Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 03:38 PM EDT

PDB ID	:	4N61
Title	:	Crystal structure of hemagglutinin from an H7N9 influenza virus in complex with LSTa, extended soaking
Authors	:	Xu, R.; Wilson, I.A.
Deposited on	:	2013-10-11
Resolution	:	2.60 Å(reported)

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

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

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

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

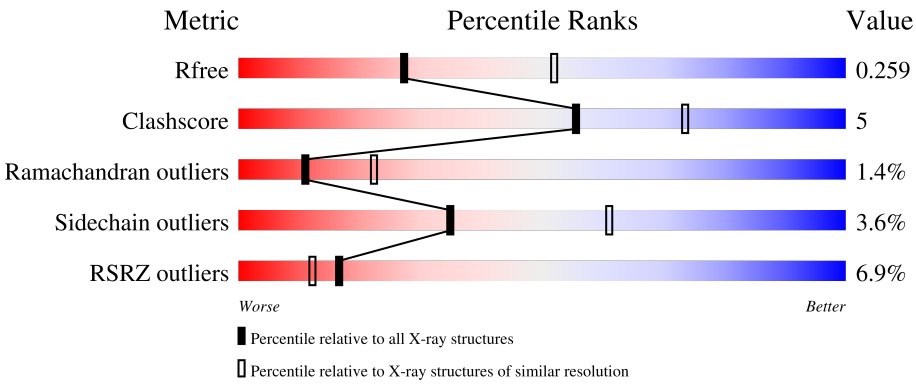
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	321	% 81% 17% ••
1	C	321	10% 82% 16% • •
2	B	179	88% • •• 6%
2	D	179	18% 85% 7% • 6%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
4	F	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7760 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2427	1509	438	465	15	0	0	0
1	C	318	2427	1509	438	465	15	0	0	0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	169	1373	845	241	280	7	0	0	0
2	D	169	1373	845	241	280	7	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

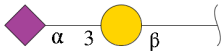
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	SER	-	expression tag	UNP R4NN21
B	174	GLY	-	expression tag	UNP R4NN21
B	175	ARG	-	expression tag	UNP R4NN21
B	176	LEU	-	expression tag	UNP R4NN21
B	177	VAL	-	expression tag	UNP R4NN21
B	178	PRO	-	expression tag	UNP R4NN21
B	179	ARG	-	expression tag	UNP R4NN21
D	173	SER	-	expression tag	UNP R4NN21
D	174	GLY	-	expression tag	UNP R4NN21
D	175	ARG	-	expression tag	UNP R4NN21
D	176	LEU	-	expression tag	UNP R4NN21
D	177	VAL	-	expression tag	UNP R4NN21
D	178	PRO	-	expression tag	UNP R4NN21
D	179	ARG	-	expression tag	UNP R4NN21

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

cetamido-2-deoxy-beta-D-glucopyranose.

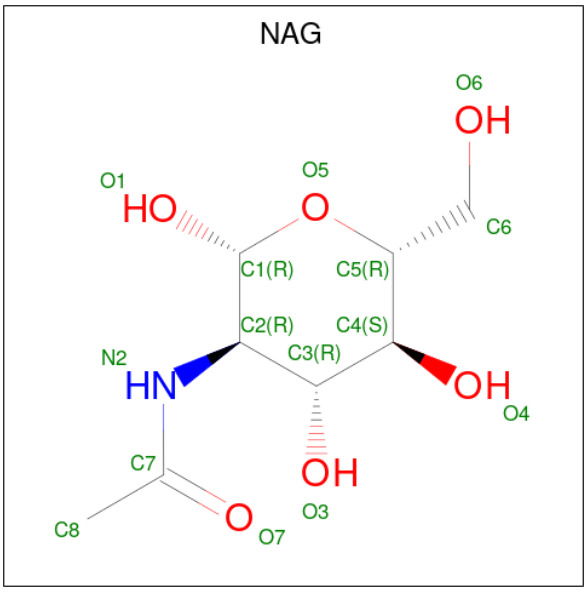
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	2	31	17	1	13	0	0	0

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



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

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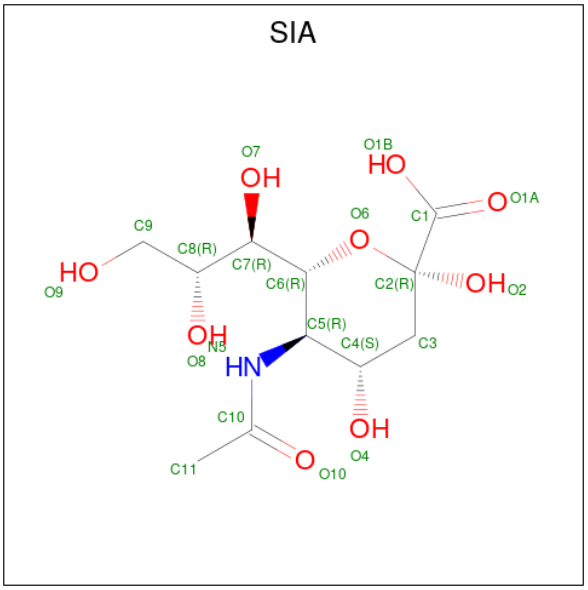
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

- Molecule 6 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	21	11	1	9	0	0

- Molecule 7 is water.

