Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 06:51 PM EDT

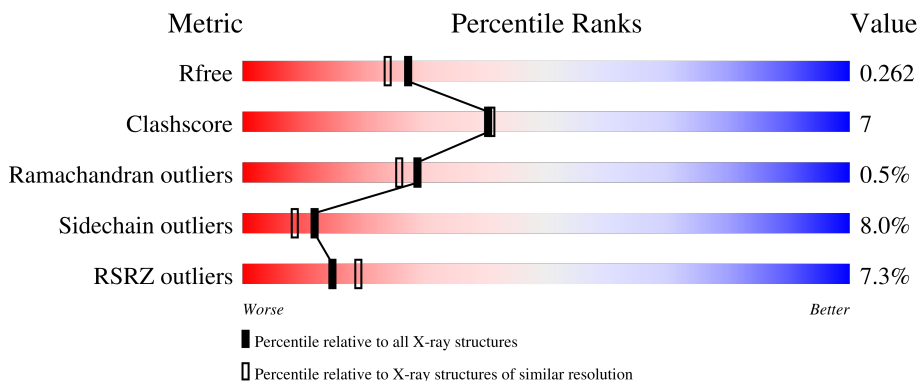|		
PDB ID	:	4R6A
Title	:	Crystal structure of human TLR8 in complex with Hybrid-2
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2014-08-22
Resolution	:	2.10 Å(reported)

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 2.10 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.
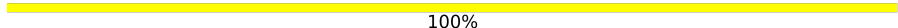
Metric	Percentile Ranks	Value
Rfree		0.262
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		8.0%
RSRZ outliers		7.3%

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	811	7% 73% 16% • 8%
1	B	811	7% 74% 15% • 9%
2	C	4	25% 50% 25%
3	D	3	33% 67%
3	E	3	100%

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Mol	Chain	Length	Quality of chain
3	G	3	100%
3	H	3	67% 33%
4	F	4	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BMA	F	3	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 12816 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	746	Total 6009	C 3844	N 1021	O 1125	S 19	0	0	0
1	B	740	Total 5964	C 3819	N 1013	O 1113	S 19	0	0	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-(1-3)-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	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
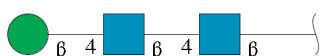
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total 39	C 22	N 2	O 15	0	0	0
3	E	3	Total 39	C 22	N 2	O 15	0	0	0
3	G	3	Total 39	C 22	N 2	O 15	0	0	0
3	H	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 4 is an oligosaccharide called alpha-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
4	F	4	Total 50	C 28	N 2	O 20	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O1
HO

O5
O

C6

C1(R)　　C5(R)

C2(R)　　C4(S)
C3(R)

N2
HN

OH
O4

C7

OH
O3

C8

O
O7

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			13	8	1	4		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 1-(4-amino-2-butyl-1H-imidazo[4,5-c]quinolin-1-yl)-2-methylpropan-2-ol (three-letter code: HB2) (formula: $C_{18}H_{24}N_4O$).

HB2

CAV

CAU CAT

OH CAN
OAW

CAU CAT

CAP

CAQ

CAS

CAL

CAO

NAM

CAD

CAJ

NAK

CAF

CAB

CAH

CAA

CAG

CAE

N

NH₂

CAC

NAI

NAR

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 23	C 18	N 4	O 1	0	0
6	B	1	Total 23	C 18	N 4	O 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	196	Total 196	O 196	0	0
7	B	206	Total 206	O 206	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Toll-like receptor 8
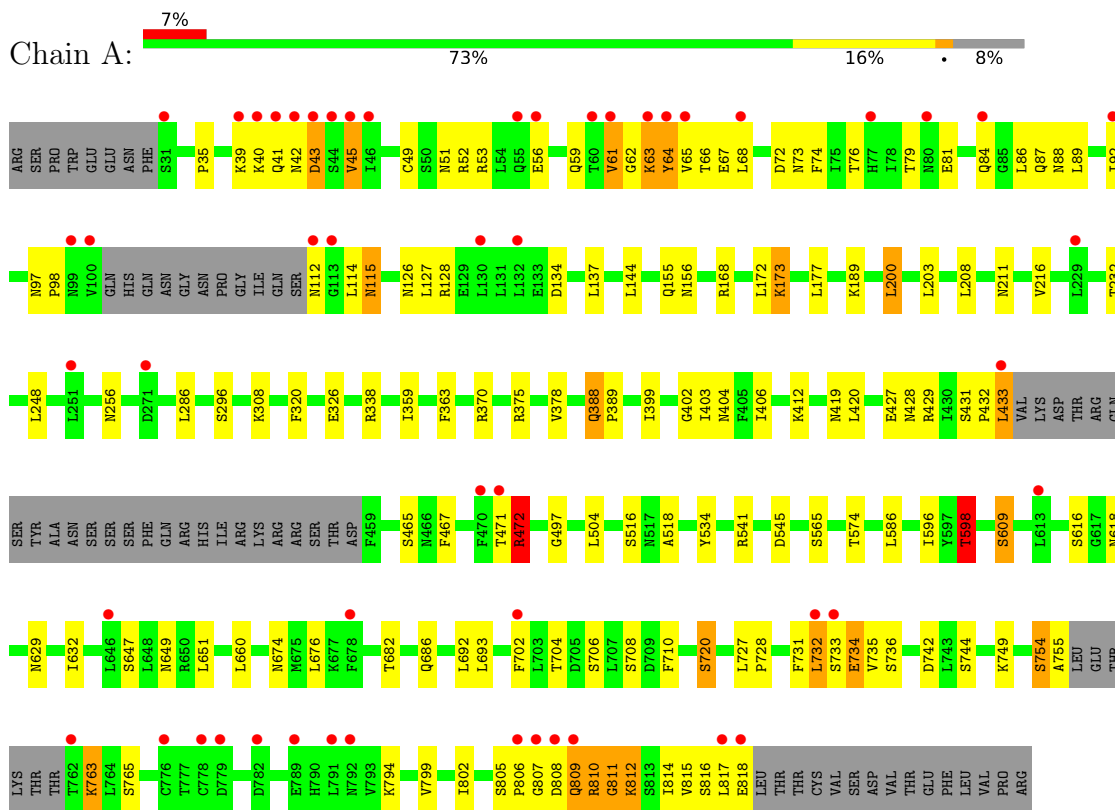
• Molecule 1: Toll-like receptor 8
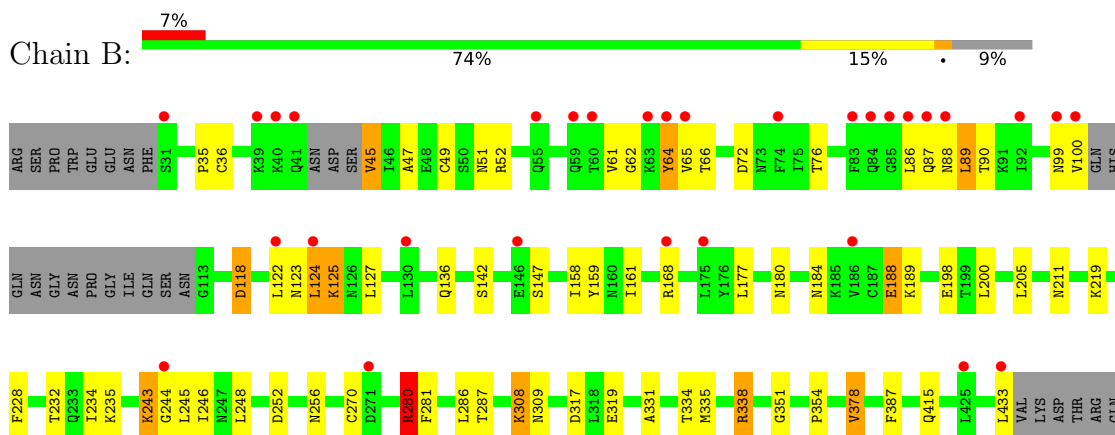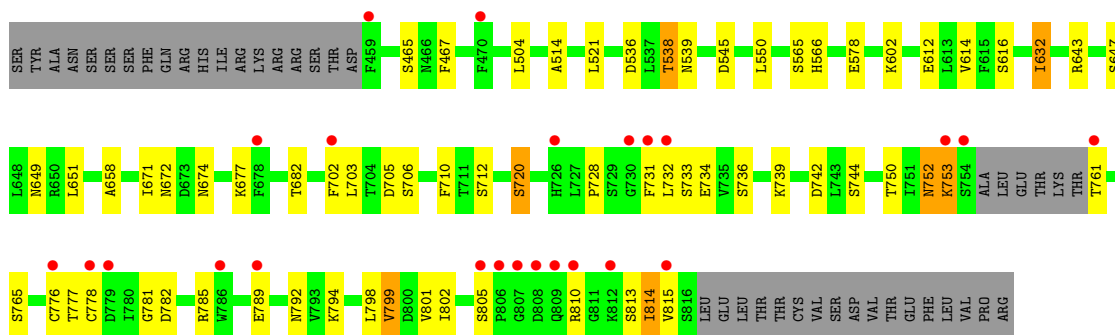
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
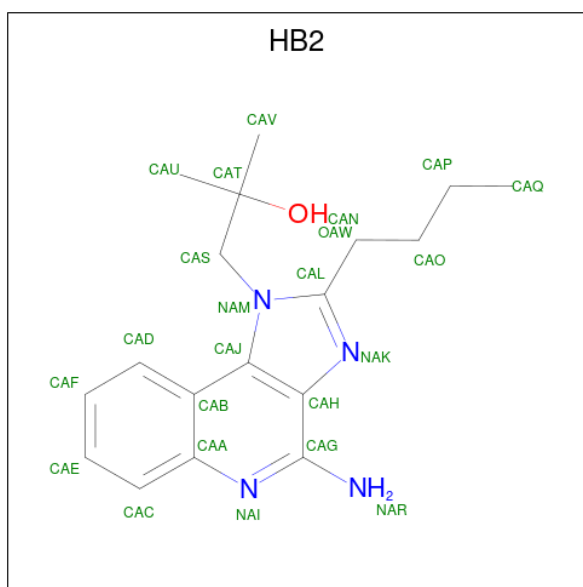
Chain C:

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

Chain D:

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

Chain E:

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

Chain G:

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

Chain H:
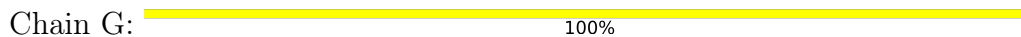
• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.14Å 122.21Å 107.78Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	26.09 – 2.10 26.09 – 2.09	Depositor EDS
% Data completeness (in resolution range)	86.7 (26.09-2.10) 86.7 (26.09-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.201 , 0.259 0.208 , 0.262	Depositor DCC
R_{free} test set	4733 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12816	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN, HB2

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	0.59	0/6133	0.77	2/8316 (0.0%)
1	B	0.58	0/6087	0.76	1/8252 (0.0%)
All	All	0.59	0/12220	0.76	3/16568 (0.0%)

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	280	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	472	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	598	THR	CB-CA-C	-5.92	95.62	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	GLY	Peptide
1	A	808	ASP	Peptide
1	A	809	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	731	PHE	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	6009	0	5988	87	0
1	B	5964	0	5949	78	1
2	C	50	0	43	1	0
3	D	39	0	34	1	0
3	E	39	0	34	0	0
3	G	39	0	34	0	0
3	H	39	0	33	2	0
4	F	50	0	43	9	0
5	A	56	0	52	1	0
5	B	83	0	78	0	0
6	A	23	0	24	6	0
6	B	23	0	24	1	0
7	A	196	0	0	7	0
7	B	206	0	0	5	0
All	All	12816	0	12336	177	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 7.

