



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:18 AM UTC

PDB ID : 9S8W / pdb_00009s8w
Title : Human heparanase in complex with neutralizing antibody A54 Fab fragment
Authors : Wu, L.
Deposited on : 2025-08-05
Resolution : 3.49 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

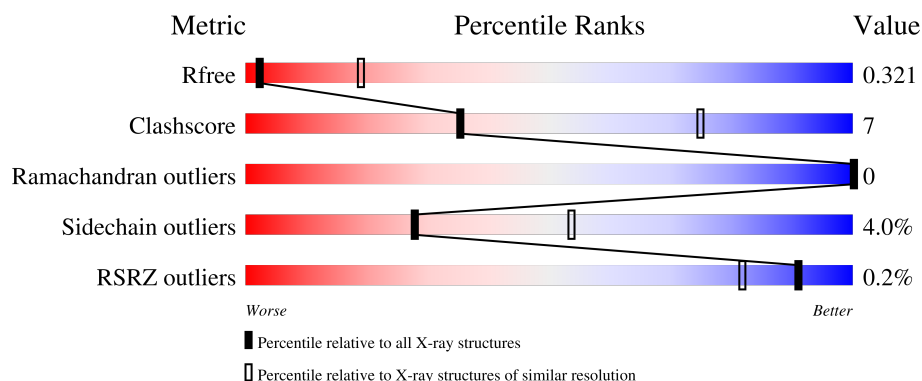
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	386	% 90% 8% .
2	B	74	80% 20%
3	H	222	72% 23% 5%
4	L	218	67% 29% .
5	C	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14031 atoms, of which 6951 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 Heparanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	H	N	O	S	82	0	0
			6097	1959	3066	515	546	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	ARG	LYS	variant	UNP Q9Y251

- Molecule 2 is a protein called Heparanase 8 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	H	N	O	14	0	0
			1187	383	601	95	108			

- Molecule 3 is a protein called A54 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	222	Total	C	H	N	O	S	74	0	0
			3296	1058	1615	274	340	9			

- Molecule 4 is a protein called A54 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	L	218	Total	C	H	N	O	S	68	0	0
			3288	1052	1603	277	349	7			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	2	Total	C	H	N	O	8	0	0
			48	14	24	1	9			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	6	0
			28	8	14	1	5		
6	A	1	Total	C	H	N	O	6	0
			28	8	14	1	5		
6	A	1	Total	C	H	N	O	6	0
			28	8	14	1	5		

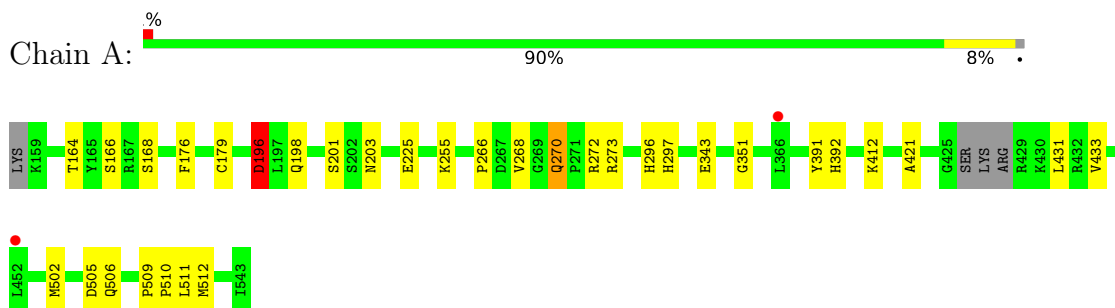
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total	O	0	0
			19	19		
7	B	2	Total	O	0	0
			2	2		
7	H	6	Total	O	0	0
			6	6		
7	L	4	Total	O	0	0
			4	4		

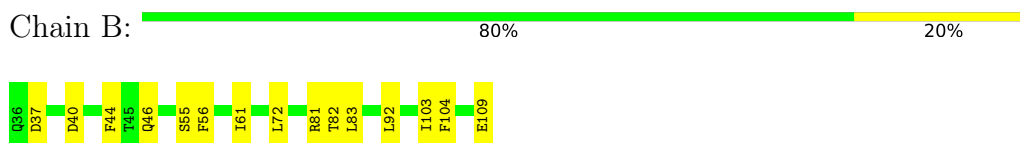
3 Residue-property plots [i](#)

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.

