



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2026 – 02:16 PM JST

PDB ID : 9W6S / pdb\_00009w6s  
Title : hCA450-21.1 Fab and GD2 complex  
Authors : Deyong, S.; Muding, R.  
Deposited on : 2025-08-05  
Resolution : 1.69 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](mailto: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	:	1.8.5 (274361), CSD as541be (2020)
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

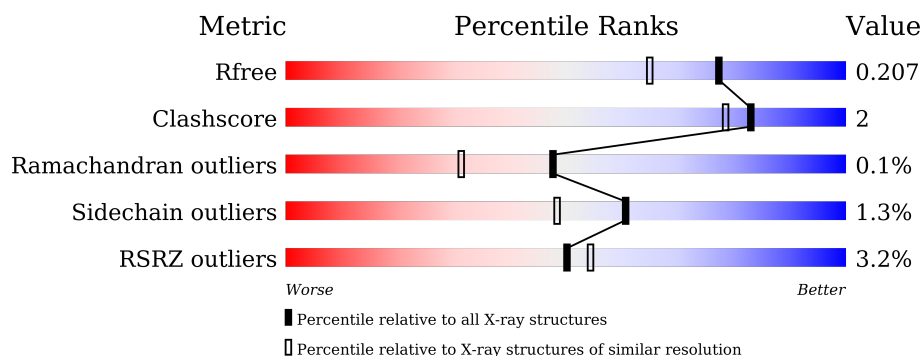
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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  $\geq 3$ , 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	213	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>93%</span> <span>7%</span> </div> </div>
1	B	213	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>95%</span> <span>..</span> </div> </div>
2	C	216	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>4%</span> <span>90%</span> <span>9%</span> </div> </div>
2	D	216	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>6%</span> <span>92%</span> <span>6% .</span> </div> </div>
3	E	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>100%</span> </div> </div>
3	F	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>100%</span> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14028 atoms, of which 6515 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.

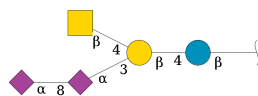
- Molecule 1 is a protein called Light chain of GD2 antibody hCA450-21.1 Fab.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	H	N	O	S	68	2	0
			3282	1042	1616	281	337	6			
1	B	210	Total	C	H	N	O	S	67	0	0
			3234	1028	1595	276	330	5			

- Molecule 2 is a protein called Heavy chain of GD2 antibody hCA450-21.1 Fab.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	216	Total	C	H	N	O	S	75	2	0
			3201	1007	1587	278	321	8			
2	D	216	Total	C	H	N	O	S	74	0	0
			3189	1004	1581	277	319	8			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-[2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	5	Total	C	H	N	O	27	0	0
			145	42	68	3	32			
3	F	5	Total	C	H	N	O	27	0	0
			145	42	68	3	32			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

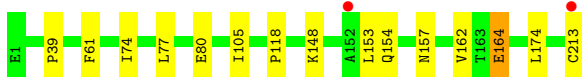
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	236	Total	O	0	0
			236	236		
5	B	206	Total	O	0	0
			206	206		
5	C	209	Total	O	0	0
			209	209		
5	D	141	Total	O	0	0
			141	141		

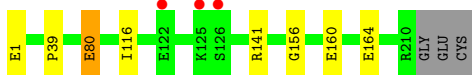
### 3 Residue-property plots [i](#)

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: Light chain of GD2 antibody hCA450-21.1 Fab



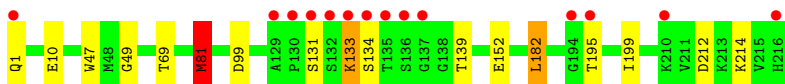
- Molecule 1: Light chain of GD2 antibody hCA450-21.1 Fab



- Molecule 2: Heavy chain of GD2 antibody hCA450-21.1 Fab



- Molecule 2: Heavy chain of GD2 antibody hCA450-21.1 Fab



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-[2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-[2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:

100%

BGC1  
GAL2  
SIA3  
SIA4  
NGA5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.48Å 109.19Å 170.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.55 – 1.69 42.55 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.55-1.69) 99.9 (42.55-1.69)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, $R_{free}$	0.181 , 0.205 0.183 , 0.207	Depositor DCC
$R_{free}$ test set	8080 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 34.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NGA, BGC, GAL, SIA, PO4