All (177) 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:720:SER:OG	1:B:742:ASP:OD2	1.75	1.02
1:B:308:LYS:HG2	1:B:335:MET:HE1	1.43	0.99
1:B:158:ILE:H	1:B:180:ASN:HD22	1.24	0.85
1:B:538:THR:CG2	1:B:539:ASN:HD22	1.93	0.82
1:B:308:LYS:HG2	1:B:335:MET:CE	2.10	0.81
4:F:3:BMA:H61	4:F:4:MAN:H5	1.63	0.80
6:A:915:HB2:H21	1:B:351:GLY:H	1.48	0.79
1:B:798:LEU:HA	1:B:801:VAL:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:THR:HG23	1:B:539:ASN:ND2	2.01	0.76
1:B:538:THR:HG22	1:B:539:ASN:HD22	1.48	0.76
1:B:124:LEU:HD12	1:B:127:LEU:HB2	1.68	0.75
1:A:63:LYS:HD3	1:A:63:LYS:H	1.50	0.75
1:B:649:ASN:H	1:B:674:ASN:HD21	1.35	0.74
1:B:538:THR:CG2	1:B:539:ASN:ND2	2.51	0.74
1:A:598:THR:HG21	7:A:1050:HOH:O	1.86	0.74
4:F:3:BMA:C6	4:F:4:MAN:H5	2.17	0.73
1:A:42:ASN:N	1:A:43:ASP:HA	2.05	0.71
4:F:3:BMA:C6	4:F:4:MAN:C5	2.69	0.70
1:A:649:ASN:H	1:A:674:ASN:HD21	1.40	0.70
1:A:211:ASN:O	1:A:232:THR:HA	1.93	0.68
4:F:2:NAG:O3	4:F:3:BMA:H2	1.93	0.68
1:A:596:ILE:H	1:A:618:ASN:HD22	1.41	0.67
6:A:915:HB2:H21	1:B:351:GLY:N	2.09	0.67
6:A:915:HB2:H16	6:A:915:HB2:H15	1.77	0.67
1:B:243:LYS:HA	7:B:1080:HOH:O	1.94	0.66
1:A:115:ASN:C	1:A:115:ASN:HD22	2.00	0.65
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.77	0.65
1:A:598:THR:HG23	7:A:1007:HOH:O	1.97	0.64
1:B:798:LEU:HA	1:B:801:VAL:CG1	2.27	0.64
1:A:598:THR:CG2	7:A:1007:HOH:O	2.45	0.64
4:F:3:BMA:H61	4:F:4:MAN:C5	2.28	0.64
1:A:799:VAL:O	1:A:802:ILE:HD11	1.98	0.64
1:A:651:LEU:H	1:A:674:ASN:HD22	1.46	0.63
1:A:763:LYS:HA	1:A:763:LYS:HE2	1.79	0.63
1:B:245:LEU:HA	7:B:1201:HOH:O	1.97	0.63
1:B:198:GLU:HG3	1:B:219:LYS:HB3	1.80	0.62
1:B:338:ARG:NH1	7:B:1110:HOH:O	2.33	0.61
1:A:586:LEU:O	1:A:609:SER:HB3	1.99	0.61
7:B:1050:HOH:O	3:H:1:NAG:H61	2.00	0.61
1:A:810:ARG:O	1:A:812:LYS:N	2.34	0.61
1:B:51:ASN:HA	1:B:72:ASP:O	2.01	0.61
1:B:159:TYR:CD2	1:B:188:GLU:HG2	2.36	0.60
1:B:536:ASP:OD1	1:B:538:THR:HB	2.00	0.60
1:B:123:ASN:O	1:B:125:LYS:HG3	2.01	0.60
4:F:3:BMA:O6	4:F:3:BMA:O4	2.12	0.60
1:A:232:THR:H	1:A:256:ASN:HD21	1.49	0.60
1:B:118:ASP:O	1:B:142:SER:O	2.19	0.59
1:B:649:ASN:H	1:B:674:ASN:ND2	2.00	0.59
6:A:915:HB2:H19	6:A:915:HB2:H8	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:O	1:B:88:ASN:N	2.37	0.58
1:A:45:VAL:HG13	1:A:66:THR:HG23	1.85	0.57
1:B:682:THR:HA	1:B:710:PHE:CD1	2.40	0.57
1:A:406:ILE:H	1:A:428:ASN:HD22	1.52	0.57
1:B:211:ASN:O	1:B:232:THR:HA	2.05	0.57
1:A:763:LYS:HA	1:A:763:LYS:CE	2.35	0.56
1:A:126:ASN:O	1:A:128:ARG:HD2	2.05	0.56
1:B:158:ILE:H	1:B:180:ASN:ND2	2.01	0.56
1:A:35:PRO:O	1:A:52:ARG:NH1	2.39	0.56
1:A:41:GLN:C	1:A:43:ASP:HA	2.27	0.56
1:B:280:ARG:HD3	1:B:281:PHE:CE2	2.41	0.55
1:A:326:GLU:CD	7:A:1168:HOH:O	2.43	0.55
1:A:433:LEU:HD13	1:A:497:GLY:HA3	1.88	0.55
1:B:651:LEU:H	1:B:674:ASN:HD22	1.53	0.55
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.42	0.55
1:A:429:ARG:HG2	7:A:1090:HOH:O	2.07	0.55
1:B:814:ILE:HG13	1:B:815:VAL:N	2.22	0.55
1:B:317:ASP:OD1	1:B:319:GLU:OE1	2.25	0.54
1:B:752:ASN:ND2	1:B:753:LYS:O	2.40	0.54
1:A:816:SER:O	1:A:817:LEU:HD12	2.08	0.54
1:B:682:THR:HG22	1:B:710:PHE:CZ	2.44	0.53
1:A:734:GLU:N	1:A:734:GLU:CD	2.63	0.52
1:B:234:ILE:O	1:B:256:ASN:HB3	2.09	0.52
1:B:467:PHE:HB3	4:F:1:NAG:H81	1.91	0.52
1:A:427:GLU:OE1	1:B:566:HIS:HE1	1.92	0.52
1:A:73:ASN:HB2	1:A:97:ASN:HD21	1.74	0.51
1:A:76:THR:HG22	1:A:98:PRO:HG3	1.91	0.51
1:B:72:ASP:OD1	1:B:99:ASN:ND2	2.43	0.51
1:A:720:SER:OG	1:A:742:ASP:OD2	2.28	0.51
1:B:47:ALA:HB2	1:B:65:VAL:HG21	1.92	0.50
1:B:616:SER:HA	1:B:647:SER:O	2.11	0.50
1:B:52:ARG:HG2	1:B:799:VAL:HG21	1.93	0.50
1:A:660:LEU:CD2	1:A:686:GLN:HG3	2.41	0.49
1:A:708:SER:HB3	1:A:734:GLU:HB2	1.94	0.49
1:B:99:ASN:O	1:B:100:VAL:C	2.51	0.49
1:B:35:PRO:O	1:B:52:ARG:NH1	2.46	0.49
1:A:732:LEU:HD13	1:A:733:SER:HA	1.94	0.49
1:A:404:ASN:H	1:A:428:ASN:ND2	2.11	0.49
1:B:66:THR:O	1:B:89:LEU:HA	2.13	0.49
1:B:100:VAL:O	1:B:100:VAL:HG13	2.13	0.49
1:A:649:ASN:H	1:A:674:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ASP:OD1	1:A:574:THR:OG1	2.25	0.48
1:B:235:LYS:HD2	1:B:270:CYS:SG	2.53	0.48
1:B:672:ASN:HD22	1:B:672:ASN:H	1.60	0.48
1:A:51:ASN:HA	1:A:72:ASP:O	2.13	0.48
1:A:404:ASN:H	1:A:428:ASN:HD21	1.61	0.48
1:A:370:ARG:HH22	5:A:905:NAG:H61	1.78	0.48
1:A:810:ARG:HG2	1:A:811:GLY:H	1.78	0.48
1:A:53:ARG:HA	1:A:74:PHE:CD2	2.48	0.48
1:A:296:SER:HA	1:A:320:PHE:O	2.13	0.48
6:B:901:HB2:H16	6:B:901:HB2:H15	1.95	0.48
1:A:177:LEU:HB2	1:A:208:LEU:HD23	1.95	0.47
1:A:807:GLY:O	1:A:810:ARG:HB3	2.13	0.47
6:A:915:HB2:H8	6:A:915:HB2:CAU	2.44	0.47
1:B:703:LEU:HD23	1:B:732:LEU:CD2	2.44	0.47
1:A:616:SER:HA	1:A:647:SER:O	2.14	0.47
1:B:62:GLY:O	1:B:65:VAL:HG12	2.15	0.47
1:B:521:LEU:HD13	1:B:550:LEU:HD21	1.96	0.47
1:A:61:VAL:CG1	1:A:86:LEU:HD11	2.45	0.47
1:A:87:GLN:N	1:A:87:GLN:CD	2.68	0.47
1:B:720:SER:HA	1:B:744:SER:O	2.15	0.47
1:B:61:VAL:HG12	1:B:86:LEU:HD22	1.97	0.47
1:A:66:THR:OG1	1:A:67:GLU:N	2.41	0.46
1:A:359:ILE:HG23	1:A:363:PHE:CD1	2.50	0.46
1:B:781:GLY:O	1:B:782:ASP:C	2.53	0.46
1:A:431:SER:HB2	1:A:432:PRO:HD2	1.97	0.46
1:B:354:PRO:HD2	1:B:378:VAL:O	2.16	0.46
1:B:415:GLN:NE2	7:B:1171:HOH:O	2.49	0.46
1:A:137:LEU:H	1:A:156:ASN:HD22	1.62	0.46
1:A:692:LEU:C	1:A:692:LEU:HD23	2.35	0.46
1:A:720:SER:HA	1:A:744:SER:O	2.15	0.46
1:B:244:GLY:HA2	1:B:245:LEU:C	2.35	0.46
1:B:813:SER:O	1:B:814:ILE:C	2.53	0.45
1:A:89:LEU:HD23	1:A:92:ILE:HD11	1.98	0.45
1:B:776:CYS:SG	1:B:814:ILE:HG22	2.57	0.45
1:B:205:LEU:C	1:B:205:LEU:HD23	2.37	0.45
1:A:728:PRO:HG2	1:A:731:PHE:HB2	1.99	0.44
1:A:754:SER:O	1:A:755:ALA:C	2.54	0.44
4:F:3:BMA:H62	4:F:4:MAN:C5	2.47	0.44
1:A:810:ARG:CG	1:A:811:GLY:N	2.80	0.44
1:B:317:ASP:OD1	1:B:319:GLU:HG3	2.16	0.44
1:A:467:PHE:HB3	2:C:1:NAG:H81	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:NAG:H62	3:D:3:BMA:C1	2.48	0.44
1:A:598:THR:HG22	7:A:1007:HOH:O	2.14	0.44
6:A:915:HB2:H15	6:A:915:HB2:CAS	2.48	0.44
1:B:36:CYS:HA	1:B:52:ARG:NH1	2.32	0.44
1:A:45:VAL:HG22	1:A:65:VAL:HA	2.00	0.44
1:A:472:ARG:CG	1:A:472:ARG:HH11	2.30	0.44
1:A:692:LEU:HD23	1:A:693:LEU:N	2.33	0.44
1:B:672:ASN:H	1:B:672:ASN:ND2	2.15	0.44
1:B:785:ARG:CZ	1:B:785:ARG:HB2	2.48	0.43
1:A:134:ASP:HA	1:A:155:GLN:O	2.19	0.43
1:B:161:ILE:HD12	1:B:177:LEU:HD13	2.00	0.43
1:A:388:GLN:N	1:A:389:PRO:CD	2.81	0.43
1:A:61:VAL:CG1	1:A:86:LEU:HD21	2.48	0.43
1:A:173:LYS:NZ	1:A:173:LYS:HB3	2.33	0.43
1:B:331:ALA:O	1:B:334:THR:HB	2.18	0.43
1:A:126:ASN:O	1:A:128:ARG:CD	2.67	0.42
1:A:81:GLU:HA	1:A:84:GLN:HB3	2.01	0.42
1:A:596:ILE:H	1:A:618:ASN:ND2	2.14	0.42
1:A:810:ARG:C	1:A:812:LYS:H	2.22	0.42
1:B:798:LEU:HD23	1:B:801:VAL:HG11	2.01	0.42
1:A:403:ILE:HA	1:A:427:GLU:O	2.18	0.42
1:B:287:THR:HA	1:B:309:ASN:O	2.19	0.42
1:A:629:ASN:ND2	1:B:184:ASN:HB3	2.35	0.42
1:B:612:GLU:OE2	1:B:643:ARG:NH1	2.52	0.42
1:B:45:VAL:CG1	1:B:64:TYR:O	2.67	0.42
1:A:518:ALA:HA	1:A:541:ARG:O	2.21	0.41
1:A:61:VAL:CG2	1:A:86:LEU:HD21	2.50	0.41
1:A:144:LEU:O	1:A:168:ARG:NH2	2.53	0.41
1:A:399:ILE:O	1:A:399:ILE:HG23	2.20	0.41
1:B:467:PHE:CB	4:F:1:NAG:H81	2.51	0.41
1:A:817:LEU:O	1:A:818:GLU:C	2.59	0.41
1:A:200:LEU:HB3	1:A:203:LEU:HB2	2.02	0.41
1:A:649:ASN:N	1:A:674:ASN:HD21	2.14	0.41
1:B:228:PHE:HA	1:B:252:ASP:HB3	2.03	0.41
1:B:244:GLY:HA2	1:B:246:ILE:N	2.36	0.41
1:A:516:SER:N	7:A:1115:HOH:O	2.45	0.41
1:B:614:VAL:HG21	3:H:1:NAG:H61	2.03	0.41
1:A:708:SER:CB	1:A:734:GLU:HB2	2.51	0.41
1:B:514:ALA:HA	1:B:539:ASN:O	2.21	0.41
1:B:578:GLU:HG2	1:B:602:LYS:HG3	2.04	0.40
1:A:814:ILE:HG13	1:A:815:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ARG:HA	1:A:402:GLY:O	2.20	0.40
1:B:632:ILE:HD13	1:B:658:ALA:HA	2.03	0.40
1:A:64:TYR:HD2	1:A:64:TYR:HA	1.78	0.40
1:A:115:ASN:C	1:A:115:ASN:ND2	2.72	0.40
1:B:705:ASP:HB3	1:B:728:PRO:HB2	2.04	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:B:280:ARG:NH2	1:B:545:ASP:OD2[2_445]	2.18	0.02

