



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:49 PM GMT

PDB ID : 4WA2
Title : The crystal structure of hemagglutinin from a H3N8 influenza virus isolated from New England harbor seals in complex with 3'SLN
Authors : Yang, H.; Villanueva, J.M.; Gubareva, L.V.; Stevens, J.
Deposited on : 2014-08-28
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

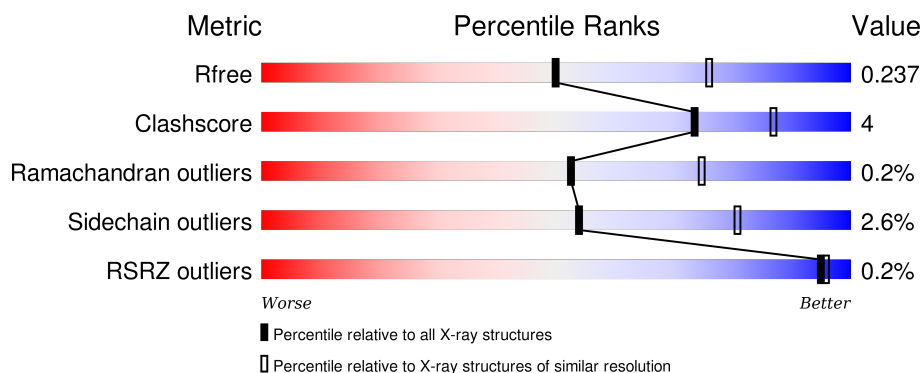
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	496	<div> <div>89%</div> <div>10% .</div> </div>
1	B	496	<div> <div>88%</div> <div>10% ..</div> </div>
1	C	496	<div> <div>87%</div> <div>10% ..</div> </div>
1	D	496	<div> <div>%</div> <div>89%</div> <div>10% .</div> </div>
1	E	496	<div> <div>86%</div> <div>11% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	496	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1007	-	-	-	X
3	NAG	C	1008	-	-	-	X
4	NAG	F	605	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24811 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	B	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	C	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	D	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	E	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	F	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			46	25	2	19		
2	B	3	Total	C	N	O	0	0
			46	25	2	19		
2	C	3	Total	C	N	O	0	0
			46	25	2	19		
2	E	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	3	Total	C	N	O	0	0
			39	22	2	15		
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

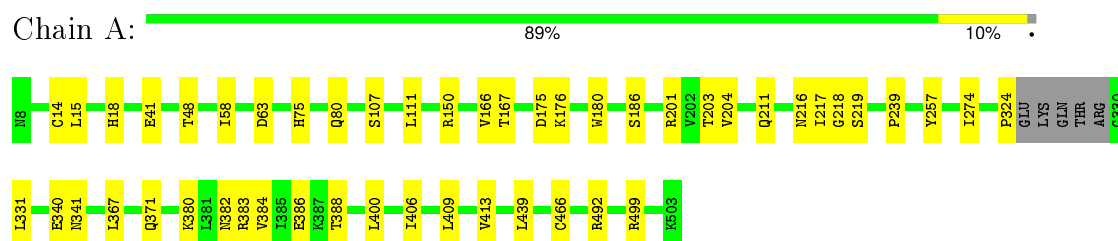
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	188	Total	O	0	0
			188	188		
6	B	171	Total	O	0	0
			171	171		
6	C	187	Total	O	0	0
			187	187		
6	D	174	Total	O	0	0
			174	174		
6	E	163	Total	O	0	0
			163	163		
6	F	170	Total	O	0	0
			170	170		

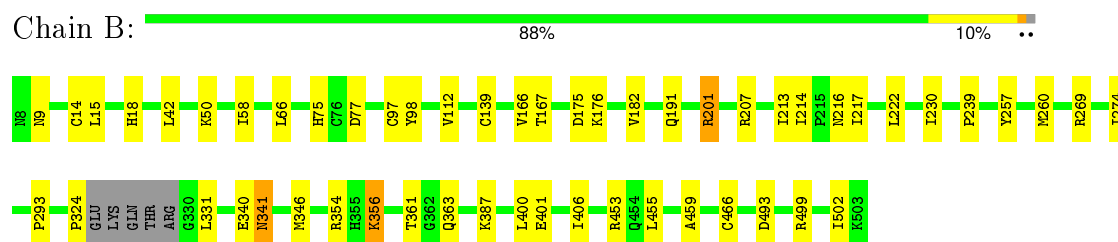
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

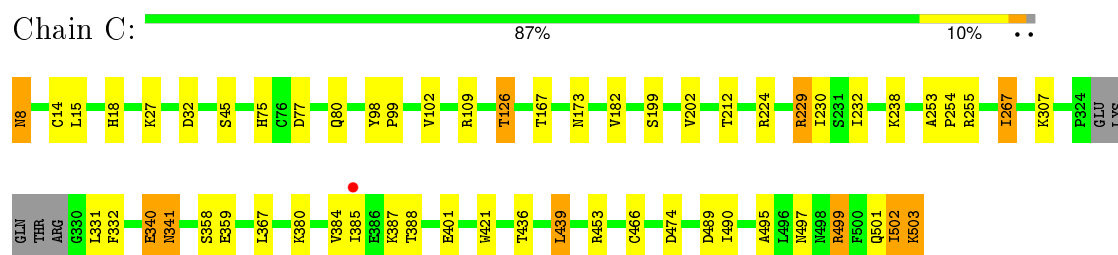
• Molecule 1: Hemagglutinin



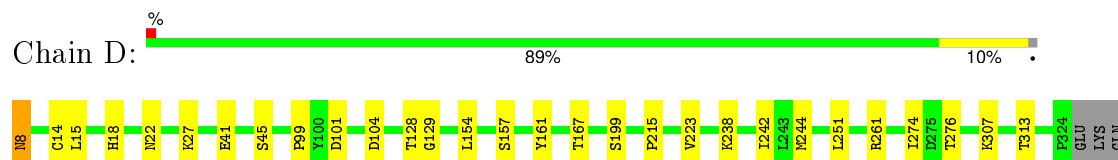
• Molecule 1: Hemagglutinin

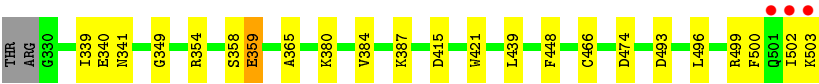


• Molecule 1: Hemagglutinin

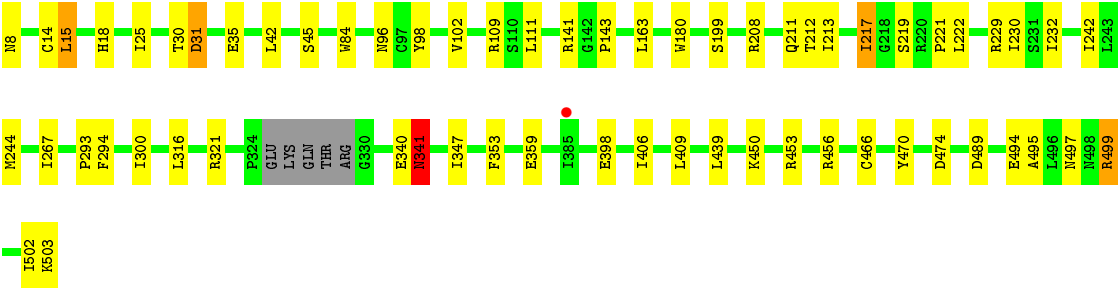
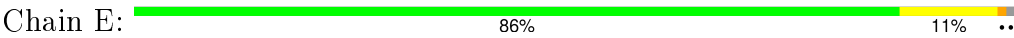


• Molecule 1: Hemagglutinin

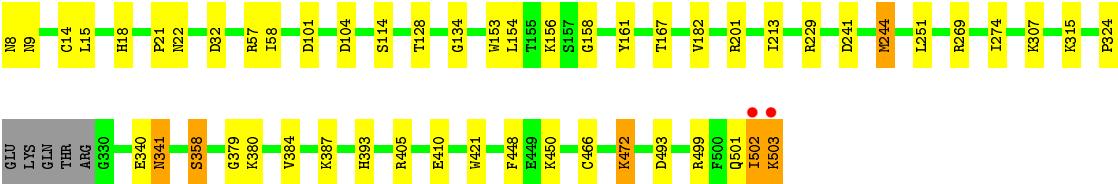
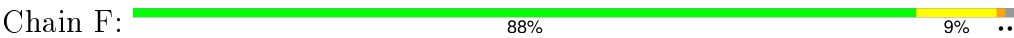




● Molecule 1: Hemagglutinin



● Molecule 1: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.54Å 102.33Å 109.67Å 90.02° 90.02° 89.51°	Depositor
Resolution (Å)	45.19 – 2.50 45.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.19-2.50) 96.5 (45.15-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.184 , 0.236 0.187 , 0.237	Depositor DCC
R_{free} test set	5793 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 6.3	EDS
Estimated twinning fraction	0.011 for h,-k,-l 0.011 for -h,k,-l 0.457 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 115418 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24811	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SIA, GAL, BMA, NAG

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	0.74	0/3937	0.86	5/5333 (0.1%)
1	B	0.75	0/3937	0.87	6/5333 (0.1%)
1	C	0.75	0/3937	0.87	4/5333 (0.1%)
1	D	0.75	0/3937	0.89	6/5333 (0.1%)
1	E	0.76	3/3937 (0.1%)	0.87	6/5333 (0.1%)
1	F	0.75	0/3937	0.88	7/5333 (0.1%)
All	All	0.75	3/23622 (0.0%)	0.87	34/31998 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	180	TRP	CB-CG	5.37	1.59	1.50
1	E	84	TRP	CB-CG	-5.27	1.40	1.50
1	E	494	GLU	CD-OE1	5.06	1.31	1.25

