



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 06:31 PM EST

PDB ID : 4BH1
Title : H5 (tyTy) Influenza Virus Haemagglutinin in Complex with Avian Receptor Analogue 3'-SLN
Authors : Xiong, X.; Coombs, P.J.; Martin, S.R.; Liu, J.; Xiao, H.; McCauley, J.W.; Locher, K.; Walker, P.A.; Collins, P.J.; Kawaoka, Y.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2013-03-29
Resolution : 2.15 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:

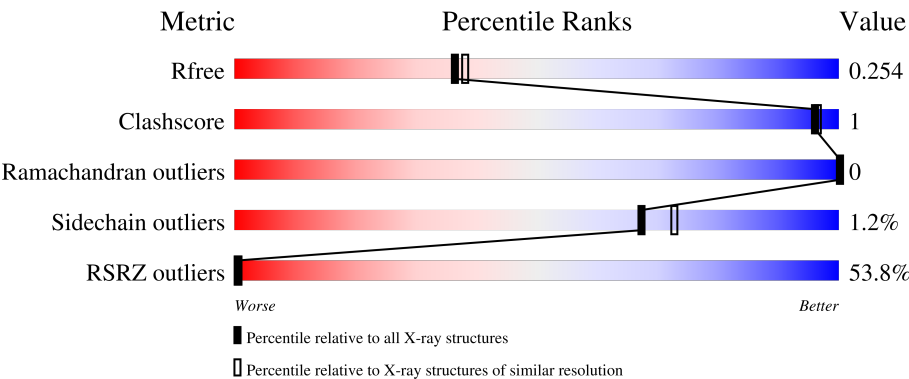
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	326	<div><div>29%</div><div>94%</div><div></div><div></div></div>
1	C	326	<div><div>26%</div><div>94%</div><div></div><div></div></div>
1	E	326	<div><div>61%</div><div>93%</div><div></div><div></div></div>
2	B	166	<div><div>72%</div><div>86%</div><div>13%</div><div></div></div>
2	D	166	<div><div>72%</div><div>84%</div><div>12%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	166	<div><div></div><div>77%</div><div></div><div>86%</div><div></div><div>13%</div></div>
3	G	3	<div><div></div><div>33%</div><div></div><div>67%</div></div>
3	H	3	<div><div></div><div>100%</div></div>
3	I	3	<div><div></div><div>33%</div><div></div><div>67%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11980 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
			2526	1592	439	481	14			
1	C	319	Total	C	N	O	S	0	0	0
			2519	1587	439	479	14			
1	E	319	Total	C	N	O	S	0	0	0
			2519	1587	439	479	14			

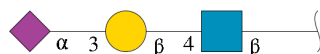
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ARG	-	expression tag	UNP Q207Z6
A	324	GLU	-	expression tag	UNP Q207Z6
A	325	THR	-	expression tag	UNP Q207Z6
A	326	ARG	-	expression tag	UNP Q207Z6
C	323	ARG	-	expression tag	UNP Q207Z6
C	324	GLU	-	expression tag	UNP Q207Z6
C	325	THR	-	expression tag	UNP Q207Z6
C	326	ARG	-	expression tag	UNP Q207Z6
E	323	ARG	-	expression tag	UNP Q207Z6
E	324	GLU	-	expression tag	UNP Q207Z6
E	325	THR	-	expression tag	UNP Q207Z6
E	326	ARG	-	expression tag	UNP Q207Z6

- Molecule 2 is a protein called HEMAGGLUTININ.

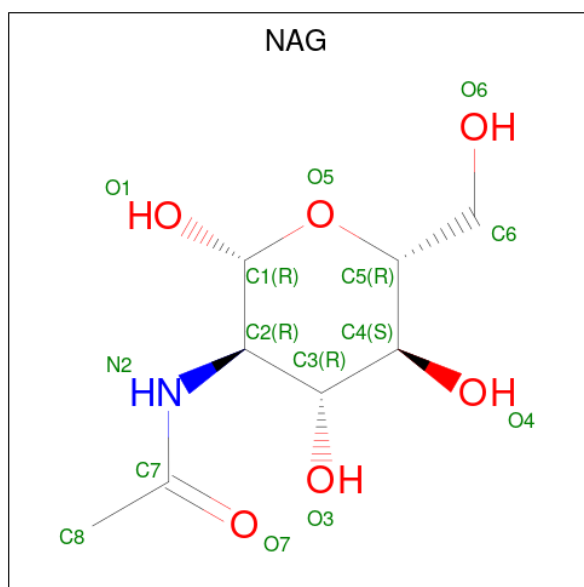
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1129	697	200	224	8			
2	D	146	Total	C	N	O	S	0	0	0
			1130	698	201	223	8			
2	F	145	Total	C	N	O	S	0	0	0
			1129	697	200	224	8			

- 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	G	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	H	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	I	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

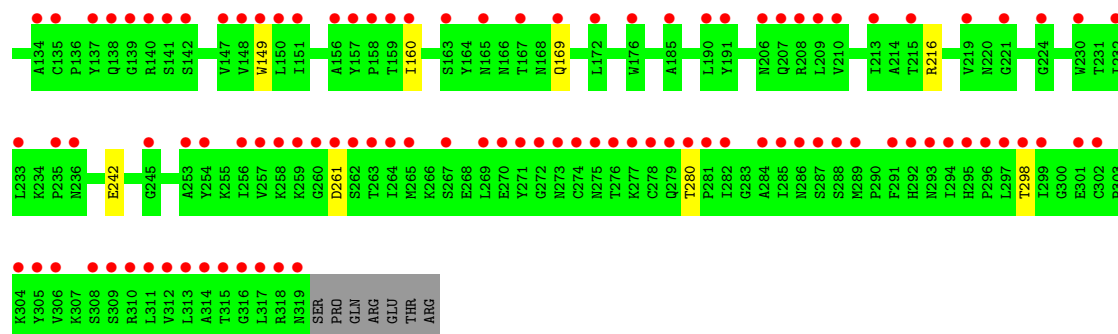
- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



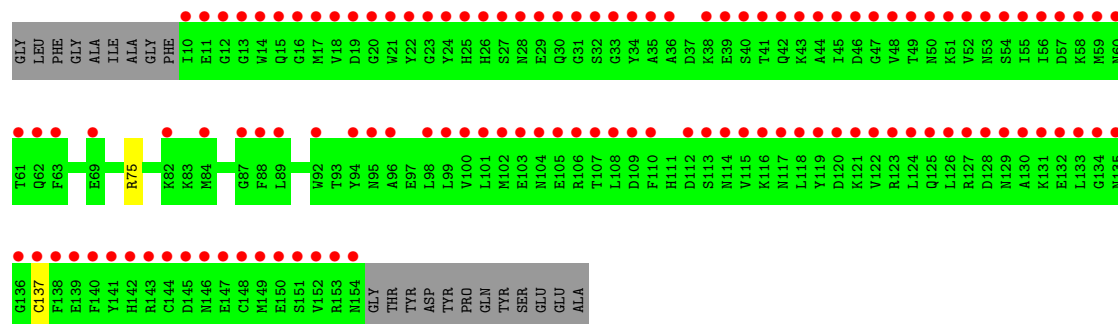
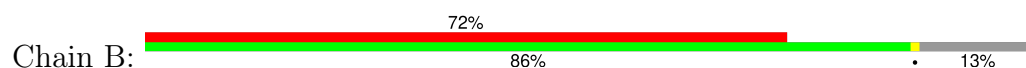
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