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	738/811 (91%)	681 (92%)	53 (7%)	4 (0%)	29	26
1	B	730/811 (90%)	671 (92%)	56 (8%)	3 (0%)	34	32
All	All	1468/1622 (90%)	1352 (92%)	109 (7%)	7 (0%)	29	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	GLY
1	A	39	LYS
1	A	806	PRO
1	B	87	GLN
1	A	378	VAL
1	B	378	VAL
1	B	814	ILE

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	692/755 (92%)	634 (92%)	58 (8%)	11	7
1	B	687/755 (91%)	634 (92%)	53 (8%)	13	9
All	All	1379/1510 (91%)	1268 (92%)	111 (8%)	12	8

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	43	ASP
1	A	45	VAL
1	A	49	CYS
1	A	56	GLU
1	A	59	GLN
1	A	61	VAL
1	A	63	LYS
1	A	64	TYR
1	A	68	LEU
1	A	79	THR
1	A	88	ASN
1	A	112	ASN
1	A	114	LEU
1	A	115	ASN
1	A	127	LEU
1	A	172	LEU
1	A	173	LYS
1	A	189	LYS
1	A	200	LEU
1	A	216	VAL
1	A	248	LEU
1	A	286	LEU
1	A	308	LYS
1	A	338	ARG
1	A	388	GLN
1	A	412	LYS

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Mol	Chain	Res	Type
1	A	419	ASN
1	A	420	LEU
1	A	433	LEU
1	A	465	SER
1	A	471	THR
1	A	472	ARG
1	A	504	LEU
1	A	534	TYR
1	A	565	SER
1	A	598	THR
1	A	609	SER
1	A	632	ILE
1	A	676	LEU
1	A	702	PHE
1	A	704	THR
1	A	706	SER
1	A	720	SER
1	A	727	LEU
1	A	732	LEU
1	A	734	GLU
1	A	735	VAL
1	A	736	SER
1	A	749	LYS
1	A	754	SER
1	A	763	LYS
1	A	765	SER
1	A	794	LYS
1	A	805	SER
1	A	809	GLN
1	A	810	ARG
1	A	812	LYS
1	B	45	VAL
1	B	49	CYS
1	B	64	TYR
1	B	76	THR
1	B	89	LEU
1	B	90	THR
1	B	118	ASP
1	B	122	LEU
1	B	124	LEU
1	B	125	LYS
1	B	136	GLN

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Mol	Chain	Res	Type
1	B	147	SER
1	B	168	ARG
1	B	188	GLU
1	B	189	LYS
1	B	200	LEU
1	B	243	LYS
1	B	248	LEU
1	B	280	ARG
1	B	286	LEU
1	B	308	LYS
1	B	338	ARG
1	B	387	PHE
1	B	433	LEU
1	B	465	SER
1	B	504	LEU
1	B	538	THR
1	B	565	SER
1	B	632	ILE
1	B	671	ILE
1	B	677	LYS
1	B	702	PHE
1	B	706	SER
1	B	712	SER
1	B	720	SER
1	B	733	SER
1	B	734	GLU
1	B	736	SER
1	B	739	LYS
1	B	750	THR
1	B	752	ASN
1	B	753	LYS
1	B	761	THR
1	B	765	SER
1	B	777	THR
1	B	778	CYS
1	B	789	GLU
1	B	792	ASN
1	B	794	LYS
1	B	799	VAL
1	B	802	ILE
1	B	805	SER
1	B	810	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	97	ASN
1	A	115	ASN
1	A	139	GLN
1	A	156	ASN
1	A	174	ASN
1	A	247	ASN
1	A	256	ASN
1	A	419	ASN
1	A	428	ASN
1	A	531	HIS
1	A	618	ASN
1	A	674	ASN
1	A	809	GLN
1	B	97	ASN
1	B	123	ASN
1	B	139	GLN
1	B	180	ASN
1	B	380	GLN
1	B	499	ASN
1	B	539	ASN
1	B	566	HIS
1	B	653	HIS
1	B	672	ASN
1	B	674	ASN

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 ⓘ

20 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	2,1	14,14,15	0.52	0	17,19,21	1.71	5 (29%)
2	NAG	C	2	2	14,14,15	0.83	0	17,19,21	1.44	3 (17%)
2	BMA	C	3	2	11,11,12	0.37	0	15,15,17	1.00	0
2	MAN	C	4	2	11,11,12	0.65	0	15,15,17	1.51	4 (26%)
3	NAG	D	1	3,1	14,14,15	1.03	1 (7%)	17,19,21	1.63	3 (17%)
3	NAG	D	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.73	5 (29%)
3	BMA	D	3	3	11,11,12	0.45	0	15,15,17	1.38	1 (6%)
3	NAG	E	1	3,1	14,14,15	0.78	0	17,19,21	1.86	5 (29%)
3	NAG	E	2	3	14,14,15	0.67	0	17,19,21	1.35	2 (11%)
3	BMA	E	3	3	11,11,12	0.71	0	15,15,17	2.20	6 (40%)
4	NAG	F	1	1,4	14,14,15	0.67	0	17,19,21	1.33	3 (17%)
4	NAG	F	2	4	14,14,15	1.01	1 (7%)	17,19,21	2.16	5 (29%)
4	BMA	F	3	4	11,11,12	0.82	0	15,15,17	3.23	7 (46%)
4	MAN	F	4	4	11,11,12	0.78	0	15,15,17	2.54	5 (33%)
3	NAG	G	1	3,1	14,14,15	0.86	0	17,19,21	1.42	3 (17%)
3	NAG	G	2	3	14,14,15	0.76	1 (7%)	17,19,21	1.80	6 (35%)
3	BMA	G	3	3	11,11,12	0.90	1 (9%)	15,15,17	2.07	7 (46%)
3	NAG	H	1	3,1	14,14,15	1.07	1 (7%)	17,19,21	2.79	6 (35%)
3	NAG	H	2	3	14,14,15	0.91	0	17,19,21	1.19	2 (11%)
3	BMA	H	3	3	11,11,12	0.63	0	15,15,17	2.40	3 (20%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	-2.56	1.39	1.43
4	F	2	NAG	O5-C1	-2.46	1.39	1.43
3	H	1	NAG	C2-N2	-2.42	1.42	1.46
3	G	3	BMA	C2-C3	2.41	1.56	1.52
3	D	1	NAG	O5-C5	-2.02	1.39	1.43
3	G	2	NAG	O5-C1	-2.02	1.40	1.43

