



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:46 PM UTC

PDB ID : 4KON / pdb_00004kon
Title : The structure of hemagglutinin from avian-origin H7N9 influenza virus in complex with human receptor analog 6'SLNLN (NeuAc<#945;2-6Gal<#946;1-4GlcNAc<#946;1-3Gal<#946;1-4Glc)
Authors : Shi, Y.; Zhang, W.; Wang, F.; Qi, J.; Song, H.; Wu, Y.; Gao, F.; Zhang, Y.; Fan, Z.; Gong, W.; Wang, D.; Shu, Y.; Wang, Y.; Yan, J.; Gao, G.F.
Deposited on : 2013-05-12
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 ⓘ 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
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

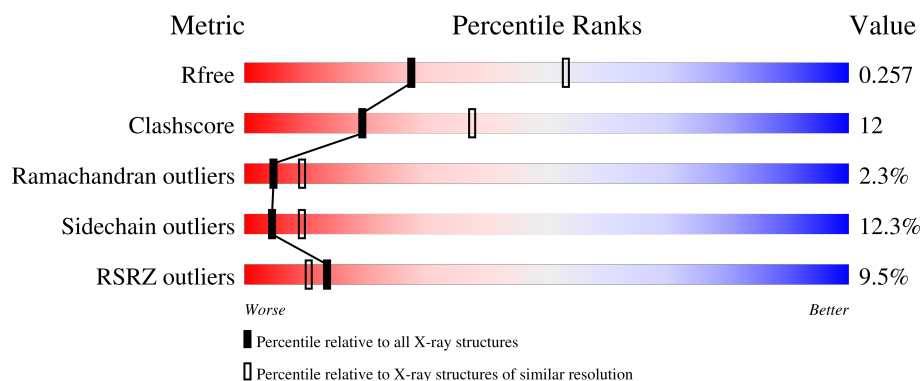
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	314	8% 69% 26% • •
2	B	169	12% 69% 22% 8% •
3	C	2	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3925 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.

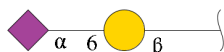
- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2395	1488	433	459	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

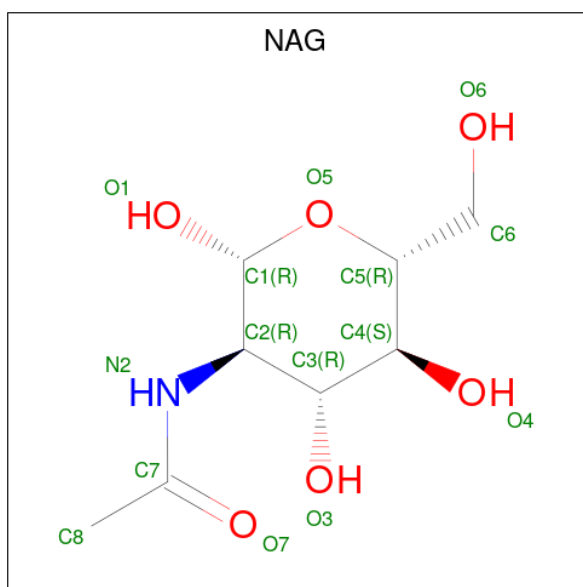
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1368	845	237	279	7			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			32	17	1	14			

- 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		

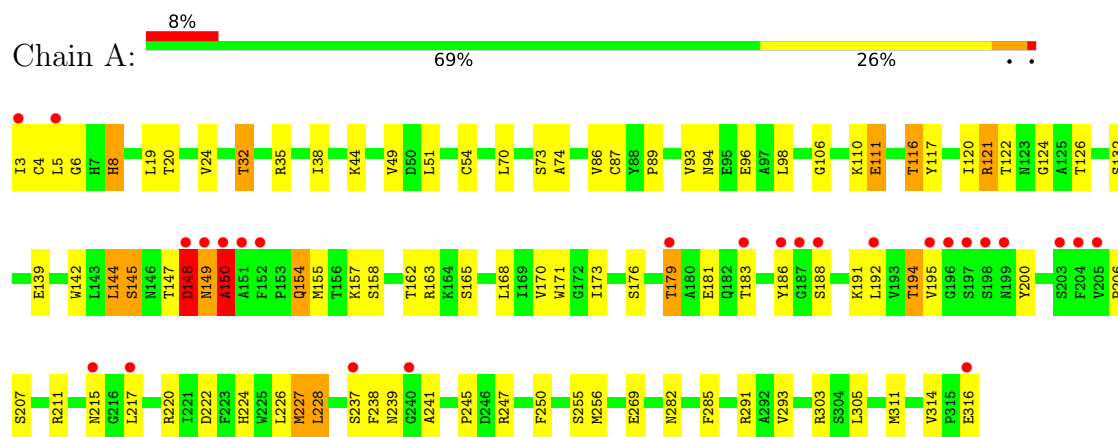
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	23	Total	O	0	0
			23	23		