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	341	ASN	N-CA-CB	-7.75	96.65	110.60
1	D	415	ASP	CB-CG-OD1	7.26	124.83	118.30
1	D	341	ASN	N-CA-CB	-7.19	97.66	110.60
1	A	499	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	341	ASN	N-CA-CB	-7.11	97.81	110.60
1	C	255	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	321	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	F	269	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	D	354	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	F	229	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	269	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	499	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	255	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	E	229	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	E	229	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	499	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	F	57	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	241	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	493	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	261	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	492	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	341	ASN	N-CA-CB	-5.34	100.99	110.60
1	C	229	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	77	ASP	CB-CG-OD1	5.28	123.06	118.30
1	A	15	LEU	CA-CB-CG	-5.28	103.16	115.30
1	D	261	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	E	141	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	383	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	E	456	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	341	ASN	N-CA-CB	-5.09	101.44	110.60
1	D	499	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	453	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	341	ASN	N-CA-CB	-5.06	101.49	110.60
1	F	405	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	GLU	Peptide
1	B	340	GLU	Peptide
1	C	340	GLU	Peptide
1	D	340	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	E	340	GLU	Peptide
1	F	340	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3860	0	3739	31	0
1	B	3860	0	3739	32	0
1	C	3860	0	3739	44	0
1	D	3860	0	3739	33	0
1	E	3860	0	3739	39	0
1	F	3860	0	3739	34	0
2	A	46	0	40	0	0
2	B	46	0	40	1	0
2	C	46	0	40	1	0
2	E	46	0	40	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	1	0
3	F	14	0	13	0	0
4	A	28	0	25	1	0
4	B	28	0	25	1	0
4	C	56	0	50	0	0
4	D	28	0	25	1	0
4	E	56	0	50	1	0
4	F	28	0	25	0	0
5	D	39	0	34	0	0
5	F	39	0	34	0	0
6	A	188	0	0	11	0
6	B	171	0	0	7	0
6	C	187	0	0	14	0
6	D	174	0	0	9	0
6	E	163	0	0	11	0
6	F	170	0	0	7	0
All	All	24811	0	22966	192	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 4.

