



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:24 AM BST

PDB ID : 6E3H
Title : Crystal structure of S9-3-37 bound to H5 influenza hemagglutinin
Authors : Wu, N.C.; Wilson, I.A.
Deposited on : 2018-07-14
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

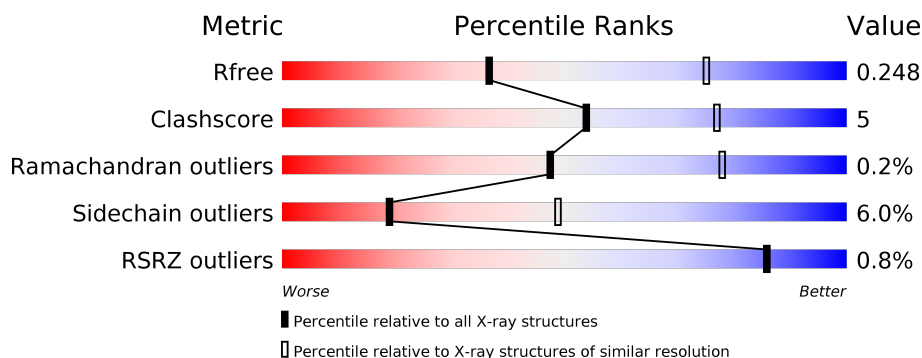
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	324	<div> <div>80%</div> <div>16%</div> <div>• •</div> </div>
2	B	175	<div> <div>88%</div> <div>11%</div> <div>•</div> </div>
3	L	219	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
4	H	233	<div> <div>2%</div> <div>82%</div> <div>12%</div> <div>• •</div> </div>
5	C	2	<div> <div>100%</div> </div>
5	E	2	<div> <div>50%</div> <div>50%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	D	4	 75% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7554 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	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP Q5EP31

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1418	881	246	283	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP Q5EP31

- Molecule 3 is a protein called antibody S9-3-37 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1687	1051	294	336	6			

- Molecule 4 is a protein called antibody S9-3-37 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	226	Total	C	N	O	S	0	0	0
			1734	1106	287	332	9			

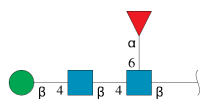
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

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



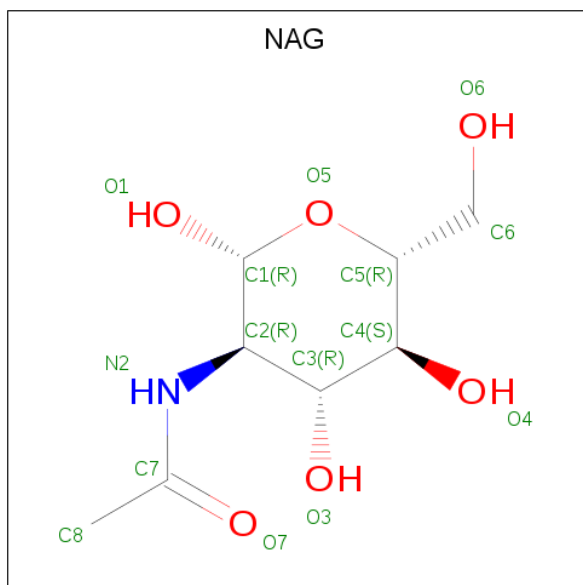
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

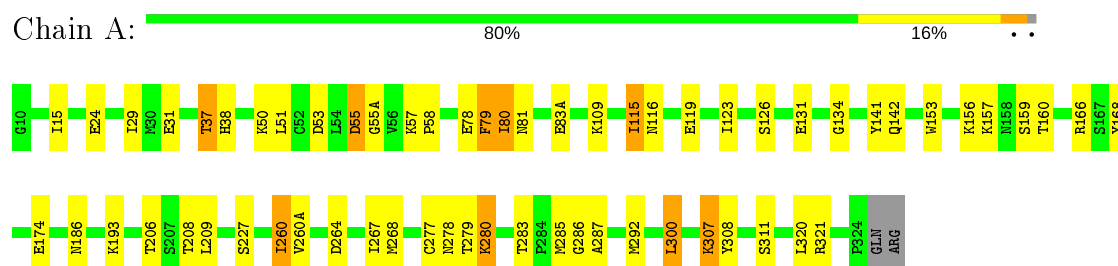
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	O	0	0
			5	5		
8	B	4	Total	O	0	0
			4	4		
8	H	6	Total	O	0	0
			6	6		