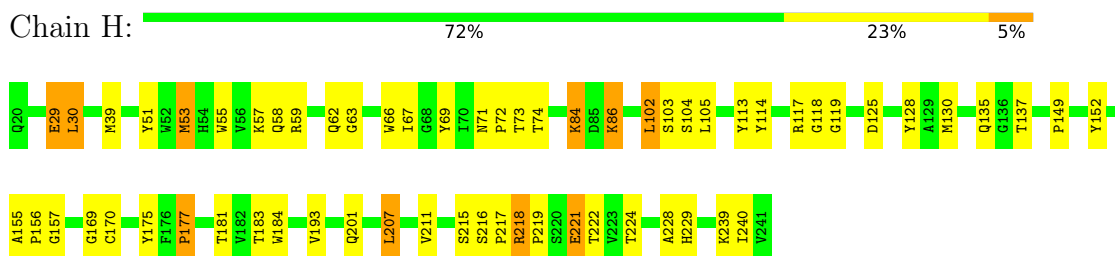
- Molecule 1: Heparanase



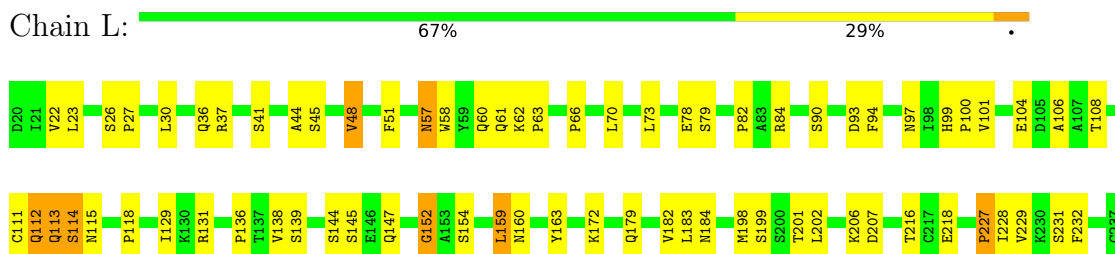
- Molecule 2: Heparanase 8 kDa subunit



- Molecule 3: A54 Fab heavy chain



- Molecule 4: A54 Fab light chain



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.74Å 69.74Å 429.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.44 – 3.49 107.44 – 3.49	Depositor EDS
% Data completeness (in resolution range)	63.4 (107.44-3.49) 63.4 (107.44-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.220 , 0.323 0.218 , 0.321	Depositor DCC
R_{free} test set	465 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 110.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14031	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.60	0/3104	1.11	6/4199 (0.1%)
2	B	0.59	0/600	1.16	2/814 (0.2%)
3	H	0.70	1/1726 (0.1%)	1.27	5/2357 (0.2%)
4	L	0.65	0/1724	1.30	11/2343 (0.5%)
All	All	0.64	1/7154 (0.0%)	1.20	24/9713 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	HIS	CE1-NE2	-5.49	1.27	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	ASP	CA-CB-CG	12.09	124.69	112.60
1	A	225	GLU	CB-CA-C	7.59	116.59	111.20
3	H	201	GLN	CB-CA-C	-7.14	100.79	111.72
4	L	57	ASN	CB-CA-C	6.20	120.49	109.65
2	B	40	ASP	CA-CB-CG	6.14	118.74	112.60
3	H	29	GLU	CB-CG-CD	6.14	123.03	112.60
4	L	51	PHE	CB-CA-C	5.72	121.79	110.42
1	A	196	ASP	CA-CB-CG	5.71	118.31	112.60
4	L	97	ASN	CB-CA-C	5.63	118.46	110.24
1	A	351	GLY	CA-C-O	-5.56	118.13	122.52
3	H	221	GLU	CB-CA-C	-5.54	99.68	109.70
3	H	86	LYS	N-CA-CB	-5.44	102.76	110.81
4	L	227	PRO	N-CA-C	5.41	119.69	111.15
4	L	179	GLN	N-CA-CB	-5.38	103.45	110.88
4	L	93	ASP	CB-CA-C	5.37	119.54	110.79
3	H	125	ASP	CA-CB-CG	5.36	117.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	LYS	CB-CA-C	-5.33	100.89	110.37
1	A	176	PHE	CA-CB-CG	-5.30	108.50	113.80
4	L	152	GLY	CA-C-O	-5.25	117.00	121.57
2	B	37	ASP	CA-CB-CG	5.10	117.70	112.60
4	L	114	SER	CA-C-N	5.10	127.82	120.38
4	L	114	SER	C-N-CA	5.10	127.82	120.38
4	L	104	GLU	CB-CG-CD	5.04	121.16	112.60
4	L	160	ASN	CA-CB-CG	-5.02	107.58	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3031	3066	3057	16	0
2	B	586	601	597	11	0
3	H	1681	1615	1609	40	0
4	L	1685	1603	1595	50	0
5	C	24	24	22	0	0
6	A	42	42	39	0	0
7	A	19	0	0	2	0
7	B	2	0	0	0	0
7	H	6	0	0	0	0
7	L	4	0	0	1	0
All	All	7080	6951	6919	103	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 7.