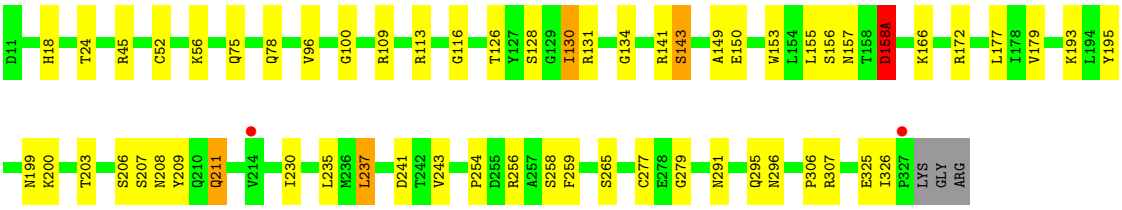
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	27	27	27	0	0
			Total	O		
7	B	21	21	21	0	0
			Total	O		
7	C	4	4	4	0	0

3 Residue-property plots (i)

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

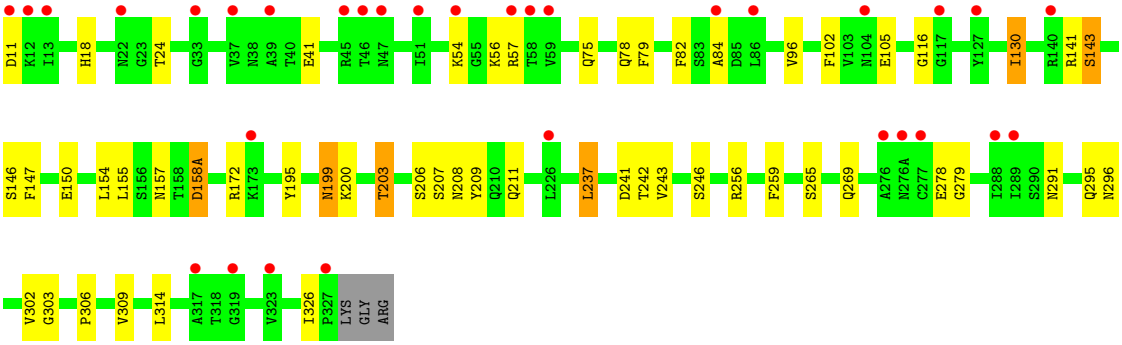
• Molecule 1: Hemagglutinin HA1

Chain A:



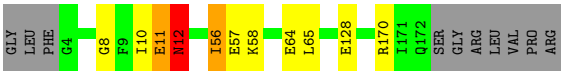
• Molecule 1: Hemagglutinin HA1

Chain C:



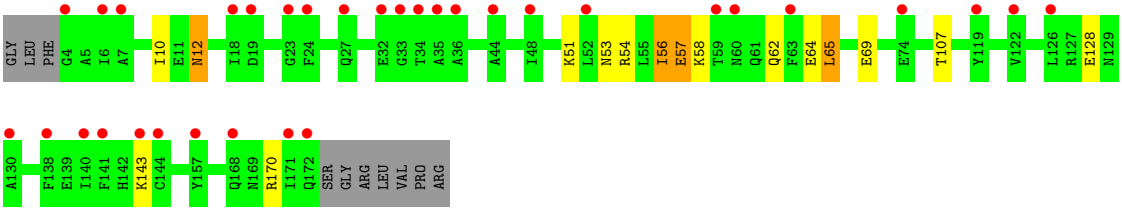
• Molecule 2: Hemagglutinin HA2

Chain B:



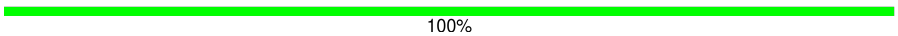
• Molecule 2: Hemagglutinin HA2

Chain D:



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

Chain E:



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	153.91Å 153.91Å 153.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 2.60 48.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.67-2.60) 99.7 (48.67-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.216 , 0.262 0.219 , 0.259	Depositor DCC
R_{free} test set	1873 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7760	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: GAL, SIA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.29	0/2474	0.48	0/3345
1	C	0.26	0/2474	0.42	0/3345
2	B	0.29	0/1396	0.44	0/1881
2	D	0.23	0/1396	0.40	0/1881
All	All	0.27	0/7740	0.44	0/10452

