Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 04:49 AM BST

PDB ID	:	4QBZ
Title	:	Crystal structure of human TLR8 in complex with DS-802
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2014-05-09
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

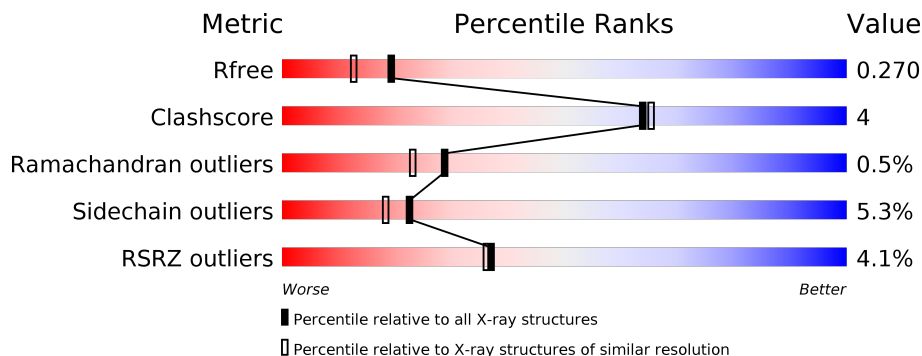|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
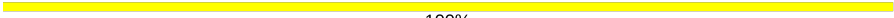
Metric	Percentile Ranks	Value
Rfree		0.270
Clashscore		4
Ramachandran outliers		0.5%
Sidechain outliers		5.3%
RSRZ outliers		4.1%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	811	4% / 81% ... 10% · 7%
1	B	811	4% / 80% ... 11% · 7%
2	C	5	80% ... 20%
3	D	2	100%
3	G	2	100%
4	E	3	67% ... 33%

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	3	100%
5	F	4	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13074 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total 6071	C 3882	N 1029	O 1141	S 19	0	0	0
1	B	751	Total 6062	C 3878	N 1031	O 1134	S 19	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
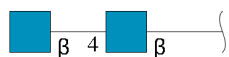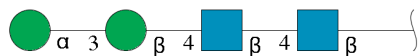

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total 28	C 16	N 2	O 10	0	0	0
3	G	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

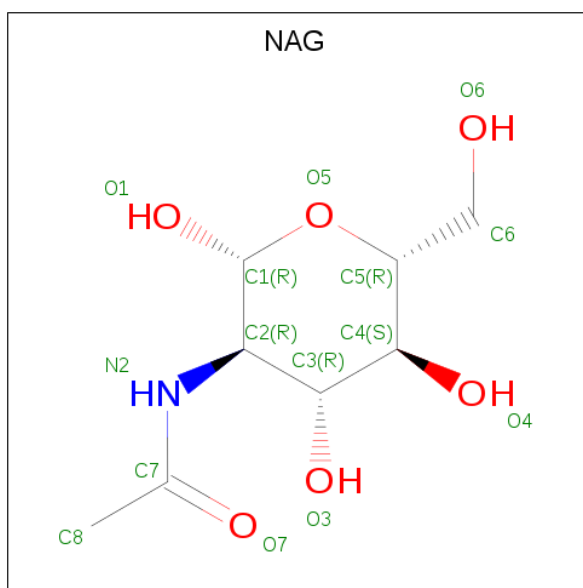| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total 39	C 22	N 2	O 15	0	0	0
4	H	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 14	C N O 8 1 5		0	0
6	A	1	Total 14	C N O 8 1 5		0	0
6	A	1	Total 14	C N O 8 1 5		0	0
6	A	1	Total 14	C N O 8 1 5		0	0
6	A	1	Total 14	C N O 8 1 5		0	0
6	A	1	Total 14	C N O 8 1 5		0	0
6	B	1	Total 14	C N O 8 1 5		0	0
6	B	1	Total 14	C N O 8 1 5		0	0
6	B	1	Total 14	C N O 8 1 5		0	0
6	B	1	Total 14	C N O 8 1 5		0	0
6	B	1	Total 14	C N O 8 1 5		0	0

- Molecule 7 is 2-butyl[1,3]oxazolo[4,5-c]quinolin-4-amine (three-letter code: D80) (formula: $C_{14}H_{15}N_3O$).

D80
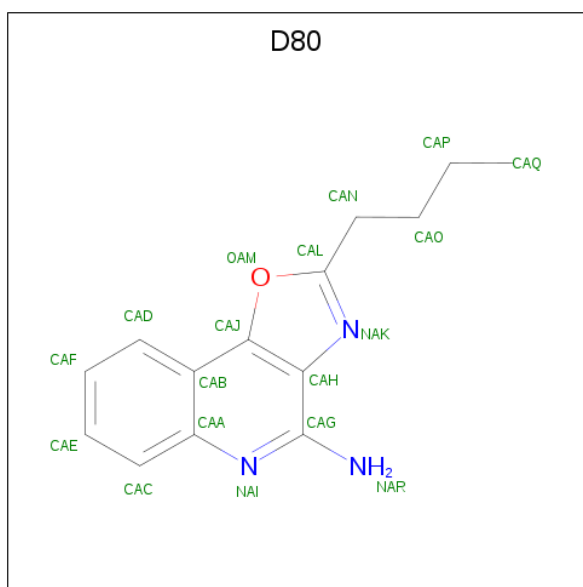
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			18	14	3	1		
7	B	1	Total	C	N	O	0	0
			18	14	3	1		

• Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	277	Total	O	0	0
			277	277		
8	B	229	Total	O	0	0
			229	229		

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 propo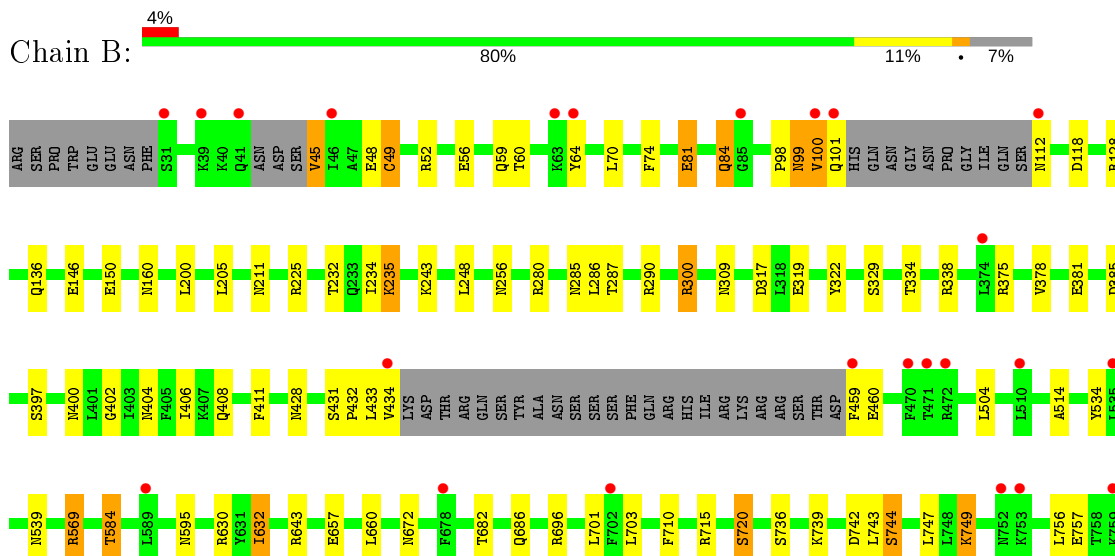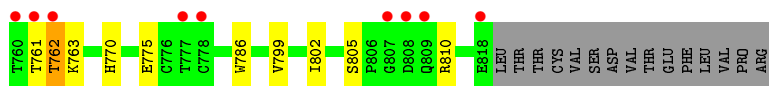rtions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, 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: Toll-like receptor 8