All (192) 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:B:406:ILE:HG22	6:B:1260:HOH:O	1.58	1.02
1:D:22:ASN:HB3	6:D:712:HOH:O	1.68	0.93
1:A:48:THR:HA	6:A:1120:HOH:O	1.79	0.83
1:A:75:HIS:CB	6:A:1228:HOH:O	2.27	0.82
1:F:22:ASN:HA	6:F:870:HOH:O	1.82	0.80
1:C:75:HIS:HB3	6:C:1107:HOH:O	1.80	0.79
1:D:215:PRO:HG2	6:D:741:HOH:O	1.82	0.79
1:B:401:GLU:HG3	6:C:1144:HOH:O	1.82	0.79
1:E:45:SER:HB2	6:E:1190:HOH:O	1.83	0.79
1:D:199:SER:HB2	6:D:794:HOH:O	1.83	0.78
1:A:406:ILE:HG22	6:A:1167:HOH:O	1.83	0.77
1:C:502:ILE:HD11	1:D:502:ILE:HD11	1.64	0.77
1:A:216:ASN:HB2	1:E:212:THR:OG1	1.84	0.76
1:D:167:THR:HG22	1:D:244:MET:HG3	1.67	0.76
1:B:216:ASN:HB2	1:C:212:THR:OG1	1.87	0.74
1:E:221:PRO:HD3	1:F:244:MET:HG3	1.69	0.74
1:A:75:HIS:HB3	6:A:1228:HOH:O	1.88	0.73
1:D:500:PHE:HB2	1:D:502:ILE:HB	1.71	0.72
1:C:109:ARG:NH2	1:C:267:ILE:HD13	2.04	0.72
1:C:502:ILE:CD1	1:D:502:ILE:HD11	2.18	0.72
1:C:45:SER:HB2	6:C:1224:HOH:O	1.90	0.71
1:E:208:ARG:HB2	6:E:1259:HOH:O	1.88	0.71
1:F:502:ILE:O	1:F:503:LYS:C	2.29	0.71
1:D:45:SER:HB2	6:D:761:HOH:O	1.90	0.70
1:F:380:LYS:O	1:F:384:VAL:HG23	1.91	0.69
1:C:388:THR:HG21	6:C:1280:HOH:O	1.92	0.68
1:F:493:ASP:HB3	1:F:503:LYS:CE	2.25	0.67
1:A:75:HIS:HB2	6:A:1228:HOH:O	1.90	0.66
1:F:502:ILE:HG23	1:F:503:LYS:N	2.11	0.66
1:B:356:LYS:HG3	1:B:361:THR:HG22	1.79	0.64
1:A:219:SER:C	1:E:244:MET:HE1	2.16	0.64
1:B:201:ARG:HG3	1:B:214:ILE:HD13	1.78	0.64
2:B:1003:NAG:H1	6:B:1179:HOH:O	1.97	0.63
1:F:324:PRO:C	6:F:805:HOH:O	2.37	0.62
1:B:502:ILE:HD11	1:D:502:ILE:HD12	1.81	0.62
1:D:276:THR:HG23	6:D:702:HOH:O	1.99	0.62
1:B:167:THR:HG21	4:B:1005:NAG:H62	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ASN:N	6:D:805:HOH:O	2.31	0.62
1:E:439:LEU:HD12	1:E:439:LEU:C	2.21	0.62
1:E:221:PRO:CD	1:F:244:MET:HG3	2.29	0.61
1:C:401:GLU:OE1	1:D:238:LYS:HE2	2.00	0.61
1:E:15:LEU:HD21	1:E:353:PHE:CE2	2.36	0.61
1:B:9:ASN:OD1	6:B:1155:HOH:O	2.16	0.61
1:F:493:ASP:HB3	1:F:503:LYS:NZ	2.14	0.61
1:A:41:GLU:HB2	6:A:1258:HOH:O	2.01	0.61
1:D:358:SER:HB2	6:D:834:HOH:O	2.00	0.61
1:F:493:ASP:HB3	1:F:503:LYS:HE3	1.83	0.60
1:D:502:ILE:HG23	1:D:503:LYS:N	2.17	0.59
1:B:75:HIS:CE1	1:E:347:ILE:HD11	2.38	0.59
1:B:176:LYS:HE2	1:B:257:TYR:CE2	2.39	0.57
1:E:502:ILE:HG22	1:E:503:LYS:HG3	1.87	0.56
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.87	0.56
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.88	0.56
1:E:359:GLU:OE2	1:E:474:ASP:HB2	2.05	0.56
1:C:340:GLU:CB	1:C:341:ASN:HB2	2.36	0.56
4:D:605:NAG:O4	6:D:866:HOH:O	2.18	0.56
1:C:359:GLU:OE2	1:C:474:ASP:HB2	2.06	0.56
1:A:382:ASN:O	1:A:386:GLU:HB2	2.06	0.56
1:A:216:ASN:CB	1:E:212:THR:OG1	2.53	0.55
1:B:207:ARG:HD2	6:B:1207:HOH:O	2.06	0.55
1:F:502:ILE:HG23	1:F:503:LYS:H	1.72	0.54
1:B:400:LEU:HD12	6:B:1256:HOH:O	2.07	0.54
1:C:307:LYS:HE2	1:C:421:TRP:CH2	2.41	0.54
1:F:167:THR:HG22	1:F:244:MET:HG2	1.90	0.54
1:F:307:LYS:HE2	1:F:421:TRP:CH2	2.42	0.53
1:B:363:GLN:HB2	1:E:143:PRO:HD3	1.91	0.53
1:C:503:LYS:HG2	6:C:1145:HOH:O	2.09	0.53
1:A:409:LEU:O	1:A:413:VAL:HG23	2.09	0.53
1:C:126:THR:HB	6:C:1263:HOH:O	2.09	0.53
1:C:173:ASN:HB3	6:C:1105:HOH:O	2.09	0.52
1:E:453:ARG:HD2	6:E:1106:HOH:O	2.09	0.52
1:A:380:LYS:O	1:A:384:VAL:HG23	2.10	0.52
1:A:386:GLU:O	1:A:388:THR:HG23	2.09	0.52
1:B:98:TYR:CD2	1:B:230:ILE:HD12	2.44	0.52
1:C:98:TYR:CD2	1:C:230:ILE:HD12	2.45	0.51
1:E:14:CYS:HA	1:E:466:CYS:HA	1.93	0.51
1:A:167:THR:HG21	4:A:1005:NAG:H62	1.91	0.51
1:C:253:ALA:HB1	1:C:254:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LEU:HD11	1:E:316:LEU:HB2	1.94	0.50
1:B:324:PRO:C	6:B:1126:HOH:O	2.49	0.50
1:D:15:LEU:HD22	1:D:448:PHE:HA	1.93	0.50
1:A:400:LEU:HD12	6:A:1283:HOH:O	2.11	0.50
1:E:31:ASP:HB3	6:E:1234:HOH:O	2.10	0.50
1:C:109:ARG:CZ	1:C:267:ILE:HD13	2.42	0.50
3:E:1008:NAG:H83	6:E:1180:HOH:O	2.12	0.50
1:F:14:CYS:HA	1:F:466:CYS:HA	1.93	0.50
1:C:340:GLU:HB2	1:C:341:ASN:HB2	1.94	0.50
1:D:502:ILE:CG2	1:D:503:LYS:N	2.74	0.49
4:E:1005:NAG:O4	6:E:1212:HOH:O	2.20	0.49
1:F:315:LYS:HD3	6:F:757:HOH:O	2.13	0.49
1:B:14:CYS:HA	1:B:466:CYS:HA	1.95	0.49
1:B:201:ARG:HG3	1:B:214:ILE:CD1	2.43	0.49
1:E:25:ILE:HD13	1:E:35:GLU:HG3	1.95	0.48
1:A:371:GLN:HG2	6:A:1216:HOH:O	2.13	0.48
1:A:80:GLN:HG2	1:A:150:ARG:NH2	2.28	0.48
1:D:349:GLY:HA3	1:D:365:ALA:HB1	1.96	0.48
6:A:1178:HOH:O	1:E:503:LYS:HE3	2.12	0.48
1:F:154:LEU:HD12	1:F:251:LEU:HD23	1.95	0.48
1:C:77:ASP:O	1:C:80:GLN:HG3	2.14	0.48
1:B:455:LEU:HD13	1:B:459:ALA:CB	2.44	0.47
1:B:216:ASN:ND2	1:C:212:THR:OG1	2.47	0.47
1:C:14:CYS:HA	1:C:466:CYS:HA	1.96	0.47
1:A:176:LYS:HE2	1:A:257:TYR:CE2	2.49	0.47
1:D:129:GLY:O	1:D:157:SER:HB3	2.15	0.47
1:D:500:PHE:CB	1:D:502:ILE:HB	2.41	0.47
1:D:167:THR:HG22	1:D:244:MET:CG	2.41	0.47
1:C:501:GLN:HG2	1:D:503:LYS:HE3	1.97	0.46
1:F:134:GLY:HA3	1:F:153:TRP:HB3	1.98	0.46
1:F:502:ILE:CG2	1:F:503:LYS:N	2.78	0.46
1:B:182:VAL:HG21	1:B:213:ILE:HB	1.98	0.46
1:D:493:ASP:OD1	1:D:503:LYS:HE2	2.16	0.46
1:C:502:ILE:CG2	6:C:1155:HOH:O	2.63	0.46
1:B:216:ASN:CB	1:C:212:THR:OG1	2.62	0.46
1:E:341:ASN:HB3	6:E:1225:HOH:O	2.15	0.46
1:D:27:LYS:HE3	6:D:788:HOH:O	2.16	0.46
1:F:450:LYS:NZ	6:F:784:HOH:O	2.48	0.46
1:E:300:ILE:HD11	1:E:398:GLU:HG3	1.96	0.46
1:F:114:SER:HB2	1:F:393:HIS:CD2	2.50	0.46
1:E:219:SER:O	1:F:244:MET:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:LEU:HD22	1:F:448:PHE:HA	1.98	0.45
1:E:30:THR:O	1:F:379:GLY:HA3	2.15	0.45
1:C:331:LEU:HD21	6:C:1136:HOH:O	2.16	0.45
1:C:495:ALA:O	1:C:499:ARG:HB2	2.15	0.45
1:A:58:ILE:HG21	1:A:274:ILE:HD12	1.97	0.45
1:A:63:ASP:HB2	6:A:1217:HOH:O	2.15	0.45
1:D:14:CYS:HA	1:D:466:CYS:HA	1.99	0.45
1:C:27:LYS:HG3	1:C:32:ASP:HA	1.99	0.45
1:F:493:ASP:O	1:F:503:LYS:HD2	2.17	0.45
1:D:307:LYS:HE2	1:D:421:TRP:CH2	2.52	0.45
1:F:472:LYS:HE2	6:F:851:HOH:O	2.17	0.45
1:A:107:SER:O	1:A:111:LEU:HD23	2.17	0.45
1:B:58:ILE:HG21	1:B:274:ILE:HD12	1.98	0.45
1:C:502:ILE:HG22	6:C:1155:HOH:O	2.17	0.44
1:C:212:THR:O	1:C:212:THR:HG23	2.16	0.44
1:B:42:LEU:O	1:B:293:PRO:HD2	2.16	0.44
1:C:503:LYS:CG	6:C:1145:HOH:O	2.65	0.44
1:B:66:LEU:HD21	1:B:112:VAL:HG12	1.99	0.44
1:F:58:ILE:HG21	1:F:274:ILE:HD12	1.99	0.44
1:B:257:TYR:CD1	1:B:257:TYR:C	2.91	0.44
1:C:401:GLU:OE1	1:D:238:LYS:CE	2.65	0.44
1:F:156:LYS:HD2	1:F:158:GLY:O	2.18	0.44
1:E:495:ALA:O	1:E:499:ARG:HB2	2.18	0.44
1:F:182:VAL:HG21	1:F:213:ILE:HG21	2.00	0.44
1:F:503:LYS:C	1:F:503:LYS:HD3	2.38	0.43
1:E:111:LEU:C	1:E:111:LEU:HD12	2.39	0.43
1:E:217:ILE:O	1:F:201:ARG:HD2	2.18	0.43
1:F:358:SER:HB2	6:F:771:HOH:O	2.17	0.43
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.53	0.43
1:A:331:LEU:HD23	6:E:1125:HOH:O	2.18	0.43
1:E:497:ASN:HB2	6:E:1131:HOH:O	2.19	0.43
1:C:453:ARG:HD2	6:C:1231:HOH:O	2.19	0.43
1:B:331:LEU:HB3	1:C:332:PHE:HZ	1.84	0.43
1:E:211:GLN:HG2	6:E:1207:HOH:O	2.19	0.43
1:A:203:THR:HA	1:A:211:GLN:O	2.19	0.43
1:C:501:GLN:CG	1:D:503:LYS:HE3	2.49	0.42
1:B:331:LEU:HB3	1:C:332:PHE:CZ	2.54	0.42
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.18	0.42
1:D:380:LYS:O	1:D:384:VAL:HG23	2.19	0.42
1:B:97:CYS:HA	1:B:139:CYS:HA	2.00	0.42
1:B:387:LYS:HB3	6:B:1264:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:CYS:HA	1:A:466:CYS:HA	2.00	0.42
1:C:497:ASN:HB2	6:C:1145:HOH:O	2.19	0.42
1:E:450:LYS:HE3	6:E:1223:HOH:O	2.18	0.42
1:E:470:TYR:O	1:E:495:ALA:HA	2.18	0.42
1:C:436:THR:HA	1:C:439:LEU:HD23	2.02	0.42
1:F:9:ASN:OD1	1:F:9:ASN:N	2.50	0.42
1:E:212:THR:C	1:E:213:ILE:HD13	2.40	0.42
1:D:154:LEU:HD12	1:D:251:LEU:HD23	2.01	0.41
1:D:99:PRO:HG3	1:D:223:VAL:HB	2.02	0.41
1:B:175:ASP:OD1	1:B:239:PRO:HD3	2.19	0.41
1:E:109:ARG:CZ	1:E:267:ILE:HD13	2.51	0.41
1:A:217:ILE:HG22	1:A:218:GLY:N	2.36	0.41
1:F:21:PRO:O	6:F:870:HOH:O	2.21	0.41
1:A:219:SER:O	1:E:244:MET:HE1	2.20	0.41
1:E:98:TYR:CD2	1:E:230:ILE:HD12	2.55	0.41
1:C:182:VAL:HG22	1:C:202:VAL:HG21	2.02	0.41
2:C:1001:SIA:O1A	2:C:1001:SIA:H6	2.19	0.41
1:D:41:GLU:OE1	1:D:313:THR:OG1	2.33	0.41
1:D:359:GLU:OE2	1:D:474:ASP:HB2	2.20	0.41
1:B:191:GLN:HG2	1:B:217:ILE:HD11	2.02	0.41
1:A:324:PRO:C	6:A:1191:HOH:O	2.60	0.41
1:D:496:LEU:HD12	1:D:503:LYS:CD	2.51	0.41
1:E:293:PRO:HG2	1:E:294:PHE:CD2	2.56	0.40
1:B:354:ARG:HD3	1:E:143:PRO:HG3	2.04	0.40
1:A:219:SER:O	1:E:244:MET:CE	2.69	0.40
1:A:386:GLU:OE1	1:A:388:THR:CG2	2.70	0.40
1:C:490:ILE:HA	1:C:490:ILE:HD13	1.85	0.40
1:C:380:LYS:O	1:C:384:VAL:HG23	2.21	0.40
1:C:238:LYS:HE2	6:C:1144:HOH:O	2.21	0.40
1:E:409:LEU:HD22	1:F:410:GLU:HG3	2.04	0.40
1:C:8:ASN:HB2	1:C:358:SER:OG	2.22	0.40
1:C:99:PRO:HB2	1:C:229:ARG:HD3	2.04	0.40

There are no symmetry-related clashes.