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	0.74	0/1710	1.11	3/2320 (0.1%)
1	B	0.73	0/1677	1.12	4/2276 (0.2%)
2	C	0.69	0/1660	1.09	6/2263 (0.3%)
2	D	0.71	0/1646	1.11	6/2244 (0.3%)
All	All	0.72	0/6693	1.11	19/9103 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLN	CB-CA-C	-8.99	92.93	109.37
2	D	81	MET	CG-SD-CE	-7.32	84.79	100.90
1	B	160	GLU	CB-CA-C	-7.11	95.87	109.66
1	B	160	GLU	CG-CD-OE2	-6.38	103.74	118.40
2	C	89	ASP	CA-CB-CG	6.37	118.97	112.60
2	C	87	ARG	CD-NE-CZ	-5.97	116.04	124.40
2	D	212	ASP	CA-CB-CG	5.80	118.40	112.60
2	D	10	GLU	CB-CA-C	-5.68	99.76	110.16
2	C	87	ARG	NE-CZ-NH1	-5.67	115.83	121.50
2	D	99	ASP	CA-CB-CG	5.64	118.24	112.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	80	GLU	CB-CG-CD	5.47	121.90	112.60
2	D	69	THR	CA-CB-OG1	-5.45	101.43	109.60
2	D	152	GLU	CG-CD-OE2	-5.43	105.92	118.40
2	C	87	ARG	CG-CD-NE	5.18	123.39	112.00
2	C	216	HIS	CA-C-O	-5.17	112.01	120.80
2	C	31	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	80	GLU	CG-CD-OE2	-5.07	106.75	118.40
1	B	1	GLU	CB-CG-CD	5.07	121.21	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	141	ARG	Sidechain
2	C	84	ARG	Sidechain

## 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	1666	1616	1606	10	0
1	B	1639	1595	1591	7	0
2	C	1614	1587	1575	9	0
2	D	1608	1581	1576	8	0
3	E	77	68	65	0	0
3	F	77	68	65	0	0
4	A	5	0	0	0	0
4	C	10	0	0	0	0
4	D	25	0	0	0	0
5	A	236	0	0	0	0
5	B	206	0	0	2	0
5	C	209	0	0	2	0
5	D	141	0	0	0	0
All	All	7513	6515	6478	32	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 2.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:87:ARG:HD3	5:C:429:HOH:O	1.84	0.77
2:C:130:PRO:HD3	2:C:142:LEU:HD23	1.79	0.66
1:B:116:ILE:O	2:D:133:LYS:HE2	1.99	0.61
2:D:81:MET:C	2:D:81:MET:HE3	2.28	0.58
2:D:199:ILE:HD13	2:D:214:LYS:HA	1.87	0.56
1:B:39:PRO:CG	1:B:164:GLU:HG3	2.37	0.55
1:B:39:PRO:HG2	1:B:164:GLU:HG3	1.90	0.54
1:B:80:GLU:HG3	5:B:306:HOH:O	2.07	0.54
1:A:148:LYS:HG2	1:A:153:LEU:HD22	1.90	0.54
2:C:207:SER:OG	2:C:209:THR:HG23	2.07	0.53
1:B:39:PRO:HG2	1:B:164:GLU:CB	2.38	0.52
2:C:131:SER:O	2:C:135:THR:HG23	2.09	0.52
1:A:157[B]:ASN:OD1	1:A:157[B]:ASN:N	2.44	0.51
1:A:148:LYS:HE2	1:A:153:LEU:CD2	2.41	0.50
1:A:153:LEU:HD12	1:B:156:GLY:HA3	1.95	0.49
1:B:164:GLU:HB2	5:B:472:HOH:O	2.12	0.49
1:A:39:PRO:CB	1:A:164:GLU:HG3	2.43	0.48
2:D:131:SER:HB2	2:D:133:LYS:HE3	1.97	0.47
2:C:182:LEU:C	2:C:182:LEU:HD12	2.41	0.46
2:C:81:MET:HE3	2:C:81:MET:HB3	1.90	0.46
2:C:1:GLN:HA	5:C:506:HOH:O	2.17	0.45
1:A:148:LYS:HE2	1:A:153:LEU:HD22	1.99	0.45
1:A:77:LEU:HD21	1:A:105:ILE:HD12	1.98	0.45
2:D:182:LEU:C	2:D:182:LEU:HD12	2.43	0.43
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.53	0.43
2:D:81:MET:HE3	2:D:81:MET:HB3	1.67	0.43
1:A:118:PRO:CG	1:A:213:CYS:HB3	2.48	0.42
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.54	0.42
2:C:205:LYS:N	2:C:206:PRO:CD	2.82	0.42
2:D:134:SER:O	2:D:139:THR:O	2.38	0.41
1:A:61:PHE:CE1	1:A:74:ILE:HG12	2.56	0.41
1:A:162:VAL:HG22	1:A:174:LEU:HD12	2.03	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/213 (100%)	209 (98%)	4 (2%)	0	100	100
1	B	208/213 (98%)	204 (98%)	4 (2%)	0	100	100
2	C	216/216 (100%)	210 (97%)	5 (2%)	1 (0%)	24	12
2	D	214/216 (99%)	209 (98%)	5 (2%)	0	100	100
All	All	851/858 (99%)	832 (98%)	18 (2%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	138	GLY