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2427	0	2387	35	0
1	C	2427	0	2389	31	0
2	B	1373	0	1273	10	0
2	D	1373	0	1274	14	0
3	E	28	0	25	0	0
4	F	31	0	26	1	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	C	21	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	27	0	0	0	0
7	B	21	0	0	0	0
7	C	4	0	0	0	0
All	All	7760	0	7418	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (77) 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:C:291:ASN:OD1	2:D:58:LYS:NZ	1.97	0.96
1:A:56:LYS:NZ	1:A:279:GLY:O	2.14	0.81
1:C:56:LYS:NZ	1:C:279:GLY:O	2.15	0.79
1:A:326:ILE:HG12	2:B:12:ASN:HB3	1.68	0.75
2:B:128:GLU:HG3	2:B:170:ARG:NH1	2.08	0.69
2:B:128:GLU:HG3	2:B:170:ARG:HH12	1.57	0.68
1:C:155:LEU:HD21	6:C:401:SIA:H111	1.77	0.67
1:A:206:SER:HB3	1:A:209:TYR:HB3	1.79	0.65
1:C:206:SER:OG	1:C:207:SER:N	2.31	0.64
1:C:291:ASN:HB3	2:D:56:ILE:HG13	1.81	0.63
1:C:199:ASN:OD1	1:C:199:ASN:N	2.30	0.62
2:D:54:ARG:HB3	2:D:54:ARG:NH1	2.15	0.62
1:A:237:LEU:HG	1:A:243:VAL:HG13	1.82	0.60
1:A:45:ARG:NH1	1:A:296:ASN:OD1	2.34	0.60
1:C:130:ILE:HD11	1:C:154:LEU:HB3	1.84	0.59
1:A:150:GLU:OE1	1:A:256:ARG:HD3	2.03	0.58
1:C:150:GLU:OE1	1:C:256:ARG:HD3	2.04	0.58
1:C:41:GLU:OE2	1:C:314:LEU:N	2.34	0.57
1:A:158(A):ASP:OD2	1:A:193:LYS:NZ	2.38	0.57
1:C:203:THR:HG23	1:C:246:SER:HB3	1.86	0.56
1:A:291:ASN:OD1	2:B:58:LYS:NZ	2.37	0.54
1:C:303:GLY:HA2	2:D:62:GLN:HG3	1.88	0.54
2:D:128:GLU:HG3	2:D:170:ARG:NH1	2.23	0.54
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.90	0.54
2:D:128:GLU:HG3	2:D:170:ARG:HH12	1.74	0.53
1:A:126:THR:O	1:A:166:LYS:NZ	2.24	0.52
1:A:206:SER:OG	1:A:207:SER:N	2.43	0.52
1:C:195:TYR:O	1:C:200:LYS:NZ	2.28	0.52
2:B:11:GLU:O	2:B:12:ASN:ND2	2.42	0.52
1:C:206:SER:HB3	1:C:209:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ARG:HD3	1:A:259:PHE:CZ	2.46	0.51
2:B:8:GLY:O	2:B:12:ASN:ND2	2.44	0.50
1:C:296:ASN:ND2	1:C:309:VAL:O	2.38	0.50
2:D:51:LYS:HZ2	2:D:107:THR:HG1	1.56	0.50
1:C:54:LYS:HD3	1:C:278:GLU:HB2	1.93	0.50
1:C:295:GLN:HG2	1:C:306:PRO:HG2	1.95	0.48
1:A:177:LEU:HB3	1:A:258:SER:HB2	1.96	0.48
1:A:291:ASN:HA	2:B:58:LYS:NZ	2.30	0.47
1:C:237:LEU:HG	1:C:243:VAL:HG13	1.97	0.47
1:A:291:ASN:HB3	2:B:56:ILE:HG13	1.97	0.46
1:C:141:ARG:O	1:C:143:SER:OG	2.30	0.46
1:A:130:ILE:HA	1:A:156:SER:O	2.15	0.46
1:A:128:SER:C	1:A:130:ILE:HG22	2.35	0.46
1:A:141:ARG:HH12	1:A:149:ALA:HB2	1.81	0.45
1:C:326:ILE:HG12	2:D:12:ASN:HB3	1.99	0.45
1:A:100:GLY:HA3	1:A:230:ILE:O	2.17	0.45
1:A:141:ARG:O	1:A:143:SER:OG	2.27	0.45
6:C:401:SIA:O6	6:C:401:SIA:O8	2.34	0.44
1:A:195:TYR:O	1:A:200:LYS:NZ	2.35	0.44
1:A:291:ASN:HA	2:B:58:LYS:HZ2	1.82	0.44
1:C:291:ASN:HA	2:D:58:LYS:NZ	2.33	0.44
1:A:130:ILE:HG12	1:A:131:ARG:N	2.33	0.44
1:C:79:PHE:HA	1:C:82:PHE:HB3	2.00	0.43
1:C:269:GLN:OE1	2:D:69:GLU:HG2	2.19	0.43
1:C:116:GLY:HA2	1:C:265:SER:HB3	1.98	0.43
1:A:109:ARG:O	1:A:113:ARG:HG3	2.19	0.43
1:C:57:ARG:HG2	1:C:84:ALA:HA	1.99	0.43
1:C:146:SER:OG	1:C:147:PHE:N	2.51	0.43
1:A:235:LEU:HD11	1:A:243:VAL:HG11	2.01	0.42
2:D:53:ASN:O	2:D:57:GLU:HG3	2.20	0.42
1:C:302:VAL:HG11	2:D:65:LEU:HD13	2.02	0.42
1:A:237:LEU:HD22	1:A:241:ASP:HB3	2.01	0.42
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.85	0.42
2:D:54:ARG:HB3	2:D:54:ARG:CZ	2.50	0.42
1:A:209:TYR:CE1	1:A:211:GLN:HB2	2.55	0.41
1:C:172:ARG:HD3	1:C:259:PHE:CZ	2.55	0.41
1:A:325:GLU:HA	2:B:12:ASN:HB2	2.02	0.41
1:C:130:ILE:HG13	1:C:155:LEU:O	2.19	0.41
1:A:141:ARG:HE	1:A:141:ARG:HB2	1.57	0.41
1:A:52:CYS:HB3	1:A:277:CYS:C	2.41	0.41
1:A:295:GLN:HG2	1:A:306:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLY:HA2	1:A:265:SER:HB3	2.02	0.41
1:A:179:VAL:O	1:A:254:PRO:HB3	2.20	0.41
1:C:11:ASP:OD2	2:D:143:LYS:HA	2.21	0.41
1:A:155:LEU:HD21	4:F:2:SIA:H111	2.02	0.41
1:C:241:ASP:OD1	1:C:242:THR:N	2.51	0.40
1:C:102:PHE:HB2	1:C:105:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	316/321 (98%)	293 (93%)	19 (6%)	4 (1%)	12 24
1	C	316/321 (98%)	294 (93%)	18 (6%)	4 (1%)	12 24
2	B	167/179 (93%)	158 (95%)	6 (4%)	3 (2%)	8 16
2	D	167/179 (93%)	156 (93%)	8 (5%)	3 (2%)	8 16
All	All	966/1000 (97%)	901 (93%)	51 (5%)	14 (1%)	11 22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	ASN
2	D	12	ASN
1	A	157	ASN
1	A	158(A)	ASP
2	B	57	GLU
1	C	157	ASN
2	D	57	GLU
1	A	143	SER
1	C	143	SER

