



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:16 PM UTC

PDB ID : 8SGM / pdb_00008sgm
Title : Crystal Structure of CD1d-lipid complexed with Beta-2-Microglobulin, TCR Alpha-Chain and TCR Beta-Chain
Authors : Chan Yew Poa, K.T.O.; Le Nours, J.; Rossjohn, J.
Deposited on : 2023-04-12
Resolution : 2.50 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

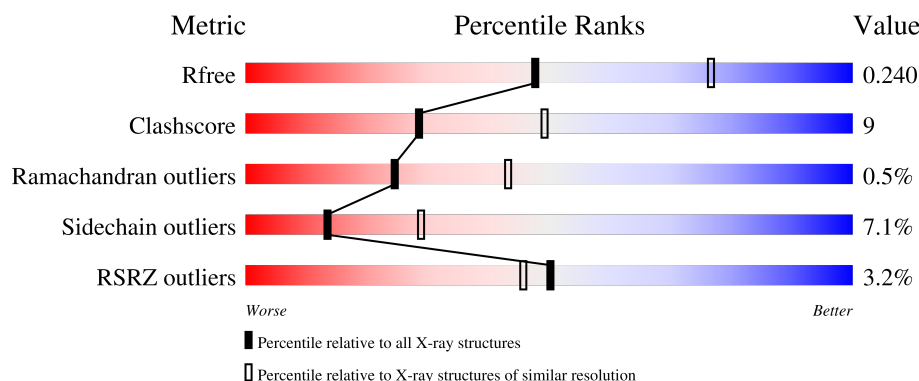
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	274	4% 74% 22% ..
2	B	100	83% 12% ..
3	C	207	4% 83% 14% ..
4	D	243	3% 74% 21% ..
5	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	3	 33% 67%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6803 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2104	1346	361	390	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P15813
A	277	GLN	-	expression tag	UNP P15813

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			813	517	138	156	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Natural killer T cell receptor TRAV26-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	203	Total	C	N	O	S	0	0	0
			1540	967	262	302	9			

- Molecule 4 is a protein called Natural killer T cell receptor TRBV19 beta chain.

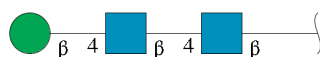
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	236	Total	C	N	O	S	0	0	0
			1847	1173	318	350	6			

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



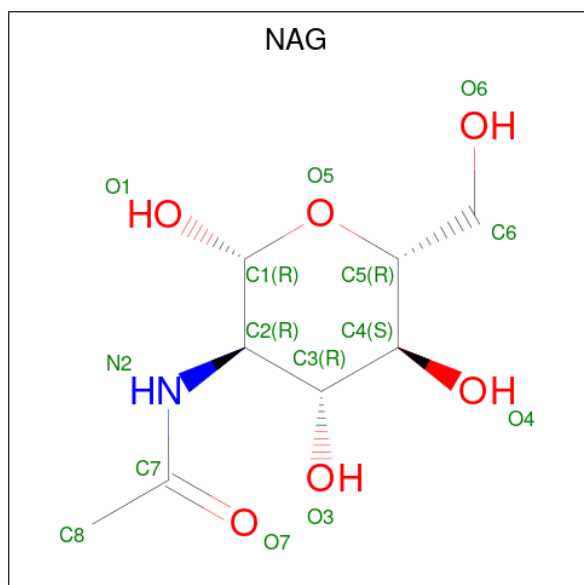
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



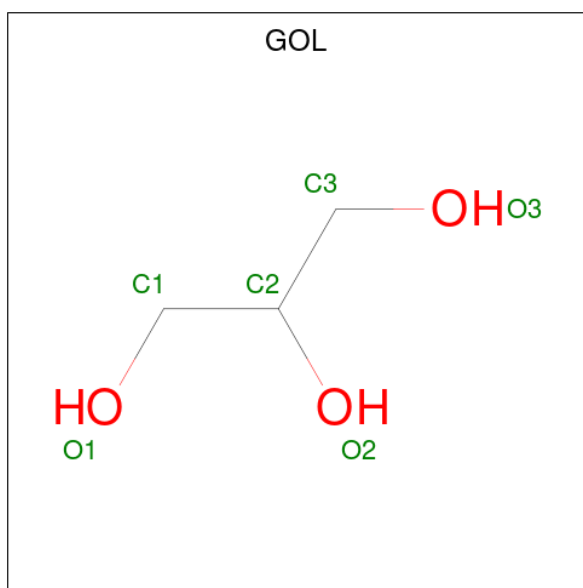
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