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	487/496 (98%)	469 (96%)	17 (4%)	1 (0%)	52	75
1	B	487/496 (98%)	468 (96%)	18 (4%)	1 (0%)	52	75
1	C	487/496 (98%)	469 (96%)	16 (3%)	2 (0%)	39	61
1	D	487/496 (98%)	464 (95%)	23 (5%)	0	100	100
1	E	487/496 (98%)	470 (96%)	16 (3%)	1 (0%)	52	75
1	F	487/496 (98%)	466 (96%)	19 (4%)	2 (0%)	39	61
All	All	2922/2976 (98%)	2806 (96%)	109 (4%)	7 (0%)	52	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ARG
1	F	341	ASN
1	F	501	GLN
1	B	201	ARG
1	C	224	ARG
1	E	341	ASN
1	C	502	ILE

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	427/432 (99%)	422 (99%)	5 (1%)	78	93
1	B	427/432 (99%)	418 (98%)	9 (2%)	61	85
1	C	427/432 (99%)	413 (97%)	14 (3%)	45	73
1	D	427/432 (99%)	415 (97%)	12 (3%)	51	78
1	E	427/432 (99%)	414 (97%)	13 (3%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	427/432 (99%)	414 (97%)	13 (3%)	48 76
All	All	2562/2592 (99%)	2496 (97%)	66 (3%)	54 81

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	166	VAL
1	A	186	SER
1	A	367	LEU
1	A	439	LEU
1	B	15	LEU
1	B	18	HIS
1	B	50	LYS
1	B	166	VAL
1	B	222	LEU
1	B	260	MET
1	B	341	ASN
1	B	346	MET
1	B	356	LYS
1	C	8	ASN
1	C	15	LEU
1	C	18	HIS
1	C	126	THR
1	C	167	THR
1	C	199	SER
1	C	267	ILE
1	C	367	LEU
1	C	385	ILE
1	C	387	LYS
1	C	439	LEU
1	C	489	ASP
1	C	499	ARG
1	C	503	LYS
1	D	8	ASN
1	D	18	HIS
1	D	101	ASP
1	D	104	ASP
1	D	128	THR
1	D	161	TYR
1	D	242	ILE
1	D	274	ILE

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Mol	Chain	Res	Type
1	D	339	ILE
1	D	359	GLU
1	D	387	LYS
1	D	439	LEU
1	E	8	ASN
1	E	15	LEU
1	E	18	HIS
1	E	31	ASP
1	E	96	ASN
1	E	163	LEU
1	E	199	SER
1	E	217	ILE
1	E	222	LEU
1	E	242	ILE
1	E	406	ILE
1	E	489	ASP
1	E	499	ARG
1	F	8	ASN
1	F	18	HIS
1	F	32	ASP
1	F	101	ASP
1	F	104	ASP
1	F	128	THR
1	F	161	TYR
1	F	244	MET
1	F	358	SER
1	F	387	LYS
1	F	472	LYS
1	F	502	ILE
1	F	503	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	216	ASN
1	A	296	ASN
1	B	22	ASN
1	B	75	HIS
1	B	216	ASN
1	B	226	GLN
1	B	296	ASN

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Mol	Chain	Res	Type
1	C	18	HIS
1	C	33	GLN
1	C	188	ASN
1	C	296	ASN
1	D	296	ASN
1	E	18	HIS
1	E	211	GLN
1	E	296	ASN
1	F	296	ASN
1	F	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

36 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	GAL	A	1002	2	11,11,12	0.72	0	14,15,17	2.05	4 (28%)
2	NAG	A	1003	2	15,15,15	0.72	0	17,21,21	2.02	5 (29%)
3	NAG	A	1004	1	14,14,15	0.95	1 (7%)	15,19,21	2.74	5 (33%)
4	NAG	A	1005	1,4	14,14,15	0.84	0	15,19,21	1.47	1 (6%)
4	NAG	A	1006	4	14,14,15	0.55	0	15,19,21	1.68	4 (26%)
3	NAG	A	1007	1	14,14,15	0.94	1 (7%)	15,19,21	1.55	2 (13%)
2	GAL	B	1002	2	11,11,12	0.86	0	14,15,17	2.32	6 (42%)
2	NAG	B	1003	2	15,15,15	0.69	0	17,21,21	1.72	5 (29%)
3	NAG	B	1004	1	14,14,15	0.72	0	15,19,21	2.32	4 (26%)
4	NAG	B	1005	1,4	14,14,15	0.68	0	15,19,21	1.78	3 (20%)
4	NAG	B	1006	4	14,14,15	0.52	0	15,19,21	2.79	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1007	1	14,14,15	0.99	1 (7%)	15,19,21	1.43	2 (13%)
2	GAL	C	1002	2	11,11,12	0.93	0	14,15,17	2.20	6 (42%)
2	NAG	C	1003	2	15,15,15	0.59	0	17,21,21	1.64	3 (17%)
4	NAG	C	1004	1,4	14,14,15	0.98	1 (7%)	15,19,21	1.95	5 (33%)
4	NAG	C	1005	4	14,14,15	0.64	0	15,19,21	1.12	1 (6%)
4	NAG	C	1006	1,4	14,14,15	1.14	1 (7%)	15,19,21	2.38	7 (46%)
4	NAG	C	1007	4	14,14,15	0.54	0	15,19,21	1.84	5 (33%)
3	NAG	C	1008	1	14,14,15	0.84	1 (7%)	15,19,21	2.17	3 (20%)
5	NAG	D	601	1,5	14,14,15	1.07	1 (7%)	15,19,21	0.95	1 (6%)
5	NAG	D	602	5	14,14,15	0.53	0	15,19,21	1.60	3 (20%)
4	NAG	D	604	1,4	14,14,15	0.75	0	15,19,21	1.66	3 (20%)
4	NAG	D	605	4	14,14,15	0.81	1 (7%)	15,19,21	2.29	4 (26%)
3	NAG	D	606	1	14,14,15	1.07	1 (7%)	15,19,21	1.92	4 (26%)
2	GAL	E	1002	2	11,11,12	0.76	0	14,15,17	2.21	6 (42%)
2	NAG	E	1003	2	15,15,15	0.44	0	17,21,21	1.85	4 (23%)
4	NAG	E	1004	1,4	14,14,15	0.45	0	15,19,21	1.61	4 (26%)
4	NAG	E	1005	4	14,14,15	0.73	0	15,19,21	1.59	3 (20%)
4	NAG	E	1006	1,4	14,14,15	0.85	1 (7%)	15,19,21	1.10	1 (6%)
4	NAG	E	1007	4	14,14,15	0.62	0	15,19,21	1.59	3 (20%)
3	NAG	E	1008	1	14,14,15	0.81	0	15,19,21	1.93	4 (26%)
5	NAG	F	601	1,5	14,14,15	0.85	0	15,19,21	1.38	3 (20%)
5	NAG	F	602	5	14,14,15	0.59	0	15,19,21	1.84	5 (33%)
4	NAG	F	604	1,4	14,14,15	1.04	2 (14%)	15,19,21	1.82	3 (20%)
4	NAG	F	605	4	14,14,15	0.81	1 (7%)	15,19,21	1.95	2 (13%)
3	NAG	F	606	1	14,14,15	1.07	1 (7%)	15,19,21	1.76	5 (33%)