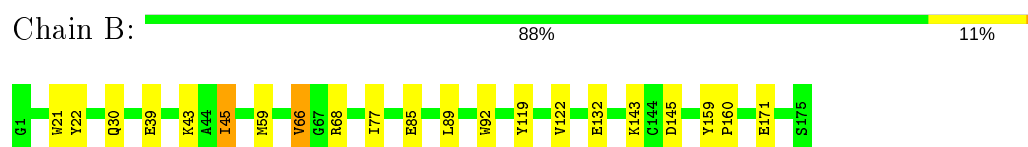
3 Residue-property plots

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.

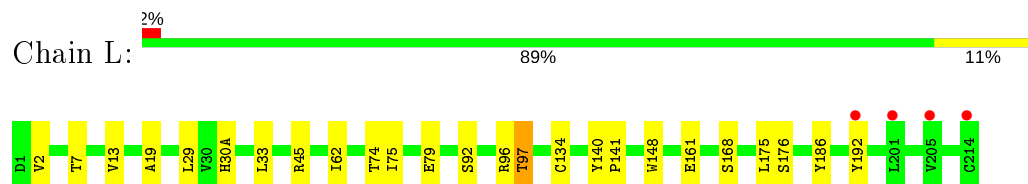
- Molecule 1: Hemagglutinin HA1



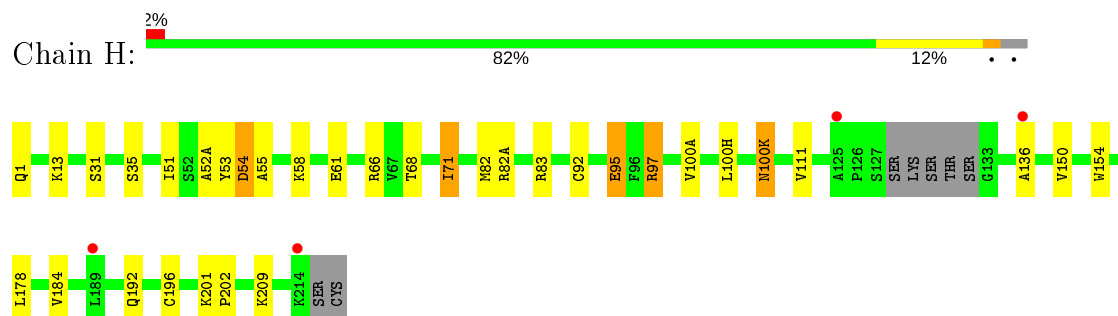
- Molecule 2: Hemagglutinin HA2



- Molecule 3: antibody S9-3-37 light chain



- Molecule 4: antibody S9-3-37 heavy chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

MAG1
MAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  75% 25%

MAG1
MAG2
BMA3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	157.27Å 157.27Å 345.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.44 – 2.90 45.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.44-2.90) 100.0 (45.40-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.205 , 0.248 0.207 , 0.248	Depositor DCC
R_{free} test set	1787 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 16.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7554	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: BMA, NAG, FUC

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	0.36	0/2615	0.59	0/3551
2	B	0.36	0/1445	0.55	0/1942
3	L	0.37	0/1722	0.57	0/2336
4	H	0.37	0/1778	0.60	0/2417
All	All	0.37	0/7560	0.58	0/10246

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2493	40	0
2	B	1418	0	1323	13	0
3	L	1687	0	1657	13	0
4	H	1734	0	1691	21	0
5	C	28	0	25	0	0
5	E	28	0	25	0	0
6	D	49	0	43	1	0
7	A	42	0	39	0	0
8	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	4	0	0	0	0
8	H	6	0	0	0	0
All	All	7554	0	7296	78	0