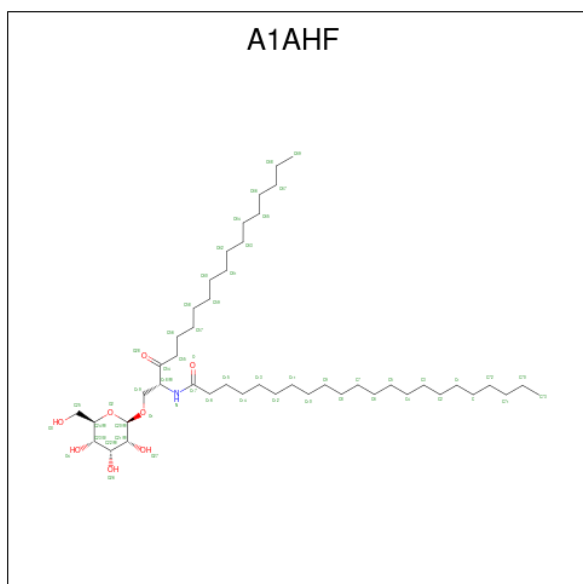
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



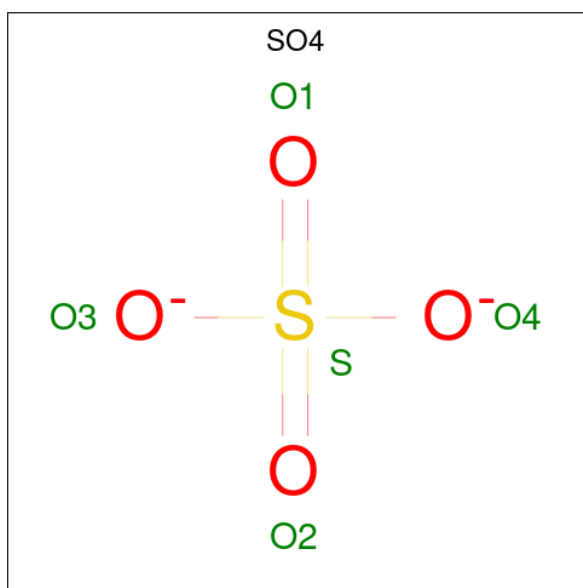
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is N-[(2S)-3-oxo-1-(beta-L-talopyranosyloxy)octadecan-2-yl]docosanamide (CCD ID: A1AHF) (formula: $C_{46}H_{89}NO_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			55	46	1	8		

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		

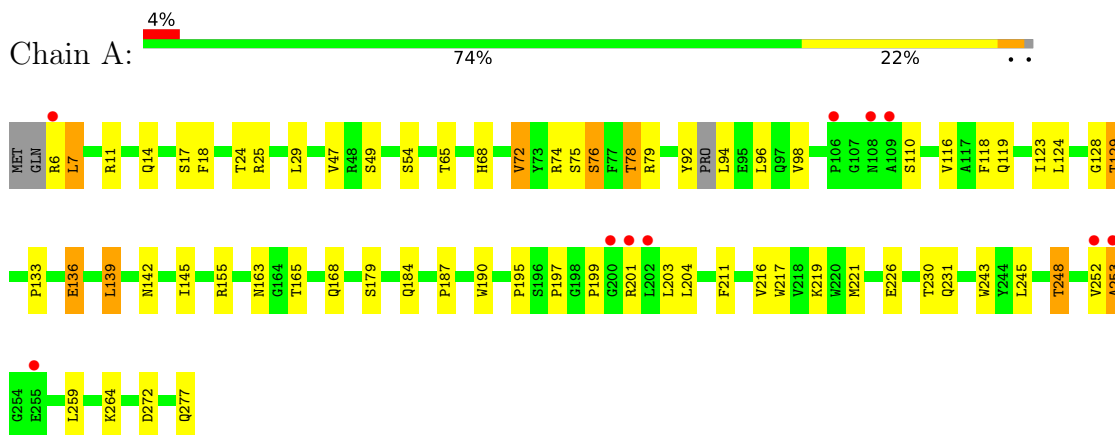
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	93	Total	O	0	0
			93	93		
11	B	71	Total	O	0	0
			71	71		
11	C	82	Total	O	0	0
			82	82		
11	D	101	Total	O	0	0
			101	101		

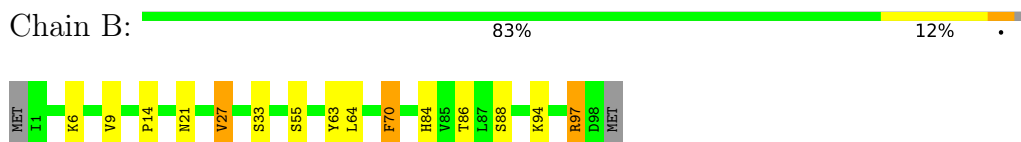
3 Residue-property plots [i](#)

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.