- Molecule 1: Toll-like receptor 8

T760 T761 T762 K763 H770 E775 C776 T777 C778 W786 V799 I802 S805 P806 G807 D808 Q809 R810 E818 LEU THR THR CYS VAL SER ASP VAL THR GLU PHE LEU VAL PRO ARG
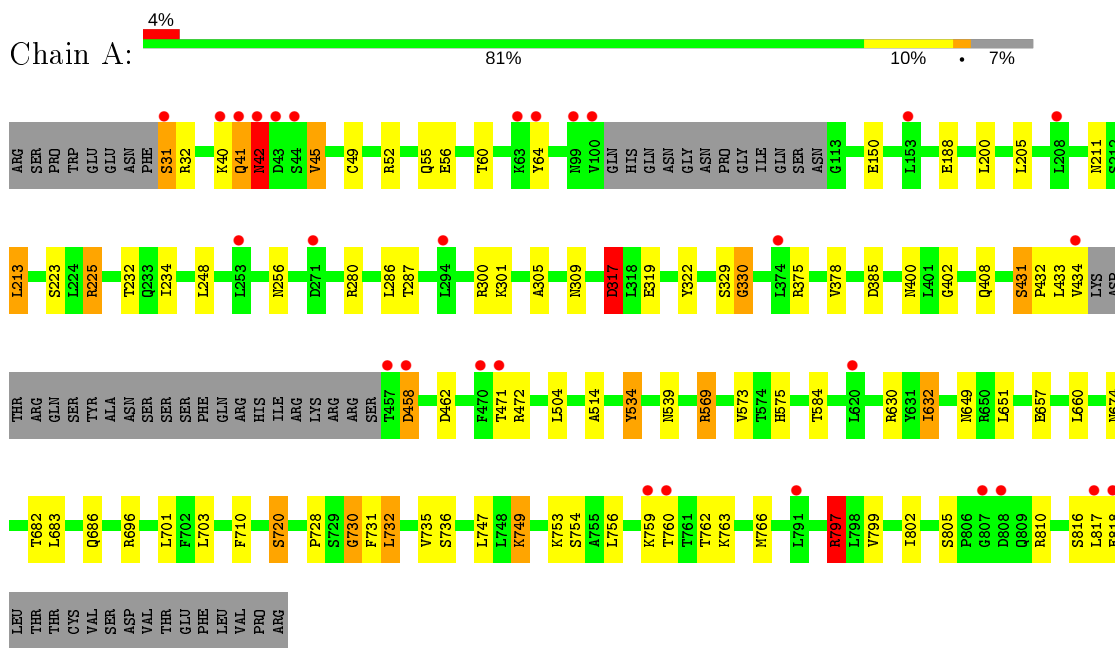
• Molecule 2: alpha-D-mannopyranose-(2-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 80% 20%

NAG1 NAG2 BMA3 MAN4 BMA5

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

NAG1 NAG2

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 67% 33%

NAG1 NAG2 BMA3

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%

NAG1 NAG2 BMA3

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1 NAG2 BMA3 MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.15Å 156.72Å 86.16Å 90.00° 77.10° 90.00°	Depositor
Resolution (Å)	26.38 – 2.00 26.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (26.38-2.00) 99.1 (26.36-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$<I/\sigma(I)>$ [1]	2.04 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.209 , 0.264 0.218 , 0.270	Depositor DCC
R_{free} test set	6273 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.1	EDS
L-test for twinning[2]	$<|L|> = 0.46, <L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13074	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: BMA, NAG, D80, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.51	0/6196	0.92	9/8404 (0.1%)
1	B	0.47	0/6186	0.90	6/8387 (0.1%)
All	All	0.49	0/12382	0.91	15/16791 (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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	569	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	643	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	630	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	290	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	730	GLY	N-CA-C	-5.74	98.74	113.10
1	A	797	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	630	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	338	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	643	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	431	SER	C-N-CD	5.29	139.51	128.40
1	A	317	ASP	CB-CG-OD2	-5.23	113.59	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	GLN	CB-CA-C	-5.16	100.09	110.40
1	A	747	LEU	CB-CG-CD2	5.04	119.56	111.00
1	A	569	ARG	CG-CD-NE	5.02	122.34	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	ASN	Peptide
1	A	458	ASP	Peptide
1	B	99	ASN	Peptide

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	6071	0	6055	48	1
1	B	6062	0	6055	58	0
2	C	61	0	52	1	0
3	D	28	0	25	0	0
3	G	28	0	25	0	0
4	E	39	0	34	2	0
4	H	39	0	34	0	0
5	F	50	0	43	0	0
6	A	84	0	78	1	0
6	B	70	0	65	1	0
7	A	18	0	15	0	0
7	B	18	0	15	0	0
8	A	277	0	0	1	1
8	B	229	0	0	2	0
All	All	13074	0	12496	104	1