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	3	BMA	C2-C3-C4	-8.46	96.25	110.89
3	H	1	NAG	C1-O5-C5	7.32	122.11	112.19
3	H	3	BMA	C1-O5-C5	6.80	121.40	112.19
4	F	4	MAN	C1-O5-C5	6.77	121.37	112.19
3	H	1	NAG	O5-C5-C6	-5.03	99.32	107.20
3	E	3	BMA	O4-C4-C3	-4.88	99.07	110.35
3	H	3	BMA	C3-C4-C5	4.73	118.68	110.24
4	F	2	NAG	O5-C1-C2	-4.73	103.83	111.29
4	F	3	BMA	C3-C4-C5	-4.72	101.83	110.24
3	E	3	BMA	C3-C4-C5	4.61	118.47	110.24
4	F	2	NAG	C1-O5-C5	-4.49	106.11	112.19
3	E	1	NAG	O5-C1-C2	-4.19	104.67	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	O6-C6-C5	-3.97	97.68	111.29
4	F	4	MAN	O3-C3-C2	3.79	117.26	109.99
2	C	1	NAG	C1-O5-C5	3.74	117.26	112.19
4	F	3	BMA	O3-C3-C4	3.70	118.90	110.35
3	D	2	NAG	C6-C5-C4	-3.68	104.39	113.00
3	H	1	NAG	C6-C5-C4	-3.66	104.42	113.00
3	D	1	NAG	O4-C4-C5	-3.64	100.27	109.30
3	G	3	BMA	C1-C2-C3	3.43	113.89	109.67
3	H	1	NAG	C1-C2-N2	-3.34	104.78	110.49
3	H	1	NAG	O5-C1-C2	-3.32	106.04	111.29
4	F	4	MAN	O2-C2-C3	3.29	116.74	110.14
3	D	2	NAG	C3-C4-C5	3.28	116.09	110.24
3	G	1	NAG	C1-O5-C5	-3.23	107.81	112.19
4	F	3	BMA	C1-O5-C5	3.20	116.53	112.19
3	H	1	NAG	O3-C3-C4	-3.18	103.00	110.35
4	F	2	NAG	O4-C4-C5	-3.14	101.51	109.30
3	G	3	BMA	O5-C5-C6	2.96	111.84	107.20
3	D	2	NAG	C1-O5-C5	2.94	116.18	112.19
3	G	3	BMA	C3-C4-C5	2.94	115.48	110.24
3	E	1	NAG	C8-C7-N2	2.92	121.05	116.10
3	G	2	NAG	C8-C7-N2	2.89	120.99	116.10
4	F	3	BMA	C6-C5-C4	-2.88	106.25	113.00
3	G	3	BMA	C1-O5-C5	2.77	115.95	112.19
4	F	1	NAG	O5-C5-C6	2.77	111.54	107.20
3	G	1	NAG	O3-C3-C4	2.76	116.72	110.35
3	E	1	NAG	O5-C5-C6	2.75	111.52	107.20
2	C	4	MAN	O5-C5-C6	2.70	111.44	107.20
4	F	2	NAG	O4-C4-C3	2.70	116.59	110.35
2	C	2	NAG	C6-C5-C4	-2.69	106.69	113.00
3	G	3	BMA	O3-C3-C2	2.66	115.09	109.99
3	G	2	NAG	O7-C7-C8	-2.66	117.12	122.06
3	E	3	BMA	O5-C5-C6	2.64	111.35	107.20
4	F	3	BMA	O3-C3-C2	2.64	115.06	109.99
2	C	4	MAN	O2-C2-C3	2.63	115.41	110.14
4	F	2	NAG	O3-C3-C2	-2.63	104.03	109.47
4	F	4	MAN	C6-C5-C4	-2.60	106.92	113.00
4	F	4	MAN	O6-C6-C5	-2.59	102.41	111.29
3	H	3	BMA	O5-C5-C4	2.56	117.05	110.83
2	C	4	MAN	O3-C3-C2	2.54	114.86	109.99
3	D	2	NAG	O7-C7-C8	-2.54	117.33	122.06
3	D	1	NAG	C4-C3-C2	-2.52	107.32	111.02
4	F	1	NAG	O4-C4-C5	-2.49	103.12	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C6-C5-C4	-2.41	107.35	113.00
3	G	2	NAG	C3-C4-C5	-2.40	105.96	110.24
3	G	2	NAG	O5-C5-C6	2.40	110.96	107.20
2	C	2	NAG	C1-O5-C5	2.39	115.43	112.19
3	D	3	BMA	C2-C3-C4	-2.39	106.77	110.89
2	C	2	NAG	O5-C1-C2	-2.37	107.55	111.29
3	E	1	NAG	O3-C3-C2	2.35	114.33	109.47
3	G	1	NAG	C4-C3-C2	-2.35	107.58	111.02
3	E	3	BMA	O5-C5-C4	2.31	116.46	110.83
3	G	3	BMA	O4-C4-C3	-2.31	105.01	110.35
3	E	1	NAG	O7-C7-C8	-2.31	117.77	122.06
2	C	1	NAG	O4-C4-C5	-2.27	103.67	109.30
4	F	1	NAG	C1-O5-C5	-2.26	109.13	112.19
3	H	2	NAG	C6-C5-C4	-2.24	107.75	113.00
4	F	3	BMA	O5-C5-C6	2.20	110.66	107.20
3	E	2	NAG	O3-C3-C2	-2.20	104.91	109.47
2	C	1	NAG	C6-C5-C4	-2.19	107.88	113.00
3	G	3	BMA	C2-C3-C4	2.16	114.64	110.89
3	E	3	BMA	C1-O5-C5	2.15	115.11	112.19
2	C	1	NAG	O5-C5-C4	2.14	116.04	110.83
3	H	2	NAG	O3-C3-C4	-2.13	105.42	110.35
3	G	2	NAG	C2-N2-C7	-2.11	119.90	122.90
3	D	1	NAG	O3-C3-C4	2.07	115.13	110.35
3	E	3	BMA	O5-C1-C2	-2.06	107.58	110.77
3	D	2	NAG	O7-C7-N2	2.05	125.71	121.95
2	C	4	MAN	C6-C5-C4	-2.02	108.26	113.00
3	G	2	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6