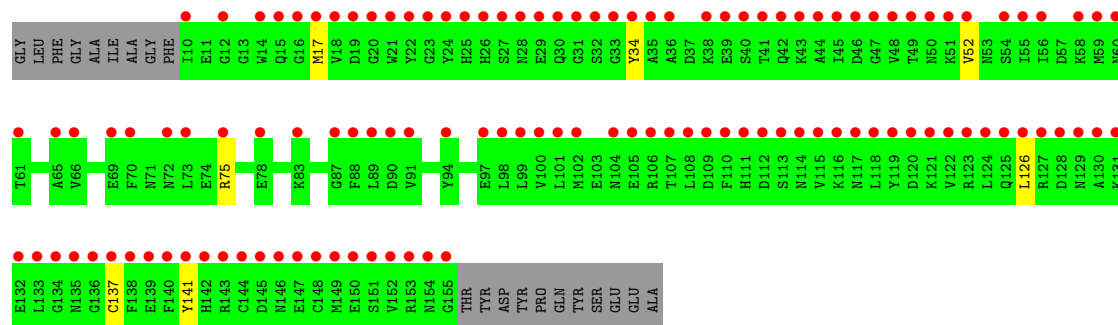
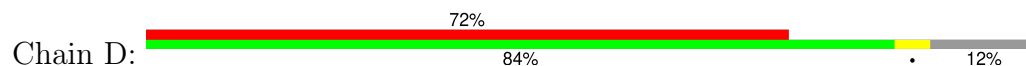
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	266	Total	O	0	0
			266	266		
6	B	36	Total	O	0	0
			36	36		
6	C	243	Total	O	0	0
			243	243		
6	D	35	Total	O	0	0
			35	35		
6	E	218	Total	O	0	0
			218	218		
6	F	30	Total	O	0	0
			30	30		



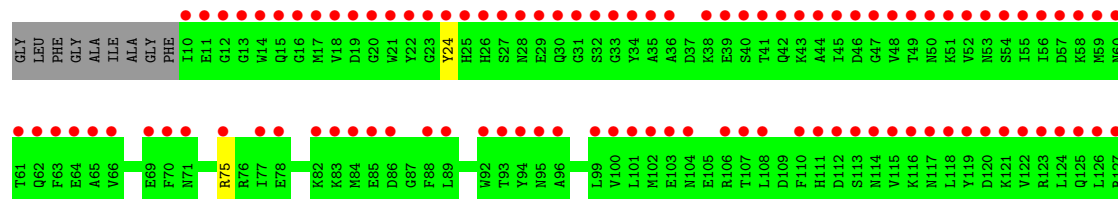
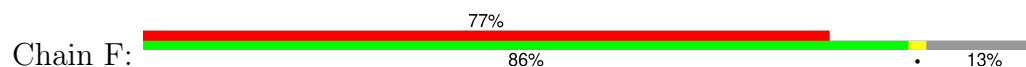
• Molecule 2: HEMAGGLUTININ

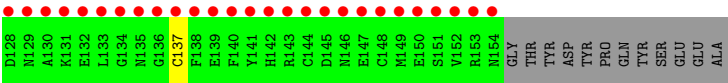


• Molecule 2: HEMAGGLUTININ

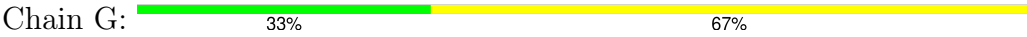


• Molecule 2: HEMAGGLUTININ

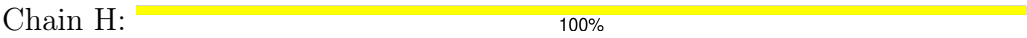




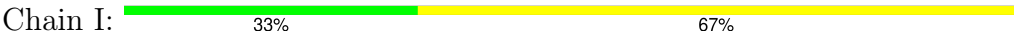
● Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.86Å 228.29Å 71.92Å 90.00° 113.71° 90.00°	Depositor
Resolution (Å)	62.48 – 2.15 62.48 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (62.48-2.15) 98.6 (62.48-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.224 0.261 , 0.254	Depositor DCC
R_{free} test set	5489 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11980	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: PO4, SIA, NAG, GAL

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	0.32	0/2586	0.55	2/3515 (0.1%)
1	C	0.32	0/2579	0.55	2/3506 (0.1%)
1	E	0.31	0/2579	0.55	1/3506 (0.0%)
2	B	0.29	0/1149	0.44	0/1551
2	D	0.30	0/1150	0.44	0/1552
2	F	0.29	0/1149	0.43	0/1551
All	All	0.31	0/11192	0.52	5/15181 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	216	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	C	216	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	216	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	216	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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	2526	0	2460	7	0
1	C	2519	0	2447	7	0
1	E	2519	0	2447	6	1
2	B	1129	0	1007	1	0
2	D	1130	0	1008	2	0
2	F	1129	0	1007	1	0
3	G	46	0	40	0	0
3	H	46	0	40	0	0
3	I	46	0	40	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
5	A	10	0	0	0	0
5	C	5	0	0	0	0
5	E	5	0	0	0	0
6	A	266	0	0	2	1
6	B	36	0	0	0	0
6	C	243	0	0	3	0
6	D	35	0	0	0	0
6	E	218	0	0	0	0
6	F	30	0	0	0	0
All	All	11980	0	10535	22	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 1.

All (22) 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:162:ARG:HD2	6:C:2149:HOH:O	2.03	0.58
1:C:84:ASN:ND2	6:C:2069:HOH:O	2.36	0.57
1:A:7:TYR:HB2	1:A:317:LEU:CD2	2.43	0.48
1:A:130:GLY:HA3	1:A:149:TRP:HB3	1.96	0.47
1:E:130:GLY:HA3	1:E:149:TRP:HB3	1.95	0.47
1:C:130:GLY:HA3	1:C:149:TRP:HB3	1.97	0.47
1:E:280:THR:HG22	1:E:298:THR:HG22	1.98	0.46
1:A:280:THR:HG22	1:A:298:THR:HG22	1.98	0.45
1:E:160:ILE:O	1:E:242:GLU:HA	2.17	0.45
1:A:94:ASN:ND2	6:A:2077:HOH:O	2.45	0.45
1:C:313:LEU:HD13	2:D:52:VAL:HG12	1.98	0.45
1:A:160:ILE:O	1:A:242:GLU:HA	2.17	0.44
1:C:160:ILE:O	1:C:242:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:MET:HG3	2:D:34:TYR:HB3	1.99	0.44
1:A:18:THR:HG22	1:A:19:ILE:N	2.33	0.43
1:C:280:THR:HG22	1:C:298:THR:HG22	1.98	0.43
1:E:18:THR:HG22	1:E:19:ILE:N	2.34	0.43
1:E:3:ILE:HD11	2:F:24:TYR:HB3	2.01	0.42
1:A:94:ASN:HB2	6:A:2078:HOH:O	2.20	0.41
1:C:18:THR:HG22	1:C:19:ILE:N	2.34	0.41
2:B:75:ARG:HG3	6:C:2090:HOH:O	2.20	0.41
1:E:104:LEU:HD13	1:E:108:ILE:HD12	2.02	0.41

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:E:169:GLN:NE2	6:A:2135:HOH:O[1_655]	2.09	0.11

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	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
1	C	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
1	E	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
2	B	143/166 (86%)	137 (96%)	6 (4%)	0	100	100
2	D	144/166 (87%)	137 (95%)	7 (5%)	0	100	100
2	F	143/166 (86%)	137 (96%)	6 (4%)	0	100	100
All	All	1381/1476 (94%)	1338 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	284/292 (97%)	282 (99%)	2 (1%)	81	86
1	C	282/292 (97%)	280 (99%)	2 (1%)	81	86
1	E	282/292 (97%)	279 (99%)	3 (1%)	70	75
2	B	113/141 (80%)	112 (99%)	1 (1%)	75	81
2	D	112/141 (79%)	108 (96%)	4 (4%)	30	29
2	F	113/141 (80%)	111 (98%)	2 (2%)	54	59
All	All	1186/1299 (91%)	1172 (99%)	14 (1%)	67	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	317	LEU
2	B	137	CYS
1	C	107	ARG
1	C	310	ARG
2	D	75	ARG
2	D	126	LEU
2	D	137	CYS
2	D	141	TYR
1	E	104	LEU
1	E	107	ARG
1	E	261	ASP
2	F	75	ARG
2	F	137	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	C	2	GLN
2	D	15	GLN