All (103) 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:L:57:ASN:HB2	4:L:112:GLN:OE1	1.76	0.85
4:L:26:SER:HB3	4:L:41:SER:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:217:PRO:O	3:H:221:GLU:HB2	1.97	0.65
3:H:66:TRP:HZ3	4:L:118:PRO:HB3	1.61	0.65
3:H:224:THR:HG22	3:H:239:LYS:HA	1.78	0.64
1:A:164:THR:HA	2:B:103:ILE:O	1.98	0.64
1:A:270:GLN:HG2	1:A:297:HIS:HA	1.81	0.63
1:A:168:SER:HB3	2:B:109:GLU:O	1.99	0.63
4:L:26:SER:HB3	4:L:27:PRO:HD3	1.82	0.61
4:L:206:LYS:O	4:L:207:ASP:HB2	2.02	0.60
4:L:172:LYS:HB2	4:L:216:THR:HB	1.84	0.59
3:H:114:TYR:CE1	4:L:66:PRO:HB3	2.37	0.59
3:H:58:GLN:OE1	4:L:61:GLN:NE2	2.36	0.59
4:L:78:GLU:HG3	4:L:79:SER:H	1.68	0.58
4:L:106:ALA:HB2	4:L:129:ILE:HD12	1.84	0.58
3:H:117:ARG:HG2	3:H:118:GLY:H	1.69	0.58
4:L:113:GLN:HG2	4:L:115:ASN:H	1.71	0.56
3:H:102:LEU:HB3	3:H:105:LEU:HD21	1.88	0.56
4:L:136:PRO:HG2	4:L:228:ILE:HD12	1.87	0.55
1:A:203:ASN:HD21	2:B:104:PHE:HB3	1.71	0.54
3:H:207:LEU:HD12	3:H:207:LEU:C	2.32	0.54
4:L:182:VAL:HG22	4:L:202:LEU:HD13	1.90	0.54
2:B:61:ILE:HG12	2:B:92:LEU:HD11	1.90	0.54
3:H:86:LYS:HD3	3:H:103:SER:O	2.08	0.54
3:H:193:VAL:HA	3:H:211:VAL:HG22	1.89	0.53
4:L:36:GLN:O	4:L:101:VAL:HG23	2.07	0.53
1:A:512:MET:HA	1:A:512:MET:HE2	1.90	0.53
3:H:152:TYR:HB3	4:L:144:SER:OG	2.09	0.52
3:H:51:TYR:HA	3:H:119:GLY:O	2.10	0.51
4:L:30:LEU:HD12	4:L:30:LEU:O	2.11	0.51
4:L:90:SER:HA	4:L:94:PHE:CE2	2.45	0.50
4:L:184:ASN:HD22	4:L:184:ASN:N	2.10	0.50
4:L:66:PRO:HD3	7:L:303:HOH:O	2.10	0.50
3:H:216:SER:N	3:H:217:PRO:HD2	2.26	0.50
1:A:166:SER:HB2	2:B:109:GLU:C	2.37	0.49
3:H:58:GLN:HG3	3:H:63:GLY:O	2.11	0.49
3:H:181:THR:HB	3:H:228:ALA:HB3	1.94	0.49
4:L:82:PRO:HB2	4:L:84:ARG:HG2	1.93	0.49
1:A:412:LYS:HD2	1:A:511:LEU:HD12	1.93	0.49
3:H:57:LYS:HB2	3:H:67:ILE:HD11	1.95	0.48
1:A:421:ALA:CB	1:A:433:VAL:HG22	2.44	0.48
4:L:37:ARG:HG2	4:L:99:HIS:HB3	1.95	0.48
3:H:58:GLN:CD	4:L:61:GLN:HE22	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:701:HOH:O	2:B:81:ARG:HB3	2.14	0.47
4:L:78:GLU:HG3	4:L:79:SER:N	2.30	0.47
1:A:510:PRO:HB2	1:A:512:MET:HE3	1.96	0.47
3:H:30:LEU:HB3	3:H:177:PRO:HG3	1.96	0.46
4:L:78:GLU:CG	4:L:79:SER:H	2.28	0.46
1:A:266:PRO:HG2	1:A:268:VAL:HG13	1.96	0.46
3:H:39:MET:HE2	3:H:55:TRP:HZ3	1.81	0.46
1:A:502:MET:HA	1:A:509:PRO:HD3	1.97	0.46
4:L:106:ALA:HB2	4:L:129:ILE:CD1	2.46	0.46
3:H:218:ARG:N	3:H:219:PRO:HD2	2.31	0.46
4:L:218:GLU:HG2	4:L:227:PRO:HB2	1.98	0.46
4:L:58:TRP:CZ3	4:L:111:CYS:HB3	2.50	0.45
2:B:72:LEU:C	2:B:72:LEU:HD23	2.42	0.45
3:H:39:MET:HE3	3:H:137:THR:HB	1.98	0.45
