2	B	29	OMG	C5-C6	3.00	1.53	1.47
2	B	24	85Y	C2-N3	2.98	1.43	1.38
2	D	29	OMG	C5-C6	2.98	1.53	1.47
2	D	1	OMC	O2-C2	-2.95	1.18	1.23
2	D	28	85Y	O21-C20	-2.92	1.18	1.23
2	B	27	85Y	O4-C4	-2.90	1.18	1.23
2	B	5	OMG	C5-C4	-2.86	1.35	1.43
2	D	3	OMC	O2-C2	-2.85	1.18	1.23
2	B	29	OMG	C5-C4	-2.85	1.35	1.43
2	D	10	85Y	C5-C20	2.85	1.58	1.49
2	D	30	OMC	C5-C4	2.84	1.49	1.42
2	B	19	OMG	C2-N1	2.84	1.44	1.37
2	D	24	85Y	O21-C20	-2.83	1.18	1.23
2	D	30	OMC	O2-C2	-2.81	1.18	1.23
2	B	24	85Y	O21-C20	-2.80	1.18	1.23
2	B	16	85Y	O3'-C3'	-2.80	1.37	1.43
2	D	29	OMG	C5-C4	-2.79	1.36	1.43
2	B	28	85Y	O21-C20	-2.75	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	OMC	O2-C2	-2.72	1.18	1.23
2	D	5	OMG	C2-N1	2.70	1.44	1.37
2	B	1	OMC	O2-C2	-2.69	1.18	1.23
2	D	19	OMG	O6-C6	-2.68	1.17	1.23
2	D	19	OMG	C2-N1	2.67	1.44	1.37
2	D	28	85Y	O4-C4	-2.65	1.18	1.23
2	D	24	85Y	O3'-C3'	-2.64	1.37	1.43
2	D	29	OMG	C2-N1	2.64	1.44	1.37
2	B	2	OMG	C2-N1	2.63	1.44	1.37
2	D	16	85Y	C2-N3	2.61	1.42	1.38
2	D	2	OMG	C2-N1	2.61	1.44	1.37
2	D	28	85Y	O3'-C3'	-2.60	1.37	1.43
2	D	1	OMC	C5-C4	2.59	1.48	1.42
2	B	4	85Y	O4-C4	-2.58	1.18	1.23
2	D	5	OMG	C5-C4	-2.57	1.36	1.43
2	D	22	85Y	O21-C20	-2.57	1.18	1.23
2	B	30	OMC	O2-C2	-2.56	1.19	1.23
2	D	19	OMG	C5-C4	-2.54	1.36	1.43
2	B	24	85Y	O3'-C3'	-2.53	1.38	1.43
2	D	3	OMC	C5-C4	2.52	1.48	1.42
2	D	4	85Y	O21-C20	-2.51	1.18	1.23
2	D	24	85Y	C2-N3	2.49	1.42	1.38
2	B	5	OMG	C2-N1	2.49	1.43	1.37
2	D	24	85Y	C23-N22	2.47	1.50	1.46
2	D	4	85Y	O4-C4	-2.46	1.18	1.23
2	B	1	OMC	C5-C4	2.46	1.48	1.42
2	D	27	85Y	O4-C4	-2.46	1.18	1.23
2	B	4	85Y	C2-N3	2.45	1.42	1.38
2	D	2	OMG	C5-C4	-2.43	1.36	1.43
2	D	18	OMG	C5-C4	-2.39	1.37	1.43
2	B	27	85Y	C32-C33	2.38	1.42	1.36
2	D	27	85Y	O3'-C3'	-2.38	1.38	1.43
2	B	29	OMG	C2-N1	2.38	1.43	1.37
2	D	16	85Y	O4-C4	-2.36	1.19	1.23
2	B	22	85Y	O4-C4	-2.35	1.19	1.23
2	B	28	85Y	O3'-C3'	-2.35	1.38	1.43
2	B	16	85Y	O4-C4	-2.32	1.19	1.23
2	D	4	85Y	C2-N3	2.30	1.42	1.38
2	B	24	85Y	C23-C24	2.30	1.56	1.51
2	D	10	85Y	C2-N3	2.30	1.42	1.38
2	B	19	OMG	C5-C4	-2.29	1.37	1.43
2	B	27	85Y	O3'-C3'	-2.28	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	22	85Y	C2-N3	2.24	1.42	1.38
2	B	10	85Y	C2-N3	2.23	1.41	1.38
2	D	16	85Y	C32-C33	2.22	1.41	1.36
2	B	27	85Y	C27-C26	-2.22	1.37	1.42
2	D	31	OMG	C5-C4	-2.20	1.37	1.43
2	B	22	85Y	O21-C20	-2.19	1.19	1.23
2	B	3	OMC	C5-C4	2.18	1.47	1.42
2	B	22	85Y	C2-N3	2.16	1.41	1.38
2	B	19	OMG	C6-N1	2.15	1.41	1.37
