



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:20 AM EDT

PDB ID : 5XL3 / pdb_00005xl3
Title : Complex structure of H4 hemagglutinin from avian influenza H4N6 virus with LSTa
Authors : Song, H.; Qi, J.; Gao, G.F.
Deposited on : 2017-05-10
Resolution : 2.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

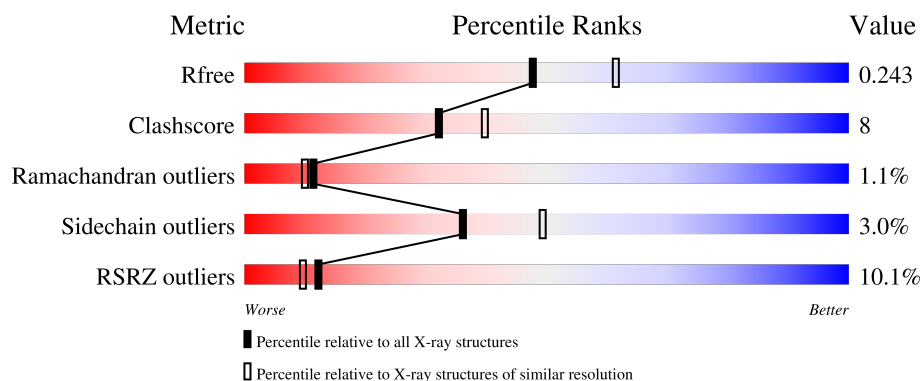
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	19% 77% 16% ...
1	B	327	9% 87% 9% ..
2	C	176	2% 89% 7% ...
2	D	176	2% 89% 7% ...
3	E	3	67% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

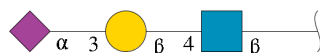
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2457	1538	437	470	12			
1	B	319	Total	C	N	O	S	0	0	0
			2457	1538	437	470	12			

- Molecule 2 is a protein called Hemagglutinin.

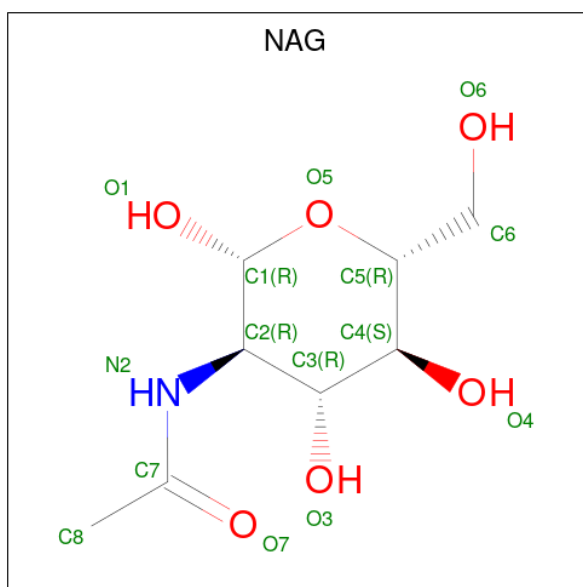
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			
2	D	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



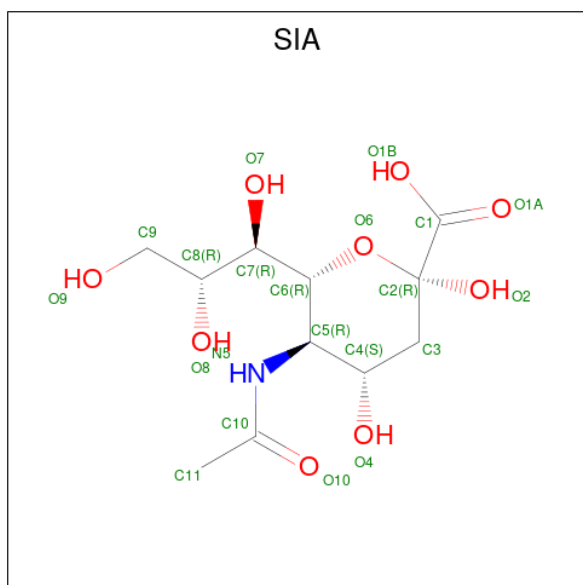
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



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

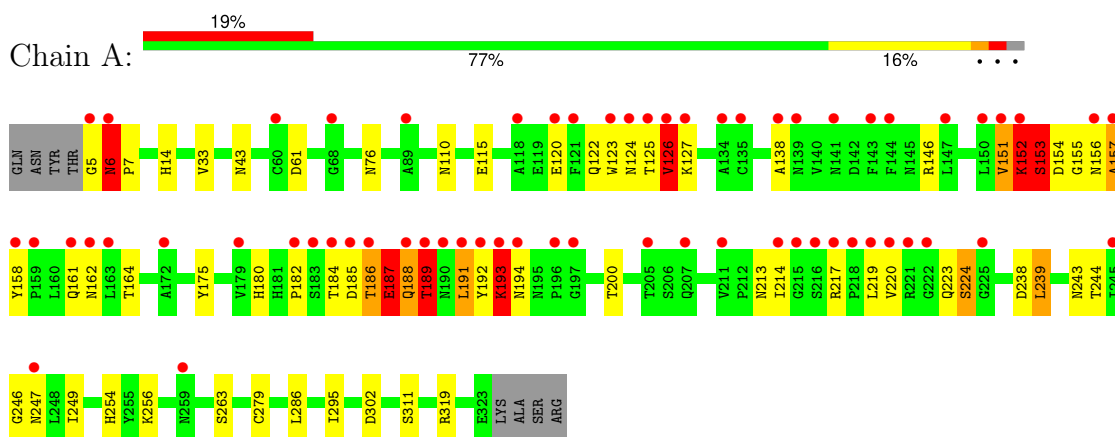
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total	O	0	0
			58	58		
6	C	101	Total	O	0	0
			101	101		
6	B	103	Total	O	0	0
			103	103		
6	D	110	Total	O	0	0
			110	110		