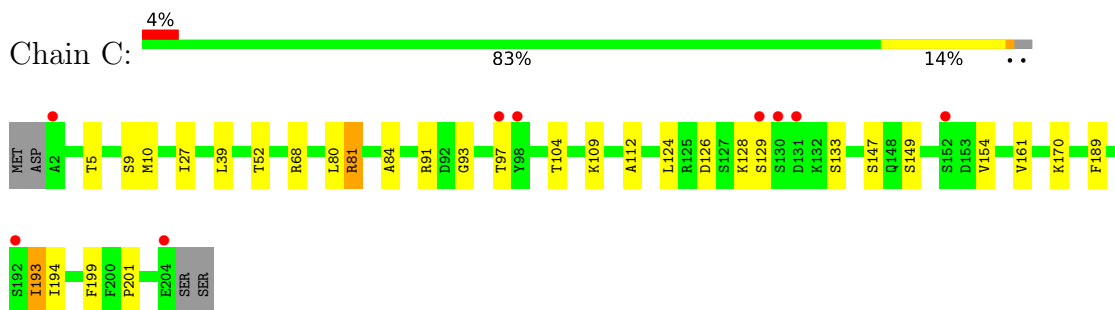
- Molecule 1: Antigen-presenting glycoprotein CD1d



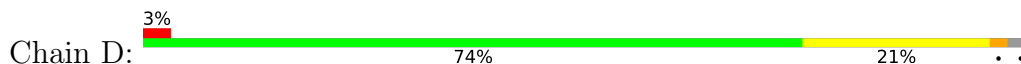
- Molecule 2: Beta-2-microglobulin

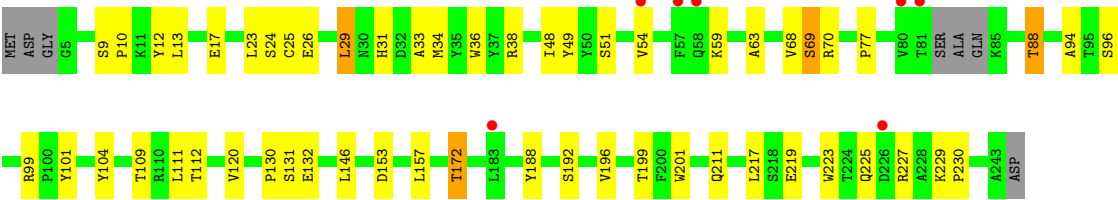


- Molecule 3: Natural killer T cell receptor TRAV26-2

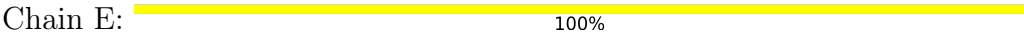


- Molecule 4: Natural killer T cell receptor TRBV19 beta chain





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



● Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	133.79Å 133.79Å 68.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.50 47.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.30-2.50) 100.0 (47.30-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.184 , 0.234 0.189 , 0.240	Depositor DCC
R_{free} test set	2145 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6803	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, SO4, GOL, A1AHF

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	0.35	0/2165	0.50	0/2956
2	B	0.41	0/836	0.56	0/1134
3	C	0.39	0/1577	0.52	0/2155
4	D	0.35	0/1898	0.56	0/2594
All	All	0.37	0/6476	0.53	0/8839

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	2104	0	1970	42	0
2	B	813	0	765	8	0
3	C	1540	0	1412	24	0
4	D	1847	0	1701	42	0
5	E	28	0	25	0	0
6	F	39	0	34	1	0
7	A	14	0	13	0	0
8	A	6	0	8	0	0
9	A	55	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	5	0	0	0	0
10	B	5	0	0	0	0
11	A	93	0	0	4	0
11	B	71	0	0	1	0
11	C	82	0	0	4	0
11	D	101	0	0	3	0
All	All	6803	0	5928	109	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 9.