2	D	22	85Y	O4-C4	-2.12	1.19	1.23
2	B	16	85Y	C5-C20	2.10	1.56	1.49
2	B	2	OMG	C5-C4	-2.10	1.37	1.43
2	D	28	85Y	C23-N22	2.09	1.50	1.46
2	D	24	85Y	C27-C26	-2.09	1.37	1.42
2	B	18	OMG	C5-C4	-2.08	1.37	1.43
2	D	10	85Y	O4-C4	-2.08	1.19	1.23
2	B	16	85Y	C32-C33	2.07	1.41	1.36
2	B	4	85Y	C32-C33	2.07	1.41	1.36
2	B	22	85Y	C23-N22	2.05	1.50	1.46
2	D	27	85Y	O21-C20	-2.05	1.19	1.23
2	D	29	OMG	O6-C6	-2.05	1.19	1.23
2	D	2	OMG	O6-C6	-2.02	1.19	1.23
2	D	4	85Y	C27-C26	-2.01	1.37	1.42
2	B	16	85Y	C23-N22	2.00	1.49	1.46
2	D	27	85Y	C27-C26	-2.00	1.37	1.42

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	28	85Y	C23-N22-C20	10.63	136.33	122.08
2	B	28	85Y	C23-C24-C25	10.33	140.01	121.51
2	B	27	85Y	C23-N22-C20	9.50	134.82	122.08
2	B	10	85Y	C23-C24-C29	-9.43	101.34	120.91
2	D	24	85Y	C23-N22-C20	9.39	134.67	122.08
2	B	27	85Y	C4-N3-C2	-9.35	115.25	127.35
2	D	4	85Y	C24-C23-N22	-9.27	93.20	113.05
2	B	27	85Y	C5-C4-N3	9.05	130.02	114.35
2	B	27	85Y	C5-C6-N1	-9.04	111.08	123.10
2	D	28	85Y	C23-C24-C25	9.02	137.66	121.51
2	B	24	85Y	C23-N22-C20	8.81	133.90	122.08
2	B	28	85Y	C5-C4-N3	8.81	129.59	114.35
2	B	28	85Y	C23-C24-C29	-8.79	102.68	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	24	85Y	C24-C23-N22	8.62	131.51	113.05
2	B	22	85Y	C24-C23-N22	-8.54	94.75	113.05
2	B	16	85Y	C23-C24-C29	-8.52	103.23	120.91
2	B	10	85Y	C5-C6-N1	-8.40	111.94	123.10
2	D	28	85Y	C23-C24-C29	-8.38	103.52	120.91
2	B	10	85Y	C23-C24-C25	8.20	136.18	121.51
2	D	27	85Y	C4-N3-C2	-7.91	117.11	127.35
2	D	27	85Y	C5-C6-N1	-7.78	112.76	123.10
2	D	10	85Y	C23-C24-C29	-7.76	104.82	120.91
2	D	4	85Y	C23-C24-C29	-7.71	104.92	120.91
2	B	4	85Y	C24-C23-N22	-7.69	96.57	113.05
2	B	16	85Y	C5-C6-N1	-7.59	113.00	123.10
2	B	10	85Y	C4-N3-C2	-7.55	117.58	127.35
2	D	24	85Y	C24-C23-N22	7.49	129.09	113.05
2	D	27	85Y	C23-C24-C29	-7.49	105.38	120.91
2	B	4	85Y	C4-N3-C2	-7.48	117.67	127.35
2	D	28	85Y	C5-C4-N3	7.47	127.28	114.35
2	B	16	85Y	C23-C24-C25	7.45	134.85	121.51
2	B	28	85Y	C4-N3-C2	-7.39	117.79	127.35
2	D	27	85Y	C23-C24-C25	7.37	134.70	121.51
2	D	28	85Y	C4-N3-C2	-7.36	117.82	127.35
2	D	27	85Y	C5-C4-N3	7.36	127.09	114.35
2	D	28	85Y	C23-N22-C20	7.25	131.81	122.08
2	B	22	85Y	C23-C24-C25	7.18	134.37	121.51
2	B	4	85Y	C5-C6-N1	-7.14	113.61	123.10
2	B	4	85Y	C23-C24-C29	-7.12	106.13	120.91
2	B	27	85Y	C23-C24-C25	7.12	134.26	121.51
2	B	22	85Y	C23-C24-C29	-7.06	106.27	120.91