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Mol	Chain	Res	Type
1	C	158(A)	ASP
1	A	208	ASN
1	C	208	ASN
2	B	10	ILE
2	D	10	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	267/269 (99%)	256 (96%)	11 (4%)	30	56
1	C	267/269 (99%)	256 (96%)	11 (4%)	30	56
2	B	145/153 (95%)	140 (97%)	5 (3%)	37	63
2	D	145/153 (95%)	142 (98%)	3 (2%)	53	77
All	All	824/844 (98%)	794 (96%)	30 (4%)	35	61

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	24	THR
1	A	75	GLN
1	A	78	GLN
1	A	96	VAL
1	A	130	ILE
1	A	158(A)	ASP
1	A	199	ASN
1	A	203	THR
1	A	211	GLN
1	A	237	LEU
2	B	11	GLU
2	B	12	ASN
2	B	56	ILE
2	B	64	GLU
2	B	65	LEU

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Mol	Chain	Res	Type
1	C	18	HIS
1	C	24	THR
1	C	75	GLN
1	C	78	GLN
1	C	96	VAL
1	C	130	ILE
1	C	158(A)	ASP
1	C	199	ASN
1	C	203	THR
1	C	211	GLN
1	C	237	LEU
2	D	56	ILE
2	D	64	GLU
2	D	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.51	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	2	3	14,14,15	0.17	0	17,19,21	0.56	0
4	GAL	F	1	4	11,11,12	0.56	0	15,15,17	0.93	1 (6%)
4	SIA	F	2	4	20,20,21	0.65	0	21,28,31	1.07	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	GAL	F	1	4	-	1/2/19/22	0/1/1/1
4	SIA	F	2	4	-	6/18/34/38	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2	SIA	O1B-C1-C2	2.50	119.20	112.71
4	F	2	SIA	O1A-C1-C2	-2.43	117.60	122.85
4	F	1	GAL	O3-C3-C4	-2.08	105.48	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	SIA	O6-C6-C7-O7
4	F	2	SIA	C6-C7-C8-O8
4	F	2	SIA	O7-C7-C8-O8
4	F	2	SIA	O7-C7-C8-C9
3	E	2	NAG	O5-C5-C6-O6
4	F	2	SIA	C6-C7-C8-C9
3	E	2	NAG	C4-C5-C6-O6
4	F	1	GAL	C4-C5-C6-O6
4	F	2	SIA	C6-C5-N5-C10

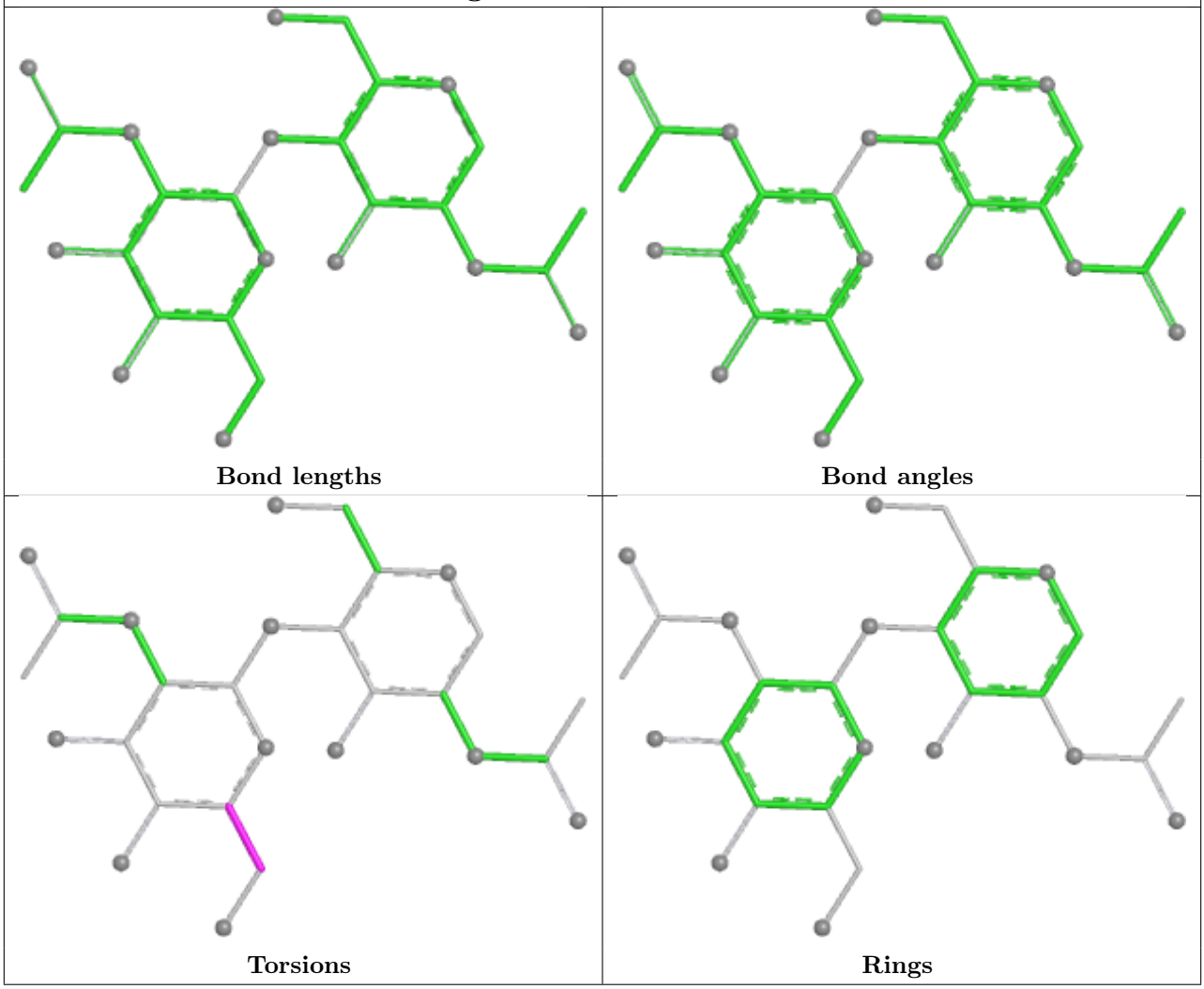
There are no ring outliers.