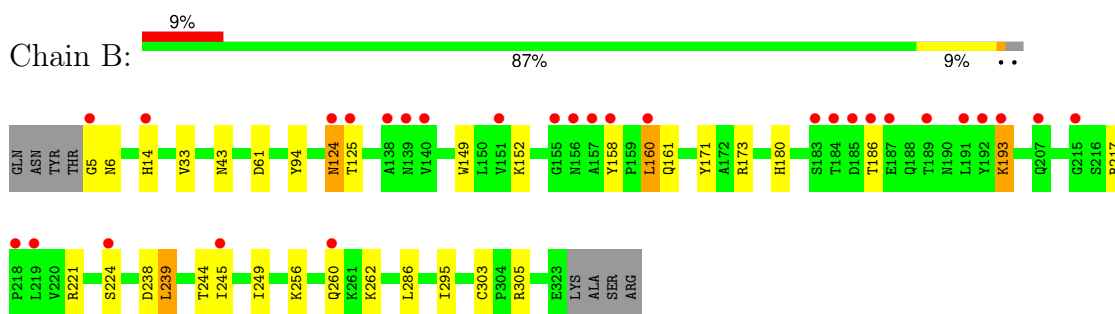
3 Residue-property plots [i](#)

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.

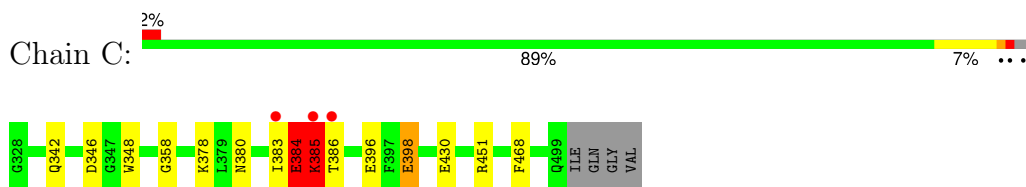
• Molecule 1: Hemagglutinin



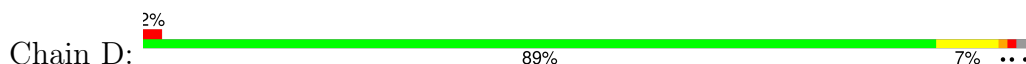
• Molecule 1: Hemagglutinin

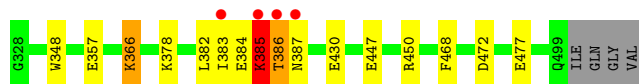


• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin





- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.53Å 100.53Å 685.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 2.20 49.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.09-2.20) 91.9 (49.09-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.213 , 0.244 0.216 , 0.243	Depositor DCC
R_{free} test set	3468 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtrriage
Anisotropy	0.458	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8217	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8585e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NAG, GAL, SIA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	2/2511 (0.1%)	0.95	10/3418 (0.3%)
1	B	0.35	0/2511	0.76	1/3418 (0.0%)
2	C	0.36	0/1428	0.77	5/1922 (0.3%)
2	D	0.41	0/1428	0.78	3/1922 (0.2%)
All	All	0.41	2/7878 (0.0%)	0.83	19/10680 (0.2%)

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
2	C	0	1
2	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	VAL	CA-CB	5.23	1.59	1.54
1	A	189	THR	N-CA	5.03	1.52	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	N-CA-C	7.58	126.93	110.80
2	D	386	THR	N-CA-C	7.10	125.92	110.80
1	A	126	VAL	CB-CA-C	-6.77	101.12	111.08
2	D	386	THR	CA-C-N	6.45	132.16	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	386	THR	C-N-CA	6.45	132.16	122.68
1	A	153	SER	N-CA-C	6.40	124.43	110.80
2	C	384	GLU	CA-C-N	6.36	133.68	121.54
2	C	384	GLU	C-N-CA	6.36	133.68	121.54
1	A	187	GLU	CA-CB-CG	6.35	126.80	114.10
1	A	187	GLU	CB-CG-CD	6.28	123.28	112.60
1	A	153	SER	CB-CA-C	-6.14	98.19	110.42
2	C	385	LYS	N-CA-C	5.76	123.07	110.80
2	C	358	GLY	N-CA-C	5.75	118.19	110.43
1	A	152	LYS	N-CA-C	5.46	117.58	110.43
1	A	157	ALA	N-CA-C	5.44	117.49	108.13
2	C	384	GLU	CB-CA-C	-5.18	100.11	110.42
1	B	186	THR	N-CA-C	-5.06	105.86	112.23
1	A	6	ASN	CA-C-N	-5.05	114.75	119.85
1	A	6	ASN	C-N-CA	-5.05	114.75	119.85

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	TRP	Peptide
1	A	186	THR	Peptide
1	A	187	GLU	Peptide
2	C	384	GLU	Peptide
2	D	385	LYS	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	2457	0	2402	73	0
1	B	2457	0	2402	26	0
2	C	1404	0	1320	10	0
2	D	1404	0	1320	19	0
3	E	46	0	40	2	0
4	A	28	0	26	1	0
4	B	28	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	21	0	18	2	0
6	A	58	0	0	5	0
6	B	103	0	0	6	0
6	C	101	0	0	3	0
6	D	110	0	0	2	0
All	All	8217	0	7554	123	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 8.