2	B	4	85Y	C23-C24-C25	7.04	134.11	121.51
2	D	16	85Y	C23-C24-C29	-6.90	106.60	120.91
2	D	10	85Y	C5-C6-N1	-6.88	113.96	123.10
2	D	27	85Y	C23-N22-C20	6.87	131.30	122.08
2	D	4	85Y	C4-N3-C2	-6.86	118.47	127.35
2	D	4	85Y	C23-C24-C25	6.85	133.78	121.51
2	B	16	85Y	C4-N3-C2	-6.84	118.49	127.35
2	D	24	85Y	C5-C6-N1	-6.74	114.14	123.10
2	D	22	85Y	C23-C24-C29	-6.74	106.93	120.91
2	D	10	85Y	C4-N3-C2	-6.73	118.64	127.35
2	D	24	85Y	C4-N3-C2	-6.73	118.64	127.35
2	D	4	85Y	C5-C4-N3	6.67	125.89	114.35
2	B	4	85Y	C5-C4-N3	6.62	125.80	114.35
2	B	27	85Y	C23-C24-C29	-6.54	107.33	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	10	85Y	C23-C24-C25	6.52	133.18	121.51
2	B	4	85Y	C23-N22-C20	6.49	130.78	122.08
2	D	16	85Y	C23-C24-C25	6.42	133.01	121.51
2	D	4	85Y	C5-C6-N1	-6.38	114.62	123.10
2	D	28	85Y	C5-C6-N1	-6.24	114.80	123.10
2	B	10	85Y	C6-C5-C4	6.22	125.31	118.19
2	D	16	85Y	C4-N3-C2	-6.19	119.34	127.35
2	D	22	85Y	C24-C23-N22	-6.17	99.82	113.05
2	B	24	85Y	C4-N3-C2	-6.13	119.42	127.35
2	B	22	85Y	C5-C4-N3	6.11	124.93	114.35
2	B	24	85Y	C5-C6-N1	-6.11	114.98	123.10
2	D	22	85Y	C23-C24-C25	6.08	132.39	121.51
2	D	16	85Y	C5-C4-N3	6.05	124.83	114.35
2	B	10	85Y	N3-C2-N1	6.01	122.87	114.89
2	D	22	85Y	C5-C6-N1	-5.98	115.15	123.10
2	D	16	85Y	C5-C6-N1	-5.97	115.17	123.10
2	D	22	85Y	C4-N3-C2	-5.90	119.71	127.35
2	B	16	85Y	C23-N22-C20	-5.80	114.31	122.08
2	D	22	85Y	C5-C4-N3	5.73	124.27	114.35
2	B	10	85Y	C23-N22-C20	-5.73	114.41	122.08
2	D	24	85Y	C5-C4-N3	5.68	124.17	114.35
2	D	10	85Y	C5-C4-N3	5.62	124.08	114.35
2	D	10	85Y	C24-C23-N22	-5.48	101.31	113.05
2	B	24	85Y	N3-C2-N1	5.44	122.11	114.89
2	B	28	85Y	O4-C4-N3	-5.34	109.88	120.12
2	D	4	85Y	C23-N22-C20	5.32	129.21	122.08
2	B	16	85Y	C5-C4-N3	5.29	123.50	114.35
2	B	27	85Y	O4-C4-N3	-5.26	110.03	120.12
2	B	16	85Y	O4'-C1'-N1	5.19	117.15	107.86
2	B	4	85Y	O2-C2-N1	-5.13	115.96	122.79
2	D	24	85Y	N3-C2-N1	5.07	121.62	114.89
2	B	22	85Y	C4-N3-C2	-5.07	120.79	127.35
2	D	27	85Y	C24-C23-N22	-5.06	102.20	113.05
2	D	16	85Y	C23-N22-C20	-5.00	115.38	122.08
2	B	22	85Y	C5-C6-N1	-4.98	116.48	123.10
2	B	28	85Y	C5-C6-N1	-4.94	116.53	123.10
2	B	4	85Y	N3-C2-N1	4.92	121.42	114.89
2	D	24	85Y	C23-C24-C29	-4.87	110.81	120.91
2	B	24	85Y	O2-C2-N1	-4.81	116.40	122.79
2	B	1	OMC	C1'-N1-C2	4.79	129.11	118.42
2	D	27	85Y	N3-C2-N1	4.79	121.25	114.89
2	B	10	85Y	C5-C4-N3	4.75	122.57	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	24	85Y	C23-C24-C29	-4.73	111.09	120.91