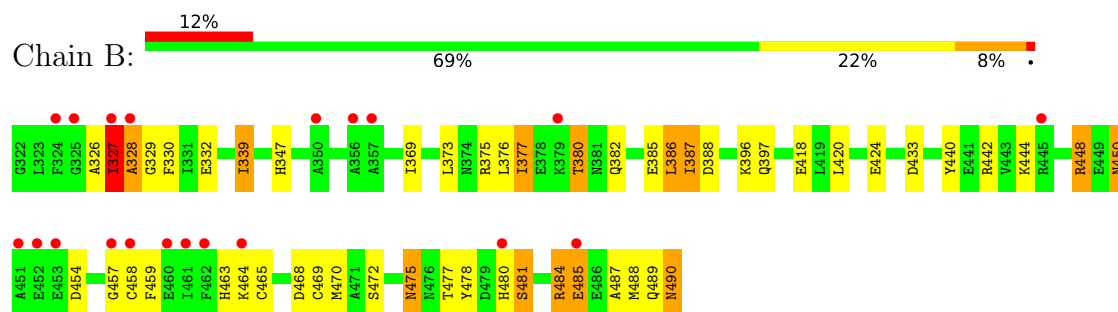
3 Residue-property plots

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: Hemagglutinin HA1



• Molecule 2: Hemagglutinin HA2



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	116.24Å 116.24Å 296.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.65 – 2.60 47.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.65-2.60) 99.8 (47.65-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.218 , 0.256 0.215 , 0.257	Depositor DCC
R_{free} test set	1229 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.021 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.007 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3925	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.46	0/2441	0.85	1/3300 (0.0%)
2	B	0.42	0/1392	0.79	0/1876
All	All	0.45	0/3833	0.83	1/5176 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ALA	CB-CA-C	7.92	126.18	110.42

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	2395	0	2352	54	0
2	B	1368	0	1264	37	0
3	C	32	0	28	0	0
4	A	28	0	26	0	0
4	B	14	0	13	2	0
5	A	65	0	0	4	0
5	B	23	0	0	4	0
All	All	3925	0	3683	87	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 12.