All (123) 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:153:SER:HB2	1:A:157:ALA:H	1.24	1.02
1:A:152:LYS:HE2	1:A:158:TYR:HB3	1.44	0.97
1:A:124:ASN:ND2	1:A:161:GLN:OE1	1.98	0.95
1:A:14:HIS:HD2	2:C:348:TRP:HA	1.32	0.94
1:B:14:HIS:HD2	2:D:348:TRP:HA	1.34	0.92
1:A:188:GLN:NE2	1:A:194:ASN:O	2.04	0.91
2:D:477:GLU:OE2	6:D:701:HOH:O	1.91	0.89
1:A:124:ASN:OD1	1:A:125:THR:N	2.04	0.88
1:A:244:THR:HG22	1:A:246:GLY:H	1.36	0.86
1:A:152:LYS:HE2	1:A:158:TYR:CB	2.05	0.85
1:A:152:LYS:HD2	1:A:193:LYS:N	1.92	0.84
2:D:385:LYS:HG3	2:D:386:THR:HB	1.58	0.83
1:A:152:LYS:HD2	1:A:193:LYS:H	1.43	0.82
1:A:14:HIS:CD2	2:C:348:TRP:HA	2.15	0.81
1:B:5:GLY:HA2	2:D:468:PHE:HA	1.63	0.81
1:A:188:GLN:O	1:A:192:TYR:N	2.15	0.78
1:B:14:HIS:CD2	2:D:348:TRP:HA	2.19	0.78
1:A:124:ASN:HB2	1:A:161:GLN:HE22	1.49	0.78
1:A:61:ASP:OD1	6:A:701:HOH:O	2.02	0.76
2:D:386:THR:OG1	2:D:387:ASN:N	2.17	0.75
1:A:311:SER:O	6:A:702:HOH:O	2.05	0.73
1:A:124:ASN:CG	1:A:125:THR:H	1.95	0.73
1:A:184:THR:O	1:A:214:ILE:HG21	1.89	0.73
1:A:127:LYS:HD3	1:A:151:VAL:HG13	1.72	0.70
1:A:5:GLY:HA2	2:C:468:PHE:HA	1.74	0.69
1:A:120:GLU:OE2	1:A:122:GLN:HG3	1.93	0.69
1:B:61:ASP:OD1	6:B:702:HOH:O	2.10	0.68
1:B:124:ASN:OD1	1:B:125:THR:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:HA	1:A:187:GLU:HG3	1.74	0.67
2:C:346:ASP:OD1	6:C:601:HOH:O	2.11	0.67
2:D:450:ARG:NH2	6:D:702:HOH:O	2.30	0.65
1:B:14:HIS:CE1	1:B:33:VAL:HG21	2.32	0.65
1:A:152:LYS:CE	1:A:158:TYR:HB3	2.25	0.64
1:A:319:ARG:NE	6:A:704:HOH:O	2.19	0.64
1:A:188:GLN:O	1:A:191:LEU:N	2.30	0.64
2:D:385:LYS:HG3	2:D:386:THR:CB	2.26	0.62
2:D:385:LYS:HE3	2:D:386:THR:HB	1.81	0.61
1:A:184:THR:O	1:A:187:GLU:HG3	2.00	0.61
1:A:120:GLU:CD	1:A:122:GLN:HG3	2.26	0.61
4:A:601:NAG:O4	6:A:703:HOH:O	2.16	0.60
2:D:386:THR:CG2	2:D:387:ASN:H	2.15	0.59
1:A:124:ASN:HB3	1:A:126:VAL:CG2	2.32	0.59
1:A:152:LYS:NZ	1:A:193:LYS:HB2	2.18	0.59
4:B:602:NAG:O4	6:B:701:HOH:O	2.01	0.59
1:A:187:GLU:OE1	1:A:189:THR:N	2.36	0.58
1:B:149:TRP:CH2	3:E:3:SIA:H7	2.38	0.58
4:B:601:NAG:H83	4:B:601:NAG:H3	1.84	0.58
2:D:383:ILE:HG13	2:D:383:ILE:O	2.04	0.57
1:A:14:HIS:CE1	1:A:33:VAL:HG21	2.40	0.57
1:B:124:ASN:O	6:B:703:HOH:O	2.17	0.57
2:D:386:THR:HG23	2:D:387:ASN:H	1.70	0.56
2:D:386:THR:HG23	2:D:387:ASN:N	2.20	0.55
1:A:154:ASP:HA	6:A:738:HOH:O	2.06	0.55
1:A:124:ASN:HB3	1:A:126:VAL:HG23	1.88	0.54
4:B:602:NAG:H83	6:B:743:HOH:O	2.07	0.54
1:B:305:ARG:NH1	6:B:707:HOH:O	2.41	0.54
1:B:94:TYR:OH	3:E:3:SIA:H91	2.08	0.54
1:B:124:ASN:OD1	1:B:124:ASN:C	2.51	0.53
1:A:152:LYS:HD3	1:A:193:LYS:HG3	1.90	0.53
1:A:14:HIS:HD2	2:C:348:TRP:CA	2.13	0.53
1:B:14:HIS:HD2	2:D:348:TRP:CA	2.13	0.53
1:A:124:ASN:HB2	1:A:161:GLN:NE2	2.20	0.52
1:B:238:ASP:OD1	1:B:239:LEU:N	2.39	0.52
1:A:43:ASN:HB3	1:A:295:ILE:HD13	1.92	0.52
1:A:152:LYS:HE3	1:A:192:TYR:HA	1.91	0.52
2:D:378:LYS:NZ	2:D:430:GLU:O	2.42	0.52