All (109) 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:A:18:PHE:HB2	1:A:94:LEU:HB2	1.63	0.81
1:A:231:GLN:HB3	1:A:248:THR:HG22	1.64	0.80
1:A:110:SER:HB3	11:A:467:HOH:O	1.87	0.74
4:D:88:THR:HB	4:D:112:THR:HA	1.72	0.72
4:D:132:GLU:OE2	4:D:132:GLU:CG	2.38	0.72
1:A:129:THR:HG23	1:A:155:ARG:HH21	1.55	0.71
3:C:133:SER:O	11:C:301:HOH:O	2.09	0.70
4:D:120:VAL:HG12	4:D:230:PRO:HB2	1.72	0.70
4:D:38:ARG:HB2	4:D:48:ILE:HD11	1.73	0.69
4:D:132:GLU:CG	4:D:132:GLU:OE1	2.43	0.67
3:C:124:LEU:O	3:C:133:SER:HB2	1.94	0.66
3:C:80:LEU:HD11	3:C:170:LYS:HD3	1.77	0.66
1:A:74:ARG:O	1:A:78:THR:HG23	1.95	0.65
3:C:27:ILE:HG21	3:C:68:ARG:O	1.96	0.65
1:A:11:ARG:NH2	11:A:404:HOH:O	2.30	0.64
4:D:223:TRP:HB2	4:D:229:LYS:HG3	1.79	0.64
3:C:189:PHE:HB2	3:C:194:ILE:HD11	1.79	0.63
4:D:54:VAL:HG13	11:D:341:HOH:O	1.98	0.63
4:D:49:TYR:CE2	4:D:63:ALA:HB1	2.33	0.63
4:D:69:SER:O	4:D:77:PRO:HD2	1.99	0.61
1:A:7:LEU:HD22	11:A:402:HOH:O	2.00	0.61
4:D:132:GLU:OE2	4:D:132:GLU:OE1	2.20	0.60
1:A:195:PRO:HD2	1:A:203:LEU:HD23	1.84	0.59
4:D:33:ALA:HB3	4:D:96:SER:HB3	1.85	0.58
4:D:120:VAL:O	4:D:227:ARG:NH2	2.36	0.58
1:A:49:SER:HB3	1:A:54:SER:HB2	1.85	0.58
4:D:172:THR:HB	4:D:192:SER:HB2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASN:HB3	3:C:52:THR:HG21	1.86	0.57
4:D:49:TYR:CE1	4:D:59:LYS:HG2	2.40	0.57
1:A:118:PHE:HB2	1:A:123:ILE:HD13	1.87	0.56
1:A:231:GLN:CB	1:A:248:THR:HG22	2.35	0.56
1:A:76:SER:HB2	9:A:303:A1AHF:O28	2.04	0.56
4:D:223:TRP:CB	4:D:229:LYS:HG3	2.36	0.56
3:C:81:ARG:HG2	11:C:364:HOH:O	2.06	0.56
1:A:221:MET:HG2	1:A:226:GLU:HA	1.88	0.55
4:D:34:MET:HE3	4:D:70:ARG:NE	2.21	0.55
1:A:129:THR:CG2	1:A:155:ARG:HH21	2.19	0.55
1:A:204:LEU:HD22	1:A:277:GLN:OE1	2.07	0.54
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.43	0.54
1:A:163:ASN:HD22	3:C:52:THR:HG22	1.72	0.53
1:A:76:SER:HA	1:A:79:ARG:HB2	1.91	0.52
1:A:98:VAL:HG22	1:A:116:VAL:HG22	1.92	0.52
4:D:96:SER:OG	11:D:301:HOH:O	2.19	0.51
3:C:93:GLY:O	4:D:99:ARG:NH1	2.42	0.51
4:D:10:PRO:HD2	4:D:13:LEU:HD13	1.93	0.50
4:D:54:VAL:HA	4:D:70:ARG:HG2	1.93	0.50
1:A:216:VAL:HG22	1:A:217:TRP:H	1.76	0.50
1:A:216:VAL:HG22	1:A:217:TRP:N	2.28	0.49
1:A:25:ARG:NH2	2:B:33:SER:OG	2.45	0.49
4:D:172:THR:HB	4:D:192:SER:CB	2.42	0.49
1:A:139:LEU:O	1:A:142:ASN:HB2	2.13	0.48
1:A:136:GLU:H	1:A:136:GLU:CD	2.21	0.48
4:D:33:ALA:HA	4:D:51:SER:O	2.12	0.48
1:A:92:TYR:O	1:A:94:LEU:N	2.47	0.48
1:A:219:LYS:HA	1:A:230:THR:HG21	1.95	0.48
1:A:133:PRO:HD3	1:A:145:ILE:HD13	1.96	0.48
4:D:49:TYR:CZ	4:D:59:LYS:HG2	2.49	0.48
4:D:157:LEU:HA	4:D:211:GLN:O	2.14	0.47