All (87) 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)
2:B:328:ALA:H	2:B:329:GLY:HA3	0.96	1.11
2:B:328:ALA:N	2:B:329:GLY:HA3	1.60	1.06
2:B:327:ILE:HG22	2:B:327:ILE:O	1.60	0.99
2:B:397:GLN:HG3	5:B:620:HOH:O	1.72	0.88
1:A:165:SER:OG	5:A:710:HOH:O	1.91	0.87
2:B:326:ALA:O	2:B:327:ILE:HB	1.75	0.85
2:B:328:ALA:N	2:B:329:GLY:CA	2.44	0.80
2:B:347:HIS:HB2	2:B:470:MET:HE3	1.63	0.79
2:B:327:ILE:O	2:B:327:ILE:CG2	2.34	0.74
1:A:121:ARG:NH1	1:A:145:SER:O	2.22	0.73
2:B:327:ILE:O	2:B:328:ALA:HB3	1.88	0.72
1:A:96:GLU:OE2	5:A:702:HOH:O	2.09	0.71
1:A:121:ARG:HB3	1:A:144:LEU:HB2	1.74	0.69
2:B:327:ILE:O	2:B:328:ALA:CB	2.41	0.67
2:B:396:LYS:HE3	4:B:501:NAG:H81	1.76	0.66
1:A:87:CYS:O	1:A:215:ASN:ND2	2.29	0.65
1:A:148:ASP:OD2	1:A:148:ASP:N	2.29	0.65
2:B:326:ALA:O	2:B:327:ILE:CB	2.46	0.64
1:A:293:VAL:HG11	2:B:386:LEU:HD13	1.80	0.63
1:A:207:SER:O	1:A:211:ARG:NH2	2.24	0.63
2:B:463:HIS:HB3	2:B:487:ALA:HB2	1.80	0.62
1:A:6:GLY:HA3	5:B:623:HOH:O	1.97	0.62
1:A:192:LEU:N	1:A:239:ASN:OD1	2.33	0.62
1:A:44:LYS:HE2	1:A:269:GLU:HB2	1.83	0.60
1:A:183:THR:HG22	1:A:188:SER:HA	1.84	0.60
1:A:282:ASN:HB3	2:B:377:ILE:HG23	1.84	0.59
1:A:195:VAL:HG23	1:A:200:TYR:HE2	1.67	0.59
1:A:291:ARG:HH21	2:B:388:ASP:HB3	1.67	0.58
1:A:191:LYS:HA	1:A:239:ASN:HD21	1.69	0.58
2:B:380:THR:HG22	2:B:382:GLN:H	1.68	0.57
2:B:475:ASN:ND2	2:B:477:THR:OG1	2.36	0.57
1:A:32:THR:HG23	1:A:285:PHE:HD1	1.69	0.57
4:B:501:NAG:H83	5:B:621:HOH:O	2.03	0.57
1:A:158:SER:HA	5:A:720:HOH:O	2.05	0.56
1:A:154:GLN:OE1	1:A:239:ASN:HB3	2.06	0.55
2:B:326:ALA:HB2	2:B:330:PHE:CE2	2.41	0.55
2:B:375:ARG:NH2	2:B:424:GLU:OE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:GLU:HA	2:B:488:MET:HB2	1.90	0.54
2:B:450:ASN:N	2:B:450:ASN:OD1	2.39	0.54
2:B:490:ASN:OD1	2:B:490:ASN:N	2.43	0.52
1:A:70:LEU:O	1:A:110:LYS:NZ	2.39	0.52
1:A:194:THR:HG23	1:A:237:SER:HB2	1.92	0.52
1:A:49:VAL:HG23	1:A:74:ALA:HB2	1.91	0.52
2:B:485:GLU:O	2:B:489:GLN:HG2	2.10	0.52
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.44	0.51
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.10	0.51
2:B:387:ILE:HD12	2:B:387:ILE:H	1.75	0.51
1:A:98:LEU:HD11	1:A:168:LEU:HD21	1.91	0.51
1:A:168:LEU:HA	1:A:227:MET:HE3	1.92	0.51
1:A:117:TYR:O	5:A:752:HOH:O	2.18	0.50
2:B:440:TYR:CE1	2:B:457:GLY:HA2	2.48	0.49
1:A:147:THR:O	1:A:149:ASN:N	2.45	0.49
2:B:376:LEU:HD22	2:B:420:LEU:HD21	1.94	0.49
2:B:481:SER:HA	2:B:484:ARG:HB2	1.94	0.49
2:B:484:ARG:NE	2:B:488:MET:SD	2.67	0.49
1:A:186:TYR:CZ	1:A:241:ALA:HA	2.48	0.48
1:A:35:ARG:HD3	1:A:303:ARG:HG2	1.95	0.47
1:A:116:THR:O	1:A:157:LYS:NZ	2.32	0.47
1:A:32:THR:HG23	1:A:285:PHE:CD1	2.50	0.47
1:A:179:THR:O	1:A:183:THR:HG23	2.15	0.46
1:A:4:CYS:HA	2:B:458:CYS:HA	1.97	0.46
1:A:120:ILE:HG12	1:A:155:MET:HE1	1.98	0.45
1:A:32:THR:HG22	1:A:305:LEU:HB2	1.97	0.45
1:A:3:ILE:O	2:B:459:PHE:N	2.37	0.45
1:A:173:ILE:HB	1:A:222:ASP:HB2	1.99	0.44
2:B:440:TYR:HE1	2:B:457:GLY:HA2	1.83	0.44
1:A:191:LYS:HA	1:A:239:ASN:ND2	2.32	0.44
1:A:124:GLY:HA3	1:A:142:TRP:HB3	2.01	0.43
2:B:469:CYS:O	2:B:472:SER:OG	2.31	0.43
1:A:51:LEU:HB3	1:A:54:CYS:O	2.19	0.42
1:A:192:LEU:O	1:A:238:PHE:HA	2.19	0.42
1:A:117:TYR:CE2	1:A:157:LYS:HE3	2.55	0.42
2:B:326:ALA:O	2:B:433:ASP:CG	2.63	0.42
1:A:170:VAL:O	1:A:245:PRO:HB3	2.20	0.41
1:A:149:ASN:HB3	1:A:150:ALA:H	1.66	0.41
1:A:93:VAL:HG21	1:A:224:HIS:CE1	2.55	0.41
1:A:6:GLY:CA	5:B:623:HOH:O	2.63	0.41
2:B:339:ILE:H	2:B:339:ILE:HG12	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.89	0.41
1:A:89:PRO:HB2	1:A:220:ARG:HD3	2.03	0.41
1:A:191:LYS:O	1:A:206:PRO:HD2	2.21	0.41
1:A:8:HIS:CE1	1:A:311:MET:HE3	2.56	0.40
1:A:111:GLU:OE2	1:A:163:ARG:NH1	2.55	0.40
1:A:171:TRP:CH2	1:A:226:LEU:HD23	2.57	0.40
1:A:106:GLY:HA2	1:A:255:SER:HB3	2.02	0.40
2:B:444:LYS:HB2	2:B:459:PHE:CZ	2.56	0.40
2:B:472:SER:O	2:B:478:TYR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/314 (99%)	290 (93%)	18 (6%)	4 (1%)	9	21
2	B	167/169 (99%)	144 (86%)	16 (10%)	7 (4%)	2	3
All	All	479/483 (99%)	434 (91%)	34 (7%)	11 (2%)	5	9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	327	ILE
2	B	328	ALA
2	B	448	ARG
1	A	148	ASP
2	B	484	ARG
1	A	132	SER
1	A	150	ALA
1	A	154	GLN
2	B	464	LYS