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Mol	Chain	Res	Type
1	E	2	GLN
1	E	87	ASN
1	E	110	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	G	1	3	15,15,15	0.38	0	21,21,21	1.37	4 (19%)
3	GAL	G	2	3	11,11,12	0.41	0	15,15,17	0.88	0
3	SIA	G	3	3	20,20,21	0.73	0	21,28,31	1.51	4 (19%)
3	NAG	H	1	3	15,15,15	0.45	0	21,21,21	1.24	2 (9%)
3	GAL	H	2	3	11,11,12	0.33	0	15,15,17	1.07	2 (13%)
3	SIA	H	3	3	20,20,21	0.70	0	21,28,31	1.19	2 (9%)
3	NAG	I	1	3	15,15,15	0.40	0	21,21,21	1.27	2 (9%)
3	GAL	I	2	3	11,11,12	0.26	0	15,15,17	0.77	0
3	SIA	I	3	3	20,20,21	0.63	0	21,28,31	1.11	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	G	1	3	-	0/6/26/26	0/1/1/1
3	GAL	G	2	3	-	1/2/19/22	0/1/1/1
3	SIA	G	3	3	-	0/18/34/38	0/1/1/1
3	NAG	H	1	3	-	0/6/26/26	0/1/1/1
3	GAL	H	2	3	-	1/2/19/22	0/1/1/1
3	SIA	H	3	3	-	0/18/34/38	0/1/1/1
3	NAG	I	1	3	-	0/6/26/26	0/1/1/1
3	GAL	I	2	3	-	0/2/19/22	0/1/1/1
3	SIA	I	3	3	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-C2-N2	-4.25	105.80	110.73
3	G	3	SIA	O6-C2-C1	3.62	114.55	107.72
3	G	1	NAG	C1-C2-N2	-3.61	106.55	110.73
3	I	1	NAG	C1-C2-N2	-3.52	106.65	110.73
3	G	3	SIA	C6-C5-N5	-2.77	106.48	110.91
3	G	3	SIA	O1B-C1-C2	2.75	119.85	112.71
3	G	1	NAG	C3-C2-N2	-2.65	105.74	110.62
3	H	3	SIA	C6-C5-N5	-2.60	106.75	110.91
3	I	1	NAG	C3-C2-N2	-2.60	105.83	110.62
3	G	1	NAG	O5-C1-C2	2.52	112.05	109.52
3	I	3	SIA	C4-C5-N5	-2.47	105.56	110.44
3	H	3	SIA	O1B-C1-C2	2.45	119.07	112.71
3	I	3	SIA	C6-C5-N5	-2.35	107.16	110.91
3	H	2	GAL	C1-C2-C3	2.28	112.97	109.64
3	G	1	NAG	C1-C2-C3	2.25	113.61	110.54
3	H	1	NAG	C3-C2-N2	-2.18	106.60	110.62
3	H	2	GAL	C1-O5-C5	2.09	114.99	112.19
3	G	3	SIA	O1A-C1-C2	-2.05	118.42	122.85

There are no chirality outliers.

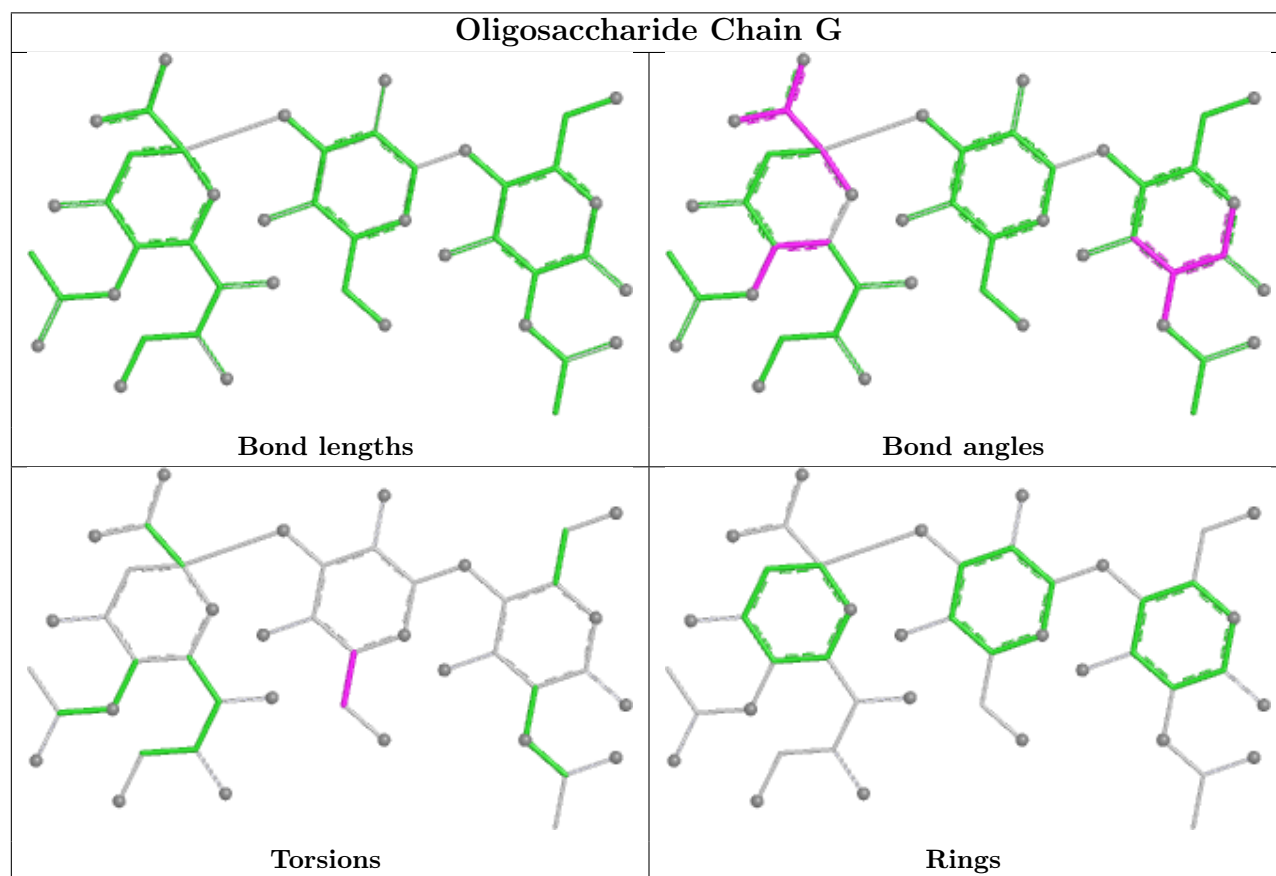
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	GAL	C4-C5-C6-O6
3	G	2	GAL	C4-C5-C6-O6

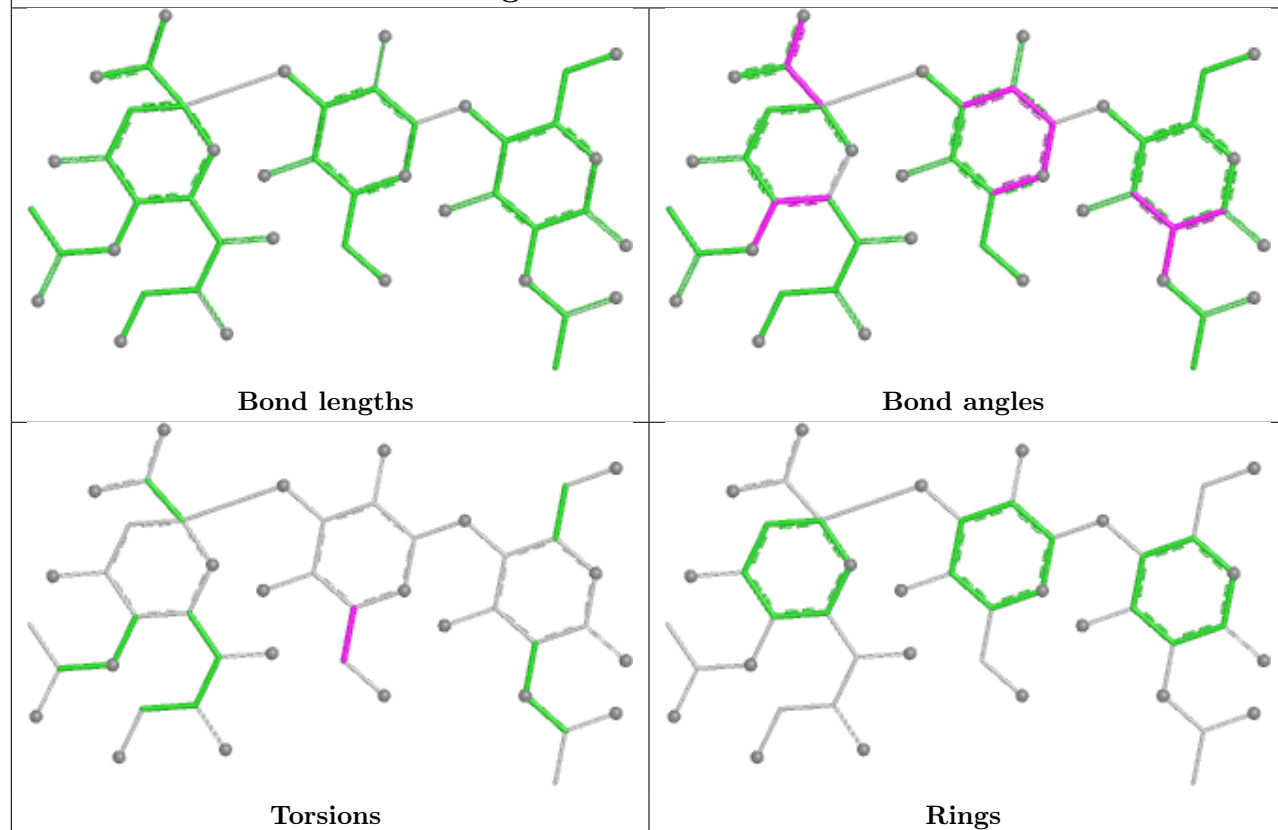
There are no ring outliers.