2	B	24	85Y	C23-C24-C25	4.67	129.87	121.51
2	B	16	85Y	O21-C20-C5	-4.65	112.46	121.05
2	D	10	85Y	N3-C2-N1	4.65	121.06	114.89
2	B	27	85Y	N3-C2-N1	4.59	120.99	114.89
2	D	24	85Y	C23-C24-C25	4.56	129.67	121.51
2	D	1	OMC	C1'-N1-C2	4.52	128.51	118.42
2	B	10	85Y	C24-C23-N22	-4.49	103.42	113.05
2	B	16	85Y	C6-C5-C4	4.44	123.28	118.19
2	B	22	85Y	O4'-C1'-N1	4.43	115.77	107.86
2	B	22	85Y	C23-N22-C20	4.42	128.01	122.08
2	B	24	85Y	C5-C4-N3	4.41	121.98	114.35
2	D	28	85Y	N3-C2-N1	4.38	120.71	114.89
2	B	5	OMG	C8-N7-C5	4.30	111.19	102.99
2	B	16	85Y	N3-C2-N1	4.29	120.59	114.89
2	B	16	85Y	C5-C20-N22	4.16	125.65	116.64
2	B	1	OMC	C1'-N1-C6	-4.06	112.00	120.84
2	D	4	85Y	N3-C2-N1	4.02	120.22	114.89
2	D	16	85Y	N3-C2-N1	3.86	120.01	114.89
2	D	27	85Y	O4-C4-N3	-3.85	112.74	120.12
2	D	16	85Y	C5-C20-N22	3.78	124.83	116.64
2	D	28	85Y	C24-C23-N22	-3.77	104.97	113.05
2	B	16	85Y	C2'-C1'-N1	-3.75	105.13	113.77
2	D	1	OMC	C1'-N1-C6	-3.72	112.72	120.84
2	D	24	85Y	O2-C2-N1	-3.71	117.86	122.79
2	B	28	85Y	N3-C2-N1	3.69	119.79	114.89
2	B	27	85Y	C24-C23-N22	-3.69	105.15	113.05
2	D	28	85Y	O4-C4-N3	-3.66	113.09	120.12
2	D	22	85Y	N3-C2-N1	3.63	119.71	114.89
2	D	5	OMG	C8-N7-C5	3.52	109.69	102.99
2	D	16	85Y	O4'-C1'-N1	3.47	114.06	107.86
2	B	27	85Y	O4'-C1'-N1	3.46	114.04	107.86
2	B	1	OMC	O2'-C2'-C1'	3.45	115.82	109.08
2	D	5	OMG	C5-C6-N1	3.45	120.05	113.95
2	B	16	85Y	O4-C4-C5	-3.44	117.94	125.99
2	B	18	OMG	O6-C6-N1	-3.42	116.61	120.65
2	B	2	OMG	C5-C6-N1	3.39	119.95	113.95
2	B	18	OMG	C5-C6-N1	3.38	119.92	113.95
2	B	31	OMG	C5-C6-N1	3.38	119.92	113.95
2	B	10	85Y	O4-C4-C5	-3.37	118.10	125.99
2	B	24	85Y	C6-C5-C4	3.36	122.04	118.19
2	B	5	OMG	C5-C6-N1	3.31	119.81	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5	OMG	CM2-O2'-C2'	3.29	123.16	114.52
2	D	10	85Y	C6-C5-C4	3.28	121.94	118.19
2	B	28	85Y	C24-C23-N22	-3.27	106.03	113.05
2	D	31	OMG	C5-C6-N1	3.27	119.72	113.95
2	B	18	OMG	N1-C2-N3	-3.26	117.22	123.32
2	B	5	OMG	C2-N1-C6	-3.26	119.10	125.10
2	B	22	85Y	C2'-C1'-N1	-3.24	106.31	113.77
2	D	2	OMG	C5-C6-N1	3.23	119.66	113.95
2	B	29	OMG	C5-C6-N1	3.20	119.60	113.95
2	B	4	85Y	O4-C4-C5	-3.20	118.50	125.99
2	D	29	OMG	C5-C6-N1	3.18	119.56	113.95
2	B	27	85Y	C1'-N1-C2	-3.17	111.39	117.64
2	D	10	85Y	O4-C4-C5	-3.17	118.56	125.99
2	B	2	OMG	C8-N7-C5	3.17	109.02	102.99
2	B	24	85Y	O4-C4-C5	-3.15	118.61	125.99
2	D	18	OMG	C5-C6-N1	3.14	119.49	113.95