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

All (78) 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)
4:H:68:THR:OG1	4:H:82(A):ARG:NH1	1.63	1.29
4:H:68:THR:CB	4:H:82(A):ARG:NH1	2.29	0.95
1:A:37:THR:HG22	1:A:38:HIS:CD2	2.09	0.88
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.55	0.88
4:H:68:THR:HG1	4:H:82(A):ARG:HH12	1.17	0.84
1:A:126:SER:OG	1:A:166:ARG:NH1	2.10	0.84
3:L:2:VAL:O	3:L:97:THR:HG21	1.85	0.76
1:A:283:THR:HB	1:A:286:GLY:O	1.91	0.70
3:L:96:ARG:NH2	4:H:95:GLU:OE2	2.25	0.69
1:A:53:ASP:HB2	1:A:278:ASN:HD22	1.58	0.68
4:H:68:THR:CB	4:H:82(A):ARG:HH11	2.04	0.68
1:A:37:THR:CG2	1:A:38:HIS:CD2	2.76	0.68
1:A:55(A):GLY:H	1:A:278:ASN:HD21	1.42	0.68
4:H:68:THR:HB	4:H:82(A):ARG:HH11	1.58	0.67
3:L:13:VAL:HG21	3:L:19:ALA:HB2	1.77	0.67
4:H:52(A):ALA:HA	4:H:71:ILE:HD13	1.77	0.66
2:B:45:ILE:HD13	4:H:100(H):LEU:HD11	1.80	0.62
1:A:80:ILE:HD12	1:A:80:ILE:H	1.66	0.61
1:A:31:GLU:OE2	1:A:321:ARG:NH2	2.37	0.58
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.84	0.58
1:A:186:ASN:HD21	1:A:227:SER:HB3	1.69	0.57
1:A:156:LYS:CE	1:A:193:LYS:O	2.53	0.57
1:A:156:LYS:HE2	1:A:193:LYS:O	2.05	0.56
1:A:186:ASN:HD21	1:A:227:SER:CB	2.19	0.55
1:A:283:THR:HG22	1:A:285:MET:H	1.72	0.54
3:L:30(A):HIS:HE1	4:H:100(A):VAL:H	1.57	0.53
1:A:109:LYS:HB3	1:A:267:ILE:CD1	2.39	0.53
1:A:116:ASN:HB3	1:A:260(A):VAL:HG23	1.91	0.52
1:A:79:PHE:C	1:A:81:ASN:H	2.11	0.51
3:L:186:TYR:CE1	3:L:192:TYR:CE2	2.98	0.51
3:L:62:ILE:HD13	3:L:75:ILE:HG23	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:161:GLU:HA	3:L:176:SER:O	2.11	0.51
1:A:307:LYS:HE3	2:B:59:MET:SD	2.51	0.51
1:A:206:THR:HB	1:A:209:LEU:HB3	1.93	0.51
4:H:154:TRP:CH2	4:H:196:CYS:HB3	2.46	0.50
1:A:279:THR:CG2	1:A:287:ALA:HB1	2.36	0.50
4:H:51:ILE:HG12	4:H:71:ILE:HD12	1.92	0.49
2:B:45:ILE:HD13	4:H:100(H):LEU:CD1	2.43	0.49
1:A:307:LYS:HG2	2:B:92:TRP:CE2	2.47	0.49
3:L:30(A):HIS:HD2	3:L:92:SER:O	1.95	0.49
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.95	0.48
1:A:51:LEU:CD2	1:A:268:MET:CE	2.92	0.48
1:A:308:TYR:CD2	2:B:89:LEU:HD12	2.49	0.48
1:A:123:ILE:HG22	1:A:168:TYR:CZ	2.49	0.47
2:B:68:ARG:HH22	2:B:85:GLU:CD	2.16	0.47
1:A:300:LEU:HA	2:B:66:VAL:HG22	1.96	0.47
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
1:A:79:PHE:C	1:A:81:ASN:N	2.68	0.46
1:A:156:LYS:HD2	1:A:159:SER:HA	1.99	0.45
4:H:35:SER:OG	4:H:95:GLU:OE1	2.26	0.45
1:A:109:LYS:HE2	1:A:267:ILE:HD13	1.98	0.45
1:A:115:ILE:HG13	1:A:260:ILE:HG22	1.98	0.45
3:L:33:LEU:HD13	3:L:33:LEU:C	2.36	0.45
2:B:119:TYR:OH	2:B:132:GLU:HG2	2.17	0.45
4:H:178:LEU:HD12	4:H:178:LEU:C	2.37	0.45
4:H:83:ARG:O	4:H:111:VAL:HG11	2.16	0.45
1:A:131:GLU:HG2	1:A:157:LYS:HD3	1.99	0.45
6:D:1:NAG:O3	6:D:1:NAG:O7	2.28	0.44
1:A:206:THR:HG22	1:A:208:THR:H	1.83	0.43
1:A:55:ASP:OD1	1:A:280:LYS:HE3	2.18	0.43
4:H:201:LYS:N	4:H:202:PRO:CD	2.80	0.43
1:A:79:PHE:O	1:A:81:ASN:N	2.51	0.43
4:H:1:GLN:OE1	4:H:1:GLN:N	2.35	0.43
3:L:175:LEU:C	3:L:175:LEU:HD23	2.39	0.43
2:B:30:GLN:HE22	2:B:145:ASP:HA	1.84	0.43
2:B:21:TRP:CZ3	2:B:45:ILE:HG13	2.54	0.43
1:A:38:HIS:CD2	2:B:21:TRP:HE1	2.37	0.43
4:H:31:SER:O	4:H:97:ARG:HG2	2.19	0.43
2:B:159:TYR:HB3	2:B:160:PRO:HD3	2.00	0.43
1:A:80:ILE:O	1:A:80:ILE:HG22	2.19	0.42
1:A:141:TYR:CD2	1:A:142:GLN:HG3	2.53	0.42
1:A:53:ASP:CB	1:A:278:ASN:HD22	2.31	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:150:VAL:CG2	4:H:178:LEU:HD21	2.50	0.41
3:L:2:VAL:HG11	3:L:29:LEU:HD21	2.03	0.41
1:A:57:LYS:HG2	1:A:58:PRO:HD2	2.02	0.41
4:H:54:ASP:O	4:H:55:ALA:HB3	2.20	0.41
4:H:136:ALA:N	4:H:184:VAL:O	2.51	0.40
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.57	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	320/324 (99%)	303 (95%)	16 (5%)	1 (0%)	41	71
2	B	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
3	L	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
4	H	222/233 (95%)	206 (93%)	15 (7%)	1 (0%)	29	61
All	All	932/951 (98%)	890 (96%)	40 (4%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	100(K)	ASN
1	A	80	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/291 (99%)	268 (93%)	21 (7%)	14	38
2	B	150/150 (100%)	142 (95%)	8 (5%)	22	54
3	L	193/193 (100%)	187 (97%)	6 (3%)	40	74
4	H	190/197 (96%)	176 (93%)	14 (7%)	13	38
All	All	822/831 (99%)	773 (94%)	49 (6%)	19	49