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 (104) 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:818:GLU:N	1:A:818:GLU:OE1	1.88	1.05
1:A:433:LEU:HD23	1:A:434:VAL:N	1.95	0.82
1:B:99:ASN:HB3	1:B:100:VAL:HG23	1.64	0.80
1:B:317:ASP:OD2	1:B:319:GLU:OE1	2.03	0.76
1:A:31:SER:OG	1:A:32:ARG:N	2.18	0.75
1:B:696:ARG:HG2	1:B:720:SER:HB2	1.69	0.74
1:A:696:ARG:HG2	1:A:720:SER:HB2	1.69	0.73
1:B:799:VAL:O	1:B:802:ILE:HD11	1.93	0.67
1:A:799:VAL:O	1:A:802:ILE:HD11	1.95	0.67
1:B:375[B]:ARG:HD2	1:B:400:ASN:HD21	1.60	0.66
1:A:651:LEU:H	1:A:674:ASN:HD22	1.47	0.63
1:A:462:ASP:OD2	2:C:4:MAN:O6	2.10	0.62
1:B:742:ASP:OD1	1:B:744:SER:HB2	2.00	0.62
1:A:632:ILE:HD11	1:A:657:GLU:HB3	1.81	0.62
1:B:744:SER:OG	1:B:770:HIS:CE1	2.54	0.61
1:A:375:ARG:HD2	1:A:400:ASN:HD21	1.66	0.61
1:B:632:ILE:HD11	1:B:657:GLU:HB3	1.83	0.61
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.37	0.60
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.21	0.59
1:A:731:PHE:O	1:A:732:LEU:HB3	2.02	0.59
1:B:736:SER:O	1:B:763:LYS:HB2	2.01	0.59
1:B:74:PHE:HE1	1:B:100:VAL:HB	1.67	0.59
1:B:682:THR:HG22	1:B:710:PHE:CZ	2.38	0.57
1:A:732:LEU:HA	1:A:735:VAL:CG1	2.35	0.57
1:B:406:ILE:H	1:B:428:ASN:HD22	1.53	0.57
1:A:649:ASN:H	1:A:674:ASN:HD21	1.54	0.56
1:A:287:THR:OG1	8:A:1158:HOH:O	2.17	0.55
1:B:411:PHE:HB3	1:B:504:LEU:HD11	1.88	0.55
1:A:433:LEU:HD23	1:A:433:LEU:C	2.27	0.54
1:A:797:ARG:HH11	1:A:797:ARG:HG2	1.72	0.54
1:B:287:THR:HA	1:B:309:ASN:O	2.08	0.53
1:B:235:LYS:HD3	1:B:235:LYS:N	2.24	0.53
1:A:287:THR:HA	1:A:309:ASN:O	2.09	0.52
1:A:797:ARG:HH11	1:A:797:ARG:CG	2.22	0.52
1:B:59:GLN:HE21	1:B:59:GLN:HA	1.75	0.52
1:B:715:ARG:HG2	1:B:739:LYS:HE2	1.91	0.52
1:B:431:SER:HB2	1:B:432:PRO:CD	2.40	0.52
1:B:404:ASN:H	1:B:428:ASN:HD21	1.58	0.52
1:A:749:LYS:N	1:A:749:LYS:HD3	2.25	0.51
1:B:98:PRO:HG2	1:B:112:ASN:OD1	2.11	0.50
1:B:300:ARG:HG3	1:B:322:TYR:HB2	1.94	0.50
1:A:60:THR:HG22	1:A:60:THR:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:VAL:HG12	1:B:101:GLN:N	2.28	0.49
1:A:329:SER:OG	1:A:330:GLY:N	2.45	0.49
1:A:234:ILE:O	1:A:256:ASN:HB3	2.12	0.49
1:B:234:ILE:O	1:B:256:ASN:HB3	2.13	0.49
1:B:761:THR:O	1:B:762:THR:HG22	2.13	0.48
6:B:909:NAG:H82	8:B:1045:HOH:O	2.14	0.48
1:B:720:SER:OG	1:B:744:SER:HB2	2.13	0.48
1:A:205:LEU:HD23	1:A:205:LEU:C	2.34	0.48
1:B:60:THR:HG22	1:B:60:THR:O	2.14	0.48
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.97	0.47
1:B:381:GLU:HG3	1:B:408:GLN:HG3	1.96	0.47
1:B:243:LYS:O	1:B:285:ASN:OD1	2.32	0.47
1:A:651:LEU:H	1:A:674:ASN:ND2	2.12	0.47
1:A:805:SER:HB3	1:B:805:SER:HB3	1.97	0.47
1:A:728:PRO:HG2	1:A:731:PHE:HB2	1.97	0.47
1:B:100:VAL:HG12	1:B:101:GLN:HG3	1.97	0.47
1:B:756:LEU:HD13	1:B:786:TRP:HB2	1.96	0.47
1:B:81:GLU:O	1:B:84:GLN:NE2	2.48	0.47
1:B:211:ASN:O	1:B:232:THR:HA	2.15	0.46
1:B:404:ASN:H	1:B:428:ASN:ND2	2.14	0.46
1:B:433:LEU:O	1:B:434:VAL:CG2	2.64	0.46
1:B:660:LEU:HD22	1:B:686:GLN:HG3	1.97	0.46
1:A:300:ARG:HG3	1:A:322:TYR:HB2	1.98	0.46
1:B:128:ARG:HA	1:B:128:ARG:HD3	1.82	0.46
1:B:584:THR:HB	8:B:1129:HOH:O	2.16	0.45
1:A:458:ASP:N	1:A:458:ASP:OD2	2.50	0.45
1:B:736:SER:O	1:B:763:LYS:CB	2.65	0.45
1:A:375:ARG:HA	1:A:402:GLY:O	2.17	0.45
1:A:534:TYR:OH	4:E:2:NAG:H81	2.16	0.44
1:B:375[B]:ARG:HA	1:B:402:GLY:O	2.17	0.44
1:A:683:LEU:HD21	6:A:916:NAG:H61	2.00	0.44
1:A:649:ASN:H	1:A:674:ASN:ND2	2.14	0.44
1:B:431:SER:HB2	1:B:432:PRO:HD2	2.00	0.44
1:B:749:LYS:HZ2	1:B:775:GLU:HB2	1.82	0.44
1:B:459:PHE:CD2	1:B:459:PHE:O	2.70	0.43
1:B:375[A]:ARG:HA	1:B:402:GLY:O	2.17	0.43
1:A:730:GLY:HA2	1:A:754:SER:O	2.18	0.43
1:B:205:LEU:HD23	1:B:205:LEU:C	2.39	0.43
1:A:213:LEU:HB2	1:A:232:THR:HB	2.00	0.43
1:A:514:ALA:HA	1:A:539:ASN:O	2.19	0.42
1:B:317:ASP:OD2	1:B:319:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:O	1:A:232:THR:HA	2.19	0.42
1:B:744:SER:HG	1:B:770:HIS:CE1	2.35	0.42
1:B:514:ALA:HA	1:B:539:ASN:O	2.19	0.42
1:A:810:ARG:CD	1:B:749:LYS:HD2	2.50	0.42
1:A:749:LYS:HD2	1:B:810:ARG:CZ	2.49	0.42
1:B:375[B]:ARG:HD2	1:B:400:ASN:ND2	2.32	0.42
1:A:45:VAL:CG1	1:A:64:TYR:O	2.68	0.42
1:A:534:TYR:CE2	4:E:2:NAG:H81	2.54	0.42
1:A:762:THR:HG22	1:A:763:LYS:N	2.35	0.41
1:B:569:ARG:HE	1:B:569:ARG:HB3	1.52	0.41
1:B:672:ASN:HA	1:B:696:ARG:O	2.19	0.41
1:B:100:VAL:HG12	1:B:101:GLN:CG	2.51	0.41
1:B:45:VAL:CG1	1:B:64:TYR:O	2.69	0.41
1:B:112:ASN:O	1:B:136:GLN:OE1	2.39	0.41
1:A:223:SER:O	1:A:225:ARG:NH1	2.54	0.41
1:A:280:ARG:CZ	1:A:305:ALA:HB1	2.52	0.41
1:A:573:VAL:O	1:A:575:HIS:CE1	2.75	0.40
1:B:49:CYS:HB3	1:B:70:LEU:HD23	2.03	0.40
1:A:431:SER:HB2	1:A:432:PRO:CD	2.50	0.40
1:A:736:SER:O	1:A:763:LYS:HG2	2.21	0.40
1:B:45:VAL:HG13	1:B:64:TYR:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LYS:NZ	8:A:1277:HOH:O[1_556]	2.02	0.18

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	748/811 (92%)	698 (93%)	46 (6%)	4 (0%)	29	23
1	B	744/811 (92%)	693 (93%)	48 (6%)	3 (0%)	34	30
All	All	1492/1622 (92%)	1391 (93%)	94 (6%)	7 (0%)	29	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	B	762	THR
1	B	100	VAL
1	A	330	GLY
1	B	378	VAL
1	A	42	ASN
1	A	378	VAL

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	701/755 (93%)	663 (95%)	38 (5%)	22	18
1	B	699/755 (93%)	663 (95%)	36 (5%)	23	19
All	All	1400/1510 (93%)	1326 (95%)	74 (5%)	22	18