1 monomer is involved in 1 short contact:

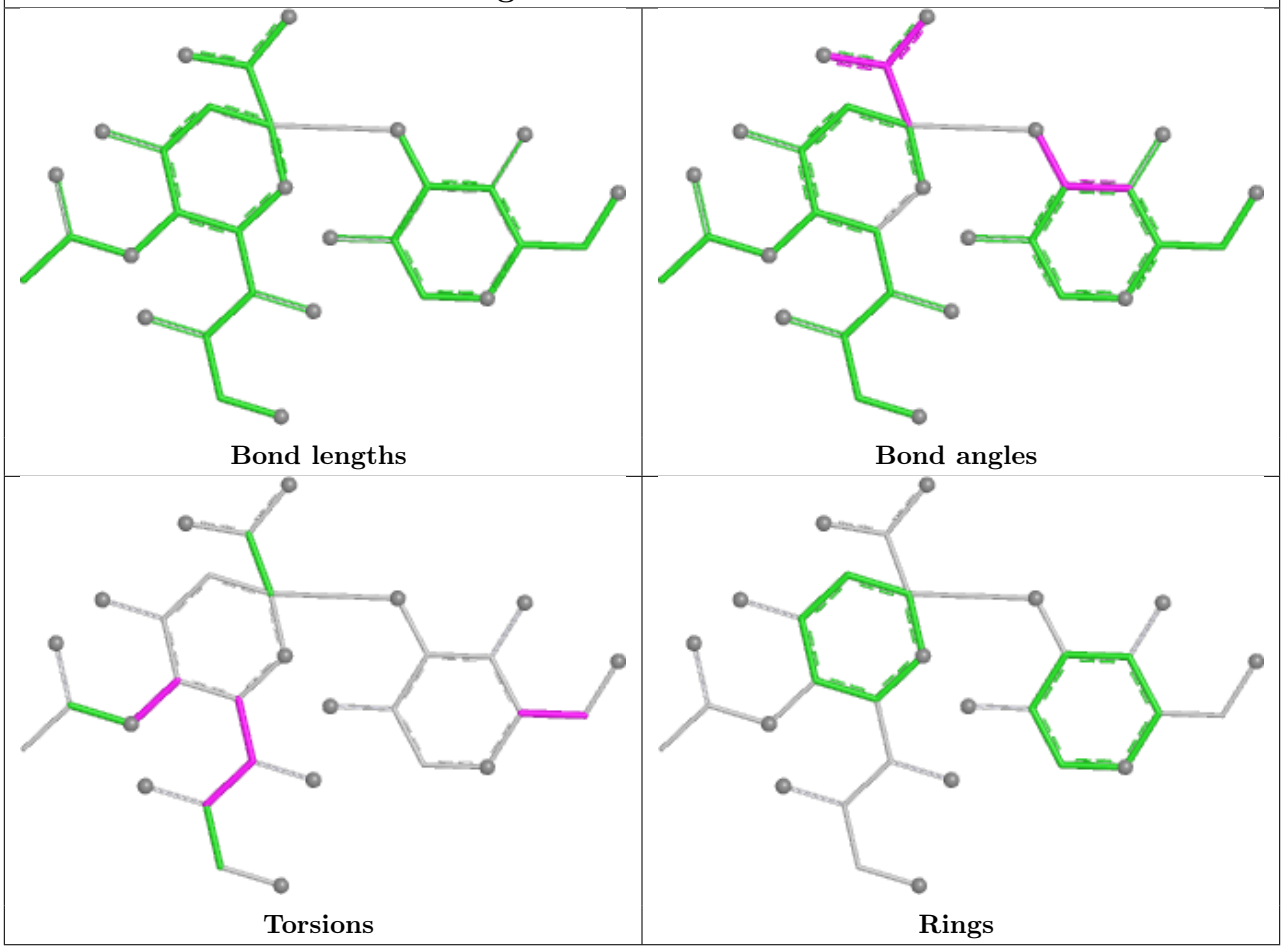
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	SIA	1	0