1:A:187:GLU:OE1	1:A:189:THR:OG1	2.26	0.51
1:A:153:SER:CB	1:A:157:ALA:H	2.10	0.51
1:A:200:THR:HB	1:A:243:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LYS:HD3	1:B:193:LYS:H	1.76	0.49
1:A:156:ASN:O	1:A:193:LYS:NZ	2.45	0.49
1:B:171:TYR:CZ	1:B:256:LYS:HD3	2.46	0.49
1:A:187:GLU:HG2	1:A:188:GLN:CB	2.42	0.48
1:A:153:SER:HB3	1:A:155:GLY:N	2.27	0.48
1:A:187:GLU:CD	1:A:189:THR:H	2.21	0.48
1:A:192:TYR:CZ	1:A:247:ASN:HA	2.49	0.48
1:B:260:GLN:NE2	1:B:262:LYS:HD2	2.28	0.48
2:C:378:LYS:NZ	2:C:430:GLU:O	2.47	0.48
1:A:152:LYS:HZ2	1:A:193:LYS:HB2	1.78	0.47
1:A:14:HIS:CE1	1:A:33:VAL:HG11	2.49	0.46
1:A:152:LYS:CE	1:A:192:TYR:HA	2.46	0.46
1:B:160:LEU:HD23	1:B:245:ILE:HG23	1.97	0.46
1:A:152:LYS:H	1:A:152:LYS:HG2	1.39	0.46
2:D:357:GLU:OE2	2:D:472:ASP:HB2	2.15	0.46
1:B:158:TYR:HE2	1:B:245:ILE:HA	1.79	0.46
1:A:76:ASN:OD1	1:A:146:ARG:NH2	2.43	0.46
2:C:451:ARG:HD2	6:C:606:HOH:O	2.16	0.46
1:B:14:HIS:HE1	1:B:33:VAL:HG21	1.77	0.46
1:A:213:ASN:O	1:A:217:ARG:NH2	2.43	0.45
1:B:303:CYS:O	2:D:387:ASN:HB3	2.16	0.45
1:A:127:LYS:HB3	1:A:151:VAL:O	2.16	0.45
1:A:186:THR:H	1:A:187:GLU:HB3	1.82	0.45
1:A:185:ASP:CA	1:A:187:GLU:HG3	2.43	0.45
2:C:342:GLN:NE2	6:C:607:HOH:O	2.48	0.45
1:A:187:GLU:CG	1:A:188:GLN:N	2.80	0.44
1:B:217:ARG:O	1:B:224:SER:OG	2.33	0.44
1:A:6:ASN:H	1:A:7:PRO:CD	2.31	0.44
1:A:182:PRO:HG2	1:A:188:GLN:HB2	2.00	0.44
1:A:217:ARG:O	1:A:224:SER:HB2	2.18	0.43
2:C:380:ASN:O	2:C:384:GLU:HG3	2.18	0.43
1:A:175:TYR:CE2	1:A:254:HIS:HB3	2.54	0.43
1:B:161:GLN:HB2	1:B:244:THR:HG23	2.00	0.43
1:A:187:GLU:HG2	1:A:188:GLN:HB2	2.01	0.42
1:A:120:GLU:OE2	1:A:122:GLN:N	2.53	0.42
1:A:180:HIS:HB2	1:A:249:ILE:HD11	2.02	0.42
1:B:14:HIS:CE1	1:B:33:VAL:HG11	2.55	0.42
2:C:398:GLU:H	2:C:398:GLU:HG3	1.62	0.42
1:A:191:LEU:HD11	5:A:603:SIA:H92	2.01	0.41
1:A:14:HIS:HE1	1:A:33:VAL:HG11	1.85	0.41
1:A:219:LEU:HA	1:A:223:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG23	1:A:239:LEU:HD23	2.02	0.41
2:D:366:LYS:HB2	2:D:366:LYS:HE3	1.68	0.41
2:D:447:GLU:OE1	2:D:450:ARG:NH1	2.54	0.41
1:A:238:ASP:OD1	1:A:239:LEU:N	2.48	0.41
1:A:110:ASN:HA	1:A:263:SER:O	2.21	0.41
1:A:120:GLU:CD	1:A:120:GLU:C	2.88	0.41
1:B:173:ARG:NE	6:B:705:HOH:O	2.50	0.41
1:A:115:GLU:CD	1:A:256:LYS:HE2	2.46	0.40
1:A:223:GLN:NE2	5:A:603:SIA:O1B	2.54	0.40
1:B:43:ASN:HB3	1:B:295:ILE:HD13	2.04	0.40
1:B:180:HIS:HB2	1:B:249:ILE:HD11	2.03	0.40
1:A:188:GLN:HG2	1:A:192:TYR:HB2	2.03	0.40
1:A:279:CYS:HB2	1:A:302:ASP:O	2.21	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	317/327 (97%)	290 (92%)	19 (6%)	8 (2%)	4	2
1	B	317/327 (97%)	301 (95%)	14 (4%)	2 (1%)	21	23
2	C	170/176 (97%)	158 (93%)	11 (6%)	1 (1%)	21	23
2	D	170/176 (97%)	159 (94%)	11 (6%)	0	100	100
All	All	974/1006 (97%)	908 (93%)	55 (6%)	11 (1%)	11	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	SER
1	A	188	GLN