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	GAL	A	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1003	2	-	0/6/26/26	0/1/1/1
3	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
2	GAL	B	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1003	2	-	0/6/26/26	0/1/1/1
3	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1006	4	-	0/6/23/26	0/1/1/1
3	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
2	GAL	C	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1003	2	-	0/6/26/26	0/1/1/1
4	NAG	C	1004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1005	4	-	0/6/23/26	0/1/1/1
4	NAG	C	1006	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1007	4	-	0/6/23/26	0/1/1/1
3	NAG	C	1008	1	-	0/6/23/26	0/1/1/1
5	NAG	D	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	602	5	-	0/6/23/26	0/1/1/1
4	NAG	D	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	605	4	-	0/6/23/26	0/1/1/1
3	NAG	D	606	1	-	0/6/23/26	0/1/1/1
2	GAL	E	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1003	2	-	0/6/26/26	0/1/1/1
4	NAG	E	1004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1005	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1006	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1007	4	-	0/6/23/26	0/1/1/1
3	NAG	E	1008	1	-	0/6/23/26	0/1/1/1
5	NAG	F	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	602	5	-	0/6/23/26	0/1/1/1
4	NAG	F	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	605	4	-	0/6/23/26	0/1/1/1
3	NAG	F	606	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1006	NAG	O5-C1	-2.99	1.38	1.43
5	D	601	NAG	O5-C1	-2.92	1.38	1.43
4	F	604	NAG	O5-C1	-2.62	1.39	1.43
4	E	1006	NAG	O5-C1	-2.32	1.39	1.43
4	F	604	NAG	O5-C5	-2.28	1.38	1.43
4	C	1004	NAG	O5-C1	-2.06	1.40	1.43
3	A	1004	NAG	O4-C4	2.16	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	605	NAG	O7-C7	2.23	1.28	1.23
4	D	605	NAG	O7-C7	2.31	1.28	1.23
3	A	1007	NAG	C1-C2	2.39	1.55	1.52
3	C	1008	NAG	C1-C2	2.44	1.55	1.52
3	B	1007	NAG	C1-C2	2.55	1.56	1.52
3	F	606	NAG	C1-C2	2.89	1.56	1.52
3	D	606	NAG	C1-C2	3.00	1.56	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1006	NAG	C1-O5-C5	-6.58	103.90	112.25
4	B	1006	NAG	C3-C4-C5	-5.03	101.44	110.20
2	A	1002	GAL	O3-C3-C2	-4.69	101.53	110.00
4	B	1005	NAG	O4-C4-C3	-4.63	99.91	110.34
2	C	1003	NAG	C3-C2-N2	-4.34	101.67	110.66
2	E	1002	GAL	O3-C3-C2	-4.11	102.57	110.00
4	D	605	NAG	C2-N2-C7	-4.09	117.78	123.04
2	E	1003	NAG	C3-C2-N2	-4.05	102.28	110.66
2	B	1002	GAL	O2-C2-C3	-4.02	102.03	110.12
4	C	1006	NAG	O4-C4-C3	-3.87	101.62	110.34
4	C	1004	NAG	O3-C3-C4	-3.80	101.79	110.34
4	C	1006	NAG	C4-C3-C2	-3.77	105.37	111.23
3	D	606	NAG	C3-C4-C5	-3.71	103.72	110.20
3	B	1007	NAG	O7-C7-C8	-3.66	115.35	122.06
4	F	604	NAG	O7-C7-C8	-3.56	115.53	122.06
4	A	1005	NAG	O4-C4-C3	-3.55	102.35	110.34
4	E	1004	NAG	O3-C3-C4	-3.52	102.41	110.34
2	B	1003	NAG	C4-C3-C2	-3.49	105.60	110.43
3	D	606	NAG	O7-C7-C8	-3.42	115.79	122.06
4	C	1007	NAG	O3-C3-C2	-3.39	102.40	109.11
5	F	602	NAG	O4-C4-C3	-3.36	102.78	110.34
2	E	1002	GAL	O2-C2-C3	-3.32	103.44	110.12
3	F	606	NAG	O7-C7-C8	-3.30	116.00	122.06
4	A	1006	NAG	C3-C4-C5	-3.25	104.53	110.20
2	A	1003	NAG	C4-C3-C2	-3.18	106.02	110.43
2	C	1002	GAL	O2-C2-C3	-3.03	104.02	110.12
5	F	602	NAG	C2-N2-C7	-3.03	119.15	123.04
3	F	606	NAG	C3-C4-C5	-3.02	104.94	110.20
2	A	1002	GAL	O2-C2-C3	-2.92	104.24	110.12
3	A	1007	NAG	O7-C7-C8	-2.92	116.71	122.06
2	B	1002	GAL	O3-C3-C2	-2.89	104.78	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1008	NAG	O7-C7-C8	-2.88	116.79	122.06
4	C	1004	NAG	C2-N2-C7	-2.82	119.42	123.04
4	C	1007	NAG	C2-N2-C7	-2.78	119.47	123.04
3	A	1004	NAG	C3-C4-C5	-2.78	105.36	110.20
4	C	1006	NAG	O3-C3-C2	-2.68	103.80	109.11
4	D	605	NAG	C3-C4-C5	-2.67	105.54	110.20
5	D	601	NAG	C4-C3-C2	-2.57	107.24	111.23
4	F	605	NAG	C3-C4-C5	-2.56	105.73	110.20
2	E	1003	NAG	C1-O5-C5	-2.55	108.76	113.47
2	A	1003	NAG	O7-C7-C8	-2.49	117.50	122.06
3	C	1008	NAG	C4-C3-C2	-2.47	107.39	111.23
4	D	604	NAG	O5-C5-C6	-2.45	102.04	107.35
2	B	1003	NAG	O7-C7-C8	-2.43	117.61	122.06
4	C	1006	NAG	O5-C5-C6	-2.42	102.12	107.35
4	E	1004	NAG	C2-N2-C7	-2.37	120.00	123.04
4	F	604	NAG	O5-C5-C6	-2.37	102.22	107.35
4	B	1006	NAG	C4-C3-C2	-2.36	107.56	111.23
5	F	601	NAG	C4-C3-C2	-2.35	107.58	111.23
4	B	1005	NAG	O4-C4-C5	-2.35	103.02	109.24
4	C	1004	NAG	O7-C7-C8	-2.33	117.79	122.06
2	C	1002	GAL	C6-C5-C4	-2.29	107.36	113.02
5	F	601	NAG	O4-C4-C3	-2.28	105.20	110.34
4	C	1006	NAG	C3-C2-N2	-2.26	105.14	110.56
4	E	1006	NAG	C3-C2-N2	-2.26	105.15	110.56
4	E	1007	NAG	O3-C3-C2	-2.16	104.84	109.11
2	C	1003	NAG	O4-C4-C3	-2.15	105.49	110.34
2	C	1002	GAL	O3-C3-C2	-2.15	106.12	110.00
2	E	1002	GAL	C6-C5-C4	-2.14	107.74	113.02
4	C	1005	NAG	C3-C4-C5	-2.13	106.48	110.20
5	D	602	NAG	O7-C7-C8	-2.13	118.16	122.06
4	C	1007	NAG	C3-C2-N2	-2.12	105.48	110.56
3	B	1004	NAG	C6-C5-C4	-2.08	107.88	113.02
3	C	1008	NAG	C6-C5-C4	-2.05	107.97	113.02
4	E	1007	NAG	C2-N2-C7	-2.03	120.43	123.04
4	D	604	NAG	C8-C7-N2	2.00	119.94	116.11
2	E	1002	GAL	O2-C2-C1	2.03	113.27	109.21
4	A	1006	NAG	O4-C4-C3	2.03	114.91	110.34
3	E	1008	NAG	O7-C7-N2	2.04	126.02	121.86
3	B	1004	NAG	C3-C2-N2	2.06	115.49	110.56
4	B	1006	NAG	C2-N2-C7	2.08	125.71	123.04
2	A	1002	GAL	C1-O5-C5	2.09	114.91	112.25
4	A	1006	NAG	O4-C4-C5	2.10	114.79	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	606	NAG	C3-C2-N2	2.11	115.60	110.56
5	F	602	NAG	C8-C7-N2	2.15	120.21	116.11
2	E	1003	NAG	O5-C5-C6	2.16	111.82	106.36
4	C	1007	NAG	O4-C4-C5	2.17	114.99	109.24
2	B	1002	GAL	C2-C3-C4	2.18	114.75	111.04
4	D	605	NAG	O4-C4-C5	2.19	115.04	109.24
3	B	1007	NAG	C8-C7-N2	2.22	120.35	116.11
2	B	1003	NAG	O5-C5-C6	2.22	111.98	106.36
3	F	606	NAG	O3-C3-C2	2.24	113.55	109.11
3	D	606	NAG	O5-C5-C6	2.25	112.23	107.35
2	C	1002	GAL	O2-C2-C1	2.29	113.79	109.21
4	E	1005	NAG	O7-C7-N2	2.29	126.53	121.86
3	E	1008	NAG	C2-N2-C7	2.31	126.00	123.04
4	E	1004	NAG	C3-C2-N2	2.31	116.09	110.56
3	F	606	NAG	O4-C4-C5	2.32	115.38	109.24
2	B	1003	NAG	O3-C3-C2	2.32	114.39	109.66
5	F	601	NAG	C3-C4-C5	2.35	114.30	110.20
4	E	1004	NAG	C1-O5-C5	2.37	115.26	112.25
2	E	1002	GAL	C1-C2-C3	2.38	112.36	109.54
4	B	1006	NAG	O4-C4-C5	2.39	115.57	109.24
5	D	602	NAG	C8-C7-N2	2.40	120.70	116.11
4	E	1005	NAG	O3-C3-C2	2.42	113.91	109.11
4	A	1006	NAG	C1-O5-C5	2.54	115.47	112.25
2	C	1003	NAG	O3-C3-C4	2.55	116.08	110.34
5	F	602	NAG	O3-C3-C2	2.62	114.29	109.11
3	D	606	NAG	O4-C4-C5	2.62	116.18	109.24
3	A	1004	NAG	O4-C4-C5	2.62	116.19	109.24
4	C	1006	NAG	O4-C4-C5	2.65	116.25	109.24
4	C	1004	NAG	O3-C3-C2	2.71	114.49	109.11
4	B	1005	NAG	O5-C5-C6	2.75	113.29	107.35
4	E	1005	NAG	C2-N2-C7	2.81	126.65	123.04
2	B	1003	NAG	O3-C3-C4	2.84	116.74	110.34
3	B	1004	NAG	O4-C4-C3	2.87	116.81	110.34
3	A	1004	NAG	C3-C2-N2	2.88	117.46	110.56
2	A	1003	NAG	O3-C3-C4	3.02	117.14	110.34
4	B	1006	NAG	O4-C4-C3	3.07	117.26	110.34
2	B	1002	GAL	C1-O5-C5	3.15	116.24	112.25
2	C	1002	GAL	C1-C2-C3	3.32	113.47	109.54
2	A	1003	NAG	C3-C2-N2	3.33	117.56	110.66
4	F	604	NAG	C1-O5-C5	3.42	116.58	112.25
5	F	602	NAG	C1-O5-C5	3.44	116.61	112.25
4	C	1007	NAG	C1-O5-C5	3.54	116.75	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1004	NAG	C3-C2-N2	3.59	119.15	110.56
4	B	1006	NAG	O5-C5-C6	3.60	115.15	107.35
2	A	1003	NAG	O3-C3-C2	3.64	117.08	109.66
2	B	1002	GAL	O2-C2-C1	3.64	116.51	109.21
4	D	604	NAG	C1-O5-C5	3.69	116.93	112.25
3	A	1007	NAG	C1-O5-C5	3.77	117.03	112.25
4	E	1007	NAG	C1-O5-C5	3.93	117.23	112.25
3	A	1004	NAG	O4-C4-C3	3.95	119.22	110.34
2	B	1002	GAL	C1-C2-C3	4.01	114.28	109.54
2	A	1002	GAL	C1-C2-C3	4.03	114.30	109.54
2	E	1003	NAG	C4-C3-C2	4.15	116.19	110.43
2	E	1002	GAL	C1-O5-C5	4.77	118.30	112.25
5	D	602	NAG	C1-O5-C5	4.82	118.36	112.25
2	C	1002	GAL	C1-O5-C5	4.90	118.47	112.25
4	C	1006	NAG	C1-O5-C5	5.12	118.75	112.25
3	E	1008	NAG	C1-O5-C5	5.26	118.92	112.25
4	F	605	NAG	C1-O5-C5	5.88	119.71	112.25
4	D	605	NAG	C1-O5-C5	6.34	120.29	112.25
3	C	1008	NAG	C1-O5-C5	6.88	120.98	112.25
3	B	1004	NAG	C1-O5-C5	7.32	121.53	112.25
3	A	1004	NAG	C1-O5-C5	7.98	122.38	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	NAG	1	0
2	B	1003	NAG	1	0
4	B	1005	NAG	1	0
4	D	605	NAG	1	0
4	E	1005	NAG	1	0
3	E	1008	NAG	1	0