2	D	4	85Y	O2-C2-N1	-3.13	118.63	122.79
2	B	18	OMG	C8-N7-C5	3.11	108.92	102.99
2	D	2	OMG	C8-N7-C5	3.09	108.88	102.99
2	D	5	OMG	C2-N1-C6	-3.07	119.45	125.10
2	B	18	OMG	O2'-C2'-C1'	3.03	115.10	109.09
2	B	18	OMG	CM2-O2'-C2'	3.02	122.45	114.52
2	B	29	OMG	C8-N7-C5	2.99	108.68	102.99
2	D	4	85Y	O4-C4-C5	-2.96	119.06	125.99
2	B	27	85Y	C2'-C1'-N1	-2.96	106.96	113.77
2	B	27	85Y	C6-N1-C2	2.94	124.28	121.30
2	D	22	85Y	O4'-C1'-N1	2.91	113.06	107.86
2	D	16	85Y	O21-C20-N22	-2.91	117.98	123.30
2	D	24	85Y	O4-C4-C5	-2.90	119.20	125.99
2	D	18	OMG	C8-N7-C5	2.87	108.46	102.99
2	B	29	OMG	N1-C2-N3	-2.83	118.04	123.32
2	D	29	OMG	C8-N7-C5	2.83	108.37	102.99
2	D	1	OMC	C2'-C1'-N1	2.79	119.65	114.22
2	D	16	85Y	O4-C4-C5	-2.79	119.46	125.99
2	B	27	85Y	C5-C20-N22	-2.79	110.61	116.64
2	B	22	85Y	O4-C4-C5	-2.76	119.52	125.99
2	D	19	OMG	C5-C6-N1	2.75	118.81	113.95
2	B	1	OMC	C2'-C1'-N1	2.75	119.56	114.22
2	B	22	85Y	C20-C5-C4	2.74	126.29	120.32
2	D	27	85Y	O4'-C1'-N1	2.73	112.75	107.86
2	B	10	85Y	C5-C20-N22	-2.73	110.73	116.64
2	D	31	OMG	C8-N7-C5	2.72	108.18	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	28	85Y	O4-C4-C5	-2.71	119.63	125.99
2	B	19	OMG	O6-C6-N1	2.68	123.82	120.65
2	B	10	85Y	C20-C5-C4	-2.68	114.48	120.32
2	B	28	85Y	C6-C5-C4	-2.65	115.16	118.19
2	D	4	85Y	O4-C4-N3	-2.65	115.04	120.12
2	D	22	85Y	O4-C4-C5	-2.64	119.79	125.99
2	D	19	OMG	O6-C6-C5	-2.62	119.25	124.37
2	B	31	OMG	C8-N7-C5	2.61	107.97	102.99
2	D	2	OMG	C2-N1-C6	-2.61	120.29	125.10
2	D	1	OMC	O2-C2-N3	-2.61	118.08	122.33
2	B	10	85Y	O2-C2-N1	-2.60	119.32	122.79
2	B	28	85Y	C33-C27-C26	2.59	123.56	118.92
2	B	28	85Y	C3'-C2'-C1'	2.58	109.00	102.54
2	B	27	85Y	O4-C4-C5	-2.58	119.95	125.99
2	B	10	85Y	C1'-N1-C2	2.57	122.70	117.64
2	B	22	85Y	N3-C2-N1	2.57	118.30	114.89
2	B	31	OMG	N2-C2-N1	2.55	122.15	116.71
2	B	22	85Y	O21-C20-C5	-2.52	116.39	121.05
2	B	19	OMG	O6-C6-C5	-2.50	119.48	124.37
2	B	28	85Y	C20-C5-C4	2.50	125.77	120.32
2	B	4	85Y	C32-C31-C30	-2.49	116.96	120.44
2	D	27	85Y	O4-C4-C5	-2.48	120.17	125.99
2	D	31	OMG	C2-N1-C6	-2.46	120.56	125.10
2	B	3	OMC	O2-C2-N3	-2.46	118.33	122.33
2	D	27	85Y	O2-C2-N1	-2.44	119.54	122.79
2	B	31	OMG	N1-C2-N3	-2.44	118.76	123.32
2	D	19	OMG	C2-N1-C6	-2.43	120.63	125.10
2	B	31	OMG	O6-C6-C5	-2.41	119.66	124.37
2	B	1	OMC	C3'-C2'-C1'	-2.41	98.36	102.89
2	D	24	85Y	C6-C5-C4	2.40	120.94	118.19
2	B	22	85Y	O4-C4-N3	-2.38	115.55	120.12