### 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	192/190 (101%)	192 (100%)	0	100	100
1	B	188/190 (99%)	188 (100%)	0	100	100
2	C	184/182 (101%)	179 (97%)	5 (3%)	39	23
2	D	182/182 (100%)	177 (97%)	5 (3%)	39	23
All	All	746/744 (100%)	736 (99%)	10 (1%)	61	48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	10	GLU
2	C	87	ARG
2	C	142	LEU
2	C	153	PRO
2	C	154	VAL
2	D	1	GLN
2	D	81	MET
2	D	133	LYS
2	D	182	LEU
2	D	195	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	37	GLN
1	A	41	GLN
1	A	136	ASN
1	A	146	GLN
1	B	37	GLN
1	B	159	GLN
2	C	1	GLN
2	C	39	GLN
2	C	59	ASN
2	D	1	GLN
2	D	3	GLN
2	D	39	GLN
2	D	65	GLN
2	D	196	GLN
2	D	203	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 ⓘ

10 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	BGC	E	1	3	12,12,12	0.52	0	17,17,17	0.85	1 (5%)
3	GAL	E	2	3	11,11,12	1.13	1 (9%)	15,15,17	1.00	1 (6%)
3	SIA	E	3	3	20,20,21	1.16	2 (10%)	24,28,31	1.25	3 (12%)
3	SIA	E	4	3	20,20,21	0.77	0	24,28,31	1.37	5 (20%)
3	NGA	E	5	3	14,14,15	0.51	0	17,19,21	1.14	2 (11%)
3	BGC	F	1	3	12,12,12	0.64	0	17,17,17	1.22	2 (11%)
3	GAL	F	2	3	11,11,12	0.68	0	15,15,17	1.34	2 (13%)
3	SIA	F	3	3	20,20,21	0.94	1 (5%)	24,28,31	1.26	3 (12%)
3	SIA	F	4	3	20,20,21	1.28	2 (10%)	24,28,31	1.06	1 (4%)
3	NGA	F	5	3	14,14,15	0.38	0	17,19,21	0.96	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
3	BGC	E	1	3	-	0/2/22/22	0/1/1/1
3	GAL	E	2	3	-	0/2/19/22	0/1/1/1
3	SIA	E	3	3	-	3/18/34/38	0/1/1/1
3	SIA	E	4	3	-	0/18/34/38	0/1/1/1
3	NGA	E	5	3	-	0/6/23/26	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	GAL	F	2	3	-	0/2/19/22	0/1/1/1
3	SIA	F	3	3	-	5/18/34/38	0/1/1/1
3	SIA	F	4	3	-	0/18/34/38	0/1/1/1
3	NGA	F	5	3	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	SIA	C2-C1	3.94	1.55	1.52
3	E	3	SIA	C2-C1	3.56	1.55	1.52
3	F	4	SIA	O6-C2	-3.11	1.39	1.43
3	E	2	GAL	C1-C2	2.44	1.57	1.52
3	F	3	SIA	O1B-C1	-2.22	1.23	1.30
3	E	3	SIA	O1B-C1	-2.03	1.23	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GAL	O2-C2-C3	3.34	116.83	110.14
3	F	3	SIA	C6-C5-N5	-2.97	105.97	110.91
3	E	3	SIA	C9-C8-C7	2.75	118.38	112.41
3	E	5	NGA	O3-C3-C2	2.60	114.85	109.47
3	E	3	SIA	O6-C2-C1	2.56	112.72	107.70
3	E	4	SIA	O1B-C1-C2	2.48	120.10	113.03
3	E	4	SIA	O6-C2-C1	2.34	112.28	107.70
3	E	4	SIA	C6-O6-C2	2.32	116.31	111.34
3	E	3	SIA	O9-C9-C8	2.28	116.05	111.07
3	E	4	SIA	C4-C5-N5	2.27	114.87	110.38
3	E	2	GAL	C1-O5-C5	2.27	115.26	112.19
3	F	4	SIA	C4-C3-C2	2.26	113.86	109.81
3	E	5	NGA	C2-N2-C7	2.25	126.10	122.90
3	E	4	SIA	O6-C2-C3	-2.19	107.44	110.46
3	E	1	BGC	O5-C1-C2	-2.17	106.41	110.28
3	F	3	SIA	C9-C8-C7	2.14	117.06	112.41
3	F	5	NGA	O3-C3-C2	2.14	113.90	109.47
3	F	2	GAL	O3-C3-C2	-2.07	106.03	109.99
3	F	1	BGC	C1-O5-C5	-2.02	109.86	113.66
3	F	3	SIA	O7-C7-C8	2.01	113.68	108.81
3	F	1	BGC	O5-C5-C4	-2.00	106.06	109.69