No monomer is involved in short contacts.

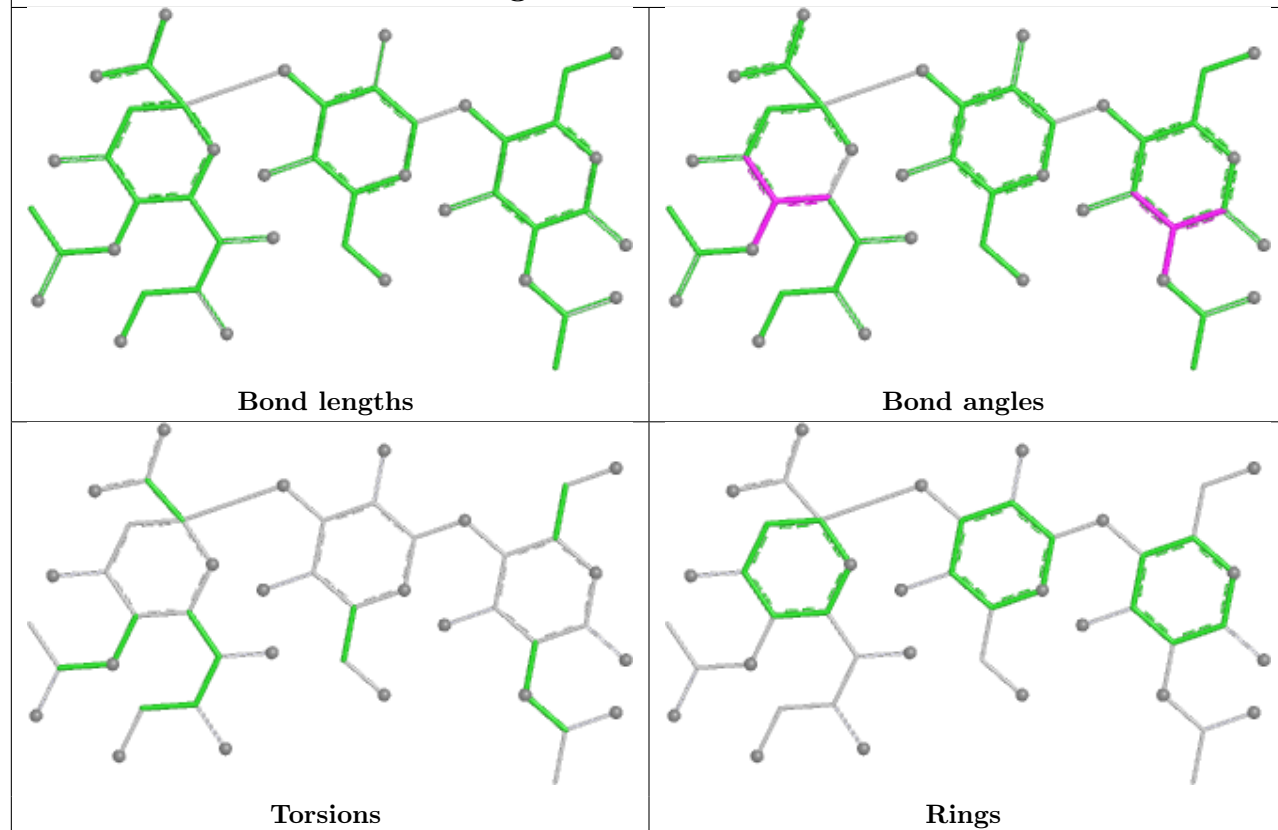
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry

7 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	PO4	C	1324	-	4,4,4	0.99	0	6,6,6	0.53	0
4	NAG	C	1320	1	14,14,15	0.55	0	17,19,21	1.38	3 (17%)
5	PO4	A	1325	-	4,4,4	0.82	0	6,6,6	0.60	0
5	PO4	E	1324	-	4,4,4	1.00	0	6,6,6	0.56	0
5	PO4	A	1324	-	4,4,4	0.92	0	6,6,6	0.57	0
4	NAG	A	1320	1	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
4	NAG	E	1320	1	14,14,15	0.37	0	17,19,21	1.06	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	1320	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1320	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1320	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1320	NAG	C1-O5-C5	3.70	117.14	112.19
4	A	1320	NAG	C1-O5-C5	3.54	116.93	112.19
4	E	1320	NAG	C1-O5-C5	2.61	115.68	112.19
4	C	1320	NAG	C1-C2-N2	2.25	113.98	110.43
4	A	1320	NAG	C3-C4-C5	-2.09	106.44	110.23
4	C	1320	NAG	C3-C4-C5	-2.03	106.55	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1320	NAG	C4-C5-C6-O6
4	A	1320	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Warning: The R factor obtained from EDS is 0.3001, which does not match the depositor's R factor of 0.20518. Please interpret the results in this section carefully.

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	319/326 (97%)	1.73	96 (30%) 1 2	23, 38, 124, 285	0
1	C	319/326 (97%)	1.54	86 (26%) 2 2	22, 40, 101, 147	0
1	E	319/326 (97%)	2.47	200 (62%) 0 0	24, 41, 129, 233	0
2	B	145/166 (87%)	3.58	119 (82%) 0 0	25, 172, 220, 245	0
2	D	146/166 (87%)	3.73	120 (82%) 0 0	29, 126, 188, 208	0
2	F	145/166 (87%)	3.79	128 (88%) 0 0	24, 166, 204, 226	0
All	All	1393/1476 (94%)	2.47	749 (53%) 0 1	22, 47, 193, 285	0

All (749) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	138	PHE	12.6
1	E	3	ILE	9.4
2	B	21	TRP	8.8
2	D	140	PHE	8.8
2	B	141	TYR	8.8
2	B	138	PHE	8.6
2	F	133	LEU	8.4
1	A	3	ILE	8.3
2	B	55	ILE	8.1
2	F	141	TYR	8.1
2	F	138	PHE	8.0
2	D	126	LEU	7.9
2	B	56	ILE	7.8
2	F	55	ILE	7.7
2	F	45	ILE	7.7
2	D	127	ARG	7.6