5.5 Carbohydrates

34 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	A	1001	2	16,20,21	0.93	1 (6%)	18,28,31	1.01	2 (11%)
2	GAL	A	1002	2	11,11,12	0.72	0	14,15,17	2.05	4 (28%)
2	NAG	A	1003	2	15,15,15	0.72	0	17,21,21	2.02	5 (29%)
4	NAG	A	1005	1,4	14,14,15	0.84	0	15,19,21	1.47	1 (6%)
4	NAG	A	1006	4	14,14,15	0.55	0	15,19,21	1.68	4 (26%)
2	SIA	B	1001	2	16,20,21	0.52	0	18,28,31	1.65	3 (16%)
2	GAL	B	1002	2	11,11,12	0.86	0	14,15,17	2.32	6 (42%)
2	NAG	B	1003	2	15,15,15	0.69	0	17,21,21	1.72	5 (29%)
4	NAG	B	1005	1,4	14,14,15	0.68	0	15,19,21	1.78	3 (20%)
4	NAG	B	1006	4	14,14,15	0.52	0	15,19,21	2.79	7 (46%)
2	SIA	C	1001	2	16,20,21	0.81	1 (6%)	18,28,31	1.43	3 (16%)
2	GAL	C	1002	2	11,11,12	0.93	0	14,15,17	2.20	6 (42%)
2	NAG	C	1003	2	15,15,15	0.59	0	17,21,21	1.64	3 (17%)
4	NAG	C	1004	1,4	14,14,15	0.98	1 (7%)	15,19,21	1.95	5 (33%)
4	NAG	C	1005	4	14,14,15	0.64	0	15,19,21	1.12	1 (6%)
4	NAG	C	1006	1,4	14,14,15	1.14	1 (7%)	15,19,21	2.38	7 (46%)
4	NAG	C	1007	4	14,14,15	0.54	0	15,19,21	1.84	5 (33%)
5	NAG	D	601	1,5	14,14,15	1.07	1 (7%)	15,19,21	0.95	1 (6%)
5	NAG	D	602	5	14,14,15	0.53	0	15,19,21	1.60	3 (20%)
5	BMA	D	603	5	11,11,12	0.70	0	14,15,17	2.81	5 (35%)
4	NAG	D	604	1,4	14,14,15	0.75	0	15,19,21	1.66	3 (20%)
4	NAG	D	605	4	14,14,15	0.81	1 (7%)	15,19,21	2.29	4 (26%)
2	SIA	E	1001	2	16,20,21	1.03	1 (6%)	18,28,31	1.84	3 (16%)
2	GAL	E	1002	2	11,11,12	0.76	0	14,15,17	2.21	6 (42%)
2	NAG	E	1003	2	15,15,15	0.44	0	17,21,21	1.85	4 (23%)
4	NAG	E	1004	1,4	14,14,15	0.45	0	15,19,21	1.61	4 (26%)
4	NAG	E	1005	4	14,14,15	0.73	0	15,19,21	1.59	3 (20%)
4	NAG	E	1006	1,4	14,14,15	0.85	1 (7%)	15,19,21	1.10	1 (6%)
4	NAG	E	1007	4	14,14,15	0.62	0	15,19,21	1.59	3 (20%)
5	NAG	F	601	1,5	14,14,15	0.85	0	15,19,21	1.38	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	602	5	14,14,15	0.59	0	15,19,21	1.84	5 (33%)
5	BMA	F	603	5	11,11,12	0.91	1 (9%)	14,15,17	2.45	4 (28%)
4	NAG	F	604	1,4	14,14,15	1.04	2 (14%)	15,19,21	1.82	3 (20%)
4	NAG	F	605	4	14,14,15	0.81	1 (7%)	15,19,21	1.95	2 (13%)