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Mol	Chain	Res	Type
2	B	481	SER
2	B	377	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/263 (100%)	233 (89%)	30 (11%)	5	11
2	B	144/144 (100%)	124 (86%)	20 (14%)	3	7
All	All	407/407 (100%)	357 (88%)	50 (12%)	4	9

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	8	HIS
1	A	19	LEU
1	A	20	THR
1	A	24	VAL
1	A	32	THR
1	A	38	ILE
1	A	73	SER
1	A	86	VAL
1	A	94	ASN
1	A	111	GLU
1	A	116	THR
1	A	121	ARG
1	A	122	THR
1	A	126	THR
1	A	144	LEU
1	A	145	SER
1	A	148	ASP
1	A	149	ASN
1	A	162	THR
1	A	176	SER

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Mol	Chain	Res	Type
1	A	179	THR
1	A	181	GLU
1	A	194	THR
1	A	217	LEU
1	A	227	MET
1	A	228	LEU
1	A	256	MET
1	A	314	VAL
1	A	316	GLU
2	B	327	ILE
2	B	332	GLU
2	B	339	ILE
2	B	369	ILE
2	B	373	LEU
2	B	380	THR
2	B	385	GLU
2	B	386	LEU
2	B	387	ILE
2	B	418	GLU
2	B	442	ARG
2	B	448	ARG
2	B	450	ASN
2	B	454	ASP
2	B	465	CYS
2	B	468	ASP
2	B	475	ASN
2	B	480	HIS
2	B	485	GLU
2	B	490	ASN

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	8	HIS
1	A	213	GLN
2	B	333	ASN
2	B	475	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 ⓘ