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Mol	Chain	Res	Type	RSRZ
2	B	122	VAL	7.5
1	A	5	ILE	7.5
2	B	136	GLY	7.4
2	F	118	LEU	7.4
2	B	52	VAL	7.3
2	F	122	VAL	7.2
2	F	152	VAL	7.2
2	B	10	ILE	7.1
2	D	141	TYR	7.1
2	F	56	ILE	7.0
2	D	61	THR	7.0
2	D	52	VAL	7.0
2	B	48	VAL	6.9
2	D	48	VAL	6.9
2	F	126	LEU	6.9
2	F	52	VAL	6.8
2	F	115	VAL	6.8
1	A	39	GLY	6.8
2	B	51	LYS	6.7
2	D	119	TYR	6.7
2	B	140	PHE	6.6
2	F	140	PHE	6.6
2	B	23	GLY	6.6
2	B	152	VAL	6.6
2	F	48	VAL	6.6
2	F	107	THR	6.5
2	B	59	MET	6.5
2	D	145	ASP	6.5
1	C	3	ILE	6.5
2	D	51	LYS	6.5
2	F	21	TRP	6.4
2	F	124	LEU	6.4
2	F	142	HIS	6.4
2	D	155	GLY	6.3
2	D	152	VAL	6.3
2	B	124	LEU	6.3
1	E	9	ALA	6.2
2	D	35	ALA	6.2
1	A	4	CYS	6.1
2	D	34	TYR	6.1
2	F	65	ALA	6.1
2	B	142	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	118	LEU	6.0
2	D	133	LEU	6.0
2	F	51	LYS	5.9
2	B	14	TRP	5.9
2	D	55	ILE	5.9
2	B	143	ARG	5.8
2	F	132	GLU	5.8
2	D	153	ARG	5.7
2	D	45	ILE	5.7
2	B	24	TYR	5.7
2	D	28	ASN	5.7
2	D	21	TRP	5.7
2	F	10	ILE	5.7
2	B	27	SER	5.6
2	D	142	HIS	5.6
2	B	137	CYS	5.6
2	D	58	LYS	5.5
2	F	136	GLY	5.5
2	D	131	LYS	5.5
2	D	16	GLY	5.5
2	F	49	THR	5.5
1	E	312	VAL	5.4
2	B	34	TYR	5.4
2	D	24	TYR	5.4
2	F	34	TYR	5.4
2	B	45	ILE	5.4
2	D	124	LEU	5.4
1	E	4	CYS	5.4
2	D	143	ARG	5.4
2	B	133	LEU	5.3
1	A	6	GLY	5.3
2	D	125	GLN	5.3
1	E	16	VAL	5.3
2	D	137	CYS	5.3
2	B	126	LEU	5.3
2	F	22	TYR	5.3
2	D	132	GLU	5.2
2	F	108	LEU	5.2
2	D	122	VAL	5.2
2	B	61	THR	5.2
1	E	32	ILE	5.2
2	D	31	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	47	GLY	5.2
2	B	22	TYR	5.2
2	D	59	MET	5.2
2	F	14	TRP	5.1
2	F	148	CYS	5.1
1	E	12	SER	5.1
2	D	30	GLN	5.1
1	E	29	ALA	5.1
2	F	25	HIS	5.0
2	F	12	GLY	5.0
1	C	7	TYR	5.0
2	B	132	GLU	5.0
1	E	20	MET	5.0
2	F	127	ARG	4.9
2	F	137	CYS	4.9
2	D	134	GLY	4.9
1	E	19	ILE	4.9
2	B	131	LYS	4.9
1	C	6	GLY	4.8
2	F	44	ALA	4.8
2	D	27	SER	4.8
2	B	115	VAL	4.8
1	C	20	MET	4.8
2	B	119	TYR	4.8
2	F	119	TYR	4.8
2	D	14	TRP	4.8
2	B	110	PHE	4.8
1	E	7	TYR	4.8
2	F	128	ASP	4.7
1	A	7	TYR	4.7
2	D	26	HIS	4.7
1	E	5	ILE	4.7
2	D	43	LYS	4.7
2	D	135	ASN	4.7
1	C	317	LEU	4.7
2	D	118	LEU	4.7
2	D	36	ALA	4.7
2	F	13	GLY	4.7
1	A	83	ILE	4.7
1	E	151	ILE	4.7
2	D	10	ILE	4.7
2	F	27	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	84	ASN	4.6
2	D	128	ASP	4.6
1	A	291	PHE	4.6
2	B	32	SER	4.6
2	F	61	THR	4.6
2	B	139	GLU	4.6
1	A	2	GLN	4.6
2	B	33	GLY	4.5
2	D	22	TYR	4.5
1	E	317	LEU	4.5
1	E	26	VAL	4.5
2	B	99	LEU	4.5
1	E	319	ASN	4.5
2	D	130	ALA	4.5
2	F	144	CYS	4.5
2	F	100	VAL	4.5
1	C	5	ILE	4.5
1	A	1	ASP	4.5
2	F	58	LYS	4.4
2	D	56	ILE	4.4
2	F	143	ARG	4.4
2	B	17	MET	4.4
1	A	311	LEU	4.4
1	E	86	ALA	4.4
2	B	25	HIS	4.4
1	E	291	PHE	4.4
2	F	110	PHE	4.4
1	E	315	THR	4.3
1	E	287	SER	4.3
2	D	32	SER	4.3
2	F	38	LYS	4.3
1	E	39	GLY	4.3
2	D	33	GLY	4.3
1	E	18	THR	4.3
2	F	11	GLU	4.3
2	F	129	ASN	4.3
2	D	144	CYS	4.3
1	E	104	LEU	4.3
2	F	31	GLY	4.3
1	C	19	ILE	4.3
2	B	12	GLY	4.2
1	E	273	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	54	SER	4.2
2	D	121	LYS	4.2
2	D	115	VAL	4.2
2	B	11	GLU	4.2
1	E	271	TYR	4.2
2	B	16	GLY	4.2
1	A	37	HIS	4.2
1	E	280	THR	4.2
1	A	30	GLN	4.1
2	D	149	MET	4.1
2	B	18	VAL	4.1
1	E	314	ALA	4.1
2	D	110	PHE	4.1
2	F	23	GLY	4.1
2	B	58	LYS	4.1
1	C	4	CYS	4.1
2	D	150	GLU	4.1
2	F	32	SER	4.1
1	E	13	THR	4.1
1	E	6	GLY	4.0
2	D	23	GLY	4.0
1	E	275	ASN	4.0
2	B	29	GLU	4.0
1	E	276	THR	4.0
2	B	103	GLU	4.0
2	F	66	VAL	4.0
2	F	120	ASP	4.0
1	C	288	SER	4.0
2	F	43	LYS	4.0
2	F	89	LEU	4.0
2	F	99	LEU	4.0
2	F	24	TYR	4.0
2	B	43	LYS	4.0
1	C	282	ILE	4.0
2	D	154	ASN	4.0
2	D	41	THR	3.9
1	A	236	ASN	3.9
2	D	60	ASN	3.9
2	F	35	ALA	3.9
2	F	139	GLU	3.9
2	D	47	GLY	3.9
2	F	33	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	288	SER	3.9
1	C	9	ALA	3.9
1	C	16	VAL	3.9
1	C	83	ILE	3.9
2	F	145	ASP	3.9
1	E	129	ALA	3.9
1	E	83	ILE	3.8
1	E	1	ASP	3.8
1	A	33	LEU	3.8
1	A	313	LEU	3.8
2	B	148	CYS	3.8
2	B	13	GLY	3.8
2	F	17	MET	3.8
2	F	54	SER	3.8
1	C	312	VAL	3.8
2	B	31	GLY	3.8
2	D	136	GLY	3.8
2	F	20	GLY	3.8
2	B	101	LEU	3.8
2	D	73	LEU	3.8
2	B	30	GLN	3.8
2	D	44	ALA	3.8
2	F	16	GLY	3.8
1	C	21	GLU	3.8
2	D	29	GLU	3.8
1	A	256	ILE	3.8
1	E	299	ILE	3.8
2	B	42	GLN	3.7
2	D	108	LEU	3.7
2	F	63	PHE	3.7
2	B	135	ASN	3.7
2	F	131	LYS	3.7
2	B	130	ALA	3.7
1	E	24	VAL	3.7
1	E	257	VAL	3.7
2	B	128	ASP	3.7
1	E	117	ILE	3.7
2	F	123	ARG	3.7
1	A	19	ILE	3.7
2	D	129	ASN	3.7
2	B	44	ALA	3.7
1	A	235	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	135	ASN	3.6
2	B	38	LYS	3.6
1	E	2	GLN	3.6
1	E	279	GLN	3.6
2	D	66	VAL	3.6
2	F	59	MET	3.6
1	A	38	ASN	3.6
1	E	33	LEU	3.6
1	A	13	THR	3.6
1	A	29	ALA	3.6
2	F	125	GLN	3.6
1	A	290	PRO	3.6
2	B	102	MET	3.6
1	E	80	VAL	3.6
1	E	38	ASN	3.6
2	D	117	ASN	3.6
1	A	264	ILE	3.6
2	B	26	HIS	3.6
1	C	29	ALA	3.6
2	F	36	ALA	3.6
2	F	70	PHE	3.6
2	D	147	GLU	3.6
2	F	40	SER	3.6
2	D	106	ARG	3.6
2	D	42	GLN	3.5
1	A	317	LEU	3.5
1	E	295	HIS	3.5
1	C	18	THR	3.5
2	D	49	THR	3.5
2	D	146	ASN	3.5
1	E	130	GLY	3.5
1	E	51	ILE	3.5
2	B	108	LEU	3.5
2	D	17	MET	3.5
2	B	35	ALA	3.5
2	B	146	ASN	3.5
2	F	28	ASN	3.5
1	A	310	ARG	3.5
2	F	18	VAL	3.5
2	F	92	TRP	3.5
1	E	316	GLY	3.5
1	E	70	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	125	GLN	3.5
1	E	8	HIS	3.5
1	E	292	HIS	3.5
2	B	20	GLY	3.5
2	B	144	CYS	3.5
2	D	38	LYS	3.5
1	A	32	ILE	3.5
1	C	294	ILE	3.5
1	A	297	LEU	3.5
1	E	313	LEU	3.5
1	E	141	SER	3.4
1	E	147	VAL	3.4
1	E	306	VAL	3.4
1	E	119	LYS	3.4
2	B	49	THR	3.4
1	A	288	SER	3.4
1	E	265	MET	3.4
1	A	306	VAL	3.4
2	F	147	GLU	3.4
1	A	36	THR	3.4
1	E	27	THR	3.4
2	F	111	HIS	3.4
2	B	121	LYS	3.4
2	B	47	GLY	3.4
2	D	98	LEU	3.4
1	E	71	LEU	3.3
1	E	264	ILE	3.3
2	B	98	LEU	3.3
1	E	127	ALA	3.3
2	D	20	GLY	3.3
2	D	94	TYR	3.3
2	F	42	GLN	3.3
1	C	51	ILE	3.3
2	F	26	HIS	3.3
2	F	39	GLU	3.3
1	C	272	GLY	3.3
1	A	24	VAL	3.3
2	F	84	MET	3.3
1	E	62	LEU	3.3
1	E	69	GLU	3.3
1	E	235	PRO	3.3
2	D	19	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	46	GLY	3.3
2	D	88	PHE	3.3
2	B	153	ARG	3.3
2	B	19	ASP	3.2
1	C	314	ALA	3.2
1	C	2	GLN	3.2
1	E	139	GLY	3.2
1	A	16	VAL	3.2
2	F	149	MET	3.2
1	E	53	ARG	3.2
2	D	101	LEU	3.2
2	B	36	ALA	3.2
2	D	65	ALA	3.2
2	D	102	MET	3.2
2	D	18	VAL	3.2
1	C	27	THR	3.2
1	E	311	LEU	3.2
1	E	42	CYS	3.2
1	E	221	GLY	3.2
1	A	11	ASN	3.2
2	B	129	ASN	3.2
2	F	50	ASN	3.2
1	C	310	ARG	3.2
1	E	66	MET	3.2
1	C	257	VAL	3.2
1	E	131	VAL	3.2
1	A	241	PHE	3.2
1	E	120	SER	3.2
1	E	116	ILE	3.2
1	E	35	LYS	3.2
2	B	149	MET	3.2
2	D	139	GLU	3.2
2	F	146	ASN	3.2
1	E	30	GLN	3.1
2	D	151	SER	3.1
2	F	15	GLN	3.1
2	F	57	ASP	3.1
1	E	105	LEU	3.1
1	E	302	CYS	3.1
2	F	62	GLN	3.1
1	A	26	VAL	3.1
1	E	57	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	142	SER	3.1
1	E	148	VAL	3.1
1	E	263	THR	3.1
1	A	277	LYS	3.1
1	E	297	LEU	3.1
2	B	147	GLU	3.1
1	C	8	HIS	3.1
1	C	37	HIS	3.1
2	D	148	CYS	3.1
2	B	145	ASP	3.1
2	F	93	THR	3.1
2	F	151	SER	3.1
1	E	73	VAL	3.1
1	A	259	LYS	3.1
2	D	116	LYS	3.1
1	C	33	LEU	3.1
1	E	41	LEU	3.1
2	B	92	TRP	3.1
1	C	84	ASN	3.1
2	F	60	ASN	3.1
1	A	184	ALA	3.1
2	D	40	SER	3.1
1	E	14	GLU	3.1
2	F	29	GLU	3.1
2	D	100	VAL	3.1
2	D	70	PHE	3.0
2	D	87	GLY	3.0
1	E	149	TRP	3.0
1	E	47	VAL	3.0
1	E	260	GLY	3.0
2	B	95	ASN	3.0
1	E	209	LEU	3.0
1	E	110	HIS	3.0
1	E	96	ASN	3.0
1	E	296	PRO	3.0
1	C	291	PHE	3.0
2	F	96	ALA	3.0
2	F	130	ALA	3.0
1	E	285	ILE	3.0
1	E	122	TRP	3.0
2	F	46	ASP	3.0
1	A	20	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	41	THR	3.0
1	E	11	ASN	3.0
1	E	286	ASN	3.0
2	D	72	ASN	3.0
1	C	24	VAL	3.0
1	E	284	ALA	3.0
2	F	116	LYS	3.0
1	A	116	ILE	2.9
1	A	285	ILE	2.9
2	F	86	ASP	2.9
2	D	25	HIS	2.9
1	A	319	ASN	2.9
1	E	272	GLY	2.9
1	A	257	VAL	2.9
2	B	127	ARG	2.9
2	D	91	VAL	2.9
1	E	50	LEU	2.9
2	D	39	GLU	2.9
1	A	314	ALA	2.9
1	E	298	THR	2.9
1	E	107	ARG	2.9
2	D	123	ARG	2.9
2	B	39	GLU	2.9
1	E	185	ALA	2.9
1	E	28	HIS	2.9
1	C	309	SER	2.9
1	E	79	ILE	2.9
1	E	282	ILE	2.9
1	E	137	TYR	2.9
1	E	157	TYR	2.9
1	E	25	THR	2.9
1	A	316	GLY	2.9
1	A	318	ARG	2.9
1	E	140	ARG	2.9
2	F	121	LYS	2.9
2	D	120	ASP	2.9
1	E	267	SER	2.9
1	C	273	ASN	2.9
1	E	293	ASN	2.9
1	C	316	GLY	2.9
2	D	105	GLU	2.9
1	C	307	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	86	ALA	2.8
2	B	15	GLN	2.8
1	A	114	ILE	2.8
1	E	236	ASN	2.8
1	A	35	LYS	2.8
2	B	94	TYR	2.8
1	E	289	MET	2.8
1	C	41	LEU	2.8
2	B	112	ASP	2.8
2	F	153	ARG	2.8
2	B	28	ASN	2.8
1	A	164	TYR	2.8
1	E	219	VAL	2.8
1	A	10	ASN	2.8
1	E	108	ILE	2.8
1	E	281	PRO	2.8
2	B	46	ASP	2.8
2	F	19	ASP	2.8
1	E	76	TRP	2.8
2	B	100	VAL	2.8
1	E	128	SER	2.8
1	E	22	LYS	2.7
2	B	53	ASN	2.7
2	B	117	ASN	2.7
1	A	300	GLY	2.7
1	A	167	THR	2.7
1	E	213	ILE	2.7
1	A	8	HIS	2.7
1	C	1	ASP	2.7
1	E	310	ARG	2.7
2	F	75	ARG	2.7
1	E	52	LEU	2.7
1	A	163	SER	2.7
2	D	50	ASN	2.7
1	A	25	THR	2.7
1	C	13	THR	2.7
1	E	215	THR	2.7
1	C	169	GLN	2.7
1	C	105	LEU	2.7
1	C	313	LEU	2.7
2	B	89	LEU	2.7
2	B	40	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	54	SER	2.7
2	F	102	MET	2.7
1	E	224	GLY	2.7
1	A	263	THR	2.7
1	A	28	HIS	2.7
2	B	150	GLU	2.7
1	E	94	ASN	2.7
1	C	12	SER	2.7
1	E	262	SER	2.7
2	D	12	GLY	2.7
1	E	232	ILE	2.7
1	E	294	ILE	2.7
2	D	104	ASN	2.6
1	C	269	LEU	2.6
1	A	9	ALA	2.6
1	A	70	PHE	2.6
2	B	63	PHE	2.6
1	A	31	ASP	2.6
1	C	31	ASP	2.6
2	D	112	ASP	2.6
1	C	278	CYS	2.6
1	A	12	SER	2.6
2	B	106	ARG	2.6
1	A	312	VAL	2.6
1	C	26	VAL	2.6
1	C	39	GLY	2.6
1	C	170	GLU	2.6
1	A	315	THR	2.6
2	F	112	ASP	2.6
2	F	53	ASN	2.6
1	C	308	SER	2.6
1	A	17	ASP	2.6
1	E	48	LYS	2.6
2	B	50	ASN	2.6
2	F	114	ASN	2.6
2	F	154	ASN	2.6
2	D	15	GLN	2.6
1	E	269	LEU	2.6
1	A	260	GLY	2.5
1	E	261	ASP	2.5
2	B	41	THR	2.5
1	C	293	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	60	ASN	2.5
1	A	213	ILE	2.5
1	E	160	ILE	2.5
1	E	37	HIS	2.5
1	E	259	LYS	2.5
2	B	96	ALA	2.5
1	C	319	ASN	2.5
1	E	111	PHE	2.5
2	F	30	GLN	2.5
2	F	95	ASN	2.5
1	E	158	PRO	2.5
1	A	282	ILE	2.5
1	A	262	SER	2.5
2	D	113	SER	2.5
2	D	99	LEU	2.5
2	D	109	ASP	2.5
2	B	84	MET	2.5
1	E	78	TYR	2.5
1	E	206	ASN	2.5
1	E	305	TYR	2.5
2	F	94	TYR	2.5
1	A	296	PRO	2.5
1	E	65	PRO	2.5
2	B	105	GLU	2.5
2	F	64	GLU	2.5
2	B	151	SER	2.5
1	E	40	LYS	2.5
2	F	82	LYS	2.5
2	B	134	GLY	2.5
2	F	134	GLY	2.5
1	E	233	LEU	2.5
1	E	17	ASP	2.5
1	E	55	CYS	2.5
1	E	115	GLN	2.5
2	B	107	THR	2.5
1	E	72	ASN	2.5
1	C	137	TYR	2.4
1	E	114	ILE	2.4
1	C	289	MET	2.4
1	C	30	GLN	2.4
1	E	156	ALA	2.4
1	C	25	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	80	VAL	2.4
1	E	112	GLU	2.4
2	B	69	GLU	2.4
2	B	116	LYS	2.4
2	F	83	LYS	2.4
1	E	191	TYR	2.4
1	A	15	GLN	2.4
1	C	89	LEU	2.4
1	E	10	ASN	2.4
1	E	270	GLU	2.4
1	E	36	THR	2.4
1	C	229	PHE	2.4
2	B	123	ARG	2.4
2	F	88	PHE	2.4
1	E	256	ILE	2.4
2	D	46	ASP	2.4
2	B	62	GLN	2.4
1	C	311	LEU	2.4
1	E	172	LEU	2.4
1	E	278	CYS	2.4
1	A	203	SER	2.4
1	C	318	ARG	2.4
1	A	111	PHE	2.4
2	F	77	ILE	2.4
2	D	89	LEU	2.3
1	E	109	ASN	2.3
1	C	22	LYS	2.3
1	C	40	LYS	2.3
1	E	253	ALA	2.3
1	E	318	ARG	2.3
1	E	138	GLN	2.3
1	A	41	LEU	2.3
1	C	292	HIS	2.3
2	D	107	THR	2.3
1	A	278	CYS	2.3
1	A	279	GLN	2.3
1	A	112	GLU	2.3
1	E	245	GLY	2.3
1	C	305	TYR	2.3
1	A	273	ASN	2.3
1	A	286	ASN	2.3
1	E	165	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	154	ASN	2.3
1	E	190	LEU	2.3
1	E	167	THR	2.3
2	F	113	SER	2.3
1	A	170	GLU	2.3
2	B	109	ASP	2.3
2	F	103	GLU	2.3
1	A	292	HIS	2.3
1	A	117	ILE	2.3
2	D	75	ARG	2.3
2	F	106	ARG	2.3
2	F	101	LEU	2.3
1	A	270	GLU	2.2
1	C	14	GLU	2.2
1	E	274	CYS	2.2
2	D	69	GLU	2.2
2	B	120	ASP	2.2
1	C	38	ASN	2.2
1	C	236	ASN	2.2
1	E	60	TRP	2.2
1	E	208	ARG	2.2
1	E	150	LEU	2.2
2	D	97	GLU	2.2
2	F	150	GLU	2.2
2	B	57	ASP	2.2
1	C	258	LYS	2.2
1	A	23	ASN	2.2
1	C	10	ASN	2.2
2	B	104	ASN	2.2
2	D	114	ASN	2.2
2	F	104	ASN	2.2
1	A	299	ILE	2.2
1	C	299	ILE	2.2
1	E	230	TRP	2.2
1	C	50	LEU	2.2
1	E	44	LEU	2.2
1	E	301	GLU	2.2
2	F	78	GLU	2.2
1	E	56	SER	2.2
2	B	113	SER	2.2
1	E	92	PRO	2.2
2	D	90	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	90	CYS	2.2
2	B	87	GLY	2.2
2	F	71	ASN	2.2
1	A	289	MET	2.2
1	E	15	GLN	2.2
1	A	301	GLU	2.2
1	E	254	TYR	2.2
1	C	284	ALA	2.2
1	E	163	SER	2.2
1	E	309	SER	2.2
1	E	258	LYS	2.2
2	D	111	HIS	2.2
1	E	207	GLN	2.2
2	D	78	GLU	2.1
1	C	263	THR	2.1
1	E	77	SER	2.1
1	E	106	SER	2.1
1	A	261	ASP	2.1
1	C	162	ARG	2.1
1	E	169	GLN	2.1
1	A	210	VAL	2.1
1	A	34	GLU	2.1
1	A	44	LEU	2.1
1	E	95	PHE	2.1
1	E	304	LYS	2.1
1	E	308	SER	2.1
1	C	185	ALA	2.1
1	E	134	ALA	2.1
1	C	49	PRO	2.1
1	E	176	TRP	2.1
1	C	139	GLY	2.1
1	C	11	ASN	2.1
1	C	23	ASN	2.1
1	C	259	LYS	2.1
2	B	82	LYS	2.1
2	D	83	LYS	2.1
1	A	269	LEU	2.1
1	E	101	LEU	2.1
1	A	18	THR	2.1
1	A	27	THR	2.1
1	A	276	THR	2.1
1	C	106	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	275	ASN	2.1
2	F	117	ASN	2.1
1	E	103	HIS	2.1
1	E	159	THR	2.1
2	B	88	PHE	2.1
1	C	279	GLN	2.1
2	B	114	ASN	2.0
2	F	69	GLU	2.0
1	E	98	TYR	2.0
1	E	210	VAL	2.0
1	C	17	ASP	2.0
1	E	43	ASP	2.0
1	C	190	LEU	2.0
2	F	85	GLU	2.0
1	E	113	LYS	2.0
1	E	277	LYS	2.0
1	E	135	CYS	2.0
1	C	28	HIS	2.0
1	E	45	ASP	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](#)