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	SIA	A	1001	2	-	0/14/34/38	0/1/1/1
2	GAL	A	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1003	2	-	0/6/26/26	0/1/1/1
4	NAG	A	1005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	4	-	0/6/23/26	0/1/1/1
2	SIA	B	1001	2	-	0/14/34/38	0/1/1/1
2	GAL	B	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1003	2	-	0/6/26/26	0/1/1/1
4	NAG	B	1005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1006	4	-	0/6/23/26	0/1/1/1
2	SIA	C	1001	2	-	0/14/34/38	0/1/1/1
2	GAL	C	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1003	2	-	0/6/26/26	0/1/1/1
4	NAG	C	1004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1005	4	-	0/6/23/26	0/1/1/1
4	NAG	C	1006	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1007	4	-	0/6/23/26	0/1/1/1
5	NAG	D	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	602	5	-	0/6/23/26	0/1/1/1
5	BMA	D	603	5	-	0/2/19/22	0/1/1/1
4	NAG	D	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	605	4	-	0/6/23/26	0/1/1/1
2	SIA	E	1001	2	-	0/14/34/38	0/1/1/1
2	GAL	E	1002	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1003	2	-	0/6/26/26	0/1/1/1
4	NAG	E	1004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1005	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1006	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1007	4	-	0/6/23/26	0/1/1/1
5	NAG	F	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	602	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	F	603	5	-	0/2/19/22	0/1/1/1
4	NAG	F	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	605	4	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1006	NAG	O5-C1	-2.99	1.38	1.43
5	D	601	NAG	O5-C1	-2.92	1.38	1.43
4	F	604	NAG	O5-C1	-2.62	1.39	1.43
4	E	1006	NAG	O5-C1	-2.32	1.39	1.43
4	F	604	NAG	O5-C5	-2.28	1.38	1.43
4	C	1004	NAG	O5-C1	-2.06	1.40	1.43
5	F	603	BMA	C2-C3	2.10	1.55	1.52
4	F	605	NAG	O7-C7	2.23	1.28	1.23
4	D	605	NAG	O7-C7	2.31	1.28	1.23
2	C	1001	SIA	C3-C2	2.44	1.56	1.52
2	E	1001	SIA	C3-C2	2.59	1.56	1.52
2	A	1001	SIA	C7-C6	2.65	1.56	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1006	NAG	C1-O5-C5	-6.58	103.90	112.25
4	B	1006	NAG	C3-C4-C5	-5.03	101.44	110.20
2	A	1002	GAL	O3-C3-C2	-4.69	101.53	110.00
4	B	1005	NAG	O4-C4-C3	-4.63	99.91	110.34
2	E	1001	SIA	C3-C4-C5	-4.48	106.48	111.47
2	C	1003	NAG	C3-C2-N2	-4.34	101.67	110.66
2	E	1002	GAL	O3-C3-C2	-4.11	102.57	110.00
4	D	605	NAG	C2-N2-C7	-4.09	117.78	123.04
2	E	1003	NAG	C3-C2-N2	-4.05	102.28	110.66
2	B	1002	GAL	O2-C2-C3	-4.02	102.03	110.12
4	C	1006	NAG	O4-C4-C3	-3.87	101.62	110.34
4	C	1004	NAG	O3-C3-C4	-3.80	101.79	110.34
4	C	1006	NAG	C4-C3-C2	-3.77	105.37	111.23
4	F	604	NAG	O7-C7-C8	-3.56	115.53	122.06
4	A	1005	NAG	O4-C4-C3	-3.55	102.35	110.34
4	E	1004	NAG	O3-C3-C4	-3.52	102.41	110.34
2	B	1003	NAG	C4-C3-C2	-3.49	105.60	110.43
2	E	1001	SIA	C4-C5-N5	-3.40	103.02	110.41
4	C	1007	NAG	O3-C3-C2	-3.39	102.40	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	602	NAG	O4-C4-C3	-3.36	102.78	110.34
2	E	1002	GAL	O2-C2-C3	-3.32	103.44	110.12
4	A	1006	NAG	C3-C4-C5	-3.25	104.53	110.20
2	A	1003	NAG	C4-C3-C2	-3.18	106.02	110.43
2	C	1002	GAL	O2-C2-C3	-3.03	104.02	110.12
5	F	602	NAG	C2-N2-C7	-3.03	119.15	123.04
2	A	1002	GAL	O2-C2-C3	-2.92	104.24	110.12
2	C	1001	SIA	C4-C5-N5	-2.90	104.11	110.41
2	B	1002	GAL	O3-C3-C2	-2.89	104.78	110.00
4	C	1004	NAG	C2-N2-C7	-2.82	119.42	123.04
4	C	1007	NAG	C2-N2-C7	-2.78	119.47	123.04
2	B	1001	SIA	C4-C5-N5	-2.74	104.45	110.41
4	C	1006	NAG	O3-C3-C2	-2.68	103.80	109.11
4	D	605	NAG	C3-C4-C5	-2.67	105.54	110.20
2	C	1001	SIA	C3-C4-C5	-2.67	108.50	111.47
5	D	603	BMA	C1-C2-C3	-2.59	106.48	109.54
5	D	601	NAG	C4-C3-C2	-2.57	107.24	111.23
4	F	605	NAG	C3-C4-C5	-2.56	105.73	110.20
2	E	1003	NAG	C1-O5-C5	-2.55	108.76	113.47
2	A	1003	NAG	O7-C7-C8	-2.49	117.50	122.06
4	D	604	NAG	O5-C5-C6	-2.45	102.04	107.35
2	B	1003	NAG	O7-C7-C8	-2.43	117.61	122.06
4	C	1006	NAG	O5-C5-C6	-2.42	102.12	107.35
4	E	1004	NAG	C2-N2-C7	-2.37	120.00	123.04
4	F	604	NAG	O5-C5-C6	-2.37	102.22	107.35
4	B	1006	NAG	C4-C3-C2	-2.36	107.56	111.23
5	F	601	NAG	C4-C3-C2	-2.35	107.58	111.23
4	B	1005	NAG	O4-C4-C5	-2.35	103.02	109.24
4	C	1004	NAG	O7-C7-C8	-2.33	117.79	122.06
2	C	1001	SIA	O8-C8-C9	-2.30	103.84	109.22
2	C	1002	GAL	C6-C5-C4	-2.29	107.36	113.02
5	F	601	NAG	O4-C4-C3	-2.28	105.20	110.34
4	C	1006	NAG	C3-C2-N2	-2.26	105.14	110.56
4	E	1006	NAG	C3-C2-N2	-2.26	105.15	110.56
2	B	1001	SIA	O8-C8-C9	-2.24	103.99	109.22
2	A	1001	SIA	C4-C5-N5	-2.23	105.56	110.41
4	E	1007	NAG	O3-C3-C2	-2.16	104.84	109.11
2	C	1003	NAG	O4-C4-C3	-2.15	105.49	110.34
2	C	1002	GAL	O3-C3-C2	-2.15	106.12	110.00
2	E	1002	GAL	C6-C5-C4	-2.14	107.74	113.02
4	C	1005	NAG	C3-C4-C5	-2.13	106.48	110.20
5	D	602	NAG	O7-C7-C8	-2.13	118.16	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1007	NAG	C3-C2-N2	-2.12	105.48	110.56
4	E	1007	NAG	C2-N2-C7	-2.03	120.43	123.04
2	A	1001	SIA	C8-C7-C6	-2.02	108.95	113.01
4	D	604	NAG	C8-C7-N2	2.00	119.94	116.11
2	E	1002	GAL	O2-C2-C1	2.03	113.27	109.21
4	A	1006	NAG	O4-C4-C3	2.03	114.91	110.34
4	B	1006	NAG	C2-N2-C7	2.08	125.71	123.04
5	D	603	BMA	O5-C5-C6	2.09	111.86	107.35
2	A	1002	GAL	C1-O5-C5	2.09	114.91	112.25
4	A	1006	NAG	O4-C4-C5	2.10	114.79	109.24
5	F	602	NAG	C8-C7-N2	2.15	120.21	116.11
2	E	1003	NAG	O5-C5-C6	2.16	111.82	106.36
4	C	1007	NAG	O4-C4-C5	2.17	114.99	109.24
2	B	1002	GAL	C2-C3-C4	2.18	114.75	111.04
4	D	605	NAG	O4-C4-C5	2.19	115.04	109.24
2	B	1003	NAG	O5-C5-C6	2.22	111.98	106.36
2	C	1002	GAL	O2-C2-C1	2.29	113.79	109.21
4	E	1005	NAG	O7-C7-N2	2.29	126.53	121.86
5	F	603	BMA	O5-C1-C2	2.30	114.59	110.86
4	E	1004	NAG	C3-C2-N2	2.31	116.09	110.56
2	B	1003	NAG	O3-C3-C2	2.32	114.39	109.66
5	F	601	NAG	C3-C4-C5	2.35	114.30	110.20
4	E	1004	NAG	C1-O5-C5	2.37	115.26	112.25
2	E	1002	GAL	C1-C2-C3	2.38	112.36	109.54
4	B	1006	NAG	O4-C4-C5	2.39	115.57	109.24
5	D	602	NAG	C8-C7-N2	2.40	120.70	116.11
4	E	1005	NAG	O3-C3-C2	2.42	113.91	109.11
4	A	1006	NAG	C1-O5-C5	2.54	115.47	112.25
2	C	1003	NAG	O3-C3-C4	2.55	116.08	110.34
5	F	602	NAG	O3-C3-C2	2.62	114.29	109.11
4	C	1006	NAG	O4-C4-C5	2.65	116.25	109.24
4	C	1004	NAG	O3-C3-C2	2.71	114.49	109.11
5	D	603	BMA	O6-C6-C5	2.72	120.34	111.33
4	B	1005	NAG	O5-C5-C6	2.75	113.29	107.35
4	E	1005	NAG	C2-N2-C7	2.81	126.65	123.04
2	B	1003	NAG	O3-C3-C4	2.84	116.74	110.34
5	D	603	BMA	O3-C3-C4	3.01	117.12	110.34
2	A	1003	NAG	O3-C3-C4	3.02	117.14	110.34
4	B	1006	NAG	O4-C4-C3	3.07	117.26	110.34
2	B	1002	GAL	C1-O5-C5	3.15	116.24	112.25
2	C	1002	GAL	C1-C2-C3	3.32	113.47	109.54
2	A	1003	NAG	C3-C2-N2	3.33	117.56	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	604	NAG	C1-O5-C5	3.42	116.58	112.25
5	F	602	NAG	C1-O5-C5	3.44	116.61	112.25
4	C	1007	NAG	C1-O5-C5	3.54	116.75	112.25
2	E	1001	SIA	O6-C6-C5	3.58	114.34	108.48
4	C	1004	NAG	C3-C2-N2	3.59	119.15	110.56
4	B	1006	NAG	O5-C5-C6	3.60	115.15	107.35
2	A	1003	NAG	O3-C3-C2	3.64	117.08	109.66
2	B	1002	GAL	O2-C2-C1	3.64	116.51	109.21
4	D	604	NAG	C1-O5-C5	3.69	116.93	112.25
4	E	1007	NAG	C1-O5-C5	3.93	117.23	112.25
2	B	1002	GAL	C1-C2-C3	4.01	114.28	109.54
2	A	1002	GAL	C1-C2-C3	4.03	114.30	109.54
2	E	1003	NAG	C4-C3-C2	4.15	116.19	110.43
5	F	603	BMA	C3-C4-C5	4.21	117.54	110.20
5	F	603	BMA	O2-C2-C3	4.64	119.45	110.12
2	E	1002	GAL	C1-O5-C5	4.77	118.30	112.25
5	D	602	NAG	C1-O5-C5	4.82	118.36	112.25
2	C	1002	GAL	C1-O5-C5	4.90	118.47	112.25
5	F	603	BMA	C1-O5-C5	4.95	118.54	112.25
2	B	1001	SIA	C3-C4-C5	5.04	117.09	111.47
4	C	1006	NAG	C1-O5-C5	5.12	118.75	112.25
4	F	605	NAG	C1-O5-C5	5.88	119.71	112.25
4	D	605	NAG	C1-O5-C5	6.34	120.29	112.25
5	D	603	BMA	C1-O5-C5	8.55	123.09	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	NAG	1	0
2	B	1003	NAG	1	0
4	B	1005	NAG	1	0
2	C	1001	SIA	1	0
4	D	605	NAG	1	0
4	E	1005	NAG	1	0

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1004	1	14,14,15	0.95	1 (7%)	15,19,21	2.74	5 (33%)
3	NAG	A	1007	1	14,14,15	0.94	1 (7%)	15,19,21	1.55	2 (13%)
3	NAG	B	1004	1	14,14,15	0.72	0	15,19,21	2.32	4 (26%)
3	NAG	B	1007	1	14,14,15	0.99	1 (7%)	15,19,21	1.43	2 (13%)
3	NAG	C	1008	1	14,14,15	0.84	1 (7%)	15,19,21	2.17	3 (20%)
3	NAG	D	606	1	14,14,15	1.07	1 (7%)	15,19,21	1.92	4 (26%)
3	NAG	E	1008	1	14,14,15	0.81	0	15,19,21	1.93	4 (26%)
3	NAG	F	606	1	14,14,15	1.07	1 (7%)	15,19,21	1.76	5 (33%)