2 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	GAL	C	1	3	12,12,12	0.58	0	17,17,17	0.98	2 (11%)
3	SIA	C	2	3	20,20,21	3.68	8 (40%)	21,28,31	3.55	6 (28%)

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	GAL	C	1	3	-	2/2/22/22	0/1/1/1
3	SIA	C	2	3	-	1/18/34/38	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	SIA	C7-C6	-9.55	1.41	1.52
3	C	2	SIA	O6-C6	6.88	1.54	1.44
3	C	2	SIA	C3-C2	-6.38	1.42	1.52
3	C	2	SIA	C3-C4	-4.77	1.43	1.52
3	C	2	SIA	C10-N5	4.61	1.49	1.34
3	C	2	SIA	C4-C5	-4.29	1.49	1.53
3	C	2	SIA	O1A-C1	2.58	1.29	1.22
3	C	2	SIA	C6-C5	-2.44	1.49	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	SIA	O6-C2-C3	-12.18	94.18	110.56
3	C	2	SIA	O6-C2-C1	8.21	123.22	107.72
3	C	2	SIA	O1B-C1-C2	3.51	121.85	112.71
3	C	2	SIA	O9-C9-C8	2.89	117.23	111.16
3	C	2	SIA	C8-C7-C6	-2.76	107.87	113.05
3	C	1	GAL	O5-C1-C2	-2.73	105.50	110.30
3	C	1	GAL	C1-O5-C5	2.18	117.86	113.65
3	C	2	SIA	O1B-C1-O1A	-2.00	119.54	124.08

There are no chirality outliers.

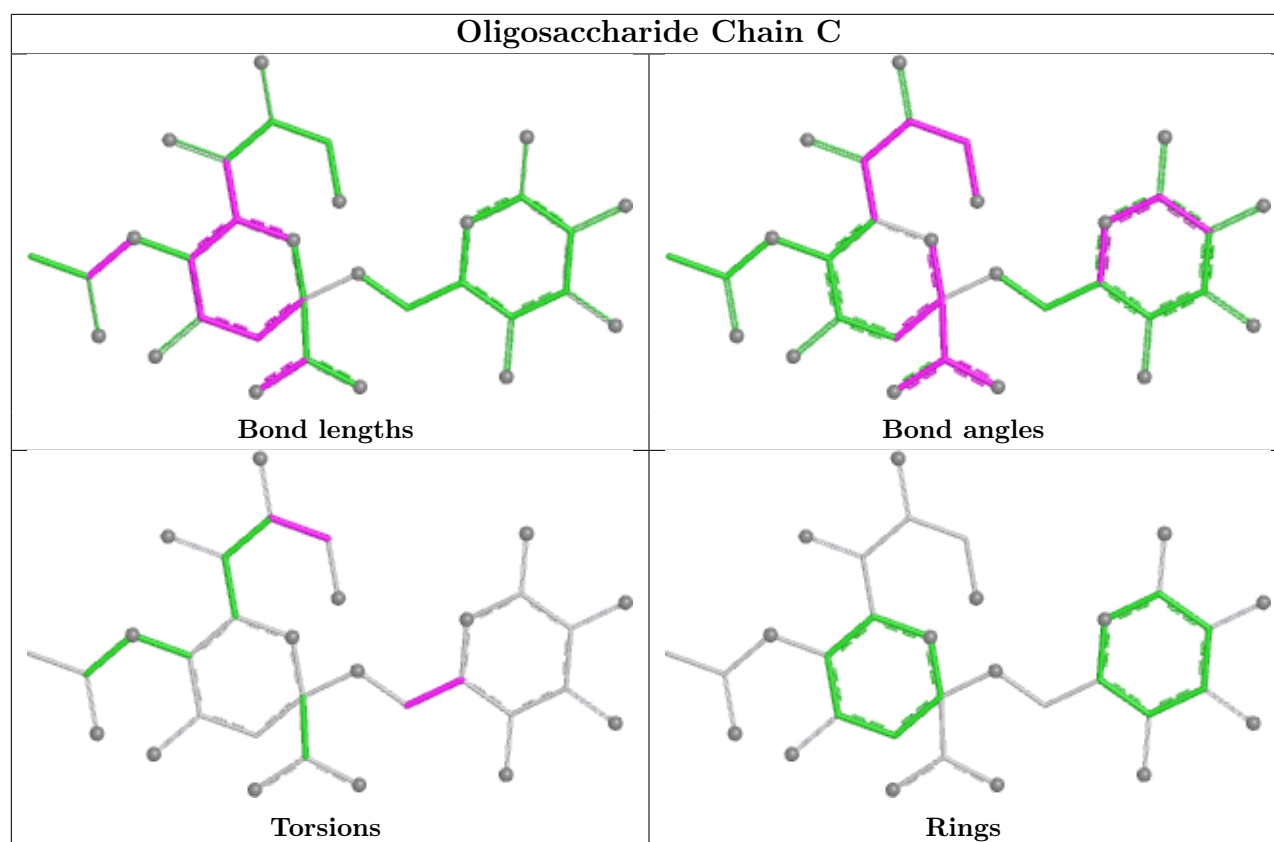
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	GAL	C4-C5-C6-O6
3	C	1	GAL	O5-C5-C6-O6
3	C	2	SIA	C7-C8-C9-O9