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	40	LYS
1	A	41	GLN
1	A	42	ASN
1	A	45	VAL
1	A	49	CYS
1	A	52	ARG
1	A	55	GLN
1	A	56	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	GLU
1	A	188	GLU
1	A	200	LEU
1	A	213	LEU
1	A	225	ARG
1	A	248	LEU
1	A	286	LEU
1	A	301	LYS
1	A	317	ASP
1	A	385	ASP
1	A	471	THR
1	A	472	ARG
1	A	504	LEU
1	A	534	TYR
1	A	569	ARG
1	A	584	THR
1	A	632	ILE
1	A	701	LEU
1	A	703	LEU
1	A	720	SER
1	A	732	LEU
1	A	749	LYS
1	A	753	LYS
1	A	756	LEU
1	A	760	THR
1	A	766	MET
1	A	797	ARG
1	A	816	SER
1	A	817	LEU
1	B	45	VAL
1	B	48	GLU
1	B	49	CYS
1	B	52	ARG
1	B	56	GLU
1	B	81	GLU
1	B	84	GLN
1	B	118	ASP
1	B	146	GLU
1	B	150	GLU
1	B	160	ASN
1	B	200	LEU
1	B	225	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	235	LYS
1	B	248	LEU
1	B	280	ARG
1	B	286	LEU
1	B	300	ARG
1	B	329	SER
1	B	334	THR
1	B	385	ASP
1	B	397	SER
1	B	460	GLU
1	B	534	TYR
1	B	569	ARG
1	B	584	THR
1	B	595	ASN
1	B	632	ILE
1	B	701	LEU
1	B	703	LEU
1	B	720	SER
1	B	743	LEU
1	B	744	SER
1	B	747	LEU
1	B	749	LYS
1	B	757	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	135	ASN
1	A	309	ASN
1	A	469	HIS
1	A	674	ASN
1	B	59	GLN
1	B	84	GLN
1	B	135	ASN
1	B	136	GLN
1	B	285	ASN
1	B	428	ASN
1	B	469	HIS
1	B	531	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	C	1	1,2	14,14,15	0.81	0	17,19,21	1.38	4 (23%)
2	NAG	C	2	2	14,14,15	0.63	0	17,19,21	1.51	3 (17%)
2	BMA	C	3	2	11,11,12	0.46	0	15,15,17	1.77	3 (20%)
2	MAN	C	4	2	11,11,12	0.71	0	13,15,17	3.42	7 (53%)
2	BMA	C	5	2	11,11,12	0.29	0	15,15,17	2.64	9 (60%)
3	NAG	D	1	1,3	14,14,15	1.03	1 (7%)	17,19,21	1.87	5 (29%)
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	1.86	5 (29%)
4	NAG	E	1	1,4	14,14,15	0.59	0	17,19,21	1.58	2 (11%)
4	NAG	E	2	4	14,14,15	0.97	1 (7%)	17,19,21	2.21	6 (35%)
4	BMA	E	3	4	11,11,12	0.45	0	15,15,17	2.03	6 (40%)
5	NAG	F	1	1,5	14,14,15	0.64	0	17,19,21	1.82	7 (41%)
5	NAG	F	2	5	14,14,15	0.93	1 (7%)	17,19,21	1.78	3 (17%)
5	BMA	F	3	5	11,11,12	0.49	0	15,15,17	1.99	5 (33%)
5	MAN	F	4	5	11,11,12	0.53	0	15,15,17	2.92	8 (53%)
3	NAG	G	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	2.01	5 (29%)
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	2.90	7 (41%)
4	NAG	H	1	1,4	14,14,15	0.80	0	17,19,21	1.52	2 (11%)
4	NAG	H	2	4	14,14,15	0.75	0	17,19,21	1.75	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	BMA	H	3	4	11,11,12	0.55	0	15,15,17	1.93	4 (26%)

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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/18/22	0/1/1/1
2	BMA	C	5	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.74	1.39	1.43
4	E	2	NAG	C8-C7	-2.32	1.45	1.50
3	G	1	NAG	O5-C1	-2.26	1.40	1.43
5	F	2	NAG	O5-C1	-2.19	1.40	1.43

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	8.67	123.94	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	C2-C3-C4	-8.12	98.89	110.69
5	F	4	MAN	O3-C3-C2	-5.74	99.00	109.99
2	C	4	MAN	C3-C4-C5	-5.61	104.38	109.97
5	F	4	MAN	O5-C1-C2	-5.55	102.20	110.77
5	F	2	NAG	O5-C5-C6	-4.92	99.50	107.20
4	E	2	NAG	O7-C7-C8	-4.89	112.97	122.06
5	F	3	BMA	O3-C3-C2	4.68	118.95	109.99
2	C	5	BMA	O5-C1-C2	-4.44	103.92	110.77
4	H	3	BMA	C2-C3-C4	-4.39	103.29	110.89
4	E	3	BMA	C2-C3-C4	-4.29	103.47	110.89
3	G	1	NAG	C4-C3-C2	-4.23	104.82	111.02
4	E	1	NAG	O4-C4-C3	-4.20	100.64	110.35
5	F	4	MAN	O5-C5-C6	4.20	113.78	107.20
3	G	2	NAG	O5-C5-C4	4.02	120.62	110.83
2	C	5	BMA	C2-C3-C4	-4.00	103.97	110.89
4	H	2	NAG	O5-C5-C6	3.94	113.37	107.20
2	C	5	BMA	C1-C2-C3	-3.93	104.84	109.67
2	C	4	MAN	C1-C2-C3	-3.90	101.92	110.91
3	D	1	NAG	C4-C3-C2	-3.84	105.40	111.02
2	C	4	MAN	O3-C3-C2	3.76	119.28	109.94
3	G	1	NAG	C1-O5-C5	-3.75	107.11	112.19
4	H	3	BMA	O3-C3-C4	3.70	118.91	110.35
2	C	3	BMA	C2-C3-C4	-3.67	104.54	110.89
3	D	2	NAG	C8-C7-N2	3.61	122.21	116.10
4	E	3	BMA	O3-C3-C4	3.50	118.44	110.35
2	C	3	BMA	O3-C3-C2	3.50	116.69	109.99
2	C	5	BMA	C3-C4-C5	3.47	116.42	110.24
3	G	2	NAG	C1-C2-N2	3.41	116.31	110.49
4	E	2	NAG	C8-C7-N2	3.33	121.73	116.10
3	D	1	NAG	O3-C3-C2	-3.23	102.79	109.47
4	E	2	NAG	C1-C2-N2	3.22	115.99	110.49
2	C	5	BMA	O4-C4-C3	-3.19	102.97	110.35
4	E	3	BMA	C1-C2-C3	3.17	113.57	109.67
3	G	1	NAG	O3-C3-C4	3.15	117.62	110.35
3	D	2	NAG	C3-C4-C5	-3.12	104.68	110.24
2	C	2	NAG	O7-C7-C8	-3.06	116.37	122.06
4	H	2	NAG	C4-C3-C2	-3.05	106.54	111.02
4	H	1	NAG	O5-C1-C2	-3.02	106.52	111.29
3	G	2	NAG	C8-C7-N2	3.01	121.19	116.10
3	D	1	NAG	C1-C2-N2	-2.98	105.40	110.49
5	F	4	MAN	C1-C2-C3	2.97	113.32	109.67
5	F	4	MAN	O2-C2-C1	-2.93	103.15	109.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	O3-C3-C4	2.92	116.00	110.14
5	F	1	NAG	C1-O5-C5	2.91	116.14	112.19
2	C	4	MAN	O4-C4-C5	2.91	116.52	109.30
2	C	5	BMA	O5-C5-C6	-2.90	102.65	107.20
5	F	3	BMA	O5-C1-C2	-2.87	106.33	110.77
4	E	2	NAG	C2-N2-C7	2.87	126.99	122.90
3	G	1	NAG	O4-C4-C3	-2.84	103.78	110.35
4	H	2	NAG	O4-C4-C3	-2.84	103.78	110.35
2	C	2	NAG	C1-C2-N2	2.80	115.28	110.49
5	F	1	NAG	O4-C4-C3	2.74	116.67	110.35
4	H	1	NAG	O5-C5-C4	-2.71	104.23	110.83
4	E	2	NAG	O3-C3-C4	-2.69	104.13	110.35
3	D	2	NAG	O5-C5-C6	2.69	111.42	107.20
5	F	3	BMA	O3-C3-C4	-2.63	104.26	110.35
2	C	1	NAG	O3-C3-C4	2.62	116.41	110.35
3	G	2	NAG	O6-C6-C5	-2.62	102.31	111.29
2	C	1	NAG	O6-C6-C5	-2.57	102.47	111.29
3	D	1	NAG	C3-C4-C5	2.55	114.80	110.24
3	G	2	NAG	O7-C7-C8	-2.50	117.41	122.06
5	F	4	MAN	C2-C3-C4	2.50	115.21	110.89
4	H	3	BMA	C1-C2-C3	2.49	112.72	109.67
2	C	3	BMA	O4-C4-C3	-2.46	104.66	110.35
5	F	1	NAG	C1-C2-N2	-2.46	106.29	110.49
4	E	2	NAG	O6-C6-C5	-2.45	102.89	111.29
5	F	3	BMA	C1-C2-C3	2.44	112.67	109.67
5	F	3	BMA	C1-O5-C5	2.41	115.46	112.19
3	G	2	NAG	O3-C3-C4	-2.41	104.78	110.35
2	C	1	NAG	C6-C5-C4	2.41	118.64	113.00
3	D	2	NAG	O7-C7-C8	-2.40	117.60	122.06
5	F	1	NAG	O7-C7-N2	2.38	126.33	121.95
3	D	2	NAG	C2-N2-C7	-2.31	119.61	122.90
2	C	2	NAG	O7-C7-N2	2.31	126.19	121.95
4	E	1	NAG	O5-C1-C2	-2.29	107.67	111.29
2	C	5	BMA	O2-C2-C1	-2.28	104.48	109.15
5	F	1	NAG	O6-C6-C5	-2.28	103.47	111.29
2	C	5	BMA	O3-C3-C4	2.28	115.61	110.35
4	H	3	BMA	C3-C4-C5	2.26	114.27	110.24
5	F	1	NAG	O4-C4-C5	-2.26	103.69	109.30
5	F	2	NAG	O5-C1-C2	-2.24	107.74	111.29
5	F	4	MAN	O3-C3-C4	2.24	115.53	110.35
2	C	1	NAG	C2-N2-C7	-2.24	119.71	122.90
5	F	2	NAG	C6-C5-C4	2.23	118.23	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C6-C5-C4	-2.22	107.81	113.00
4	E	3	BMA	O4-C4-C5	-2.22	103.79	109.30
2	C	5	BMA	O5-C5-C4	2.21	116.21	110.83
4	E	3	BMA	O2-C2-C3	-2.19	105.74	110.14
3	G	1	NAG	O6-C6-C5	-2.18	103.82	111.29
5	F	4	MAN	O4-C4-C3	2.16	115.35	110.35
4	H	2	NAG	O7-C7-N2	2.10	125.82	121.95
5	F	1	NAG	O5-C1-C2	-2.04	108.07	111.29
4	E	3	BMA	O4-C4-C3	-2.03	105.65	110.35
2	C	4	MAN	O6-C6-C5	-2.00	104.42	111.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	H	3	BMA	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	5	BMA	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