3:C:9:SER:HB2	11:C:369:HOH:O	2.14	0.47
3:C:193:ILE:HD11	11:C:344:HOH:O	2.15	0.47
4:D:223:TRP:CG	4:D:229:LYS:HG3	2.50	0.47
3:C:80:LEU:CD1	3:C:170:LYS:HD3	2.45	0.47
4:D:25:CYS:HB2	4:D:36:TRP:CZ2	2.50	0.47
3:C:81:ARG:HB2	3:C:81:ARG:NH1	2.30	0.46
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.97	0.46
1:A:190:TRP:CD2	2:B:14:PRO:HG3	2.50	0.46
1:A:68:HIS:O	1:A:72:VAL:HG12	2.16	0.46
3:C:147:SER:H	3:C:193:ILE:HD12	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:HA	1:A:119:GLN:OE1	2.15	0.46
1:A:197:PRO:HG2	1:A:201:ARG:CB	2.47	0.45
4:D:54:VAL:HA	4:D:70:ARG:CG	2.47	0.45
1:A:163:ASN:HB3	3:C:52:THR:CG2	2.47	0.45
4:D:130:PRO:HD2	4:D:201:TRP:CZ2	2.52	0.44
4:D:120:VAL:HG21	4:D:217:LEU:HD21	1.98	0.44
2:B:97:ARG:HD2	11:B:233:HOH:O	2.18	0.44
1:A:252:VAL:O	1:A:253:ALA:C	2.59	0.44
9:A:303:A1AHF:O27	9:A:303:A1AHF:C19	2.65	0.44
4:D:10:PRO:CD	4:D:13:LEU:HD13	2.48	0.44
6:F:2:NAG:H4	6:F:3:BMA:O2	2.19	0.43
1:A:14:GLN:HB3	1:A:98:VAL:HB	2.00	0.43
3:C:10:MET:HE3	3:C:10:MET:HB2	1.97	0.43
3:C:39:LEU:HD23	3:C:84:ALA:HB2	2.01	0.43
2:B:55:SER:HB3	2:B:63:TYR:CZ	2.53	0.43
3:C:199:PHE:CZ	3:C:201:PRO:HB3	2.54	0.43
1:A:124:LEU:C	1:A:124:LEU:HD12	2.43	0.43
4:D:10:PRO:HG2	4:D:12:TYR:O	2.19	0.43
1:A:190:TRP:CE3	2:B:14:PRO:HG3	2.53	0.43
4:D:9:SER:HA	4:D:10:PRO:HA	1.78	0.43
3:C:128:LYS:O	3:C:129:SER:C	2.62	0.42
4:D:13:LEU:O	4:D:111:LEU:HD12	2.19	0.42
1:A:264:LYS:HG2	1:A:272:ASP:CG	2.44	0.42
4:D:146:LEU:HA	4:D:146:LEU:HD23	1.82	0.42
3:C:149:SER:OG	3:C:154:VAL:O	2.31	0.42
1:A:184:GLN:NE2	11:A:401:HOH:O	2.20	0.42
4:D:34:MET:HE2	4:D:70:ARG:NH2	2.35	0.42
3:C:91:ARG:HG2	4:D:101:TYR:HB2	2.02	0.42
3:C:112:ALA:HB2	3:C:161:VAL:HG21	2.00	0.42
4:D:153:ASP:HB3	4:D:188:TYR:CD2	2.55	0.41
4:D:199:THR:HG23	11:D:362:HOH:O	2.19	0.41
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.56	0.41
4:D:59:LYS:HD2	4:D:63:ALA:HB3	2.03	0.41
2:B:6:LYS:O	2:B:27:VAL:HA	2.21	0.41
4:D:94:ALA:HA	4:D:104:TYR:O	2.20	0.41
3:C:126:ASP:HB3	3:C:129:SER:O	2.20	0.41
4:D:29:LEU:H	4:D:29:LEU:HG	1.39	0.41
1:A:6:ARG:O	1:A:7:LEU:HD22	2.22	0.40
3:C:91:ARG:HD3	4:D:101:TYR:HB3	2.02	0.40
1:A:211:PHE:CE2	1:A:243:TRP:HB2	2.56	0.40
1:A:264:LYS:HG2	1:A:272:ASP:OD2	2.21	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	267/274 (97%)	252 (94%)	12 (4%)	3 (1%)	11	22
2	B	96/100 (96%)	92 (96%)	4 (4%)	0	100	100
3	C	201/207 (97%)	189 (94%)	12 (6%)	0	100	100
4	D	232/243 (96%)	214 (92%)	17 (7%)	1 (0%)	30	49
All	All	796/824 (97%)	747 (94%)	45 (6%)	4 (0%)	24	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	A	199	PRO
1	A	253	ALA
4	D	17	GLU