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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$
4	NAG	A	602	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
4	NAG	B	501	2	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
4	NAG	A	601	1	14,14,15	0.45	0	17,19,21	1.57	1 (5%)

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	A	602	1	-	2/6/23/26	0/1/1/1
4	NAG	B	501	2	-	3/6/23/26	0/1/1/1
4	NAG	A	601	1	-	1/6/23/26	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(°)
4	A	601	NAG	C1-O5-C5	5.18	119.14	112.19
4	A	602	NAG	C1-O5-C5	2.75	115.87	112.19
4	B	501	NAG	C1-O5-C5	2.20	115.14	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	NAG	C8-C7-N2-C2
4	A	602	NAG	O7-C7-N2-C2
4	B	501	NAG	C8-C7-N2-C2
4	A	601	NAG	O5-C5-C6-O6
4	B	501	NAG	O7-C7-N2-C2
4	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	314/314 (100%)	0.22	26 (8%) 17 13	29, 57, 101, 134	0
2	B	169/169 (100%)	0.58	20 (11%) 9 7	24, 83, 130, 158	0
All	All	483/483 (100%)	0.35	46 (9%) 14 10	24, 64, 119, 158	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	480	HIS	5.4
1	A	149	ASN	3.8
2	B	462	PHE	3.7
1	A	148	ASP	3.7
1	A	195	VAL	3.7
1	A	203	SER	3.5
1	A	198	SER	3.3
2	B	457	GLY	3.3
1	A	187	GLY	3.1
2	B	328	ALA	3.1
2	B	464	LYS	3.1
2	B	350	ALA	3.0
1	A	179	THR	2.9
1	A	217	LEU	2.8
1	A	192	LEU	2.8
1	A	151	ALA	2.7
2	B	327	ILE	2.7
1	A	199	ASN	2.6
1	A	204	PHE	2.6
1	A	186	TYR	2.6
1	A	150	ALA	2.6
2	B	458	CYS	2.5
2	B	451	ALA	2.5
1	A	152	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	485	GLU	2.4
1	A	205	VAL	2.4
2	B	445	ARG	2.3
1	A	215	ASN	2.3
1	A	188	SER	2.3
2	B	461	ILE	2.3
1	A	196	GLY	2.3
1	A	183	THR	2.2
1	A	316	GLU	2.2
1	A	197	SER	2.2
1	A	237	SER	2.2
2	B	357	ALA	2.2
2	B	379	LYS	2.2
1	A	240	GLY	2.2
2	B	325	GLY	2.2
2	B	356	ALA	2.1
2	B	460	GLU	2.1
2	B	452	GLU	2.1
2	B	324	PHE	2.1
1	A	3	ILE	2.1
1	A	5	LEU	2.0
2	B	453	GLU	2.0