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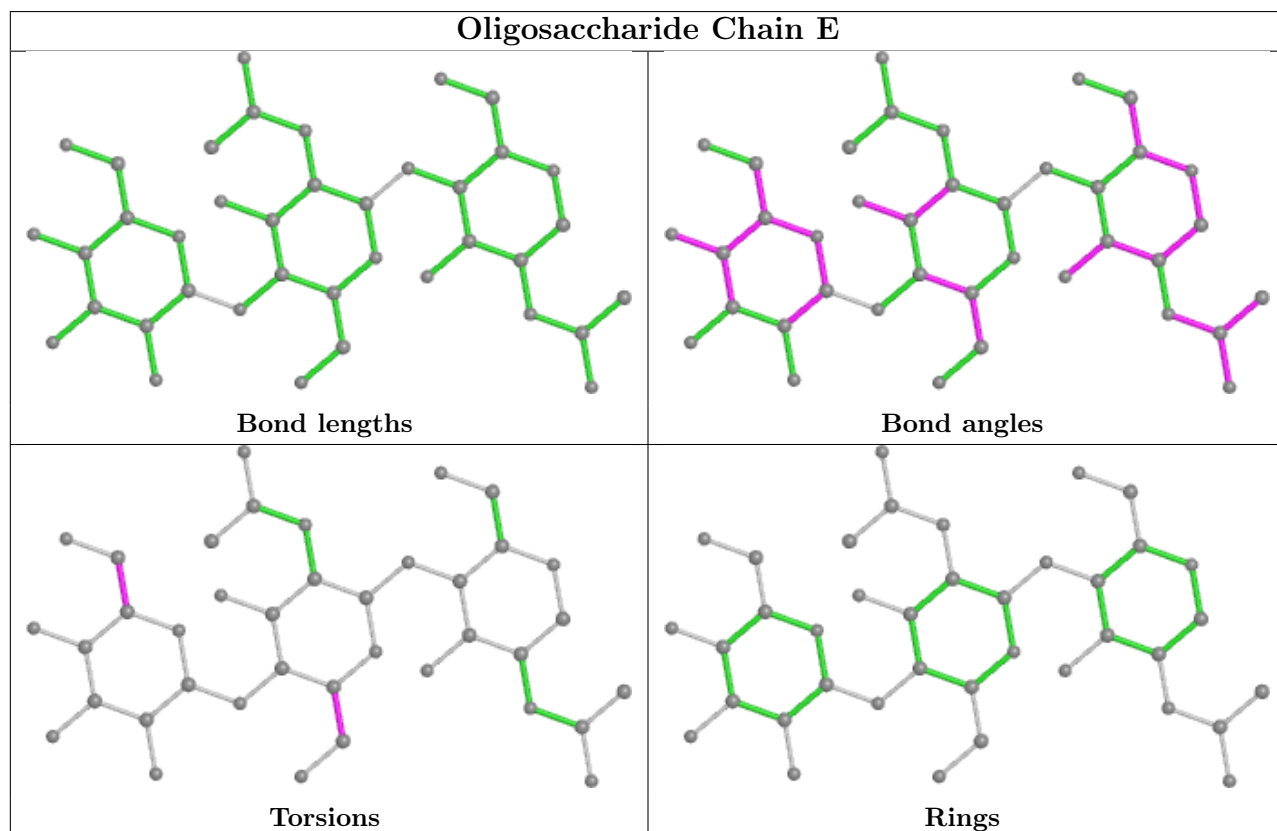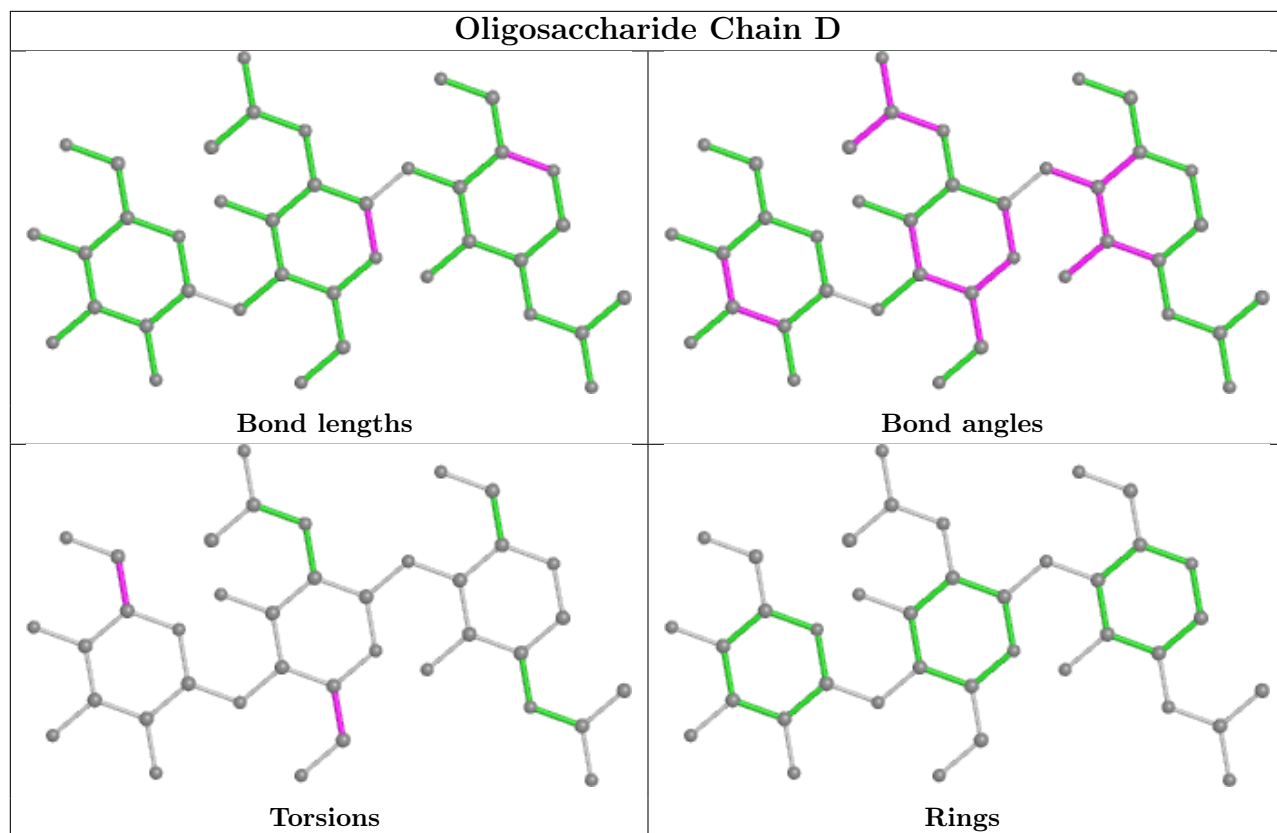| Mol	Chain	Res	Type	Atoms
3	G	3	BMA	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.
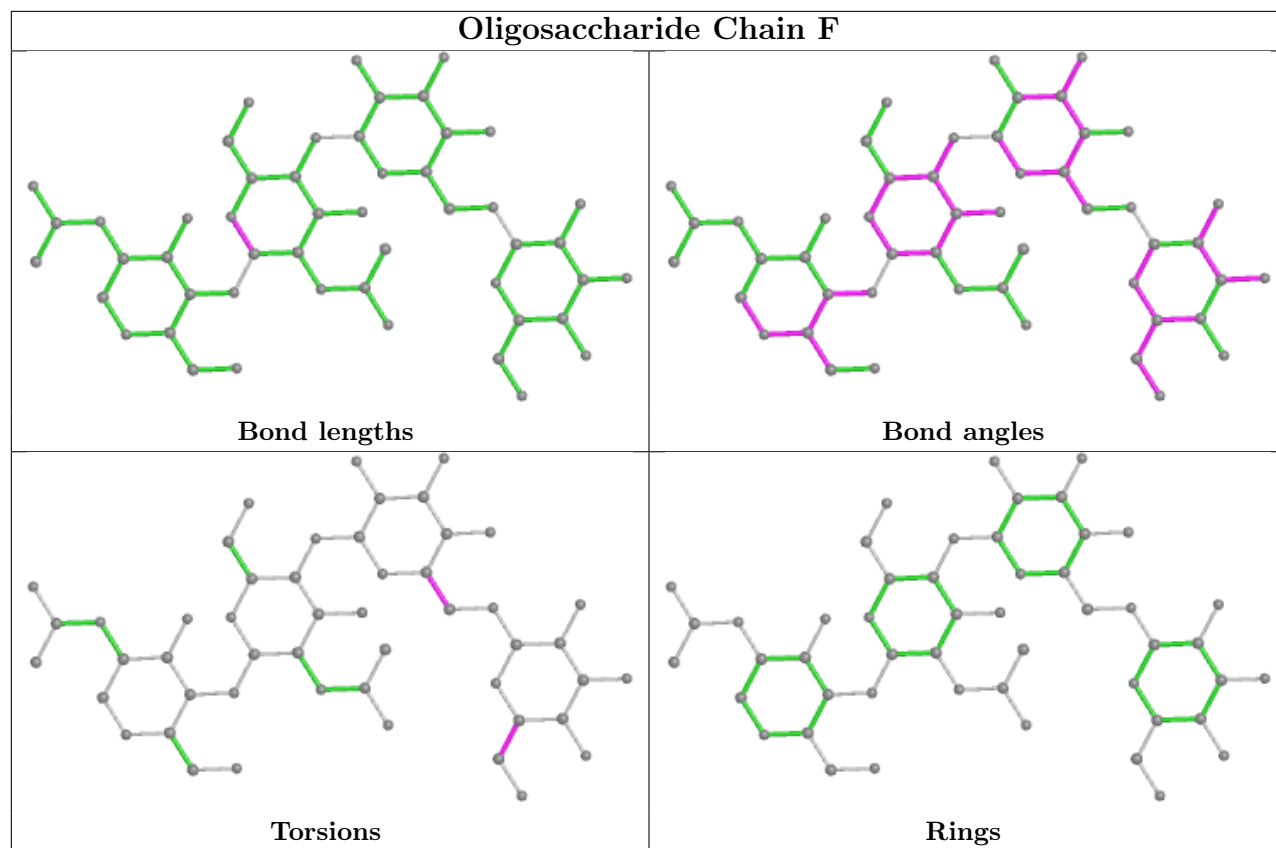
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	2	0
2	C	1	NAG	1	0
4	F	1	NAG	2	0
3	D	2	NAG	1	0
3	D	3	BMA	1	0
4	F	2	NAG	1	0
4	F	4	MAN	5	0
4	F	3	BMA	7	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 E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

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 (i)

12 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	#$|Z| > 2$
5	NAG	A	913	1	14,14,15	0.57	0	17,19,21	1.13	3 (17%)
5	NAG	A	905	1	14,14,15	0.68	0	17,19,21	1.66	3 (17%)
5	NAG	A	909	1	14,14,15	1.24	2 (14%)	17,19,21	2.83	6 (35%)
5	NAG	B	912	1	13,13,15	0.79	0	16,17,21	2.56	6 (37%)
6	HB2	B	901	-	21,25,25	1.11	1 (4%)	27,37,37	1.31	3 (11%)
5	NAG	A	914	1	14,14,15	0.72	0	17,19,21	1.80	6 (35%)
5	NAG	B	916	1	14,14,15	0.73	0	17,19,21	1.06	0
5	NAG	B	907	1	14,14,15	0.86	1 (7%)	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	B	911	1	14,14,15	1.04	1 (7%)	17,19,21	1.72	2 (11%)
6	HB2	A	915	-	21,25,25	1.15	1 (4%)	27,37,37	1.47	4 (14%)
5	NAG	B	917	1	14,14,15	0.60	0	17,19,21	1.40	2 (11%)
5	NAG	B	902	1	14,14,15	0.72	0	17,19,21	1.46	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	913	1	-	0/6/23/26	0/1/1/1
5	NAG	A	905	1	-	2/6/23/26	0/1/1/1
5	NAG	A	909	1	-	2/6/23/26	0/1/1/1
5	NAG	B	912	1	-	2/5/22/26	0/1/1/1
6	HB2	B	901	-	-	2/7/9/9	0/3/3/3
5	NAG	A	914	1	-	2/6/23/26	0/1/1/1
5	NAG	B	916	1	-	0/6/23/26	0/1/1/1
5	NAG	B	907	1	-	0/6/23/26	0/1/1/1
5	NAG	B	911	1	-	0/6/23/26	0/1/1/1
6	HB2	A	915	-	-	1/7/9/9	0/3/3/3
5	NAG	B	917	1	-	2/6/23/26	0/1/1/1
5	NAG	B	902	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	HB2	CAS-CAT	3.49	1.58	1.54
6	A	915	HB2	CAS-CAT	3.17	1.57	1.54
5	B	911	NAG	O5-C1	-2.99	1.38	1.43
5	A	909	NAG	C2-N2	-2.70	1.41	1.46
5	B	907	NAG	C1-C2	2.16	1.55	1.52
5	A	909	NAG	O5-C1	-2.14	1.40	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	912	NAG	C7-N2-C2	6.93	124.76	114.57
5	A	909	NAG	C2-N2-C7	6.28	131.85	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	911	NAG	C1-O5-C5	5.32	119.40	112.19
5	A	909	NAG	C1-C2-N2	-5.23	101.55	110.49
5	A	909	NAG	O7-C7-N2	-5.20	112.40	121.95
5	A	905	NAG	C1-O5-C5	4.10	117.74	112.19
5	A	909	NAG	C8-C7-N2	3.57	122.14	116.10
6	B	901	HB2	CAJ-CAB-CAA	-3.56	116.94	119.65
5	B	912	NAG	C1-O5-C5	3.56	117.02	112.19
5	B	917	NAG	C1-O5-C5	3.53	116.97	112.19
5	B	917	NAG	O5-C1-C2	-3.51	105.74	111.29
5	A	905	NAG	C3-C4-C5	3.42	116.35	110.24
5	B	912	NAG	C6-C5-C4	-3.40	105.03	113.00
6	A	915	HB2	CAJ-CAB-CAA	-3.26	117.17	119.65
5	A	914	NAG	C6-C5-C4	3.21	120.53	113.00
5	B	912	NAG	C1-C2-N2	3.20	115.82	110.32
5	A	914	NAG	O5-C5-C4	-3.16	103.14	110.83
5	A	914	NAG	O5-C5-C6	3.08	112.04	107.20
5	B	912	NAG	O5-C5-C4	3.06	118.27	110.83
5	B	907	NAG	C4-C3-C2	-3.03	106.58	111.02
5	B	912	NAG	C3-C4-C5	2.78	115.19	110.24
6	A	915	HB2	CAU-CAT-CAS	2.75	117.10	110.13
5	B	902	NAG	C3-C4-C5	2.72	115.08	110.24
5	A	914	NAG	C3-C4-C5	-2.67	105.47	110.24
5	B	902	NAG	C1-O5-C5	2.65	115.79	112.19
5	A	909	NAG	O5-C5-C4	-2.57	104.58	110.83
6	A	915	HB2	CAB-CAA-NAI	-2.53	120.58	123.01
5	B	911	NAG	C6-C5-C4	-2.50	107.14	113.00
6	B	901	HB2	CAH-CAG-NAI	-2.44	119.41	121.01
6	A	915	HB2	CAF-CAE-CAC	-2.43	117.03	120.44
5	A	914	NAG	C1-O5-C5	-2.41	108.93	112.19
5	A	909	NAG	C1-O5-C5	-2.39	108.96	112.19
5	A	913	NAG	C1-O5-C5	2.36	115.38	112.19
5	A	913	NAG	C4-C3-C2	-2.26	107.70	111.02
6	B	901	HB2	NAR-CAG-NAI	2.15	122.81	117.09
5	A	905	NAG	C6-C5-C4	-2.11	108.05	113.00
5	A	913	NAG	C1-C2-N2	-2.11	106.88	110.49
5	A	914	NAG	C1-C2-N2	-2.01	107.05	110.49