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	29	ILE
1	A	37	THR
1	A	50	LYS
1	A	55	ASP
1	A	78	GLU
1	A	79	PHE
1	A	83(A)	GLU
1	A	115	ILE
1	A	119	GLU
1	A	160	THR
1	A	174	GLU
1	A	260	ILE
1	A	264	ASP
1	A	277	CYS
1	A	280	LYS
1	A	292	MET
1	A	300	LEU
1	A	307	LYS
1	A	311	SER
1	A	320	LEU
2	B	22	TYR
2	B	39	GLU
2	B	43	LYS
2	B	45	ILE
2	B	66	VAL
2	B	77	ILE
2	B	143	LYS
2	B	171	GLU
3	L	7	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	45	ARG
3	L	74	THR
3	L	79	GLU
3	L	97	THR
3	L	168	SER
4	H	13	LYS
4	H	53	TYR
4	H	54	ASP
4	H	58	LYS
4	H	61	GLU
4	H	66	ARG
4	H	71	ILE
4	H	82	MET
4	H	92	CYS
4	H	95	GLU
4	H	97	ARG
4	H	100(K)	ASN
4	H	192	GLN
4	H	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	186	ASN
1	A	196	GLN
1	A	278	ASN
2	B	30	GLN
2	B	79	ASN
2	B	117	ASN
2	B	142	HIS
2	B	146	ASN
3	L	30(A)	HIS
3	L	37	HIS
4	H	99	GLN
4	H	100(K)	ASN
4	H	164	HIS
4	H	192	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 ⓘ