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Mol	Chain	Res	Type
1	A	193	LYS
1	B	6	ASN
1	B	193	LYS
1	A	138	ALA
1	A	162	ASN
1	A	187	GLU
1	A	189	THR
2	C	385	LYS
1	A	6	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/282 (97%)	264 (96%)	10 (4%)	31	42
1	B	274/282 (97%)	269 (98%)	5 (2%)	51	68
2	C	147/150 (98%)	141 (96%)	6 (4%)	27	37
2	D	147/150 (98%)	143 (97%)	4 (3%)	39	53
All	All	842/864 (98%)	817 (97%)	25 (3%)	36	49

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	151	VAL
1	A	152	LYS
1	A	187	GLU
1	A	191	LEU
1	A	193	LYS
1	A	220	VAL
1	A	224	SER
1	A	239	LEU
1	A	286	LEU
2	C	383	ILE
2	C	384	GLU

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Mol	Chain	Res	Type
2	C	385	LYS
2	C	386	THR
2	C	396	GLU
2	C	398	GLU
1	B	124	ASN
1	B	160	LEU
1	B	221	ARG
1	B	239	LEU
1	B	286	LEU
2	D	366	LYS
2	D	382	LEU
2	D	384	GLU
2	D	385	LYS

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

Mol	Chain	Res	Type
1	A	74	HIS
1	B	42	GLN
1	B	168	ASN
2	D	369	GLN

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 ⓘ

3 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	15,15,15	0.41	0	21,21,21	0.67	1 (4%)
3	GAL	E	2	3	11,11,12	0.54	0	15,15,17	1.02	1 (6%)
3	SIA	E	3	3	20,20,21	0.55	0	21,28,31	0.86	1 (4%)

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	-	4/6/26/26	0/1/1/1
3	GAL	E	2	3	-	2/2/19/22	0/1/1/1
3	SIA	E	3	3	-	2/18/34/38	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(°)	Ideal(°)
3	E	2	GAL	O5-C5-C4	-2.34	105.14	110.83
3	E	3	SIA	O1B-C1-C2	2.31	118.71	112.71
3	E	1	NAG	O4-C4-C5	2.23	114.82	109.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

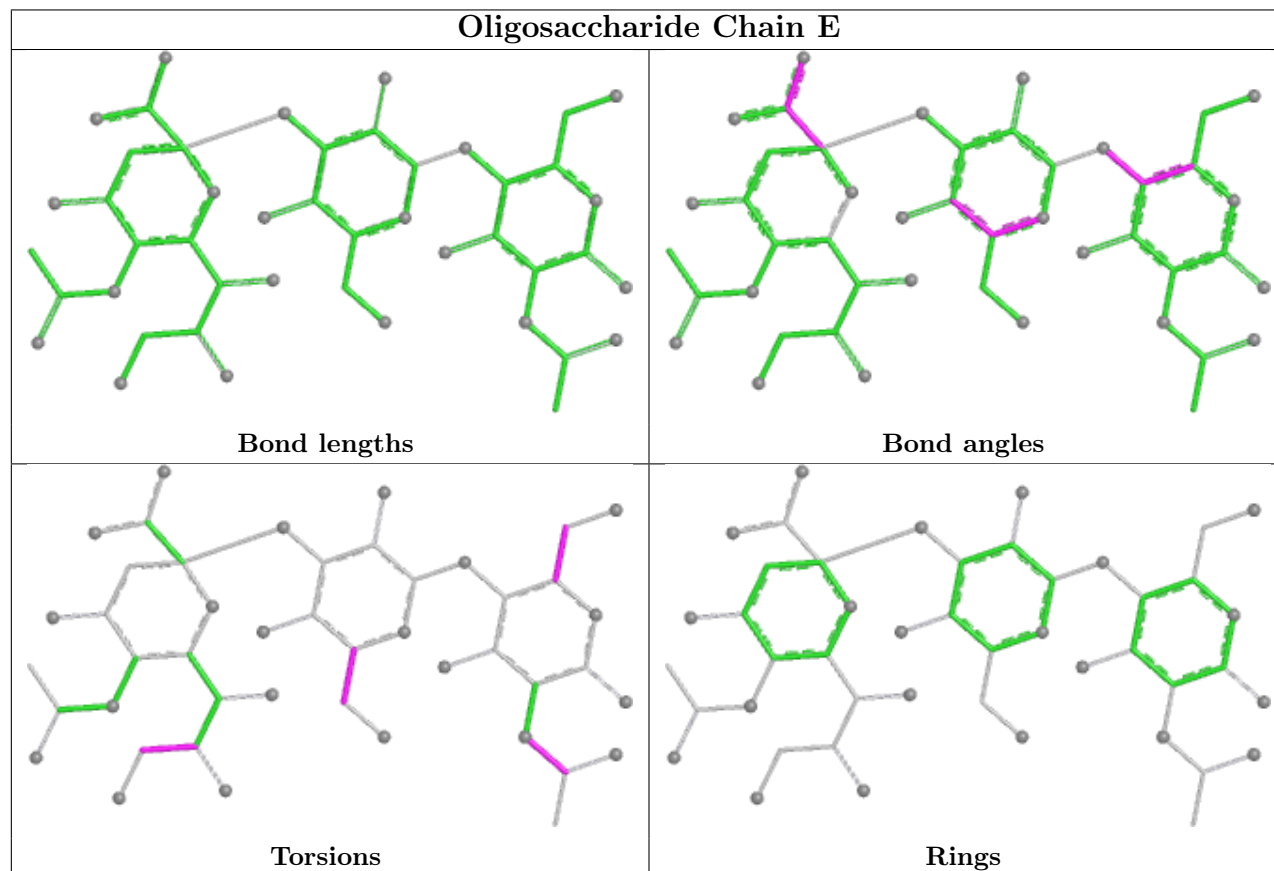
Mol	Chain	Res	Type	Atoms
3	E	2	GAL	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	2	GAL	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	E	3	SIA	O8-C8-C9-O9
3	E	3	SIA	C7-C8-C9-O9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	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 oligosaccharide.