3:H:59:ARG:HB2	3:H:62:GLN:HB2	1.99	0.45
4:L:112:GLN:HG2	4:L:113:GLN:N	2.31	0.45
3:H:39:MET:HE1	3:H:113:TYR:HB2	1.99	0.45
4:L:172:LYS:HE2	4:L:218:GLU:OE1	2.16	0.45
4:L:138:VAL:HG22	4:L:159:LEU:HD12	1.98	0.45
3:H:117:ARG:O	3:H:130:MET:HA	2.17	0.45
1:A:196:ASP:HB2	1:A:198:GLN:HG2	2.00	0.44
3:H:149:PRO:HB3	3:H:175:TYR:HB3	2.00	0.44
1:A:502:MET:SD	2:B:83:LEU:HD21	2.58	0.44
3:H:128:TYR:C	4:L:114:SER:HG	2.24	0.44
3:H:222:THR:HG22	3:H:239:LYS:HE3	1.99	0.44
3:H:135:GLN:H	3:H:135:GLN:HG2	1.57	0.43
4:L:36:GLN:HG2	4:L:37:ARG:H	1.82	0.43
4:L:48:VAL:HG13	4:L:115:ASN:HB2	2.00	0.43
2:B:44:PHE:CZ	2:B:46:GLN:HB2	2.53	0.43
3:H:71:ASN:HB3	3:H:74:THR:OG1	2.19	0.43
3:H:128:TYR:O	4:L:114:SER:OG	2.32	0.43
4:L:22:VAL:O	4:L:44:ALA:HA	2.19	0.43
4:L:23:LEU:HD11	4:L:113:GLN:HB3	2.00	0.43
3:H:104:SER:O	3:H:104:SER:OG	2.35	0.42
4:L:147:GLN:HG2	4:L:152:GLY:O	2.19	0.42
4:L:159:LEU:HD22	4:L:159:LEU:H	1.84	0.42
1:A:179:CYS:C	7:A:701:HOH:O	2.62	0.42
3:H:117:ARG:HG2	3:H:118:GLY:N	2.33	0.42
4:L:60:GLN:HB2	4:L:70:LEU:HD11	2.01	0.42
3:H:84:LYS:HB2	3:H:84:LYS:HE3	1.81	0.42
3:H:130:MET:HE3	4:L:112:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:206:LYS:O	4:L:207:ASP:CB	2.68	0.42
3:H:155:ALA:HB2	3:H:240:ILE:CG2	2.49	0.41
4:L:198:MET:HG2	4:L:199:SER:N	2.35	0.41
4:L:22:VAL:H	4:L:45:SER:HB3	1.86	0.41
1:A:296:HIS:CG	1:A:343:GLU:HB3	2.56	0.41
3:H:169:GLY:C	3:H:184:TRP:HH2	2.29	0.41
4:L:62:LYS:O	4:L:63:PRO:C	2.63	0.41
4:L:231:SER:OG	4:L:232:PHE:N	2.53	0.41
2:B:55:SER:O	2:B:56:PHE:C	2.64	0.41
3:H:155:ALA:HB1	3:H:156:PRO:HD2	2.02	0.41
4:L:159:LEU:HD22	4:L:159:LEU:N	2.36	0.41
1:A:506:GLN:C	2:B:82:THR:HG21	2.46	0.41
3:H:71:ASN:HA	3:H:72:PRO:HD3	1.92	0.41
4:L:147:GLN:OE1	4:L:154:SER:HB3	2.21	0.41
4:L:138:VAL:HG12	4:L:139:SER:N	2.35	0.41
4:L:131:ARG:HD3	4:L:163:TYR:HB2	2.03	0.40
4:L:216:THR:CG2	4:L:229:VAL:HG13	2.52	0.40
3:H:156:PRO:O	3:H:157:GLY:C	2.65	0.40
3:H:53:MET:HE3	3:H:53:MET:HB2	1.81	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	378/386 (98%)	371 (98%)	7 (2%)	0	100	100
2	B	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
3	H	220/222 (99%)	199 (90%)	21 (10%)	0	100	100
4	L	216/218 (99%)	202 (94%)	14 (6%)	0	100	100
All	All	886/900 (98%)	843 (95%)	43 (5%)	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	332/336 (99%)	324 (98%)	8 (2%)	43	64
2	B	66/66 (100%)	66 (100%)	0	100	100
3	H	187/187 (100%)	174 (93%)	13 (7%)	14	39
4	L	190/191 (100%)	180 (95%)	10 (5%)	20	47
All	All	775/780 (99%)	744 (96%)	31 (4%)	28	54