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 E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

3 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	SIA	C	401	-	21,21,21	0.97	1 (4%)	24,31,31	1.25	3 (12%)
5	NAG	A	403	1	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	B	201	2	14,14,15	0.53	0	17,19,21	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SIA	C	401	-	-	8/20/38/38	0/1/1/1
5	NAG	A	403	1	-	4/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	SIA	O2-C2	3.05	1.44	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	401	SIA	O1A-C1-C2	-3.22	118.48	123.85
6	C	401	SIA	O6-C6-C7	3.08	111.46	106.65
6	C	401	SIA	C3-C2-C1	-2.05	109.02	112.84

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	401	SIA	C6-C7-C8-O8
6	C	401	SIA	O7-C7-C8-O8
6	C	401	SIA	O7-C7-C8-C9
6	C	401	SIA	C6-C7-C8-C9
5	A	403	NAG	O5-C5-C6-O6
5	A	403	NAG	C4-C5-C6-O6
5	A	403	NAG	C3-C2-N2-C7
5	A	403	NAG	C1-C2-N2-C7
6	C	401	SIA	C6-C5-N5-C10
6	C	401	SIA	O1B-C1-C2-O2
6	C	401	SIA	O1A-C1-C2-C3
6	C	401	SIA	O1B-C1-C2-C3

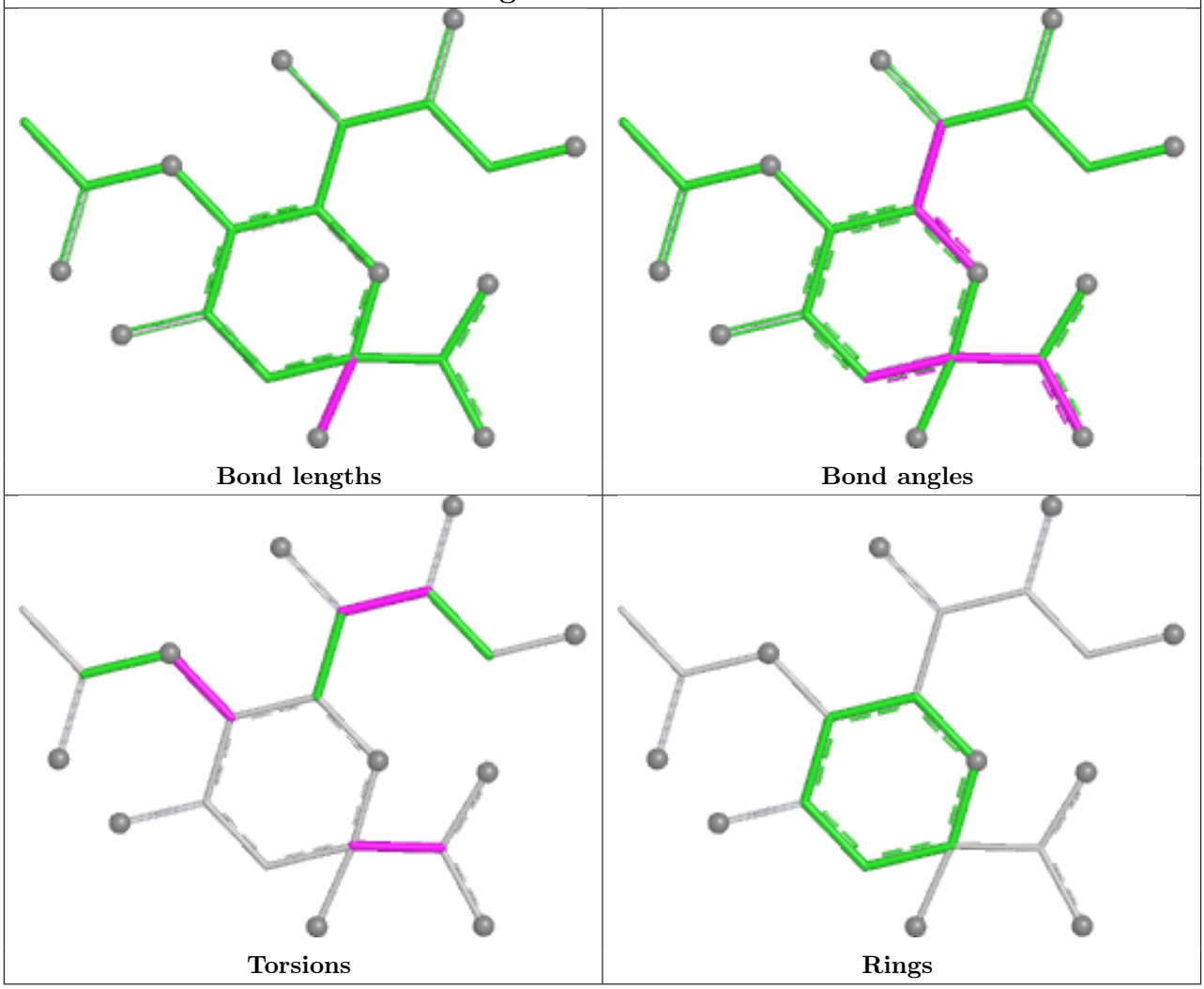
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	SIA	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 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 SIA C 401