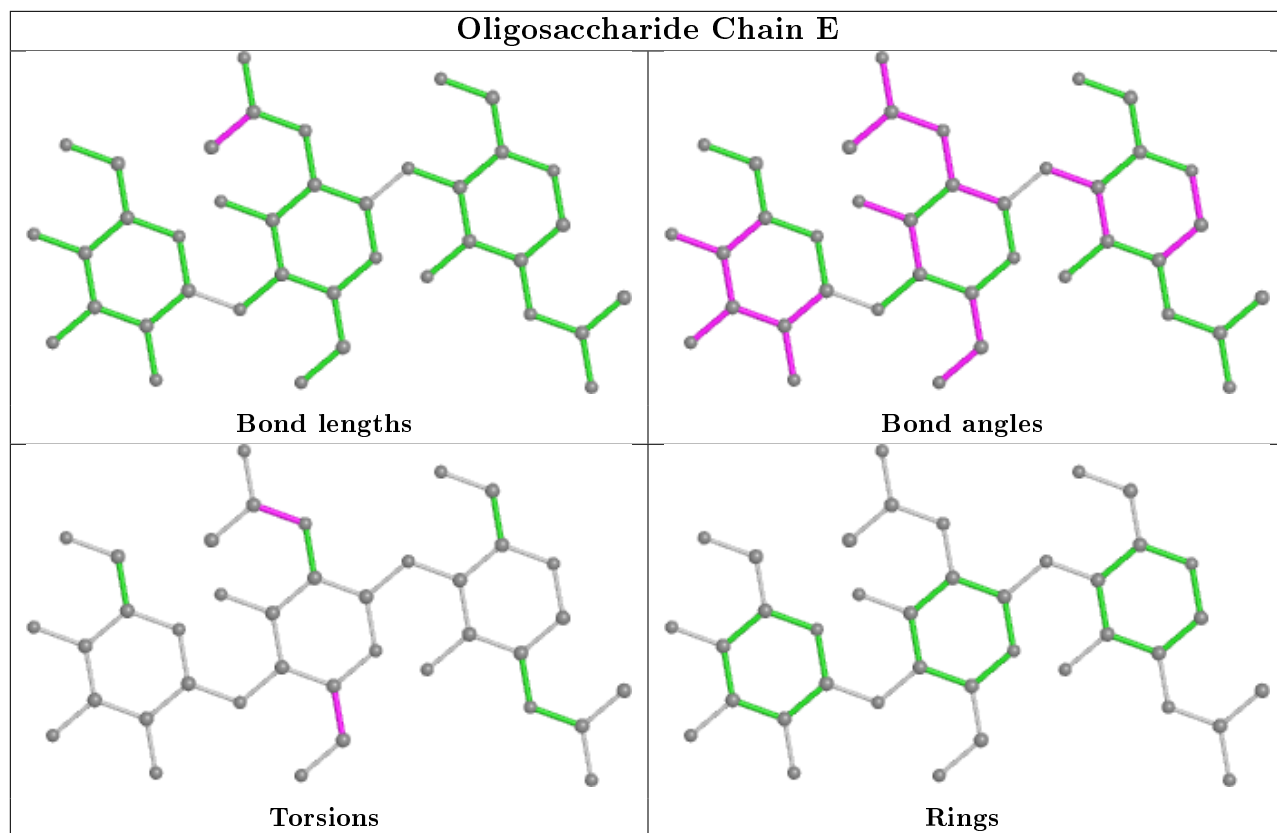| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	MAN	1	0
4	E	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C	
Bond lengths	Bond angles
Torsions	Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

13 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	$\#|Z| > 2$
6	NAG	B	914	1	14,14,15	0.74	0	17,19,21	2.21	8 (47%)
6	NAG	A	901	1	14,14,15	0.65	0	17,19,21	1.56	4 (23%)
6	NAG	B	910	1	14,14,15	0.38	0	17,19,21	2.18	3 (17%)
6	NAG	A	910	1	14,14,15	0.78	0	17,19,21	1.67	3 (17%)
6	NAG	A	907	1	14,14,15	0.47	0	17,19,21	1.09	2 (11%)
7	D80	A	917	-	16,20,20	1.03	1 (6%)	17,28,28	1.57	2 (11%)
7	D80	B	901	-	16,20,20	1.13	1 (6%)	17,28,28	1.12	1 (5%)
6	NAG	B	915	1	14,14,15	0.52	0	17,19,21	3.42	8 (47%)
6	NAG	A	915	1	14,14,15	0.92	1 (7%)	17,19,21	2.78	6 (35%)
6	NAG	A	911	1	14,14,15	0.41	0	17,19,21	2.68	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
6	NAG	A	916	1	14,14,15	0.63	0	17,19,21	2.98	7 (41%)
6	NAG	B	909	1	14,14,15	0.54	0	17,19,21	2.03	6 (35%)
6	NAG	B	906	1	14,14,15	0.43	0	17,19,21	2.32	9 (52%)