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	915	HB2	CAL-CAN-CAO-CAP

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Mol	Chain	Res	Type	Atoms
6	B	901	HB2	CAL-CAN-CAO-CAP
5	B	917	NAG	C4-C5-C6-O6
5	A	909	NAG	C8-C7-N2-C2
5	A	909	NAG	O7-C7-N2-C2
5	B	902	NAG	C8-C7-N2-C2
5	B	902	NAG	O7-C7-N2-C2
5	B	917	NAG	O5-C5-C6-O6
5	A	905	NAG	C4-C5-C6-O6
5	B	912	NAG	C1-C2-N2-C7
5	B	912	NAG	C3-C2-N2-C7
5	A	905	NAG	O5-C5-C6-O6
5	A	914	NAG	C4-C5-C6-O6
6	B	901	HB2	NAM-CAS-CAT-OAW
5	A	914	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905	NAG	1	0
6	B	901	HB2	1	0
6	A	915	HB2	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HB2 B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand HB2 A 915

Bond lengths

Bond angles

Torsions

Rings
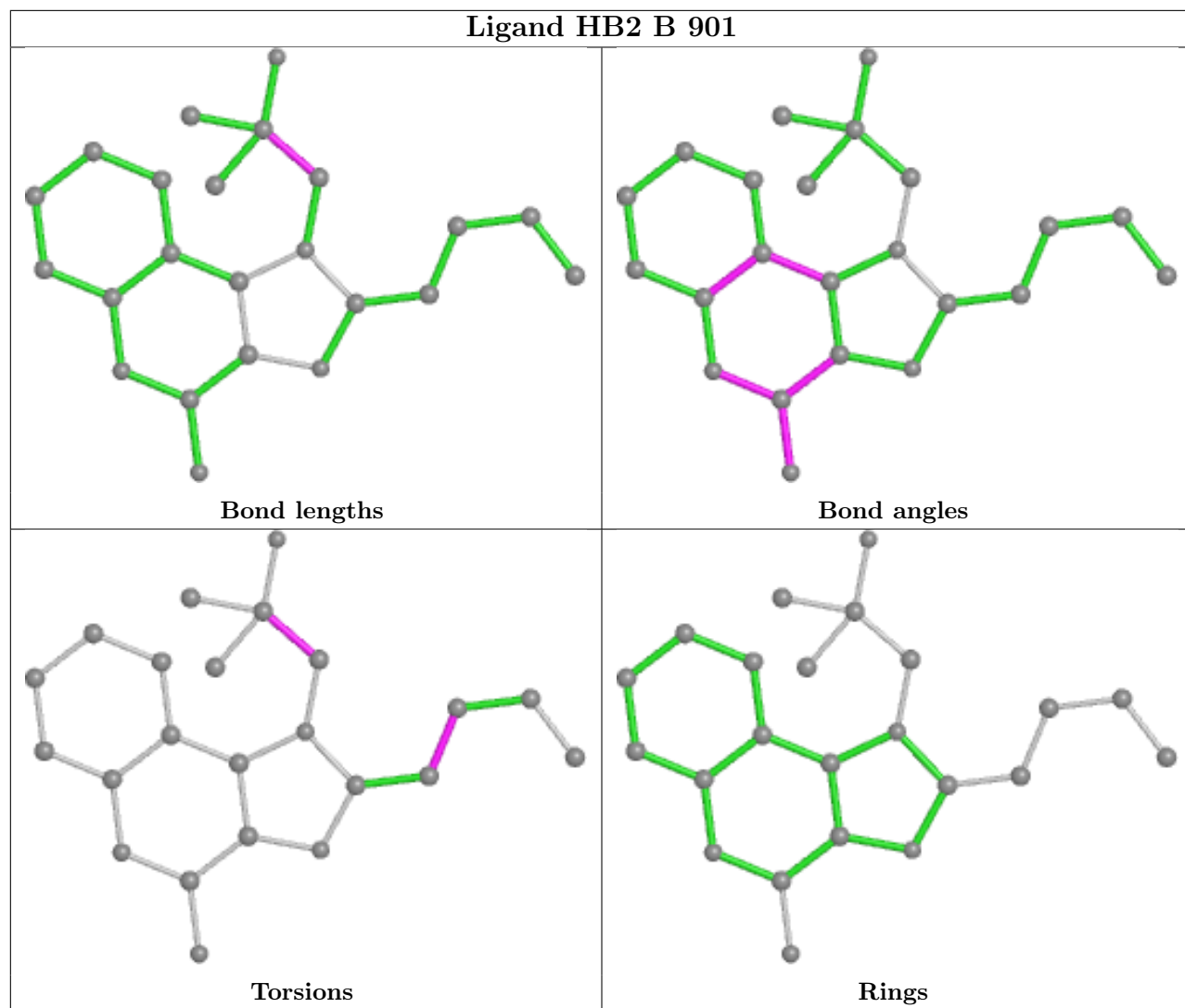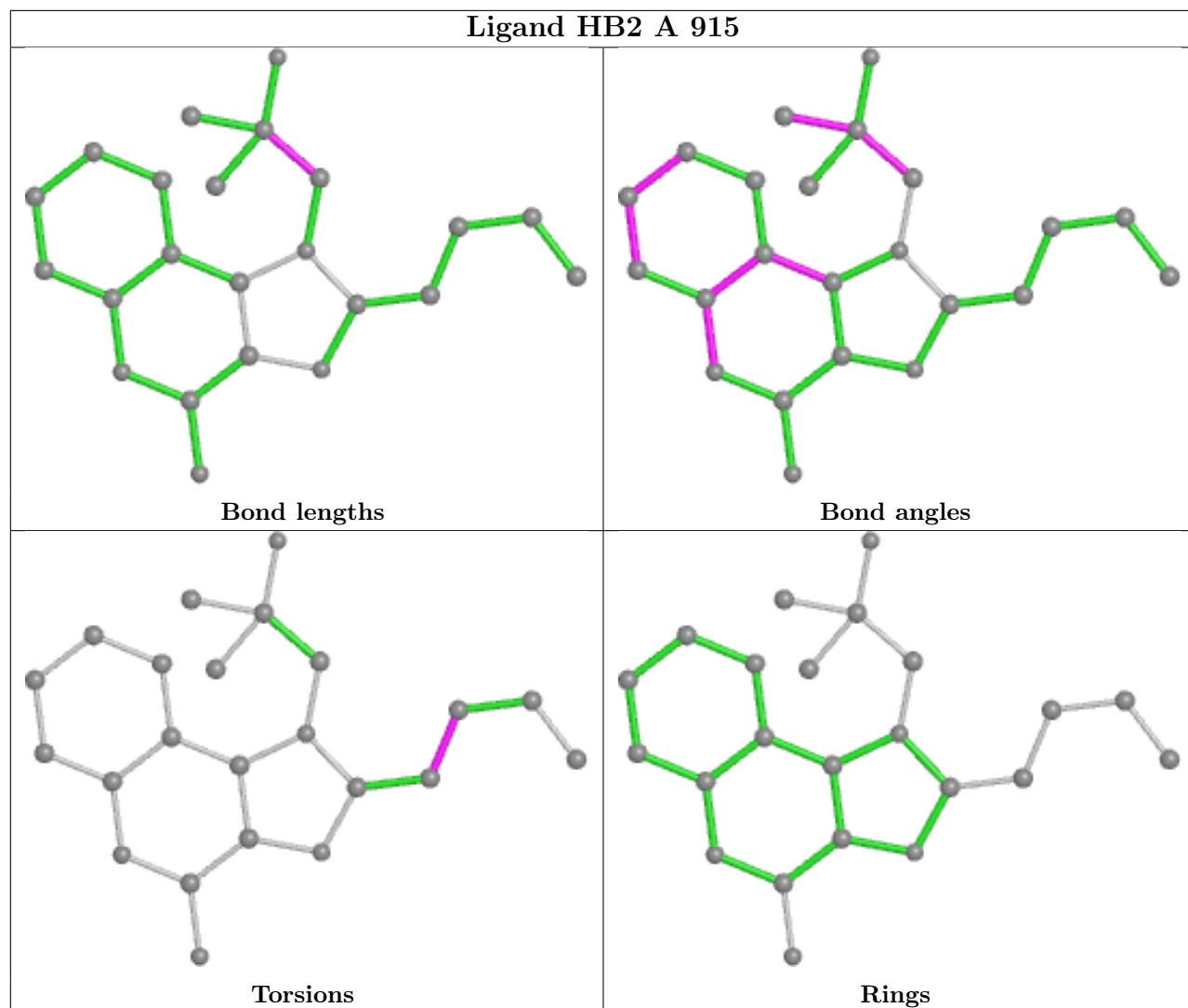
5.7 Other polymers ⓘ