5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	NAG	B	601	1	14,14,15	0.55	0	17,19,21	1.36	2 (11%)
5	SIA	A	603	-	21,21,21	0.85	1 (4%)	24,31,31	1.14	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	601	1	14,14,15	0.80	1 (7%)	17,19,21	0.51	0
4	NAG	A	602	1	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	B	602	1	14,14,15	0.36	0	17,19,21	0.54	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
4	NAG	B	601	1	-	6/6/23/26	0/1/1/1
5	SIA	A	603	-	-	3/20/38/38	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	602	1	-	2/6/23/26	0/1/1/1
4	NAG	B	602	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	SIA	O2-C2	2.77	1.43	1.39
4	A	601	NAG	O5-C1	-2.33	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	NAG	C2-N2-C7	4.55	129.00	122.90
5	A	603	SIA	O1A-C1-C2	-3.53	117.95	123.85
4	B	601	NAG	C1-C2-N2	2.26	113.99	110.43
5	A	603	SIA	O6-C6-C7	2.15	110.02	106.65
5	A	603	SIA	C8-C7-C6	-2.05	109.21	113.05

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O5-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6
4	A	602	NAG	C8-C7-N2-C2
4	A	602	NAG	O7-C7-N2-C2
4	B	601	NAG	C8-C7-N2-C2

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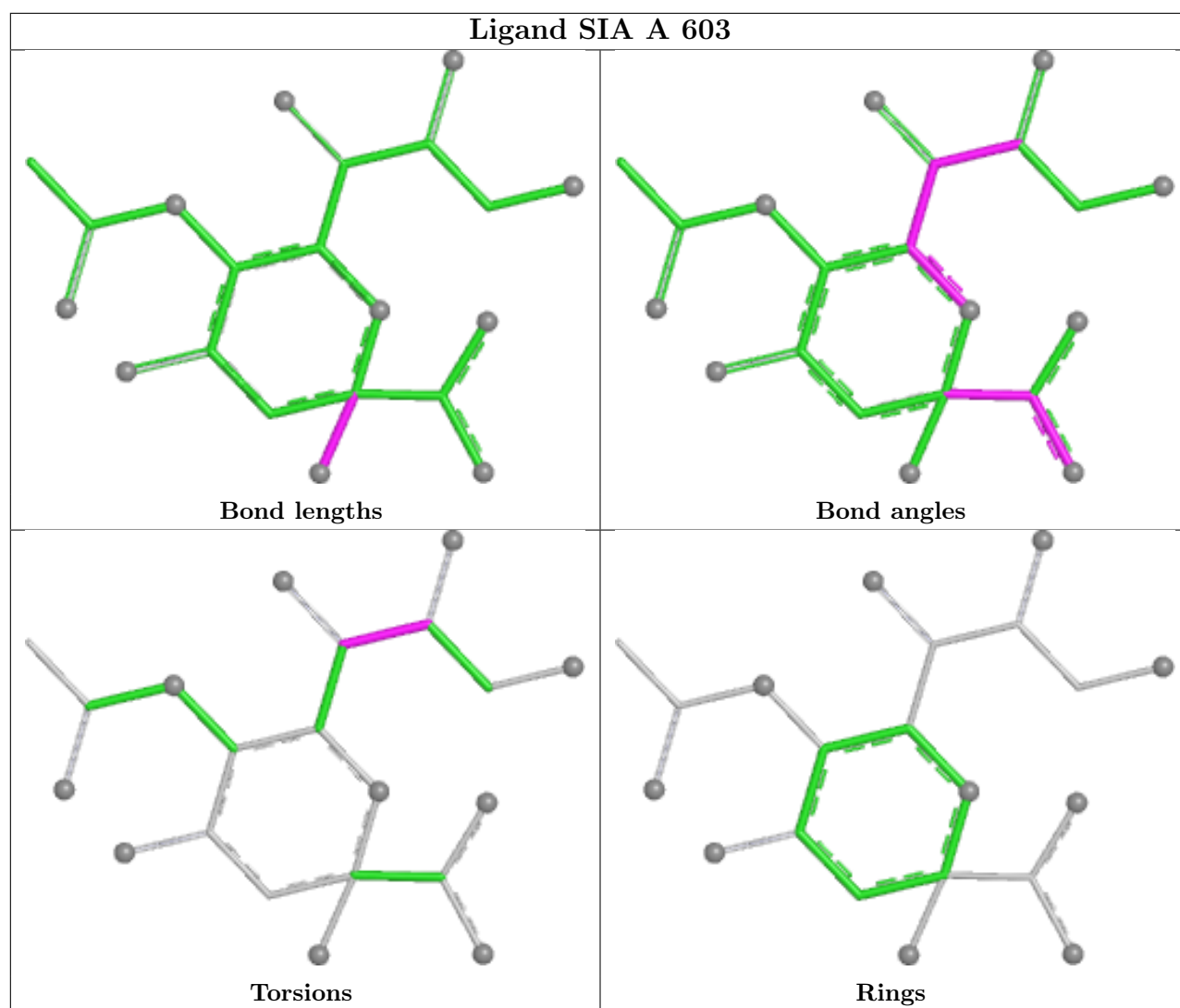
Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O7-C7-N2-C2
4	B	602	NAG	C8-C7-N2-C2
4	B	602	NAG	O7-C7-N2-C2
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6
5	A	603	SIA	C6-C7-C8-O8
4	B	601	NAG	C1-C2-N2-C7
4	B	601	NAG	C3-C2-N2-C7
5	A	603	SIA	O7-C7-C8-C9
5	A	603	SIA	O7-C7-C8-O8

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	1	0
5	A	603	SIA	2	0
4	A	601	NAG	1	0
4	B	602	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 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 than 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.