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	220/240 (92%)	200 (91%)	20 (9%)	9	19
2	B	91/95 (96%)	84 (92%)	7 (8%)	12	25
3	C	163/185 (88%)	157 (96%)	6 (4%)	30	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	191/212 (90%)	177 (93%)	14 (7%)	13	27
All	All	665/732 (91%)	618 (93%)	47 (7%)	13	29

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	SER
1	A	24	THR
1	A	29	LEU
1	A	47	VAL
1	A	65	THR
1	A	72	VAL
1	A	75	SER
1	A	76	SER
1	A	78	THR
1	A	96	LEU
1	A	129	THR
1	A	136	GLU
1	A	139	LEU
1	A	165	THR
1	A	168	GLN
1	A	179	SER
1	A	245	LEU
1	A	248	THR
1	A	259	LEU
2	B	9	VAL
2	B	27	VAL
2	B	64	LEU
2	B	70	PHE
2	B	88	SER
2	B	94	LYS
2	B	97	ARG
3	C	5	THR
3	C	81	ARG
3	C	97	THR
3	C	104	THR
3	C	109	LYS
3	C	193	ILE
4	D	23	LEU
4	D	24	SER
4	D	26	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	29	LEU
4	D	31	HIS
4	D	68	VAL
4	D	69	SER
4	D	88	THR
4	D	109	THR
4	D	131	SER
4	D	172	THR
4	D	196	VAL
4	D	219	GLU
4	D	225	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	23	ASN
4	D	20	ASN
4	D	167	HIS
4	D	213	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

5 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	E	1	5,1	14,14,15	0.74	1 (7%)	17,19,21	0.63	0
5	NAG	E	2	5	14,14,15	0.42	0	17,19,21	0.66	1 (5%)
6	NAG	F	1	6,1	14,14,15	0.27	0	17,19,21	0.78	0
6	NAG	F	2	6	14,14,15	0.78	1 (7%)	17,19,21	0.93	1 (5%)
6	BMA	F	3	6	11,11,12	1.24	1 (9%)	15,15,17	0.95	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	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	C1-C2	2.71	1.56	1.52
6	F	2	NAG	O5-C1	-2.70	1.39	1.43
6	F	3	BMA	C4-C3	2.27	1.58	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	2	NAG	O4-C4-C5	-2.31	103.64	109.32
5	E	2	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
6	F	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