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
6	NAG	B	914	1	-	0/6/23/26	0/1/1/1
6	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	NAG	B	910	1	-	3/6/23/26	0/1/1/1
6	NAG	A	910	1	-	2/6/23/26	0/1/1/1
6	NAG	A	907	1	-	0/6/23/26	0/1/1/1
7	D80	A	917	-	-	1/3/4/4	0/3/3/3
7	D80	B	901	-	-	2/3/4/4	0/3/3/3
6	NAG	B	915	1	-	0/6/23/26	0/1/1/1
6	NAG	A	915	1	-	2/6/23/26	0/1/1/1
6	NAG	A	911	1	-	2/6/23/26	0/1/1/1
6	NAG	A	916	1	-	2/6/23/26	0/1/1/1
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	B	906	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	917	D80	CAB-CAJ	-2.37	1.38	1.41
6	A	915	NAG	O5-C1	-2.15	1.40	1.43
7	B	901	D80	CAC-CAA	-2.07	1.38	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	915	NAG	C1-O5-C5	10.93	127.00	112.19
6	A	911	NAG	C1-O5-C5	9.45	125.00	112.19
6	A	916	NAG	C1-O5-C5	-6.84	102.93	112.19
6	A	916	NAG	C1-C2-N2	5.76	120.32	110.49
6	A	915	NAG	O3-C3-C4	-5.70	97.17	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	910	NAG	O5-C5-C6	5.20	115.36	107.20
6	B	910	NAG	C1-C2-N2	5.17	119.33	110.49
7	A	917	D80	CAD-CAB-CAJ	-4.94	118.74	122.59
6	A	915	NAG	O5-C1-C2	-4.56	104.08	111.29
6	A	916	NAG	O5-C5-C6	4.54	114.32	107.20
6	A	915	NAG	C1-O5-C5	4.49	118.28	112.19
6	A	916	NAG	O5-C1-C2	-4.46	104.25	111.29
6	B	909	NAG	C6-C5-C4	-4.35	102.81	113.00
6	B	914	NAG	C1-O5-C5	4.31	118.03	112.19
6	A	915	NAG	O6-C6-C5	-4.22	96.83	111.29
6	B	914	NAG	C2-N2-C7	4.17	128.85	122.90
6	B	906	NAG	C3-C4-C5	4.06	117.49	110.24
6	B	906	NAG	C6-C5-C4	-4.02	103.58	113.00
6	B	915	NAG	C2-N2-C7	-3.78	117.52	122.90
6	A	910	NAG	C1-O5-C5	3.74	117.27	112.19
6	A	910	NAG	O5-C1-C2	-3.67	105.49	111.29
6	A	915	NAG	O4-C4-C3	-3.67	101.88	110.35
6	B	910	NAG	C2-N2-C7	3.66	128.12	122.90
6	B	906	NAG	O4-C4-C5	3.59	118.22	109.30
6	B	915	NAG	O5-C1-C2	-3.53	105.72	111.29
6	B	909	NAG	C1-C2-N2	3.39	116.28	110.49
6	B	915	NAG	C4-C3-C2	-3.30	106.18	111.02
6	B	909	NAG	O6-C6-C5	-3.17	100.43	111.29
6	B	915	NAG	O5-C5-C4	3.16	118.53	110.83
6	B	914	NAG	O4-C4-C3	-3.15	103.06	110.35
6	B	909	NAG	C2-N2-C7	-3.14	118.43	122.90
6	B	915	NAG	O5-C5-C6	3.00	111.90	107.20
6	B	914	NAG	C1-C2-N2	-2.99	105.38	110.49
6	B	906	NAG	C1-O5-C5	2.94	116.18	112.19
6	A	901	NAG	O6-C6-C5	-2.88	101.42	111.29
6	B	915	NAG	C6-C5-C4	-2.83	106.37	113.00
6	A	911	NAG	O5-C1-C2	2.81	115.73	111.29
6	A	916	NAG	O7-C7-C8	-2.69	117.05	122.06
6	B	906	NAG	C8-C7-N2	-2.68	111.56	116.10
6	A	916	NAG	O3-C3-C4	-2.62	104.30	110.35
6	A	910	NAG	O6-C6-C5	-2.60	102.37	111.29
6	B	914	NAG	O7-C7-C8	-2.59	117.24	122.06
7	A	917	D80	CAD-CAB-CAA	2.51	121.20	117.55
6	A	901	NAG	C6-C5-C4	-2.50	107.14	113.00
6	B	915	NAG	O3-C3-C4	-2.50	104.56	110.35
6	A	915	NAG	C1-C2-N2	-2.48	106.25	110.49
6	A	907	NAG	O7-C7-C8	-2.47	117.47	122.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	901	D80	CAH-CAG-NAI	-2.46	119.40	121.01
6	A	911	NAG	O4-C4-C3	-2.45	104.67	110.35
6	B	906	NAG	C4-C3-C2	-2.43	107.46	111.02
6	B	906	NAG	C1-C2-N2	-2.41	106.37	110.49
6	B	909	NAG	C4-C3-C2	-2.34	107.59	111.02
6	B	914	NAG	O5-C1-C2	-2.34	107.60	111.29
6	A	901	NAG	C1-O5-C5	2.33	115.35	112.19
6	B	914	NAG	O7-C7-N2	2.29	126.16	121.95
6	A	907	NAG	C1-C2-N2	-2.29	106.58	110.49
6	B	914	NAG	O3-C3-C4	-2.25	105.14	110.35
6	B	906	NAG	O3-C3-C4	-2.22	105.21	110.35
6	A	901	NAG	O5-C5-C4	2.18	116.13	110.83
6	A	911	NAG	C3-C4-C5	2.09	113.96	110.24
6	B	906	NAG	O7-C7-N2	2.08	125.78	121.95
6	A	911	NAG	O5-C5-C6	-2.06	103.98	107.20
6	A	916	NAG	O6-C6-C5	-2.01	104.40	111.29
6	B	909	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	917	D80	NAK-CAL-CAN-CAO
7	B	901	D80	NAK-CAL-CAN-CAO
6	A	911	NAG	O5-C5-C6-O6
6	A	915	NAG	C4-C5-C6-O6
6	A	916	NAG	O5-C5-C6-O6
6	A	915	NAG	O5-C5-C6-O6
6	A	910	NAG	O5-C5-C6-O6
6	B	910	NAG	C4-C5-C6-O6
6	A	910	NAG	C4-C5-C6-O6
6	A	916	NAG	C4-C5-C6-O6
6	B	910	NAG	O5-C5-C6-O6
6	A	901	NAG	C4-C5-C6-O6
6	A	911	NAG	C4-C5-C6-O6
6	B	906	NAG	O5-C5-C6-O6
6	B	906	NAG	C4-C5-C6-O6
6	A	901	NAG	O5-C5-C6-O6
6	B	910	NAG	C3-C2-N2-C7
7	B	901	D80	CAL-CAN-CAO-CAP