2	B	10	85Y	O4'-C4'-C3'	-2.38	100.12	105.67
2	D	31	OMG	O6-C6-C5	-2.37	119.74	124.37
2	D	18	OMG	C2-N1-C6	-2.36	120.75	125.10
2	D	16	85Y	C2'-C1'-N1	-2.35	108.36	113.77
2	D	16	85Y	C32-C31-C30	-2.35	117.15	120.44
2	B	28	85Y	O4-C4-C5	-2.33	120.52	125.99
2	B	2	OMG	C2-N1-C6	-2.33	120.81	125.10
2	D	27	85Y	C3'-C2'-C1'	2.33	108.37	102.54
2	B	4	85Y	O4-C4-N3	-2.33	115.66	120.12
2	D	29	OMG	N1-C2-N3	-2.32	118.98	123.32
2	D	1	OMC	O2'-C2'-C1'	2.31	113.59	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	27	85Y	C6-C5-C20	2.30	124.70	114.34
2	D	16	85Y	O4-C4-N3	-2.30	115.72	120.12
2	B	4	85Y	O4'-C4'-C3'	-2.29	100.32	105.67
2	D	1	OMC	O2-C2-N1	2.23	123.50	118.89
2	D	28	85Y	O2-C2-N1	-2.19	119.87	122.79
2	B	3	OMC	C2'-C3'-C4'	2.19	106.75	101.99
2	D	22	85Y	O4-C4-N3	-2.18	115.93	120.12
2	B	1	OMC	N4-C4-N3	2.18	121.80	117.97
2	D	18	OMG	N1-C2-N3	-2.18	119.25	123.32
2	B	2	OMG	N1-C2-N3	-2.17	119.26	123.32
2	B	29	OMG	CM2-O2'-C2'	2.16	120.20	114.52
2	B	31	OMG	C2-N1-C6	-2.16	121.12	125.10
2	B	18	OMG	N2-C2-N1	2.15	121.28	116.71
2	B	19	OMG	C2-N1-C6	-2.15	121.15	125.10
2	B	10	85Y	C33-C27-C26	2.14	122.76	118.92
2	D	5	OMG	O6-C6-C5	-2.14	120.19	124.37
2	D	10	85Y	O4'-C4'-C3'	-2.13	100.71	105.67
2	B	27	85Y	C3'-C2'-C1'	2.12	107.85	102.54
2	B	10	85Y	C32-C33-C27	-2.10	117.16	120.44
2	D	16	85Y	O21-C20-C5	-2.09	117.19	121.05
2	D	1	OMC	C3'-C2'-C1'	-2.08	98.98	102.89
2	D	31	OMG	N1-C2-N3	-2.07	119.45	123.32
2	D	29	OMG	O6-C6-C5	-2.07	120.34	124.37
2	B	27	85Y	C1'-N1-C6	2.06	124.33	120.77
2	D	29	OMG	C2-N1-C6	-2.05	121.33	125.10
2	D	27	85Y	C2'-C1'-N1	-2.05	109.06	113.77
2	B	10	85Y	C28-C27-C33	-2.04	118.42	123.19
2	D	19	OMG	C8-N7-C5	2.04	106.88	102.99
2	B	28	85Y	O2-C2-N3	-2.03	117.71	121.50
2	D	16	85Y	C31-C30-C26	2.03	123.61	120.44
2	B	16	85Y	C24-C25-C26	-2.02	117.24	121.22
2	B	16	85Y	C3'-C2'-C1'	2.02	107.60	102.54
2	B	1	OMC	O2-C2-N1	2.01	123.04	118.89

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	OMC	O4'-C4'-C5'-O5'
2	B	2	OMG	C1'-C2'-O2'-CM2
2	D	2	OMG	C1'-C2'-O2'-CM2
2	B	3	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	4	85Y	O4'-C4'-C5'-O5'
2	B	4	85Y	C3'-C4'-C5'-O5'
2	D	4	85Y	O4'-C4'-C5'-O5'
2	D	4	85Y	C3'-C4'-C5'-O5'
2	B	5	OMG	C1'-C2'-O2'-CM2
2	B	10	85Y	O21-C20-C5-C6
2	B	10	85Y	N22-C20-C5-C6
2	B	10	85Y	C3'-C4'-C5'-O5'
2	D	10	85Y	C3'-C4'-C5'-O5'
2	B	16	85Y	O21-C20-C5-C6
2	B	16	85Y	N22-C20-C5-C6
2	B	18	OMG	C1'-C2'-O2'-CM2