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	746/811 (91%)	0.30	53 (7%)	16	20	15, 33, 74, 122	0
1	B	740/811 (91%)	0.38	55 (7%)	14	18	17, 33, 81, 105	0
All	All	1486/1622 (91%)	0.34	108 (7%)	15	19	15, 33, 77, 122	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	ASN	7.5
1	A	809	GLN	7.4
1	B	100	VAL	6.8
1	A	42	ASN	6.7
1	A	818	GLU	6.4
1	B	808	ASP	6.1
1	A	41	GLN	5.7
1	A	64	TYR	5.4
1	B	806	PRO	5.3
1	B	776	CYS	5.2
1	A	791	LEU	5.0
1	B	64	TYR	5.0
1	B	41	GLN	5.0
1	B	807	GLY	4.7
1	B	40	LYS	4.5
1	B	810	ARG	4.5
1	A	817	LEU	4.5
1	B	731	PHE	4.5
1	B	732	LEU	4.1
1	A	43	ASP	4.1
1	B	470	PHE	4.1
1	B	761	THR	4.0
1	A	732	LEU	3.9
1	B	753	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	39	LYS	3.7
1	A	100	VAL	3.7
1	B	805	SER	3.7
1	A	433	LEU	3.6
1	A	44	SER	3.5
1	A	808	ASP	3.5
1	A	45	VAL	3.4
1	A	84	GLN	3.4
1	A	792	ASN	3.3
1	B	702	PHE	3.3
1	A	782	ASP	3.3
1	A	733	SER	3.3
1	A	39	LYS	3.2
1	B	86	LEU	3.1
1	A	470	PHE	3.1
1	A	778	CYS	3.0
1	A	40	LYS	3.0
1	B	59	GLN	3.0
1	B	244	GLY	3.0
1	A	613	LEU	3.0
1	B	812	LYS	3.0
1	A	779	ASP	2.9
1	B	809	GLN	2.9
1	B	65	VAL	2.9
1	B	130	LEU	2.9
1	A	61	VAL	2.9
1	B	678	PHE	2.8
1	A	113	GLY	2.8
1	B	92	ILE	2.8
1	B	63	LYS	2.8
1	B	433	LEU	2.8
1	B	168	ARG	2.8
1	A	702	PHE	2.8
1	A	776	CYS	2.7
1	B	84	GLN	2.7
1	B	779	ASP	2.7
1	A	31	SER	2.7
1	A	678	PHE	2.7
1	B	175	LEU	2.6
1	A	762	THR	2.6
1	A	130	LEU	2.6
1	B	124	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	229	LEU	2.6
1	B	74	PHE	2.5
1	B	31	SER	2.5
1	A	471	THR	2.5
1	A	99	ASN	2.5
1	B	85	GLY	2.5
1	A	63	LYS	2.5
1	B	459	PHE	2.4
1	B	88	ASN	2.4
1	B	754	SER	2.4
1	B	778	CYS	2.4
1	B	60	THR	2.4
1	B	146	GLU	2.4
1	A	806	PRO	2.4
1	A	55	GLN	2.4
1	A	807	GLY	2.4
1	A	646	LEU	2.3
1	B	87	GLN	2.3
1	B	786	TRP	2.3
1	B	815	VAL	2.3
1	A	271	ASP	2.3
1	A	65	VAL	2.3
1	A	46	ILE	2.3
1	B	186	VAL	2.3
1	B	55	GLN	2.3
1	A	92	ILE	2.3
1	A	68	LEU	2.2
1	B	99	ASN	2.2
1	B	726	HIS	2.2
1	B	425	LEU	2.2
1	B	83	PHE	2.2
1	A	77	HIS	2.2
1	A	80	ASN	2.1
1	B	789	GLU	2.1
1	B	122	LEU	2.1
1	A	60	THR	2.1
1	B	730	GLY	2.1
1	A	132	LEU	2.1
1	B	271	ASP	2.1
1	A	56	GLU	2.0
1	A	251	LEU	2.0
1	A	789	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	G	3	11/12	0.80	0.28	46,53,57,66	0
4	MAN	F	4	11/12	0.80	0.32	41,50,58,58	0
4	BMA	F	3	11/12	0.82	0.25	41,45,55,56	0
3	BMA	H	3	11/12	0.82	0.22	40,47,54,59	0
3	BMA	D	3	11/12	0.83	0.40	59,67,74,78	0
3	BMA	E	3	11/12	0.83	0.31	47,54,63,73	0
2	MAN	C	4	11/12	0.83	0.30	39,43,46,49	0
2	BMA	C	3	11/12	0.92	0.20	32,38,42,42	0
3	NAG	D	2	14/15	0.92	0.18	35,43,48,52	0
3	NAG	H	2	14/15	0.93	0.11	25,28,33,36	0
3	NAG	G	2	14/15	0.94	0.21	33,42,50,51	0
3	NAG	G	1	14/15	0.95	0.10	17,20,24,26	0
3	NAG	H	1	14/15	0.95	0.09	20,23,24,29	0
3	NAG	E	2	14/15	0.95	0.10	23,28,41,42	0
2	NAG	C	2	14/15	0.96	0.12	19,27,32,39	0
4	NAG	F	2	14/15	0.96	0.12	25,30,35,35	0
3	NAG	E	1	14/15	0.96	0.09	20,22,25,26	0
2	NAG	C	1	14/15	0.96	0.09	21,22,23,29	0
3	NAG	D	1	14/15	0.97	0.08	18,22,26,28	0
4	NAG	F	1	14/15	0.98	0.08	19,22,25,30	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:

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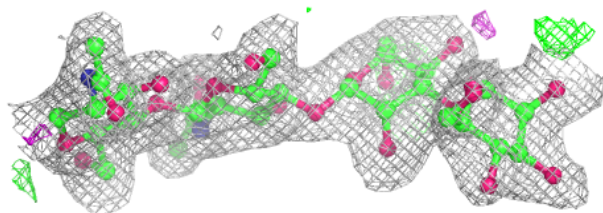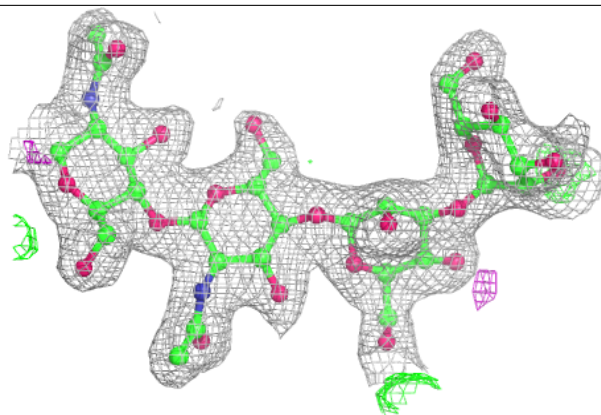
Electron density around Chain D:

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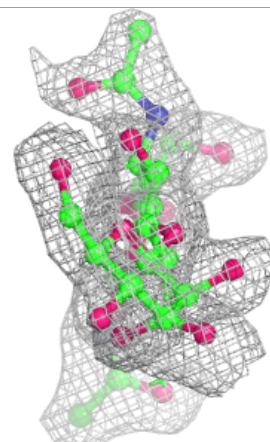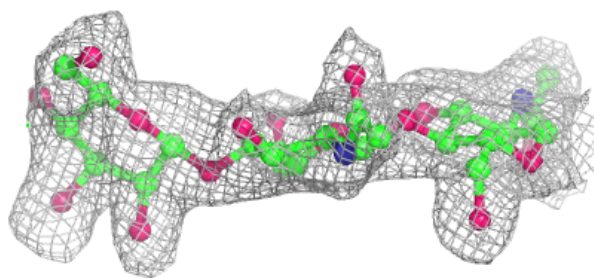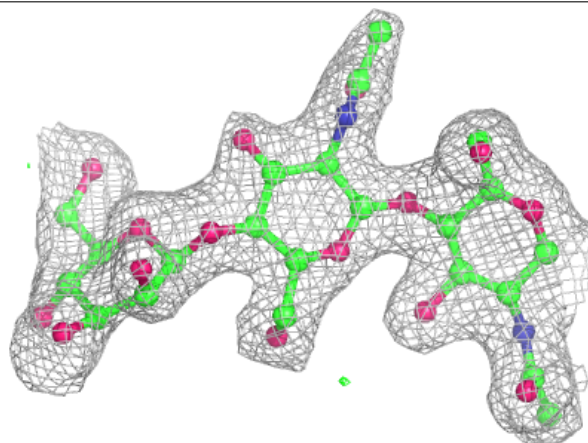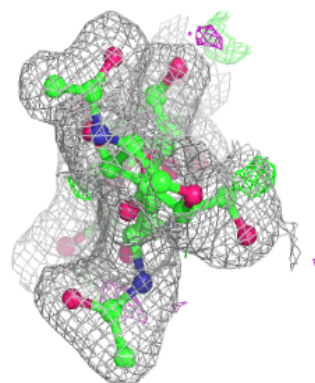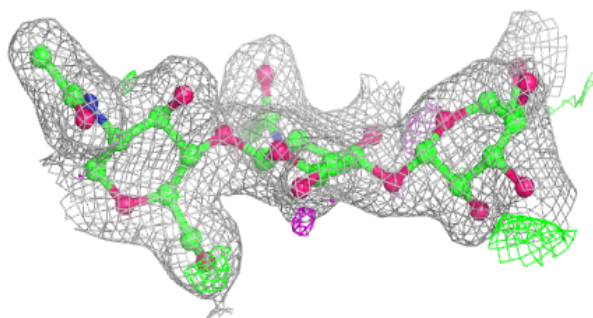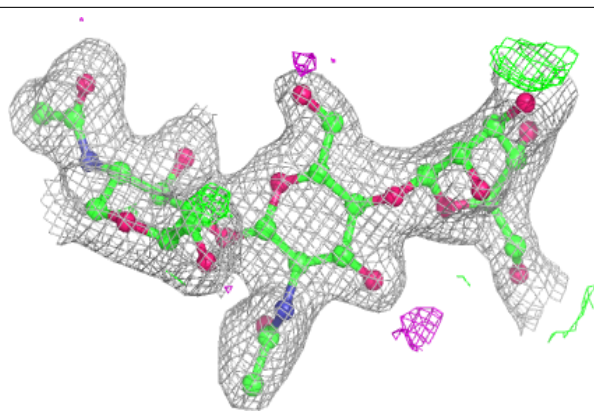$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
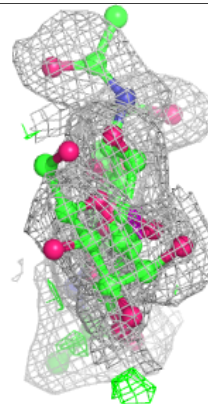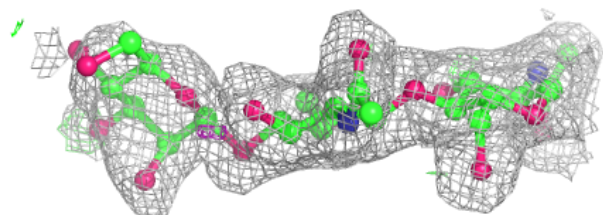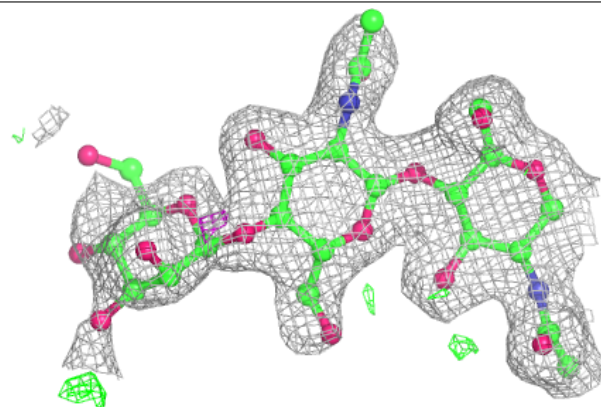
Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
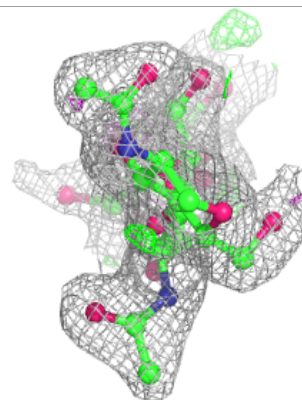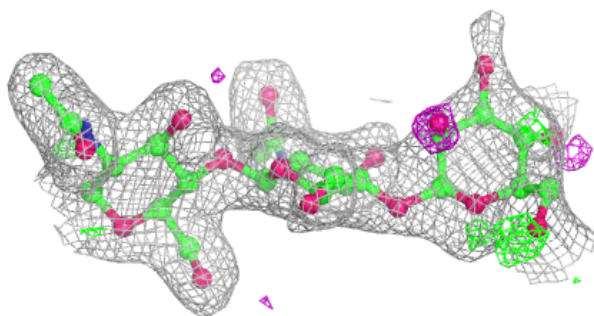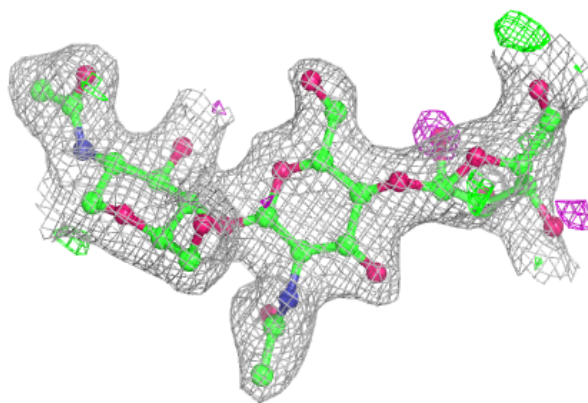
Electron density around Chain G:

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 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)
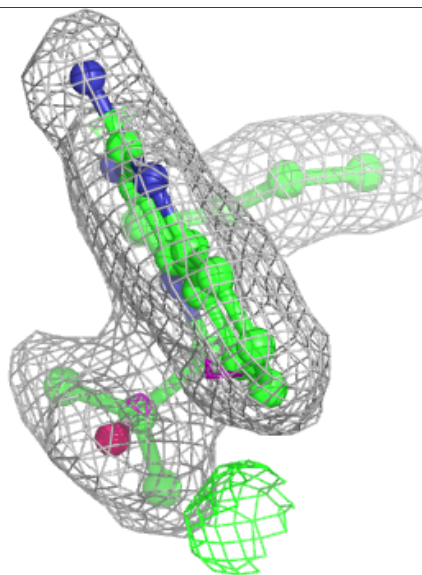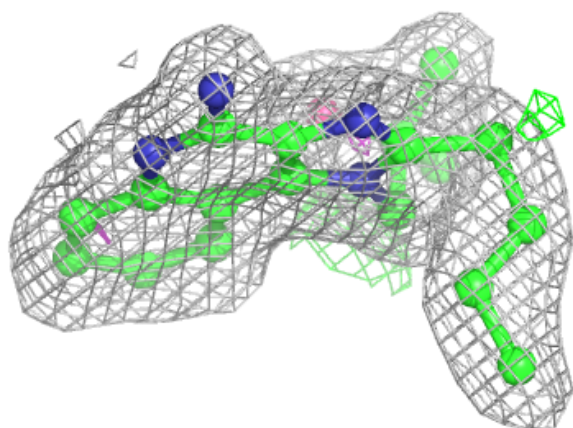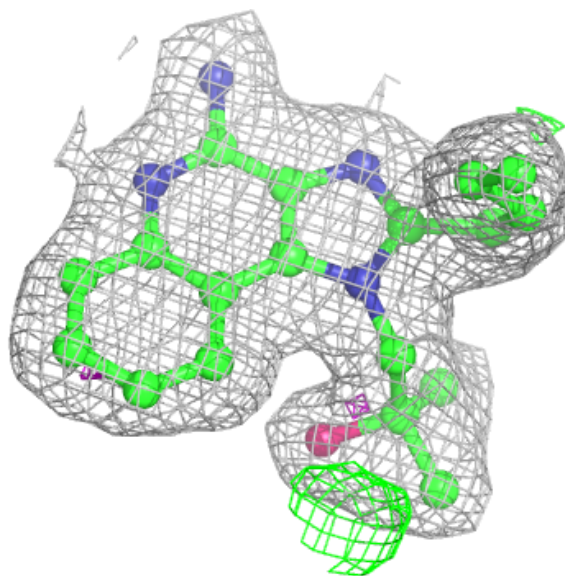and green (positive)
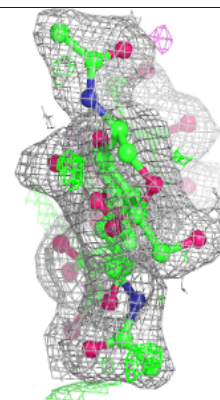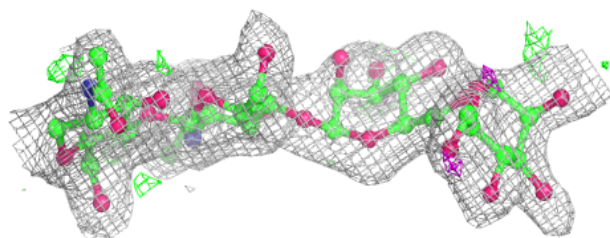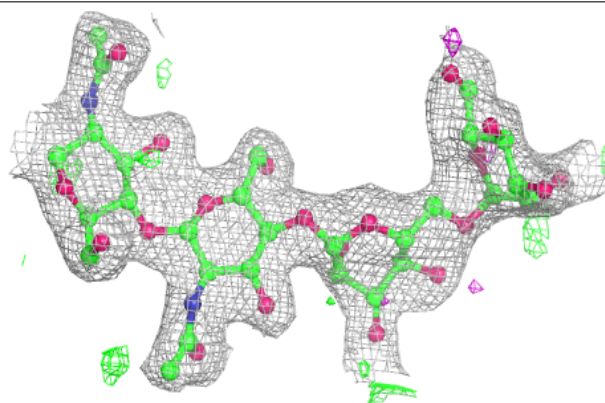
6.4 Ligands ⓘ

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.
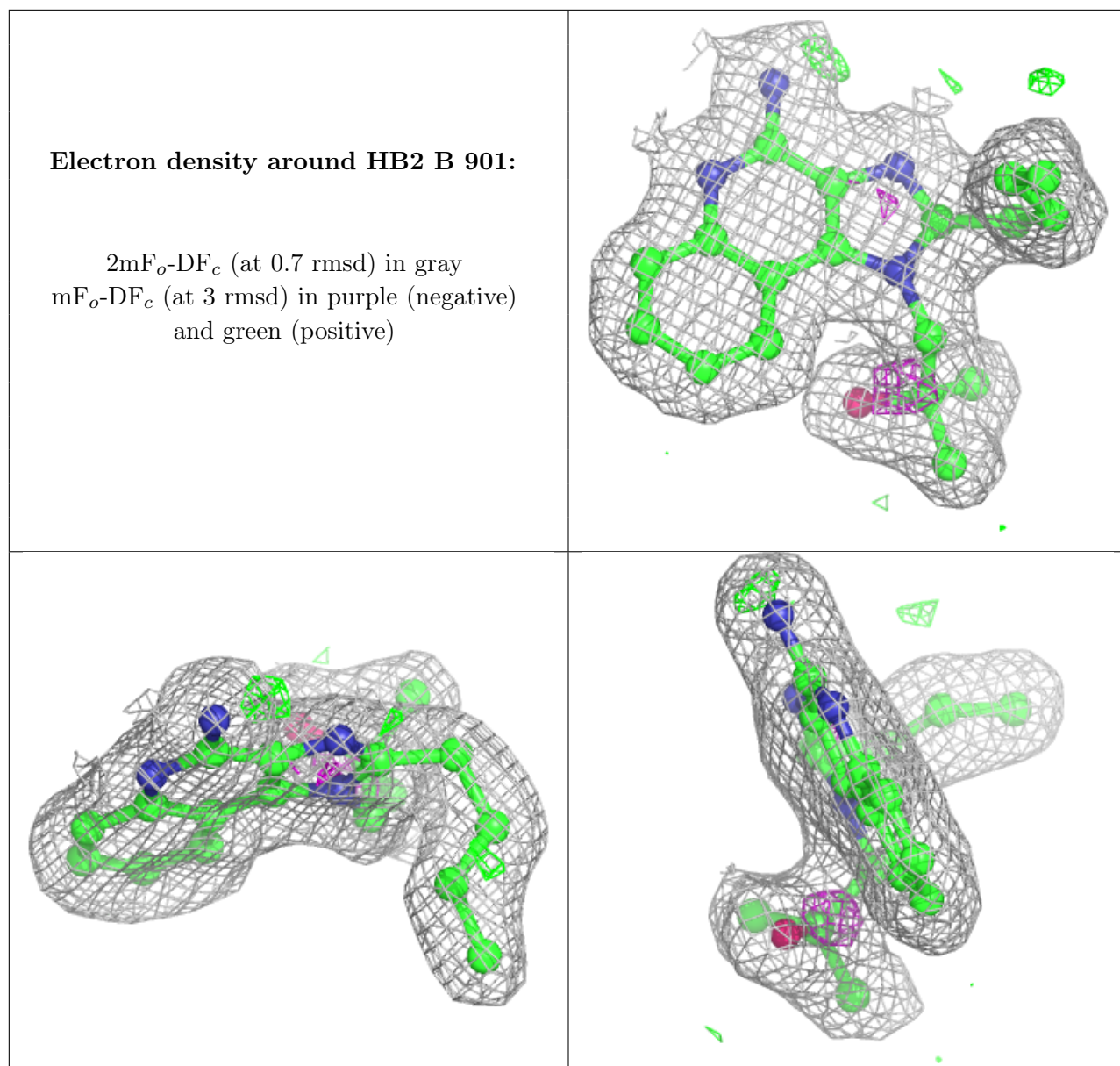
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	912	13/15	0.80	0.29	37,52,66,77	0
5	NAG	B	902	14/15	0.83	0.20	38,45,49,50	0
5	NAG	B	917	14/15	0.83	0.28	54,61,66,67	0
5	NAG	A	905	14/15	0.89	0.21	40,46,55,55	0
5	NAG	B	916	14/15	0.90	0.14	28,37,40,44	0
5	NAG	A	914	14/15	0.90	0.23	44,50,54,56	0
5	NAG	B	907	14/15	0.91	0.20	31,41,43,44	0
5	NAG	A	909	14/15	0.91	0.11	29,34,41,43	0
5	NAG	B	911	14/15	0.94	0.11	26,31,36,40	0
5	NAG	A	913	14/15	0.94	0.15	28,34,41,51	0
6	HB2	A	915	23/23	0.96	0.10	15,19,23,29	0
6	HB2	B	901	23/23	0.96	0.11	12,14,22,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HB2 A 915:

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 HB2 B 901:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.