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	318/321 (99%)	-0.15	2 (0%) 89 88	47, 72, 109, 163	0
1	C	318/321 (99%)	0.60	32 (10%) 7 4	72, 126, 176, 223	0
2	B	169/179 (94%)	-0.09	0 100 100	43, 64, 103, 160	0
2	D	169/179 (94%)	1.09	33 (19%) 1 0	91, 159, 200, 270	0
All	All	974/1000 (97%)	0.32	67 (6%) 16 12	43, 97, 181, 270	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	GLY	10.2
1	C	58	THR	7.0
2	D	7	ALA	6.9
2	D	23	GLY	6.4
2	D	172	GLN	6.0
2	D	4	GLY	5.9
1	C	327	PRO	5.8
2	D	32	GLU	5.0
1	C	289	ILE	4.9
2	D	143	LYS	4.8
2	D	6	ILE	4.7
2	D	171	ILE	4.7
2	D	33	GLY	4.6
2	D	35	ALA	4.5
1	C	86	LEU	4.1
1	A	327	PRO	4.0
2	D	168	GLN	4.0
2	D	48	ILE	4.0
1	C	288	ILE	3.7
1	C	51	ILE	3.7
2	D	60	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	13	ILE	3.5
1	C	173	LYS	3.4
1	C	12	LYS	3.3
2	D	27	GLN	3.3
1	C	37	VAL	3.2
2	D	18	ILE	3.2
2	D	140	ILE	3.1
2	D	138	PHE	3.1
2	D	63	PHE	3.0
1	C	104	ASN	3.0
1	C	45	ARG	3.0
2	D	141	PHE	2.9
2	D	126	LEU	2.9
1	C	47	ASN	2.9
1	C	276(A)	ASN	2.9
1	C	317	ALA	2.8
1	C	84	ALA	2.8
1	A	214	VAL	2.8
2	D	122	VAL	2.7
1	C	11	ASP	2.7
1	C	22	ASN	2.7
2	D	144	CYS	2.6
2	D	52	LEU	2.5
2	D	130	ALA	2.5
1	C	54	LYS	2.4
2	D	34	THR	2.3
1	C	140	ARG	2.3
2	D	24	PHE	2.3
2	D	157	TYR	2.3
1	C	59	VAL	2.3
1	C	46	THR	2.2
1	C	57	ARG	2.2
1	C	33	GLY	2.2
2	D	74	GLU	2.2
2	D	36	ALA	2.2
2	D	59	THR	2.2
2	D	19	ASP	2.2
2	D	119	TYR	2.1
2	D	44	ALA	2.1
1	C	39	ALA	2.1
1	C	276	ALA	2.1
1	C	127	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	117	GLY	2.1
1	C	323	VAL	2.1
1	C	277	CYS	2.1
1	C	226	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)

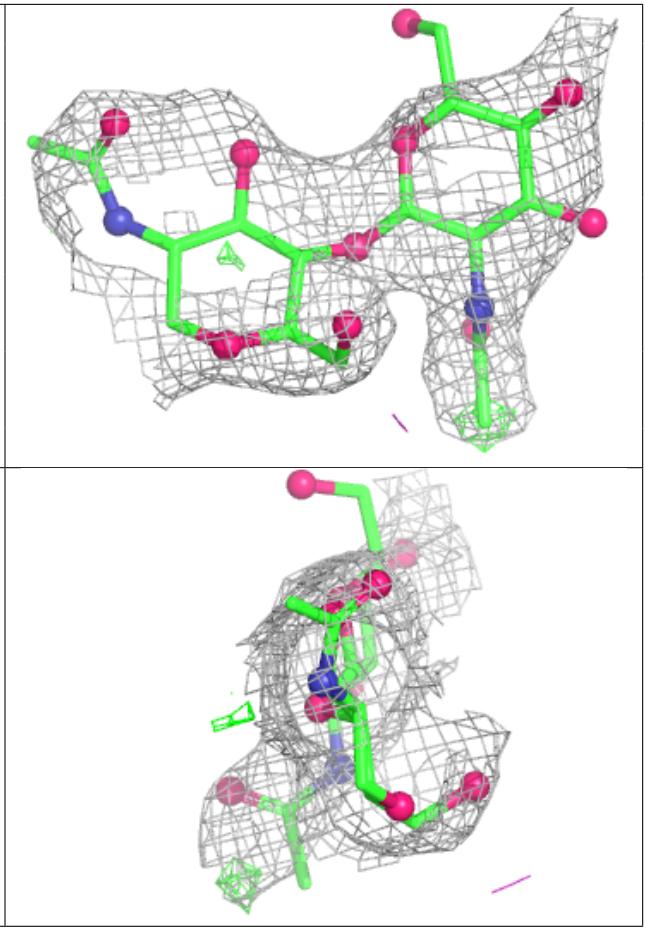
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GAL	F	1	11/12	0.75	0.25	165,182,186,188	0
3	NAG	E	2	14/15	0.77	0.30	140,148,150,150	0
4	SIA	F	2	20/21	0.88	0.23	81,100,120,120	0
3	NAG	E	1	14/15	0.94	0.16	91,112,124,133	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.