8 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$
5	NAG	C	1	1,5	14,14,15	0.44	0	17,19,21	1.45	4 (23%)
5	NAG	C	2	5	14,14,15	0.51	0	17,19,21	1.90	4 (23%)
6	NAG	D	1	1,6	14,14,15	0.25	0	17,19,21	0.92	0
6	NAG	D	2	6	14,14,15	0.23	0	17,19,21	0.56	0
6	BMA	D	3	6	11,11,12	0.33	0	15,15,17	0.60	0
6	FUC	D	4	6	10,10,11	0.24	0	14,14,16	0.56	0
5	NAG	E	1	2,5	14,14,15	0.50	0	17,19,21	1.05	1 (5%)
5	NAG	E	2	5	14,14,15	0.35	0	17,19,21	0.83	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
5	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
6	NAG	D	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	1/2/19/22	0/1/1/1
6	FUC	D	4	6	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	NAG	C1-O5-C5	5.12	119.13	112.19
5	C	1	NAG	O5-C1-C2	3.65	117.06	111.29
5	C	2	NAG	O5-C5-C6	3.27	112.33	107.20
5	C	1	NAG	C1-O5-C5	2.89	116.10	112.19
5	E	1	NAG	C4-C3-C2	2.81	115.13	111.02
5	C	2	NAG	C8-C7-N2	2.61	120.51	116.10
5	C	2	NAG	C2-N2-C7	2.60	126.60	122.90
5	C	1	NAG	C6-C5-C4	-2.33	107.54	113.00
5	C	1	NAG	C3-C4-C5	2.18	114.13	110.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

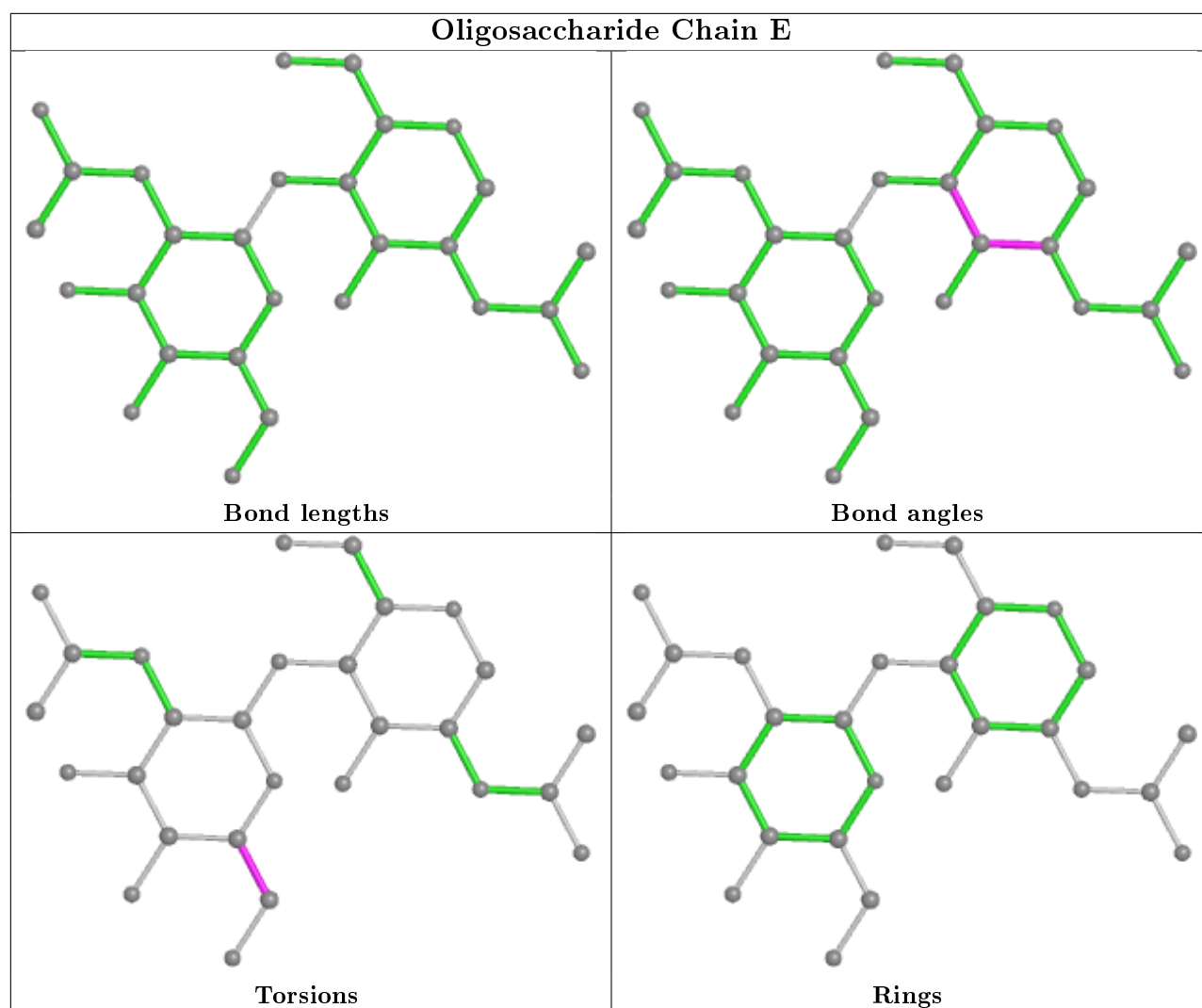
Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C1-C2-N2-C7
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
6	D	1	NAG	C3-C2-N2-C7
6	D	3	BMA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1	NAG	1	0