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	SIA	O1A-C1-C2-C3
3	F	3	SIA	O1B-C1-C2-C3
3	F	3	SIA	C7-C8-C9-O9
3	F	3	SIA	O8-C8-C9-O9
3	F	3	SIA	O1A-C1-C2-O6
3	E	3	SIA	O8-C8-C9-O9

*Continued on next page...*

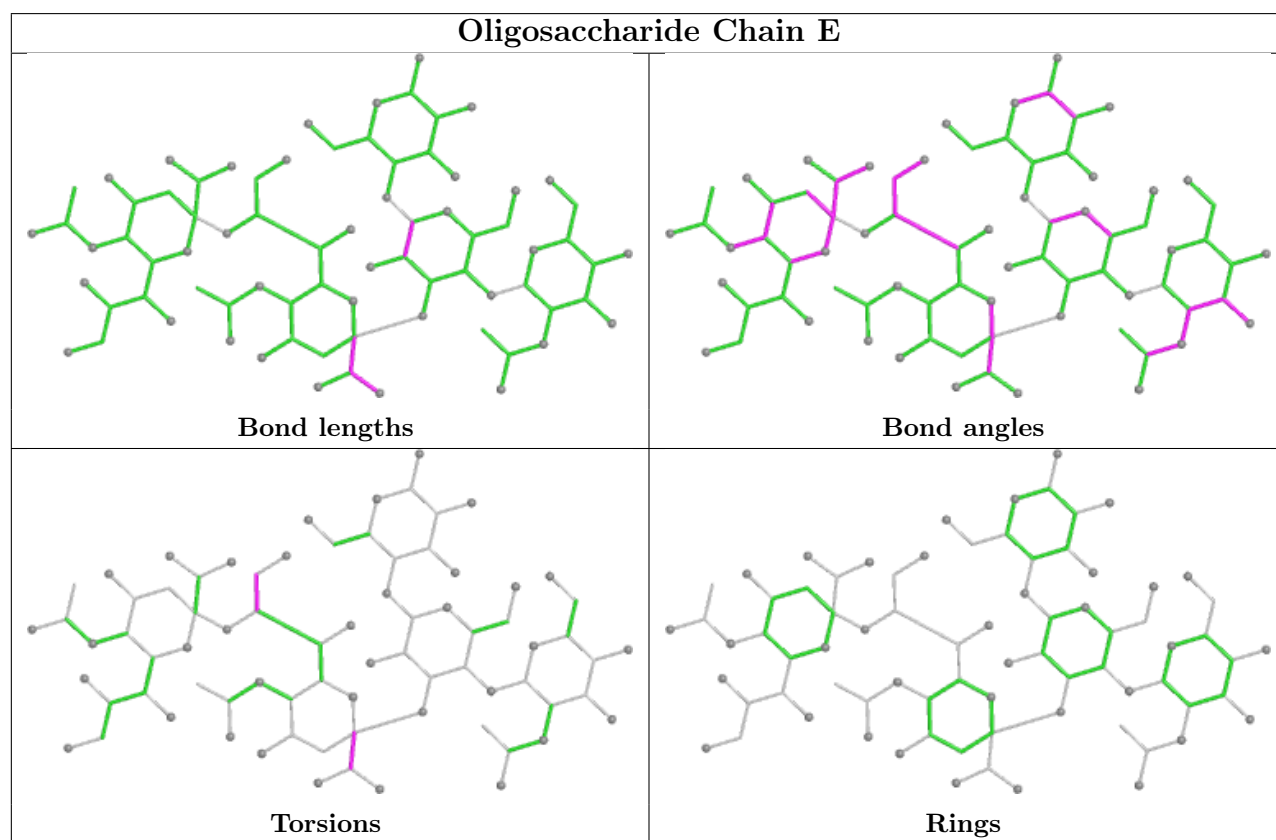
*Continued from previous page...*

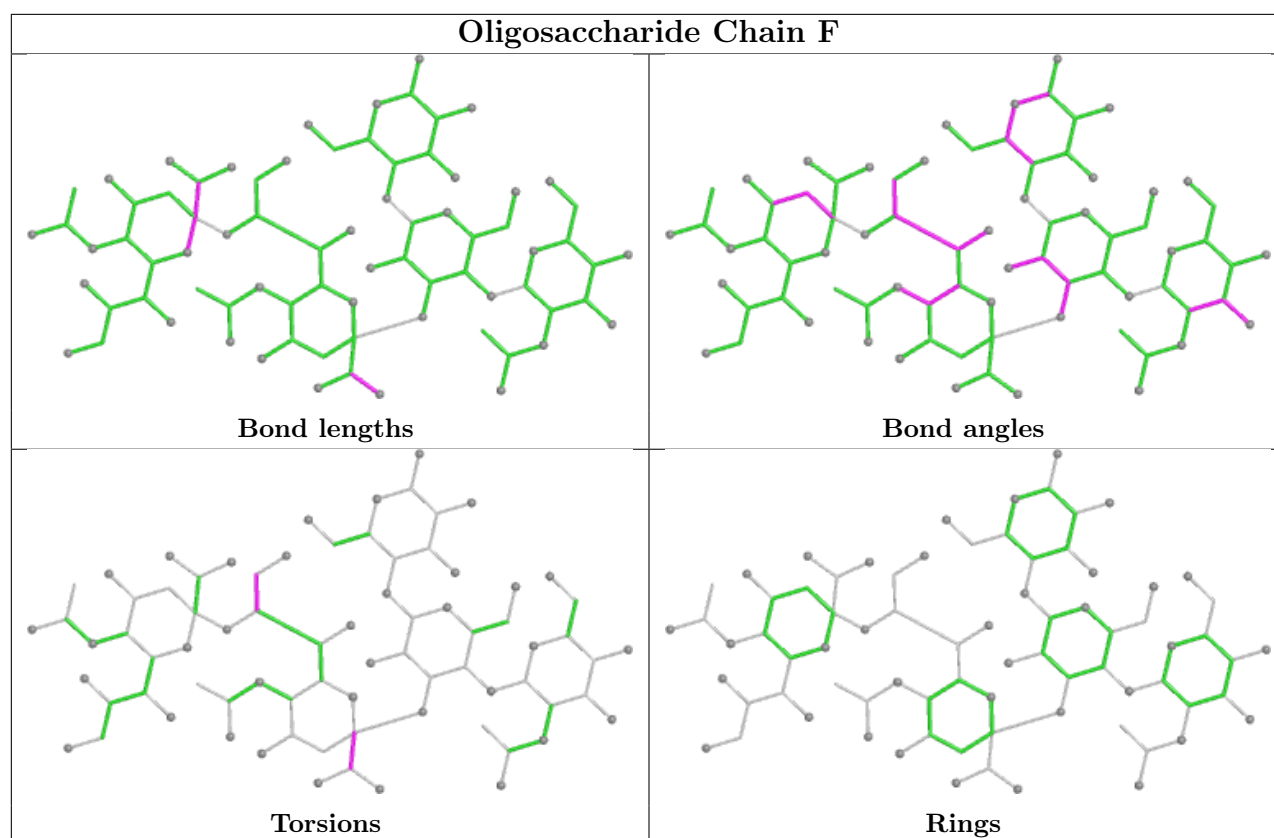
Mol	Chain	Res	Type	Atoms
3	E	3	SIA	O1A-C1-C2-O6
3	E	3	SIA	O1A-C1-C2-C3