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

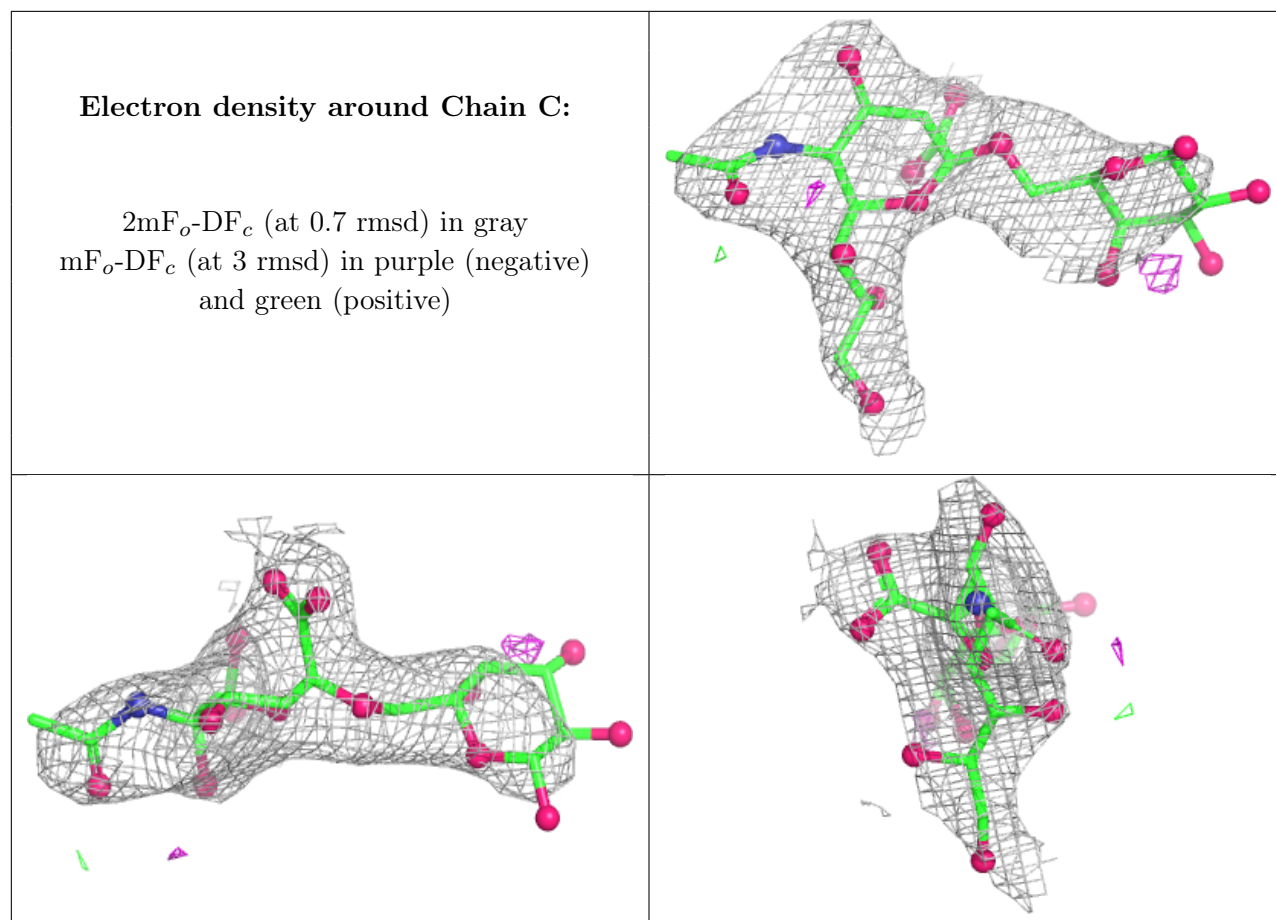
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	GAL	C	1	12/12	0.65	0.17	103,139,162,171	0
3	SIA	C	2	20/21	0.91	0.13	84,90,101,108	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(Å ²)	Q<0.9
4	NAG	A	602	14/15	0.58	0.14	110,118,121,121	0
4	NAG	A	601	14/15	0.72	0.19	103,112,120,122	0
4	NAG	B	501	14/15	0.84	0.16	67,84,93,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.