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



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	$\# Z > 2$
7	NAG	A	405	1	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
7	NAG	A	402	1	14,14,15	0.48	0	17,19,21	1.48	2 (11%)
7	NAG	A	401	1	14,14,15	0.43	0	17,19,21	0.88	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
7	NAG	A	405	1	-	3/6/23/26	0/1/1/1
7	NAG	A	402	1	-	2/6/23/26	0/1/1/1
7	NAG	A	401	1	-	2/6/23/26	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(°)
7	A	402	NAG	C2-N2-C7	3.78	128.28	122.90
7	A	402	NAG	C1-O5-C5	3.61	117.08	112.19
7	A	405	NAG	O5-C5-C6	2.04	110.41	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	402	NAG	C3-C2-N2-C7
7	A	401	NAG	O5-C5-C6-O6
7	A	401	NAG	C4-C5-C6-O6
7	A	402	NAG	O5-C5-C6-O6
7	A	405	NAG	C4-C5-C6-O6
7	A	405	NAG	O5-C5-C6-O6
7	A	405	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/324 (99%)	-0.38	0 100 100	46, 71, 97, 141	0
2	B	175/175 (100%)	-0.33	0 100 100	42, 60, 81, 114	0
3	L	219/219 (100%)	-0.19	4 (1%) 68 67	48, 78, 143, 162	0
4	H	226/233 (96%)	-0.20	4 (1%) 68 67	46, 73, 126, 147	0
All	All	942/951 (99%)	-0.28	8 (0%) 86 86	42, 70, 126, 162	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	136	ALA	3.1
3	L	201	LEU	2.9
4	H	125	ALA	2.5
4	H	214	LYS	2.4
3	L	214	CYS	2.4
3	L	205	VAL	2.4
3	L	192	TYR	2.4
4	H	189	LEU	2.3