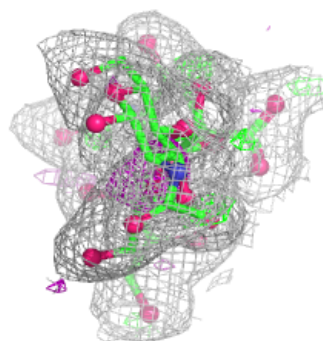
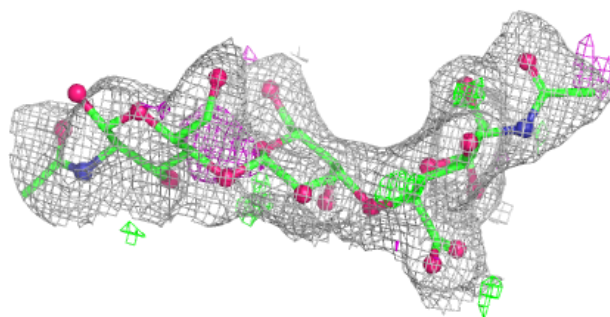
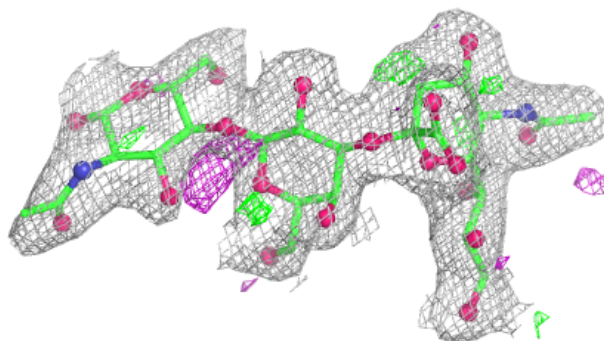
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	G	1	15/15	0.71	0.18	46,56,64,66	0
3	NAG	H	1	15/15	0.81	0.14	43,56,66,68	0
3	GAL	I	2	11/12	0.82	0.12	47,50,54,56	0
3	SIA	I	3	20/21	0.82	0.13	34,40,46,46	0
3	NAG	I	1	15/15	0.83	0.13	62,73,76,78	0
3	GAL	G	2	11/12	0.86	0.12	30,36,37,40	0
3	SIA	H	3	20/21	0.87	0.11	23,25,29,30	0
3	SIA	G	3	20/21	0.88	0.10	26,31,33,34	0
3	GAL	H	2	11/12	0.90	0.09	28,32,34,36	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.