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 ⓘ

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	319/327 (97%)	0.98	63 (19%) 3 2	26, 68, 122, 168	0
1	B	319/327 (97%)	0.49	29 (9%) 15 12	23, 49, 92, 127	0
2	C	172/176 (97%)	-0.01	3 (1%) 69 66	27, 37, 64, 123	0
2	D	172/176 (97%)	-0.08	4 (2%) 61 58	23, 34, 56, 135	0
All	All	982/1006 (97%)	0.46	99 (10%) 12 10	23, 47, 107, 168	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	383	ILE	6.6
2	C	385	LYS	6.6
1	B	158	TYR	5.5
2	C	386	THR	5.3
2	D	386	THR	5.0
1	A	191	LEU	4.9
1	A	158	TYR	4.7
1	A	5	GLY	4.6
1	B	192	TYR	4.6
1	A	192	TYR	4.3
1	A	127	LYS	4.0
1	A	193	LYS	4.0
2	C	383	ILE	4.0
1	B	193	LYS	3.8
1	A	157	ALA	3.8
1	A	156	ASN	3.8
1	B	186	THR	3.7
1	A	139	ASN	3.7
1	A	143	PHE	3.6
1	A	134	ALA	3.6
1	A	163	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	218	PRO	3.6
1	A	188	GLN	3.6
1	B	207	GLN	3.5
1	A	183	SER	3.4
1	B	219	LEU	3.4
1	B	157	ALA	3.4
1	A	126	VAL	3.3
1	A	221	ARG	3.3
1	B	156	ASN	3.3
1	A	144	PHE	3.2
1	B	155	GLY	3.1
1	B	185	ASP	3.1
1	A	125	THR	3.1
1	A	215	GLY	3.1
1	B	215	GLY	3.1
1	A	197	GLY	3.1
1	B	124	ASN	3.1
1	A	138	ALA	3.1
1	A	159	PRO	3.0
1	A	190	ASN	3.0
1	B	5	GLY	3.0
1	B	189	THR	2.9
1	A	68	GLY	2.9
1	A	123	TRP	2.9
1	B	125	THR	2.8
1	A	219	LEU	2.8
1	A	185	ASP	2.8
1	A	152	LYS	2.8
1	A	189	THR	2.7
1	A	247	ASN	2.7
1	A	207	GLN	2.6
1	A	205	THR	2.6
1	B	151	VAL	2.6
1	A	216	SER	2.6
1	A	162	ASN	2.6
1	A	214	ILE	2.6
1	B	183	SER	2.6
1	B	245	ILE	2.6
1	A	194	ASN	2.5
1	A	151	VAL	2.5
1	B	260	GLN	2.5
1	B	139	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	182	PRO	2.5
1	A	121	PHE	2.4
1	A	245	ILE	2.4
1	B	191	LEU	2.4
1	A	124	ASN	2.4
1	B	187	GLU	2.4
1	A	118	ALA	2.4
1	B	14	HIS	2.4
1	A	6	ASN	2.3
1	A	225	GLY	2.3
1	A	141	ASN	2.3
1	A	60	CYS	2.3
1	A	220	VAL	2.3
1	B	160	LEU	2.3
2	D	385	LYS	2.3
1	A	184	THR	2.3
1	B	224	SER	2.2
1	A	196	PRO	2.2
1	A	120	GLU	2.2
1	A	186	THR	2.2
1	A	135	CYS	2.2
1	A	150	LEU	2.1
1	A	222	GLY	2.1
1	A	259	ASN	2.1
1	B	218	PRO	2.1
1	B	184	THR	2.1
1	A	89	ALA	2.1
1	A	211	VAL	2.1
1	A	172	ALA	2.1
1	A	147	LEU	2.1
2	D	387	ASN	2.1
1	A	179	VAL	2.1
1	B	138	ALA	2.0
1	A	161	GLN	2.0
1	A	217	ARG	2.0
1	B	140	VAL	2.0

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

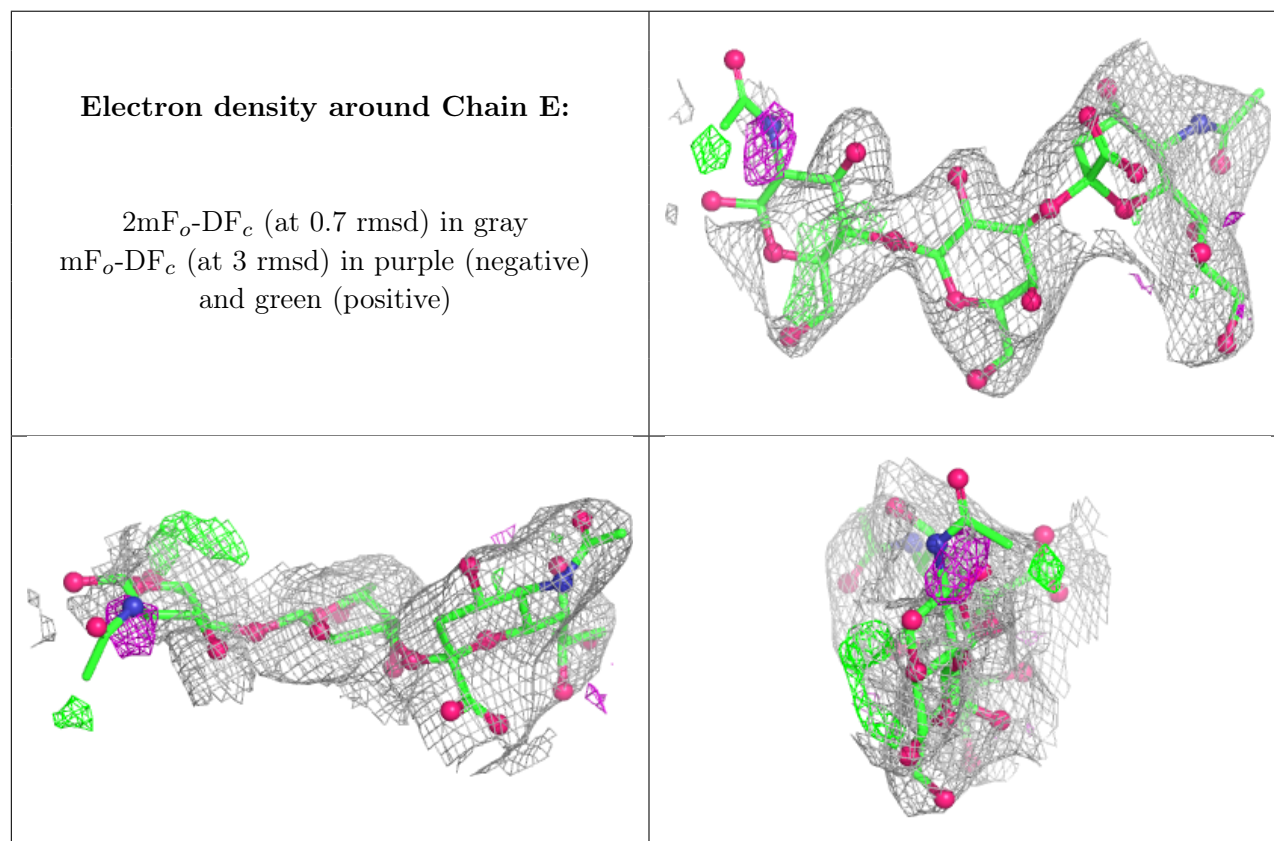
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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
3	NAG	E	1	15/15	0.17	0.20	133,146,155,157	0
3	GAL	E	2	11/12	0.71	0.13	92,101,115,120	0
3	SIA	E	3	20/21	0.83	0.15	72,80,86,87	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.