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	A	201	SER
1	A	270	GLN
1	A	272	ARG
1	A	273	ARG
1	A	391	TYR
1	A	392	HIS
1	A	431	LEU
3	H	29	GLU
3	H	30	LEU
3	H	53	MET
3	H	69	TYR
3	H	73	THR
3	H	84	LYS
3	H	102	LEU
3	H	170	CYS
3	H	177	PRO
3	H	183	THR
3	H	207	LEU
3	H	215	SER
3	H	218	ARG
4	L	48	VAL

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Mol	Chain	Res	Type
4	L	73	LEU
4	L	100	PRO
4	L	108	THR
4	L	112	GLN
4	L	113	GLN
4	L	145	SER
4	L	159	LEU
4	L	183	LEU
4	L	201	THR

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	324	GLN
3	H	135	GLN
4	L	61	GLN
4	L	168	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$
5	NAG	C	1	5,1	14,14,15	0.75	0	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	C	2	5	10,10,11	0.56	0	14,14,16	1.37	1 (7%)

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	5,1	-	4/6/23/26	0/1/1/1
5	FUC	C	2	5	-	-	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(°)
5	C	2	FUC	C1-O5-C5	2.92	119.86	112.97
5	C	1	NAG	C3-C4-C5	-2.86	105.05	110.23
5	C	1	NAG	O5-C5-C4	-2.19	105.50	110.83

There are no chirality outliers.