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	916	NAG	1	0
6	B	909	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	754/811 (92%)	0.00	29 (3%)	40	39	20, 34, 59, 90	0
1	B	751/811 (92%)	0.10	33 (4%)	34	33	22, 38, 68, 96	0
All	All	1505/1622 (92%)	0.05	62 (4%)	37	36	20, 36, 63, 96	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	LEU	6.3
1	B	760	THR	6.1
1	B	100	VAL	6.0
1	A	100	VAL	5.3
1	B	459	PHE	5.3
1	B	434	VAL	4.9
1	A	470	PHE	4.8
1	B	808	ASP	4.7
1	B	41	GLN	4.6
1	A	43	ASP	4.6
1	A	64	TYR	4.6
1	A	457	THR	4.6
1	B	761	THR	4.2
1	A	434	VAL	4.0
1	B	112	ASN	4.0
1	B	31	SER	3.9
1	A	818	GLU	3.9
1	A	808	ASP	3.8
1	B	818	GLU	3.6
1	B	759	LYS	3.6
1	A	31	SER	3.6
1	B	472	ARG	3.4
1	A	40	LYS	3.4
1	B	778	CYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	470	PHE	3.2
1	B	762	THR	3.2
1	B	678	PHE	3.1
1	B	39	LYS	3.1
1	A	42	ASN	3.1
1	A	41	GLN	3.0
1	A	374	LEU	3.0
1	B	702	PHE	3.0
1	B	101	GLN	2.8
1	B	63	LYS	2.8
1	B	85	GLY	2.8
1	A	253	LEU	2.7
1	B	46	ILE	2.7
1	A	294	LEU	2.6
1	A	791	LEU	2.6
1	B	589	LEU	2.6
1	A	99	ASN	2.5
1	A	759	LYS	2.5
1	A	44	SER	2.5
1	A	807	GLY	2.4
1	B	374	LEU	2.3
1	B	753	LYS	2.3
1	A	153	LEU	2.3
1	B	752	ASN	2.3
1	B	809	GLN	2.3
1	B	471	THR	2.2
1	B	510	LEU	2.2
1	B	535	LEU	2.2
1	B	807	GLY	2.2
1	A	458	ASP	2.1
1	A	760	THR	2.1
1	A	208	LEU	2.1
1	A	271	ASP	2.1
1	A	63	LYS	2.1
1	A	471	THR	2.1
1	B	777	THR	2.1
1	B	64	TYR	2.1
1	A	620	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	F	4	11/12	0.60	0.24	58,67,77,79	0
2	MAN	C	4	11/12	0.76	0.29	44,63,72,94	0
4	BMA	H	3	11/12	0.85	0.21	44,51,61,63	0
4	BMA	E	3	11/12	0.87	0.20	42,47,50,61	0
3	NAG	G	2	14/15	0.87	0.22	40,51,56,56	0
5	BMA	F	3	11/12	0.89	0.20	41,46,48,52	0
3	NAG	D	2	14/15	0.90	0.17	36,44,54,55	0
2	BMA	C	5	11/12	0.90	0.27	59,65,68,70	0
5	NAG	F	2	14/15	0.92	0.10	29,35,42,44	0
4	NAG	H	2	14/15	0.93	0.12	31,33,39,45	0
4	NAG	E	2	14/15	0.93	0.12	25,30,38,38	0
5	NAG	F	1	14/15	0.94	0.10	28,31,37,47	0
2	BMA	C	3	11/12	0.95	0.23	42,46,51,55	0
4	NAG	H	1	14/15	0.95	0.07	24,28,29,30	0
2	NAG	C	2	14/15	0.95	0.12	27,33,39,48	0
2	NAG	C	1	14/15	0.96	0.08	23,26,30,38	0
3	NAG	G	1	14/15	0.96	0.09	24,26,30,32	0
3	NAG	D	1	14/15	0.96	0.08	22,25,30,32	0
4	NAG	E	1	14/15	0.97	0.06	20,23,27,27	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
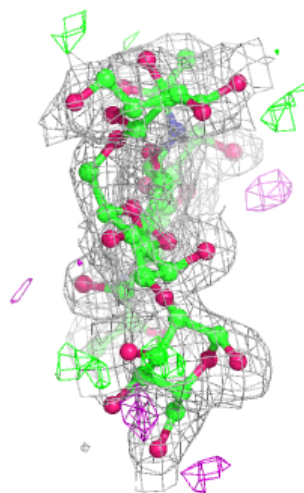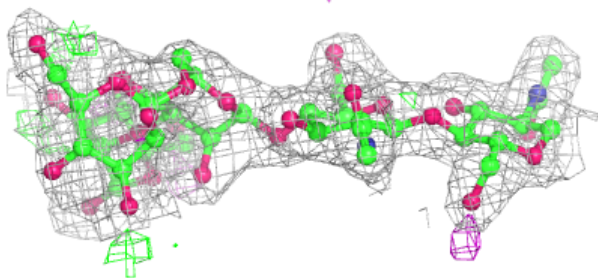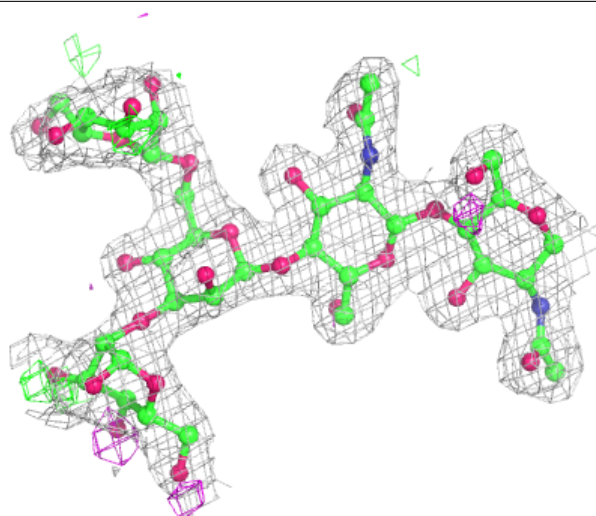
Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
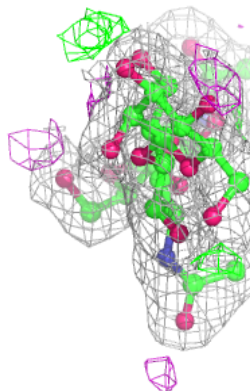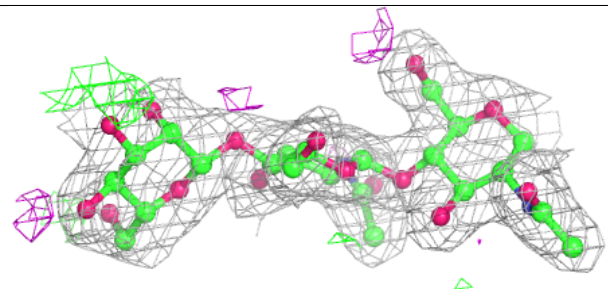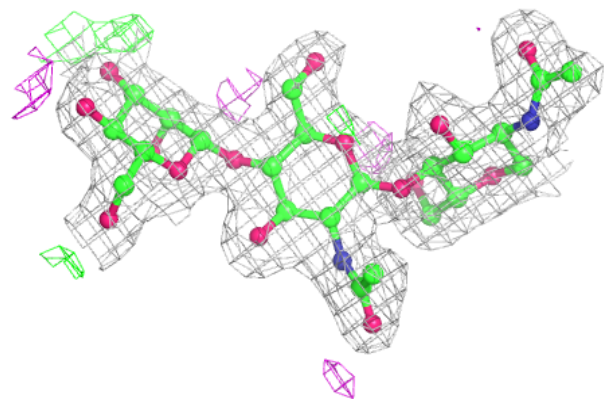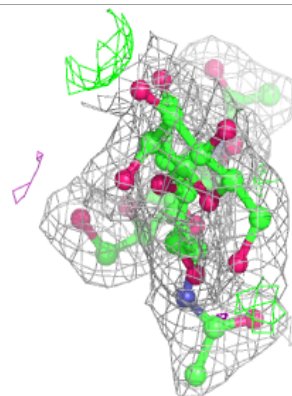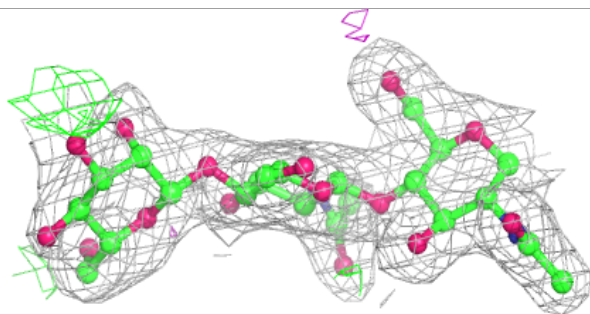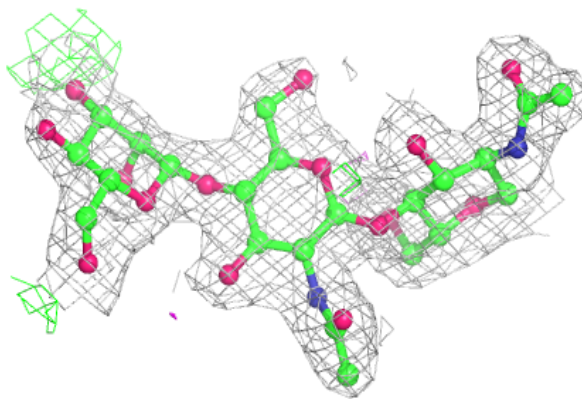and green (positive)
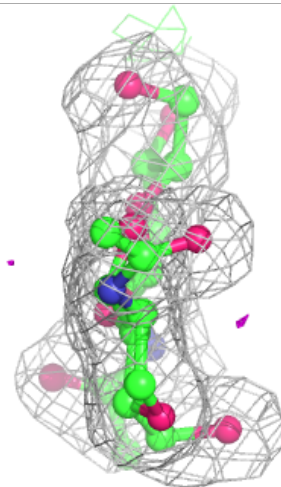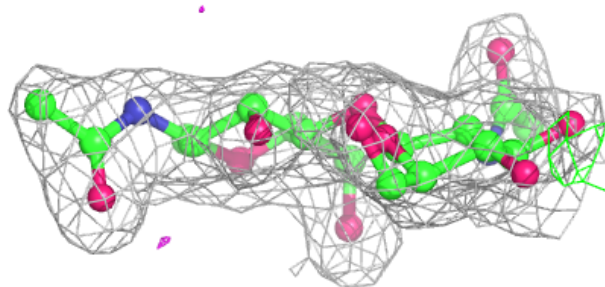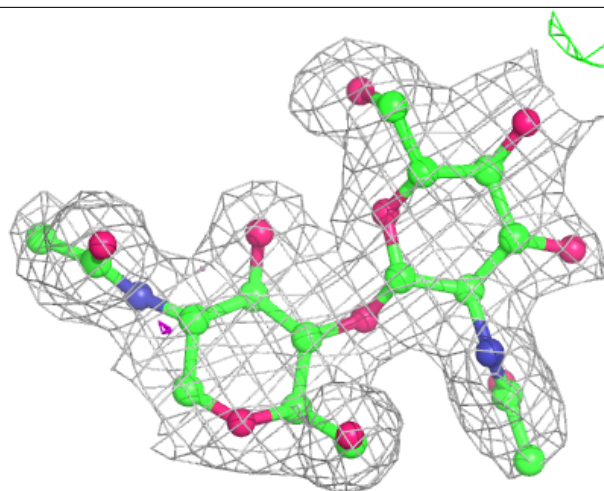
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
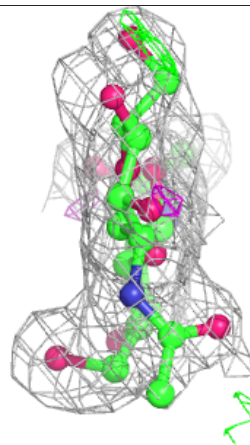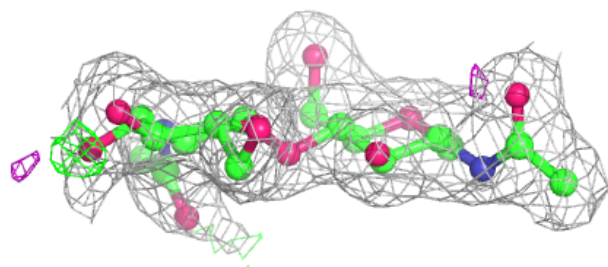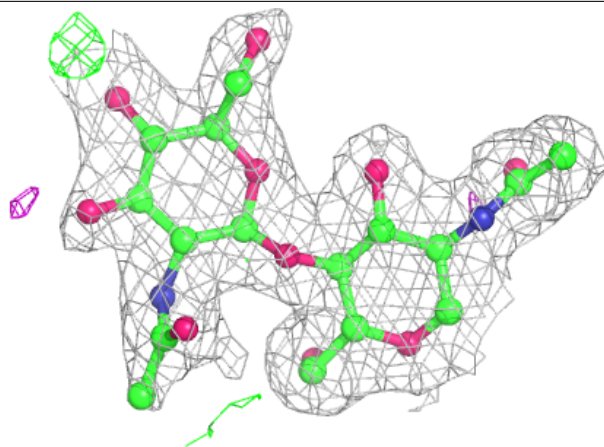
Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