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PO4	D	301	-	4,4,4	1.35	1 (25%)	6,6,6	0.49	0
4	PO4	A	301	-	4,4,4	1.00	0	6,6,6	0.70	0
4	PO4	D	302	-	4,4,4	0.68	0	6,6,6	0.56	0
4	PO4	D	304	-	4,4,4	0.94	0	6,6,6	0.62	0
4	PO4	D	303	-	4,4,4	0.89	0	6,6,6	0.43	0
4	PO4	C	301	-	4,4,4	1.33	1 (25%)	6,6,6	0.68	0
4	PO4	C	302	-	4,4,4	0.73	0	6,6,6	0.39	0
4	PO4	D	305	-	4,4,4	0.91	0	6,6,6	0.46	0



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	PO4	P-O3	-2.30	1.47	1.54
4	C	301	PO4	P-O1	-2.16	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/213 (100%)	-0.57	2 (0%) 81 83	10, 17, 34, 52	1 (0%)
1	B	210/213 (98%)	-0.46	3 (1%) 73 77	11, 19, 41, 57	0
2	C	216/216 (100%)	-0.37	8 (3%) 45 49	6, 18, 37, 76	1 (0%)
2	D	216/216 (100%)	0.27	14 (6%) 25 27	14, 25, 52, 111	0
All	All	855/858 (99%)	-0.28	27 (3%) 50 54	6, 20, 42, 111	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	135	THR	9.6
2	D	133	LYS	9.2
2	D	134	SER	8.7
2	C	137	GLY	8.3
2	D	132	SER	6.2
2	D	131	SER	5.9
1	A	213	CYS	5.1
2	D	194	GLY	5.0
2	D	137	GLY	4.9
2	D	136	SER	4.9
2	D	130	PRO	4.5
2	C	135	THR	4.5
2	C	136	SER	4.1
2	C	134	SER	3.8
2	D	195	THR	3.7
2	D	1	GLN	3.5
2	C	132	SER	3.2
2	D	216	HIS	2.9
2	C	133	LYS	2.8
2	D	129	ALA	2.8
1	B	125	LYS	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	1	GLN	2.5
1	B	126	SER	2.3
2	C	142	LEU	2.3
2	D	210	LYS	2.2
1	B	122	GLU	2.2
1	A	152	ALA	2.1