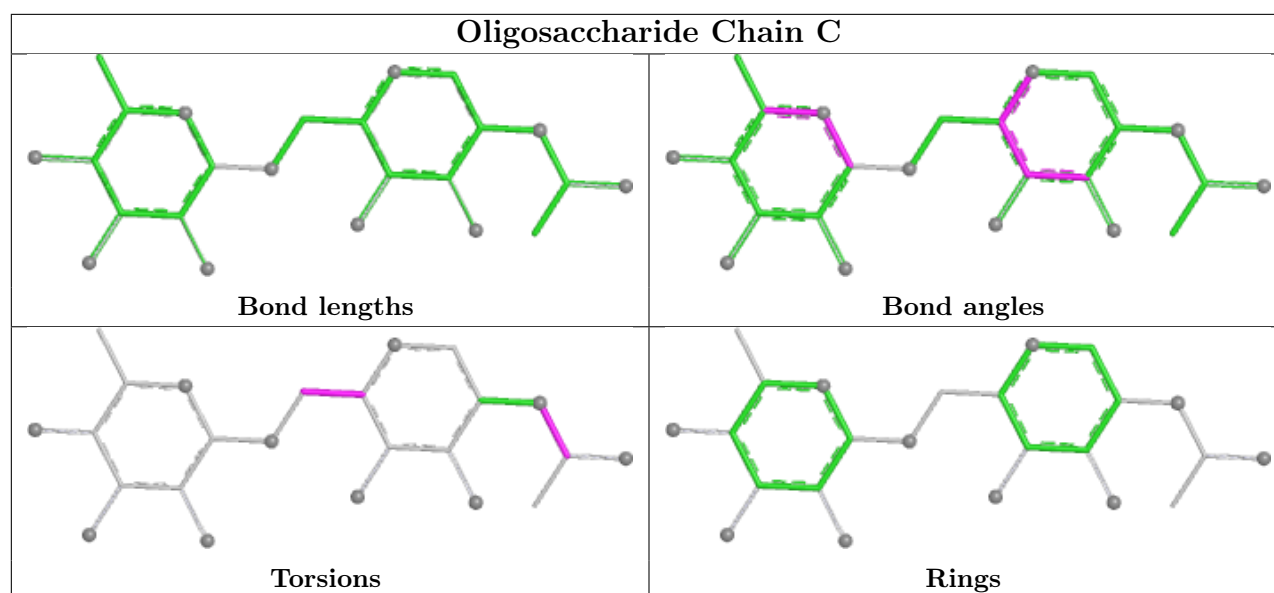
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
5	C	1	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-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.



5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	601	1	14,14,15	0.56	0	17,19,21	0.83	1 (5%)
6	NAG	A	602	1	14,14,15	0.49	0	17,19,21	0.79	0
6	NAG	A	603	1	14,14,15	0.74	0	17,19,21	1.26	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	601	1	-	4/6/23/26	0/1/1/1
6	NAG	A	602	1	-	4/6/23/26	0/1/1/1
6	NAG	A	603	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($^{\circ}$)	Ideal($^{\circ}$)
6	A	603	NAG	C1-O5-C5	2.72	115.83	112.19
6	A	601	NAG	C1-O5-C5	2.30	115.27	112.19
6	A	603	NAG	O3-C3-C2	2.13	113.83	109.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	NAG	C8-C7-N2-C2
6	A	601	NAG	O7-C7-N2-C2
6	A	603	NAG	O5-C5-C6-O6
6	A	603	NAG	C4-C5-C6-O6
6	A	602	NAG	C8-C7-N2-C2
6	A	602	NAG	O7-C7-N2-C2
6	A	601	NAG	O5-C5-C6-O6
6	A	602	NAG	O5-C5-C6-O6
6	A	602	NAG	C4-C5-C6-O6
6	A	601	NAG	C4-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 [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	382/386 (98%)	-0.56	2 (0%) 87 68	84, 131, 176, 223	0
2	B	74/74 (100%)	-0.58	0 100 100	102, 139, 166, 187	0
3	H	222/222 (100%)	-0.43	0 100 100	76, 138, 292, 356	0
4	L	218/218 (100%)	-0.69	0 100 100	84, 139, 221, 251	0
All	All	896/900 (99%)	-0.56	2 (0%) 91 82	76, 135, 217, 356	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	LEU	2.6
1	A	452	LEU	2.4