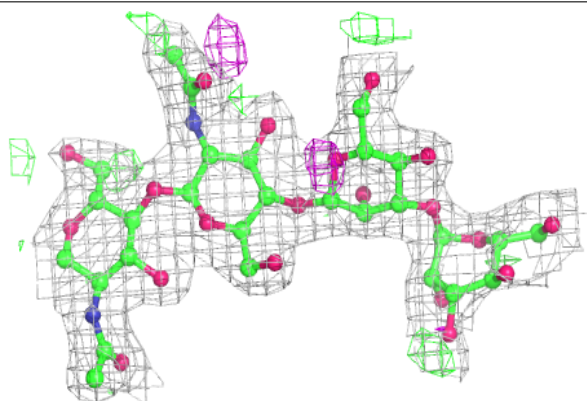**Electron density around Chain H:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
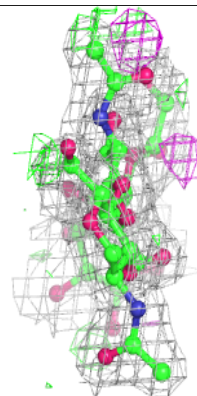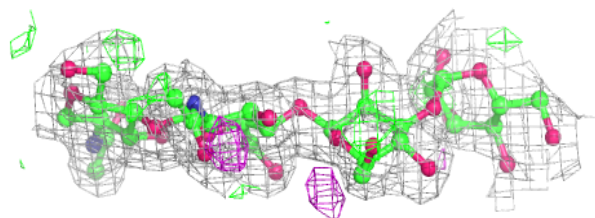
6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	901	14/15	0.79	0.27	48,57,63,66	0
6	NAG	A	911	14/15	0.86	0.29	57,62,68,71	0
6	NAG	B	915	14/15	0.87	0.19	48,54,64,65	0
6	NAG	B	910	14/15	0.87	0.27	55,62,65,66	0
6	NAG	B	906	14/15	0.89	0.19	33,43,46,57	0
6	NAG	A	916	14/15	0.91	0.23	45,51,63,67	0
6	NAG	B	909	14/15	0.91	0.18	41,54,64,67	0
6	NAG	A	915	14/15	0.91	0.13	33,43,48,50	0
6	NAG	B	914	14/15	0.94	0.12	27,40,53,55	0
6	NAG	A	910	14/15	0.94	0.19	45,56,60,67	0
6	NAG	A	907	14/15	0.94	0.15	33,39,44,47	0
7	D80	A	917	18/18	0.96	0.08	21,25,28,28	0
7	D80	B	901	18/18	0.96	0.09	21,24,28,30	0

6.5 Other polymers (i)

There are no such residues in this entry.