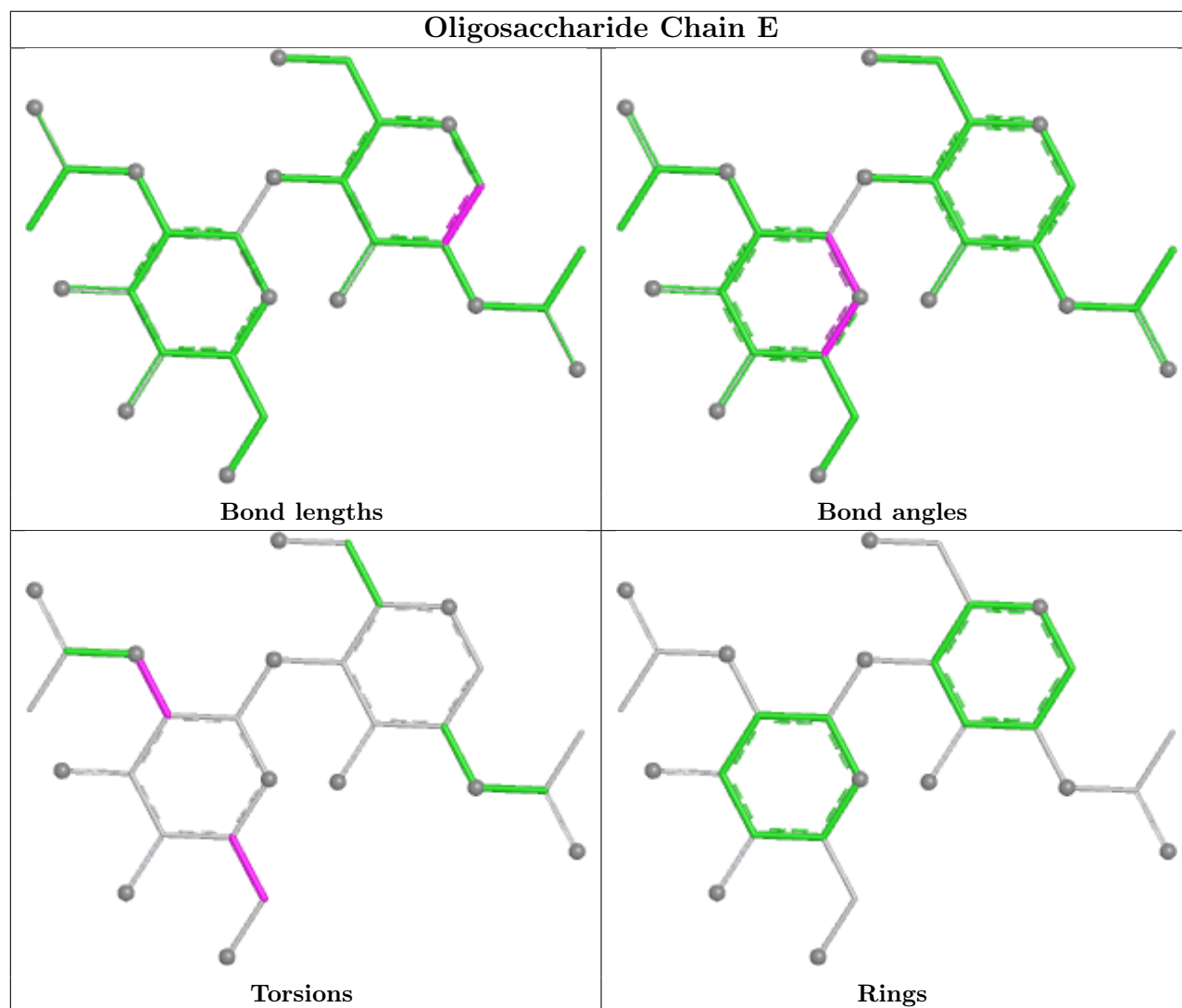
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C3-C2-N2-C7