## 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](#)

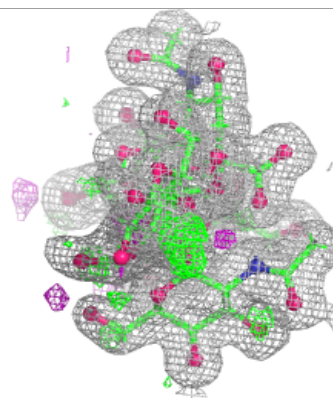
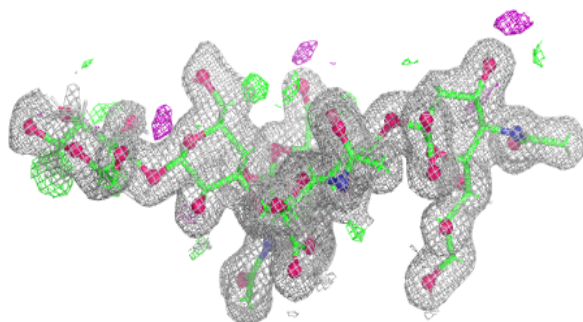
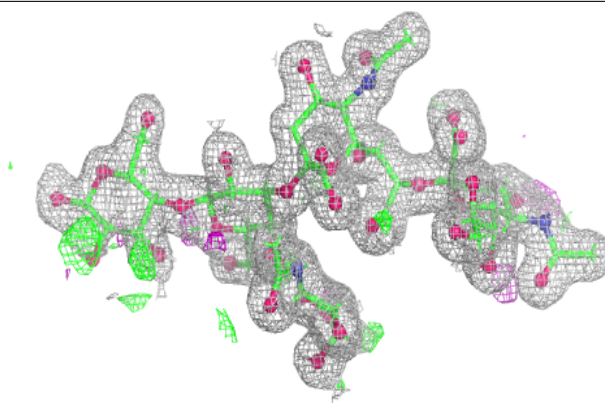
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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
3	BGC	E	1	12/12	0.84	0.16	29,44,58,66	5
3	BGC	F	1	12/12	0.90	0.12	26,35,46,49	5
3	NGA	E	5	14/15	0.97	0.06	15,17,26,33	6
3	GAL	E	2	11/12	0.97	0.06	15,19,36,37	3
3	GAL	F	2	11/12	0.97	0.06	18,21,25,26	3
3	SIA	E	3	20/21	0.98	0.04	13,15,18,19	6
3	SIA	F	3	20/21	0.98	0.05	17,19,21,22	6
3	SIA	F	4	20/21	0.98	0.04	15,17,20,22	7
3	NGA	F	5	14/15	0.98	0.06	17,19,21,23	6
3	SIA	E	4	20/21	0.99	0.03	14,15,17,18	7

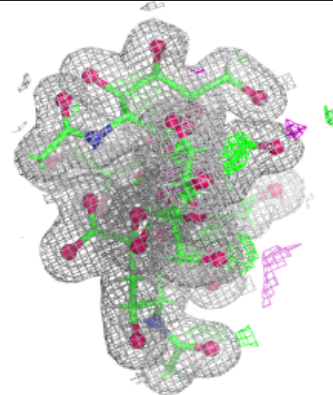
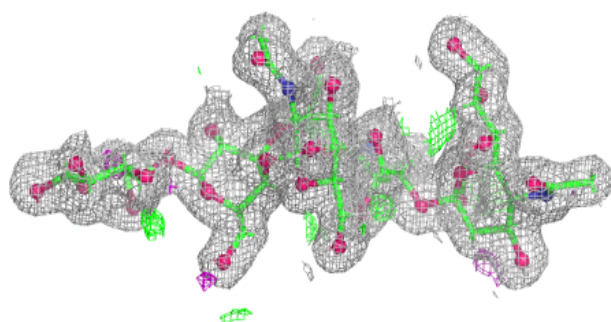
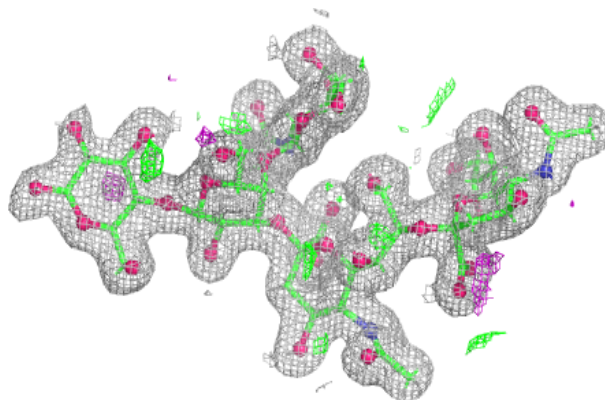
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

**Electron density around Chain F:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PO4	D	303	5/5	0.79	0.16	69,71,81,83	0
4	PO4	D	305	5/5	0.80	0.15	49,62,68,76	0
4	PO4	C	302	5/5	0.88	0.12	54,55,57,60	0
4	PO4	D	302	5/5	0.90	0.11	46,49,51,60	0
4	PO4	D	304	5/5	0.91	0.10	41,54,55,67	0
4	PO4	C	301	5/5	0.96	0.10	32,38,46,48	0
4	PO4	D	301	5/5	0.97	0.07	31,36,39,40	0
4	PO4	A	301	5/5	0.99	0.05	19,20,24,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.