2	D	18	OMG	C1'-C2'-O2'-CM2
2	B	19	OMG	C4'-C5'-O5'-P
2	B	19	OMG	C1'-C2'-O2'-CM2
2	D	19	OMG	C4'-C5'-O5'-P
2	D	19	OMG	C3'-C4'-C5'-O5'
2	B	22	85Y	O21-C20-C5-C6
2	B	22	85Y	N22-C20-C5-C6
2	D	22	85Y	O21-C20-C5-C6
2	D	22	85Y	N22-C20-C5-C6
2	B	24	85Y	C24-C23-N22-C20
2	D	24	85Y	C24-C23-N22-C20
2	B	27	85Y	C3'-C4'-C5'-O5'
2	B	28	85Y	O21-C20-C5-C4
2	B	28	85Y	O21-C20-C5-C6
2	B	28	85Y	N22-C20-C5-C6
2	D	28	85Y	O21-C20-C5-C6
2	D	28	85Y	N22-C20-C5-C6
2	B	29	OMG	C4'-C5'-O5'-P
2	B	29	OMG	C1'-C2'-O2'-CM2
2	D	29	OMG	C4'-C5'-O5'-P
2	D	29	OMG	C1'-C2'-O2'-CM2
2	B	30	OMC	C1'-C2'-O2'-CM2
2	B	30	OMC	C3'-C4'-C5'-O5'
2	D	30	OMC	C1'-C2'-O2'-CM2
2	D	30	OMC	C3'-C4'-C5'-O5'
2	B	31	OMG	C3'-C4'-C5'-O5'
2	D	31	OMG	C4'-C5'-O5'-P
2	D	31	OMG	C3'-C4'-C5'-O5'
2	B	18	OMG	C4'-C5'-O5'-P
2	B	1	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	D	2	OMG	O4'-C4'-C5'-O5'
2	B	5	OMG	O4'-C4'-C5'-O5'
2	D	5	OMG	O4'-C4'-C5'-O5'
2	D	5	OMG	C3'-C4'-C5'-O5'
2	B	19	OMG	C3'-C4'-C5'-O5'
2	D	27	85Y	C3'-C4'-C5'-O5'
2	B	28	85Y	O4'-C4'-C5'-O5'
2	B	28	85Y	C3'-C4'-C5'-O5'
2	D	28	85Y	O4'-C4'-C5'-O5'
2	D	28	85Y	C3'-C4'-C5'-O5'
2	B	30	OMC	O4'-C4'-C5'-O5'
2	D	30	OMC	O4'-C4'-C5'-O5'
2	B	1	OMC	O4'-C4'-C5'-O5'
2	D	1	OMC	C3'-C4'-C5'-O5'
2	D	2	OMG	C3'-C4'-C5'-O5'
2	B	5	OMG	C3'-C4'-C5'-O5'
2	B	10	85Y	O4'-C4'-C5'-O5'
2	D	10	85Y	O4'-C4'-C5'-O5'
2	B	18	OMG	C3'-C4'-C5'-O5'
2	B	22	85Y	O4'-C4'-C5'-O5'
2	B	27	85Y	O4'-C4'-C5'-O5'
2	B	31	OMG	O4'-C4'-C5'-O5'
2	D	1	OMC	C2'-C1'-N1-C6
2	D	1	OMC	C2'-C1'-N1-C2
2	B	10	85Y	C4'-C5'-O5'-P
2	D	18	OMG	C4'-C5'-O5'-P
2	B	31	OMG	C4'-C5'-O5'-P
2	D	31	OMG	O4'-C4'-C5'-O5'
2	B	3	OMC	O4'-C4'-C5'-O5'
2	D	18	OMG	C3'-C4'-C5'-O5'
2	B	22	85Y	C3'-C4'-C5'-O5'
2	B	19	OMG	O4'-C4'-C5'-O5'
2	D	19	OMG	O4'-C4'-C5'-O5'
2	B	28	85Y	N22-C20-C5-C4
2	D	10	85Y	C4'-C5'-O5'-P
2	D	22	85Y	O4'-C4'-C5'-O5'
2	B	1	OMC	C2'-C1'-N1-C6
2	D	27	85Y	O4'-C4'-C5'-O5'
2	B	10	85Y	O21-C20-C5-C4
2	B	22	85Y	O21-C20-C5-C4
2	D	28	85Y	O21-C20-C5-C4
2	B	1	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	B	1	OMC	C4'-C5'-O5'-P
2	D	1	OMC	C4'-C5'-O5'-P
2	D	28	85Y	C4'-C5'-O5'-P
2	B	18	OMG	O4'-C4'-C5'-O5'
2	D	18	OMG	O4'-C4'-C5'-O5'
2	B	28	85Y	C4'-C5'-O5'-P
2	B	30	OMC	C4'-C5'-O5'-P
2	D	30	OMC	C4'-C5'-O5'-P
2	D	29	OMG	C3'-C4'-C5'-O5'
2	B	22	85Y	N22-C20-C5-C4
2	B	2	OMG	O4'-C4'-C5'-O5'
2	D	22	85Y	C3'-C4'-C5'-O5'
2	B	10	85Y	N22-C20-C5-C4
2	B	16	85Y	N22-C20-C5-C4
2	D	28	85Y	N22-C20-C5-C4

There are no ring outliers.