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

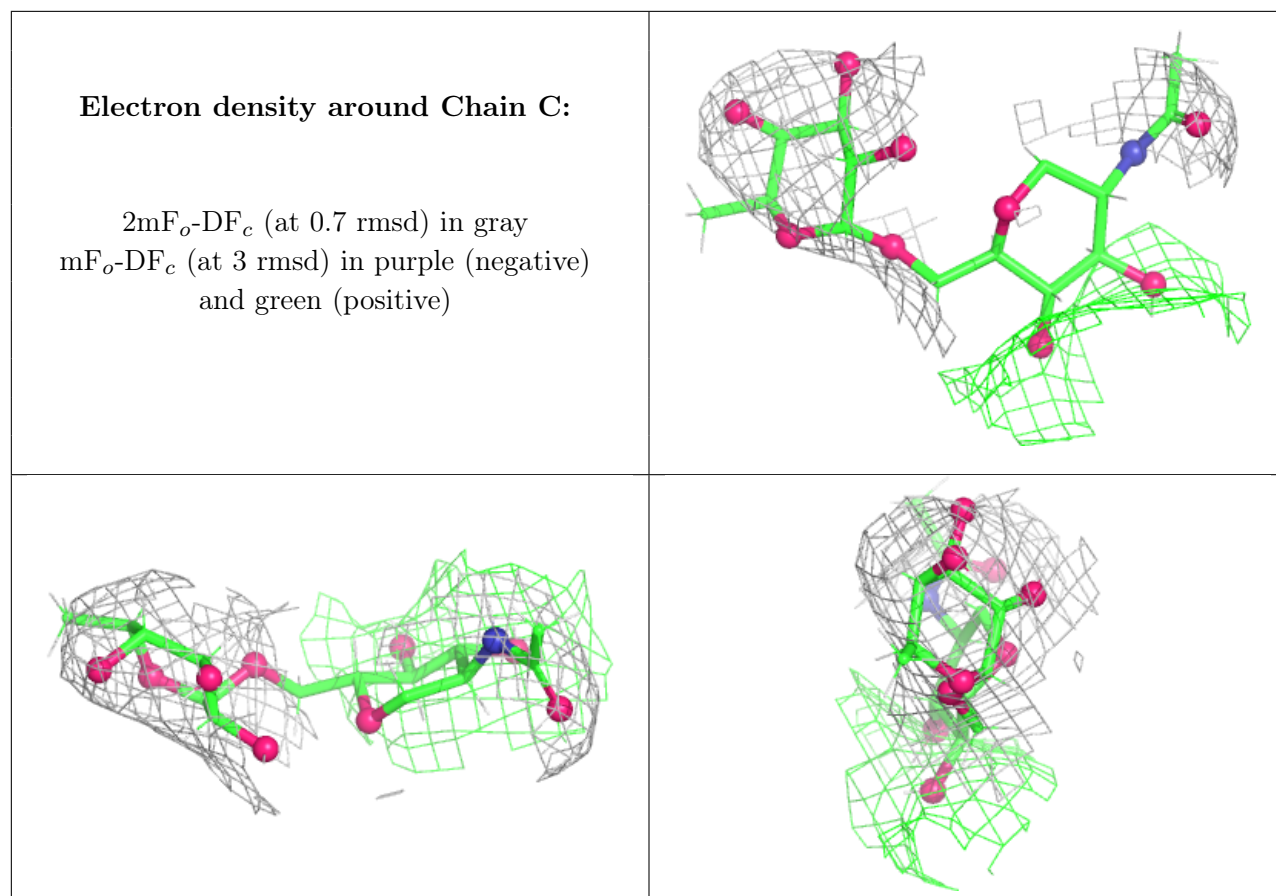
There are no non-standard protein/DNA/RNA residues in this entry.

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
5	NAG	C	1	14/15	-	-	30,153,177,186	5
5	FUC	C	2	10/11	-	-	30,163,182,190	3

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
6	NAG	A	601	14/15	0.58	0.10	30,134,142,150	6
6	NAG	A	603	14/15	0.60	0.08	30,169,178,178	6
6	NAG	A	602	14/15	0.77	0.06	30,156,172,172	6

6.5 Other polymers [i](#)

There are no such residues in this entry.