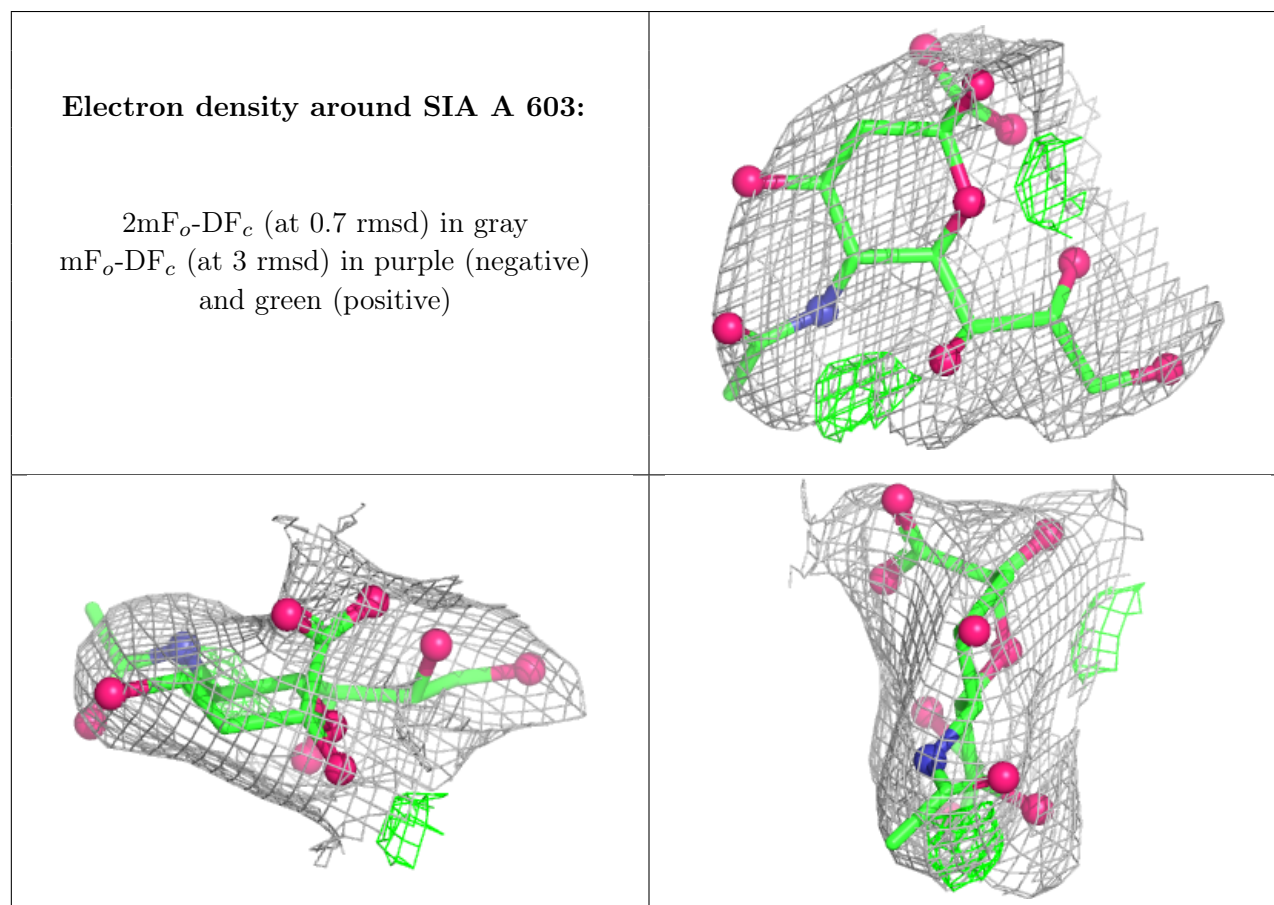


6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	NAG	A	601	14/15	0.63	0.20	116,123,128,133	0
4	NAG	B	601	14/15	0.64	0.17	108,114,117,118	0
5	SIA	A	603	21/21	0.82	0.14	92,96,99,106	0
4	NAG	A	602	14/15	0.88	0.09	40,45,48,60	0
4	NAG	B	602	14/15	0.90	0.09	30,36,40,50	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.