21 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	22	85Y	3	0
2	B	3	OMC	3	0
2	B	1	OMC	1	0
2	D	18	OMG	4	0
2	B	4	85Y	1	0
2	D	10	85Y	1	0
2	B	16	85Y	2	0
2	B	29	OMG	1	0
2	D	19	OMG	4	0
2	D	3	OMC	2	0
2	B	5	OMG	1	0
2	B	18	OMG	3	0
2	B	27	85Y	1	0
2	D	16	85Y	2	0
2	B	19	OMG	5	0
2	D	2	OMG	1	0
2	D	29	OMG	2	0
2	B	30	OMC	1	0
2	D	5	OMG	1	0
2	B	10	85Y	3	0
2	B	2	OMG	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	703/764 (92%)	-0.05	4 (0%)	89	86	43, 78, 122, 157	0
1	C	703/764 (92%)	-0.06	3 (0%)	92	90	45, 80, 124, 162	0
2	B	15/32 (46%)	-0.45	0	100	100	61, 69, 81, 85	0
2	D	15/32 (46%)	-0.39	0	100	100	67, 73, 80, 86	0
All	All	1436/1592 (90%)	-0.06	7 (0%)	91	88	43, 79, 122, 162	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	LYS	2.9
1	C	707	LYS	2.7
1	A	217	ILE	2.5
1	A	137	ALA	2.2
1	C	346	ASP	2.2
1	C	217	ILE	2.1
1	A	481	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OMG	D	31	24/25	0.79	0.22	104,139,152,157	0
2	OMC	D	1	21/22	0.81	0.25	118,138,161,186	0
2	OMG	B	31	24/25	0.83	0.18	116,130,143,147	0
2	OMC	B	1	21/22	0.85	0.29	125,149,165,173	0
2	OMG	D	18	24/25	0.86	0.27	83,102,118,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	85Y	D	28	33/34	0.87	0.32	62,77,91,112	0
2	OMG	D	29	24/25	0.87	0.24	101,109,129,138	0
2	OMG	B	29	24/25	0.88	0.20	89,110,129,138	0
2	85Y	B	28	33/34	0.88	0.27	54,70,97,119	0
2	OMC	D	30	21/22	0.89	0.17	102,118,130,143	0
2	OMG	B	2	24/25	0.89	0.17	100,122,134,157	0
2	85Y	D	27	33/34	0.89	0.24	64,74,102,105	0
2	OMG	B	18	24/25	0.90	0.26	74,89,112,119	0
2	OMG	D	2	24/25	0.90	0.18	102,121,143,187	0
2	OMC	B	30	21/22	0.91	0.12	95,112,138,159	0
2	85Y	D	16	33/34	0.91	0.24	59,75,143,154	0
2	85Y	B	16	33/34	0.92	0.18	55,77,108,111	0
2	OMG	D	5	24/25	0.92	0.22	59,74,91,102	0
2	OMG	D	19	24/25	0.92	0.22	62,86,98,101	0
2	85Y	D	22	33/34	0.93	0.32	56,74,84,94	0
2	85Y	D	24	33/34	0.93	0.28	61,71,77,86	0
2	85Y	B	27	33/34	0.93	0.24	57,71,90,92	0
2	85Y	D	4	33/34	0.93	0.27	61,84,100,114	0
2	OMC	D	3	21/22	0.94	0.20	89,99,115,140	0
2	OMG	B	19	24/25	0.94	0.18	61,82,93,95	0
2	85Y	B	4	33/34	0.94	0.24	62,76,101,108	0
2	OMC	B	3	21/22	0.94	0.22	82,92,109,120	0
2	OMG	B	5	24/25	0.94	0.21	66,76,89,96	0
2	85Y	B	24	33/34	0.95	0.21	63,70,82,89	0
2	85Y	D	10	33/34	0.95	0.29	50,71,110,115	0
2	85Y	B	22	33/34	0.95	0.28	52,71,89,96	0
2	85Y	B	10	33/34	0.95	0.26	55,68,108,119	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.