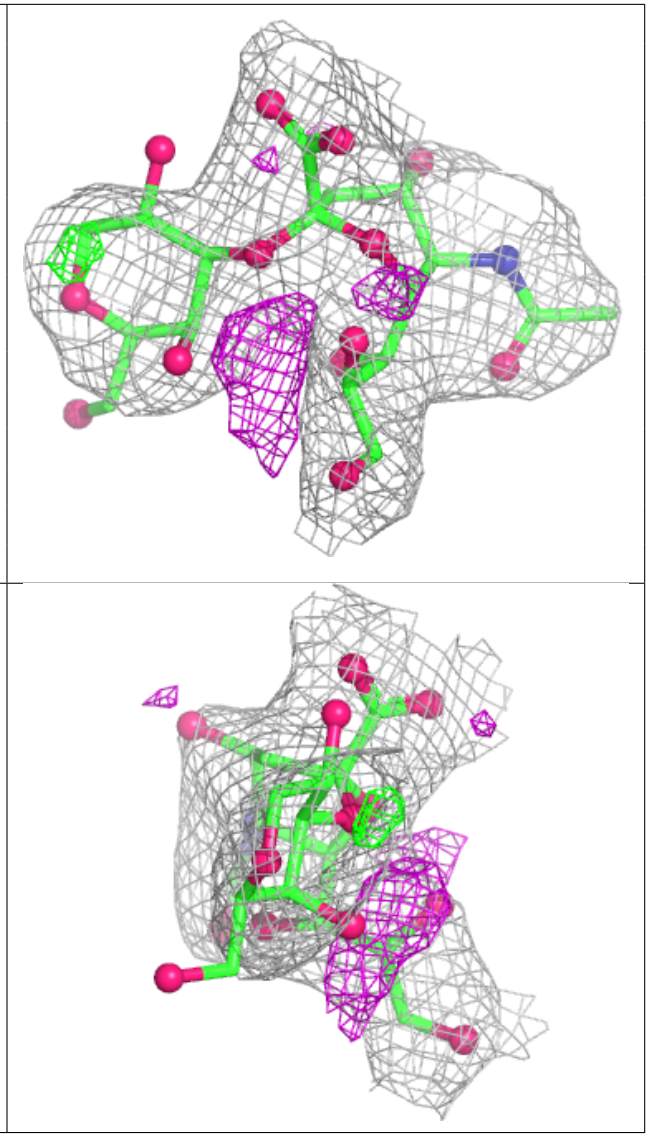
Electron density around Chain E:

$2mF_o$-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 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.

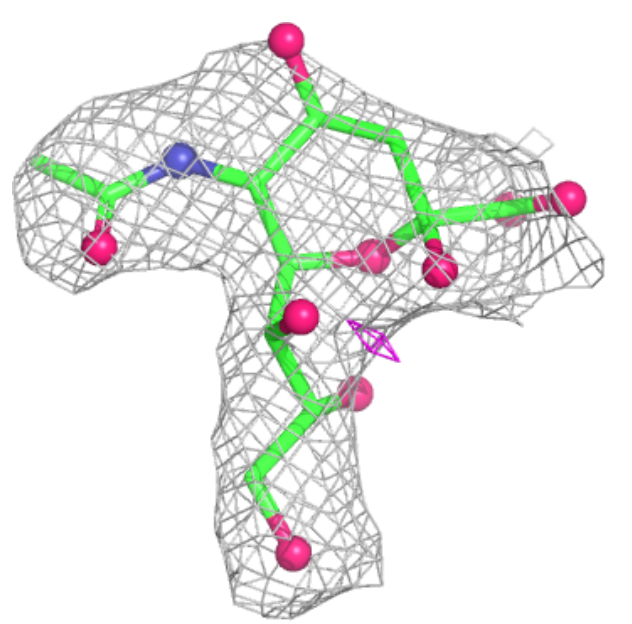
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SIA	C	401	21/21	0.81	0.30	99,127,144,150	0
5	NAG	A	403	14/15	0.84	0.18	138,151,157,158	0
5	NAG	B	201	14/15	0.86	0.16	72,92,96,101	0

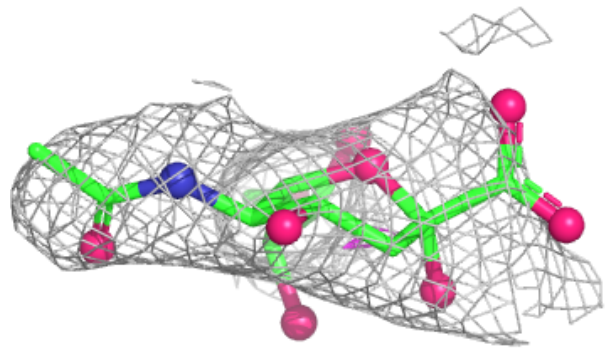
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

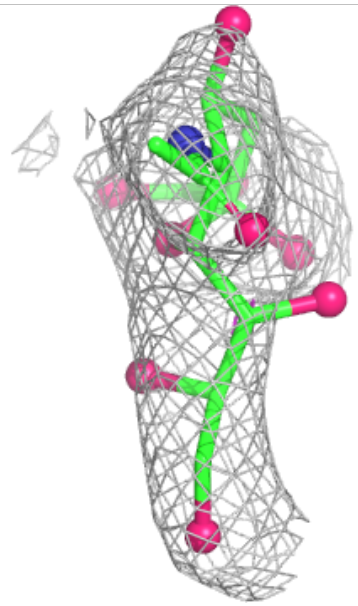
orientation to approximate a three-dimensional view.

Electron density around SIA C 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.