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	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1008	1	-	0/6/23/26	0/1/1/1
3	NAG	D	606	1	-	0/6/23/26	0/1/1/1
3	NAG	E	1008	1	-	0/6/23/26	0/1/1/1
3	NAG	F	606	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	NAG	O4-C4	2.16	1.48	1.43
3	A	1007	NAG	C1-C2	2.39	1.55	1.52
3	C	1008	NAG	C1-C2	2.44	1.55	1.52
3	B	1007	NAG	C1-C2	2.55	1.56	1.52
3	F	606	NAG	C1-C2	2.89	1.56	1.52
3	D	606	NAG	C1-C2	3.00	1.56	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	606	NAG	C3-C4-C5	-3.71	103.72	110.20
3	B	1007	NAG	O7-C7-C8	-3.66	115.35	122.06
3	D	606	NAG	O7-C7-C8	-3.42	115.79	122.06
3	F	606	NAG	O7-C7-C8	-3.30	116.00	122.06
3	F	606	NAG	C3-C4-C5	-3.02	104.94	110.20
3	A	1007	NAG	O7-C7-C8	-2.92	116.71	122.06
3	E	1008	NAG	O7-C7-C8	-2.88	116.79	122.06
3	A	1004	NAG	C3-C4-C5	-2.78	105.36	110.20
3	C	1008	NAG	C4-C3-C2	-2.47	107.39	111.23
3	B	1004	NAG	C6-C5-C4	-2.08	107.88	113.02
3	C	1008	NAG	C6-C5-C4	-2.05	107.97	113.02
3	E	1008	NAG	O7-C7-N2	2.04	126.02	121.86
3	B	1004	NAG	C3-C2-N2	2.06	115.49	110.56
3	F	606	NAG	C3-C2-N2	2.11	115.60	110.56
3	B	1007	NAG	C8-C7-N2	2.22	120.35	116.11
3	F	606	NAG	O3-C3-C2	2.24	113.55	109.11
3	D	606	NAG	O5-C5-C6	2.25	112.23	107.35
3	E	1008	NAG	C2-N2-C7	2.31	126.00	123.04
3	F	606	NAG	O4-C4-C5	2.32	115.38	109.24
3	D	606	NAG	O4-C4-C5	2.62	116.18	109.24
3	A	1004	NAG	O4-C4-C5	2.62	116.19	109.24
3	B	1004	NAG	O4-C4-C3	2.87	116.81	110.34
3	A	1004	NAG	C3-C2-N2	2.88	117.46	110.56
3	A	1007	NAG	C1-O5-C5	3.77	117.03	112.25
3	A	1004	NAG	O4-C4-C3	3.95	119.22	110.34
3	E	1008	NAG	C1-O5-C5	5.26	118.92	112.25
3	C	1008	NAG	C1-O5-C5	6.88	120.98	112.25
3	B	1004	NAG	C1-O5-C5	7.32	121.53	112.25
3	A	1004	NAG	C1-O5-C5	7.98	122.38	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1008	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	491/496 (98%)	-0.69	0	100 100	20, 34, 52, 85	0
1	B	491/496 (98%)	-0.69	0	100 100	21, 33, 52, 90	0
1	C	491/496 (98%)	-0.70	1 (0%)	95 96	23, 35, 53, 95	0
1	D	491/496 (98%)	-0.68	3 (0%)	90 91	21, 34, 56, 119	0
1	E	491/496 (98%)	-0.67	1 (0%)	95 96	20, 35, 53, 90	0
1	F	491/496 (98%)	-0.67	2 (0%)	93 93	22, 33, 54, 136	0
All	All	2946/2976 (98%)	-0.68	7 (0%)	95 96	20, 34, 53, 136	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	502	ILE	10.1
1	F	503	LYS	7.8
1	F	502	ILE	7.1
1	D	503	LYS	6.5
1	C	385	ILE	4.1
1	D	501	GLN	2.9
1	E	385	ILE	2.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	F	605	14/15	0.93	0.13	3.11	37,44,53,54	0
3	NAG	C	1008	14/15	0.92	0.19	2.87	49,60,66,69	0
3	NAG	A	1007	14/15	0.92	0.14	2.85	49,56,60,64	0
3	NAG	B	1007	14/15	0.94	0.12	1.75	43,50,59,60	0
3	NAG	A	1004	14/15	0.92	0.16	1.74	46,55,62,64	0
4	NAG	E	1006	14/15	0.97	0.12	0.78	39,43,56,60	0
4	NAG	D	605	14/15	0.91	0.12	0.74	35,40,45,48	0
3	NAG	B	1004	14/15	0.90	0.15	0.69	51,59,68,69	0
4	NAG	B	1006	14/15	0.97	0.12	0.49	37,49,59,67	0
4	NAG	A	1006	14/15	0.92	0.14	0.29	41,54,64,66	0
4	NAG	B	1005	14/15	0.95	0.11	0.22	35,39,43,46	0
5	NAG	F	601	14/15	0.97	0.10	-0.09	37,46,53,54	0
5	NAG	D	601	14/15	0.96	0.10	-0.32	36,41,46,48	0
4	NAG	C	1006	14/15	0.97	0.11	-0.40	42,47,54,54	0
4	NAG	C	1007	14/15	0.95	0.10	-0.64	37,47,50,50	0
4	NAG	E	1007	14/15	0.96	0.09	-1.18	33,42,49,54	0
3	NAG	E	1008	14/15	0.92	0.23	-	53,64,75,79	0
2	GAL	C	1002	11/12	0.97	0.09	-	29,32,38,42	0
2	GAL	E	1002	11/12	0.96	0.10	-	30,38,44,46	0
3	NAG	D	606	14/15	0.91	0.19	-	57,64,73,76	0
2	NAG	A	1003	15/15	0.87	0.20	-	58,79,87,89	0
4	NAG	C	1004	14/15	0.92	0.16	-	47,53,59,60	0
4	NAG	E	1005	14/15	0.92	0.17	-	55,61,67,72	0
2	GAL	B	1002	11/12	0.96	0.10	-	42,50,60,64	0
5	NAG	D	602	14/15	0.92	0.14	-	50,55,64,68	0
4	NAG	A	1005	14/15	0.96	0.12	-	35,40,43,43	0
2	NAG	C	1003	15/15	0.90	0.16	-	50,66,80,82	0
4	NAG	E	1004	14/15	0.95	0.14	-	57,60,65,69	0
2	NAG	E	1003	15/15	0.93	0.16	-	53,67,85,97	0
5	NAG	F	602	14/15	0.94	0.15	-	46,55,62,66	0
2	NAG	B	1003	15/15	0.81	0.29	-	67,88,106,108	0
4	NAG	D	604	14/15	0.96	0.11	-	38,42,47,49	0
2	GAL	A	1002	11/12	0.96	0.09	-	45,52,58,60	0
4	NAG	F	604	14/15	0.96	0.11	-	34,38,44,44	0
4	NAG	C	1005	14/15	0.84	0.18	-	53,64,74,76	0
3	NAG	F	606	14/15	0.87	0.15	-	52,61,66,72	0

6.3 Carbohydrates

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	F	605	14/15	0.93	0.13	3.11	37,44,53,54	0
4	NAG	E	1006	14/15	0.97	0.12	0.78	39,43,56,60	0
4	NAG	D	605	14/15	0.91	0.12	0.74	35,40,45,48	0
4	NAG	B	1006	14/15	0.97	0.12	0.49	37,49,59,67	0
2	SIA	C	1001	20/21	0.97	0.11	0.37	25,27,29,32	0
4	NAG	A	1006	14/15	0.92	0.14	0.29	41,54,64,66	0
4	NAG	B	1005	14/15	0.95	0.11	0.22	35,39,43,46	0
5	NAG	F	601	14/15	0.97	0.10	-0.09	37,46,53,54	0
2	SIA	E	1001	20/21	0.97	0.10	-0.30	24,28,31,31	0
5	NAG	D	601	14/15	0.96	0.10	-0.32	36,41,46,48	0
4	NAG	C	1006	14/15	0.97	0.11	-0.40	42,47,54,54	0
4	NAG	C	1007	14/15	0.95	0.10	-0.64	37,47,50,50	0
2	SIA	B	1001	20/21	0.97	0.10	-0.73	30,35,38,38	0
4	NAG	E	1007	14/15	0.96	0.09	-1.18	33,42,49,54	0
2	SIA	A	1001	20/21	0.96	0.09	-1.93	30,35,40,41	0
4	NAG	A	1005	14/15	0.96	0.12	-	35,40,43,43	0
4	NAG	F	604	14/15	0.96	0.11	-	34,38,44,44	0
2	GAL	C	1002	11/12	0.97	0.09	-	29,32,38,42	0
2	GAL	E	1002	11/12	0.96	0.10	-	30,38,44,46	0
5	BMA	D	603	11/12	0.86	0.14	-	63,77,81,81	0
4	NAG	E	1005	14/15	0.92	0.17	-	55,61,67,72	0
2	GAL	B	1002	11/12	0.96	0.10	-	42,50,60,64	0
2	NAG	A	1003	15/15	0.87	0.20	-	58,79,87,89	0
2	NAG	C	1003	15/15	0.90	0.16	-	50,66,80,82	0
5	BMA	F	603	11/12	0.74	0.15	-	71,73,78,79	0
5	NAG	D	602	14/15	0.92	0.14	-	50,55,64,68	0
4	NAG	C	1004	14/15	0.92	0.16	-	47,53,59,60	0
4	NAG	E	1004	14/15	0.95	0.14	-	57,60,65,69	0
5	NAG	F	602	14/15	0.94	0.15	-	46,55,62,66	0
2	NAG	E	1003	15/15	0.93	0.16	-	53,67,85,97	0
4	NAG	D	604	14/15	0.96	0.11	-	38,42,47,49	0
2	NAG	B	1003	15/15	0.81	0.29	-	67,88,106,108	0
2	GAL	A	1002	11/12	0.96	0.09	-	45,52,58,60	0
4	NAG	C	1005	14/15	0.84	0.18	-	53,64,74,76	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	1008	14/15	0.92	0.19	2.87	49,60,66,69	0
3	NAG	A	1007	14/15	0.92	0.14	2.85	49,56,60,64	0
3	NAG	B	1007	14/15	0.94	0.12	1.75	43,50,59,60	0
3	NAG	A	1004	14/15	0.92	0.16	1.74	46,55,62,64	0
3	NAG	B	1004	14/15	0.90	0.15	0.69	51,59,68,69	0
3	NAG	D	606	14/15	0.91	0.19	-	57,64,73,76	0
3	NAG	E	1008	14/15	0.92	0.23	-	53,64,75,79	0
3	NAG	F	606	14/15	0.87	0.15	-	52,61,66,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.