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

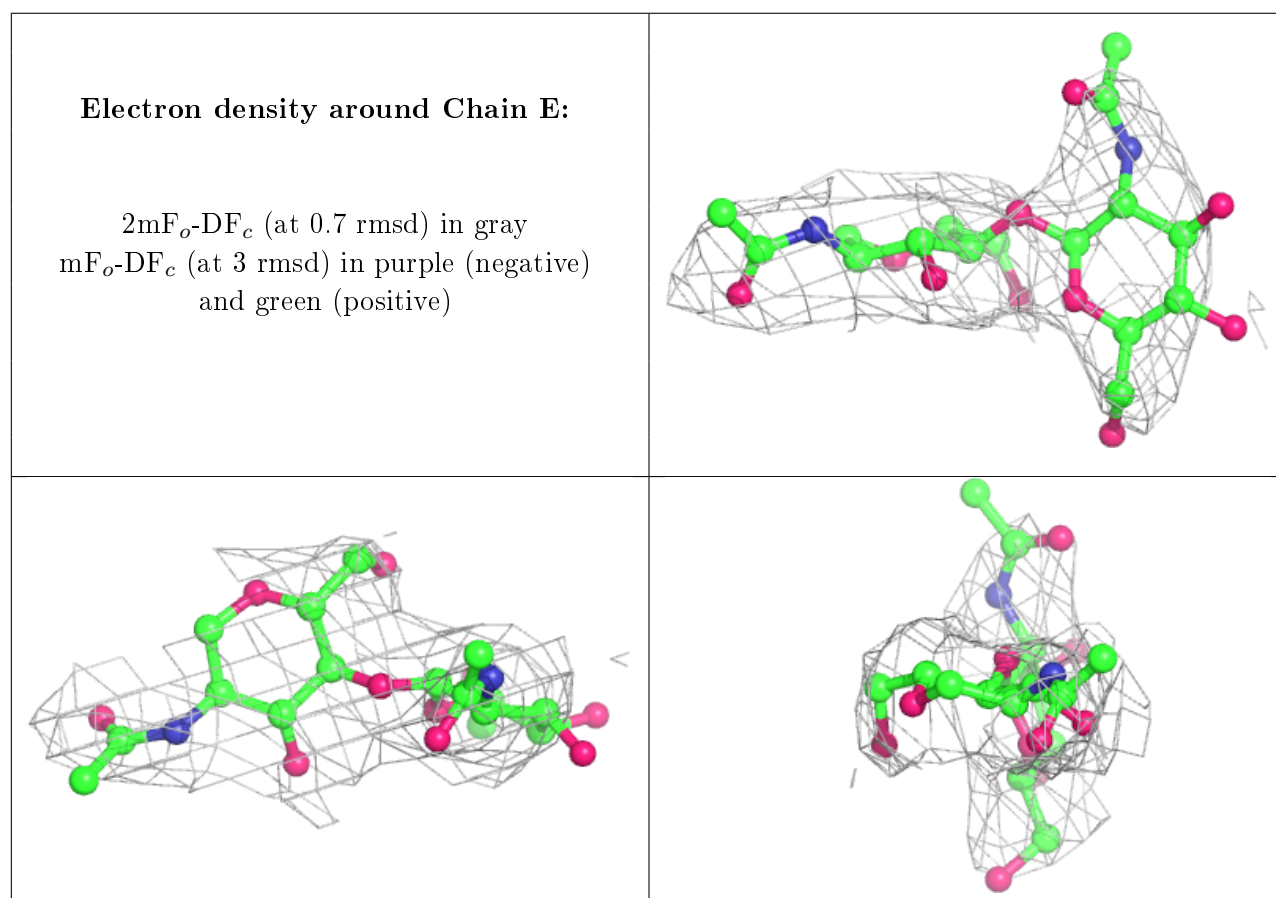
There are no non-standard protein/DNA/RNA residues in this entry.

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
5	NAG	C	1	14/15	0.81	0.39	99,110,118,118	0
5	NAG	C	2	14/15	0.83	0.42	104,119,122,123	0
6	BMA	D	3	11/12	0.85	0.31	129,135,136,136	0
6	NAG	D	1	14/15	0.87	0.13	81,88,104,108	0
5	NAG	E	2	14/15	0.87	0.38	120,129,137,141	0
5	NAG	E	1	14/15	0.89	0.26	94,102,111,121	0
6	NAG	D	2	14/15	0.91	0.19	101,112,121,131	0
6	FUC	D	4	10/11	0.92	0.29	107,112,113,113	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 ⓘ

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
7	NAG	A	401	14/15	0.77	0.19	84,93,101,101	0
7	NAG	A	402	14/15	0.78	0.32	110,121,123,125	0
7	NAG	A	405	14/15	0.82	0.20	112,122,127,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.