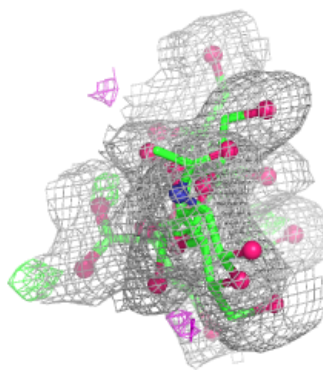
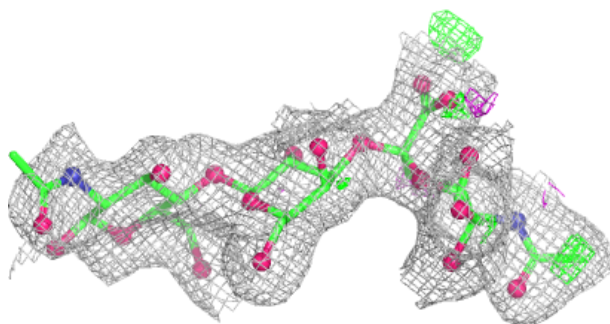
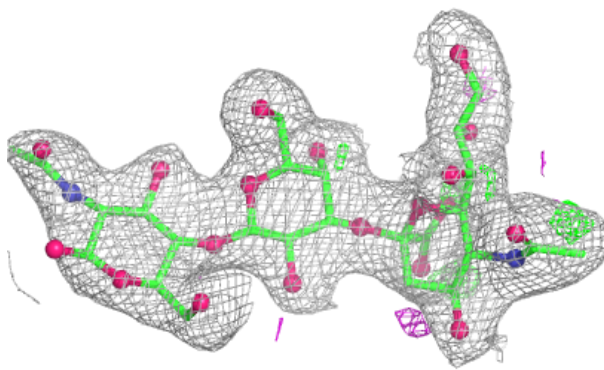
Electron density around Chain G:

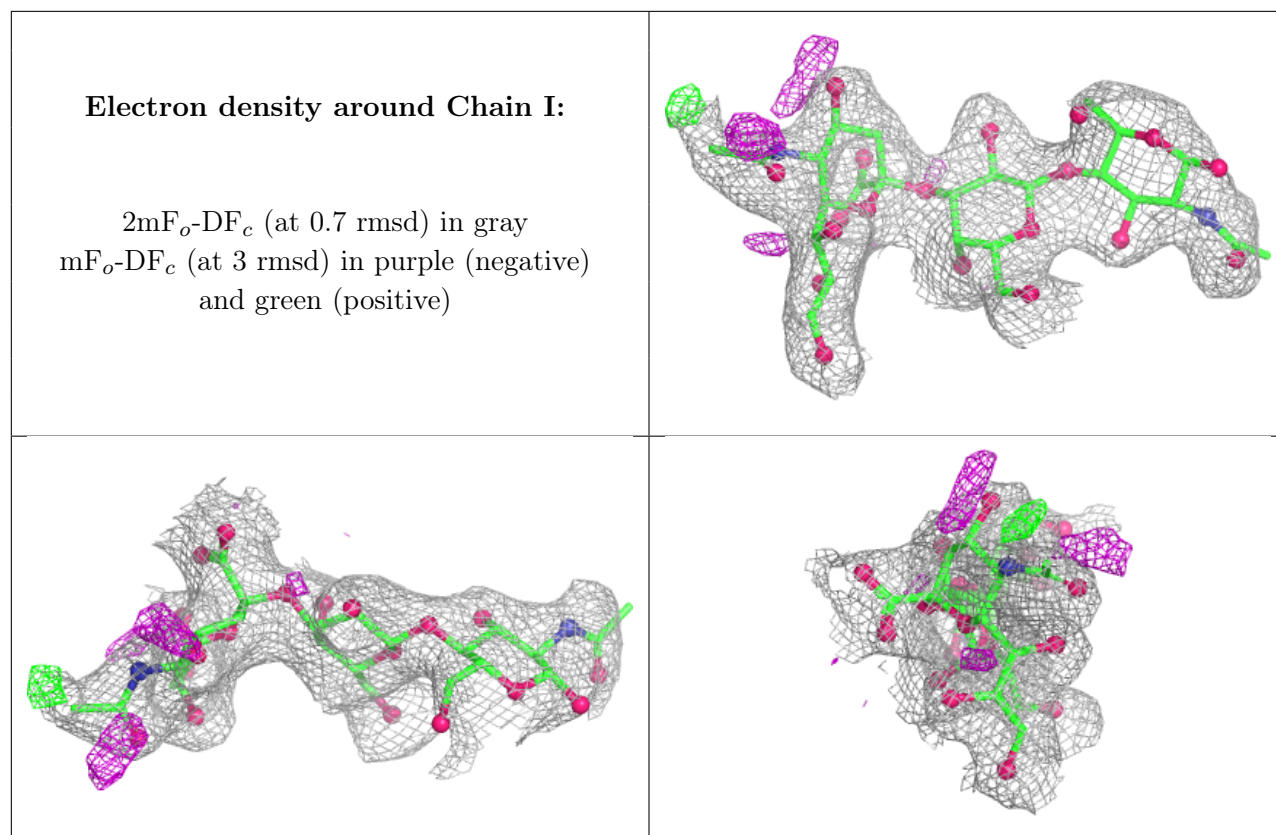
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
5	PO4	E	1324	5/5	0.58	0.17	64,71,74,75	0
5	PO4	A	1325	5/5	0.59	0.21	66,71,78,80	0
5	PO4	C	1324	5/5	0.67	0.18	53,65,67,67	0
4	NAG	C	1320	14/15	0.79	0.13	37,40,47,49	0
4	NAG	E	1320	14/15	0.84	0.12	35,37,46,50	0
5	PO4	A	1324	5/5	0.86	0.16	63,63,67,68	0
4	NAG	A	1320	14/15	0.86	0.10	36,39,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.