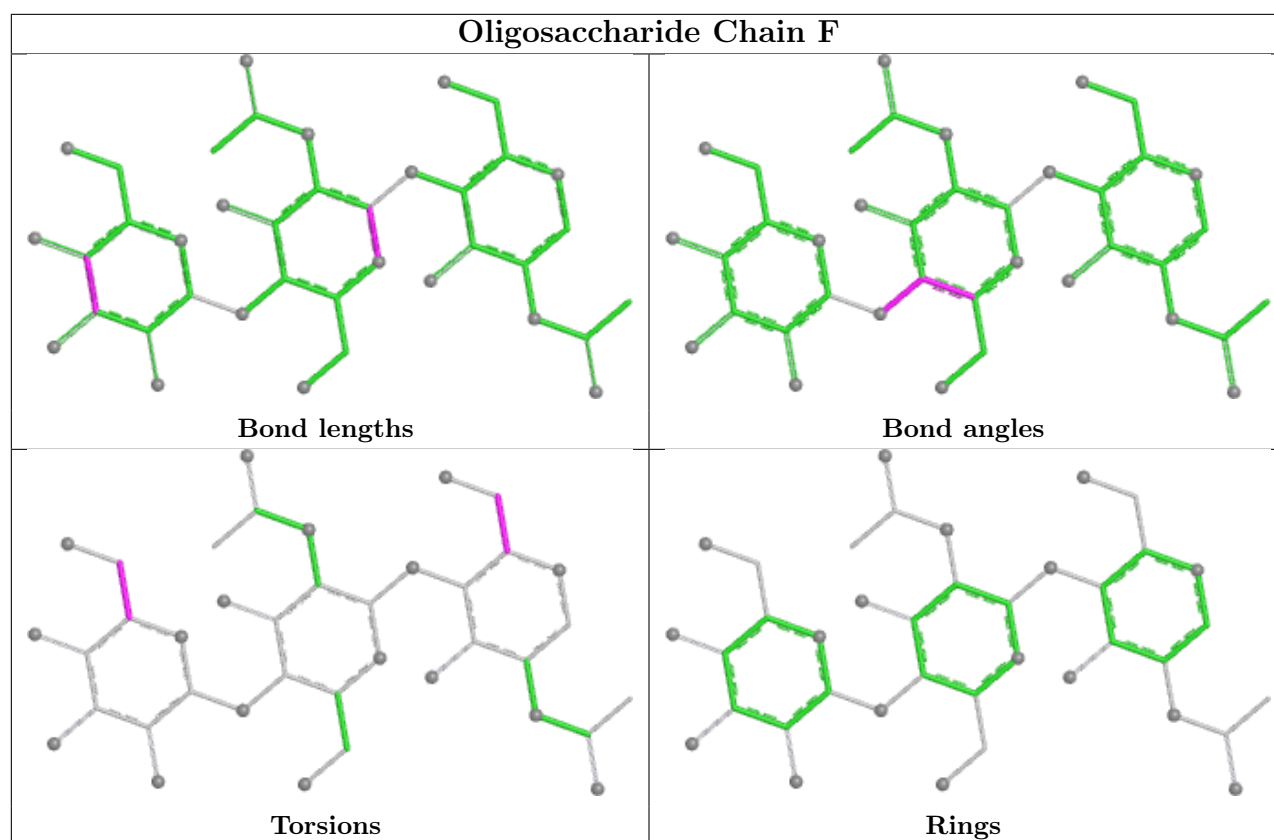
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	NAG	1	0
6	F	3	BMA	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](#)

5 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	$\# Z > 2$
10	SO4	A	304	-	4,4,4	0.27	0	6,6,6	0.22	0
8	GOL	A	302	-	5,5,5	0.48	0	5,5,5	0.41	0
7	NAG	A	301	1	14,14,15	0.60	0	17,19,21	0.77	1 (5%)
10	SO4	B	101	-	4,4,4	0.30	0	6,6,6	0.14	0
9	A1AHF	A	303	-	54,55,55	1.35	4 (7%)	60,63,63	1.58	12 (20%)

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	301	1	-	2/6/23/26	0/1/1/1
9	A1AHF	A	303	-	-	24/51/71/71	0/1/1/1
8	GOL	A	302	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	303	A1AHF	C17-N	6.66	1.48	1.34
9	A	303	A1AHF	O-C17	-2.62	1.18	1.23
9	A	303	A1AHF	O26-C22	2.17	1.48	1.43
9	A	303	A1AHF	O2-C20	2.05	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	303	A1AHF	C16-C17-N	5.93	126.31	115.86
9	A	303	A1AHF	C23-C22-C21	3.40	116.81	110.83
9	A	303	A1AHF	C22-C23-C24	3.36	116.32	110.23
9	A	303	A1AHF	O-C17-N	-3.30	117.37	122.95
9	A	303	A1AHF	O-C17-C16	-3.15	116.32	122.02
7	A	301	NAG	C1-O5-C5	2.67	115.76	112.19
9	A	303	A1AHF	O2-C20-O1	-2.66	103.75	110.04
9	A	303	A1AHF	O28-C54-C55	-2.66	117.18	121.68
9	A	303	A1AHF	C15-C16-C17	-2.63	105.88	113.19
9	A	303	A1AHF	C19-C18-N	-2.38	106.05	111.31
9	A	303	A1AHF	O2-C24-C23	2.35	113.94	109.70
9	A	303	A1AHF	C57-C56-C55	-2.01	105.73	113.13
9	A	303	A1AHF	C20-C21-C22	2.01	114.23	110.01

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	303	A1AHF	N-C18-C19-O1
9	A	303	A1AHF	C54-C18-C19-O1
9	A	303	A1AHF	N-C18-C54-C55
9	A	303	A1AHF	O2-C20-O1-C19
9	A	303	A1AHF	C18-C54-C55-C56
9	A	303	A1AHF	O28-C54-C55-C56
9	A	303	A1AHF	C16-C17-N-C18

Continued on next page...

Continued from previous page...

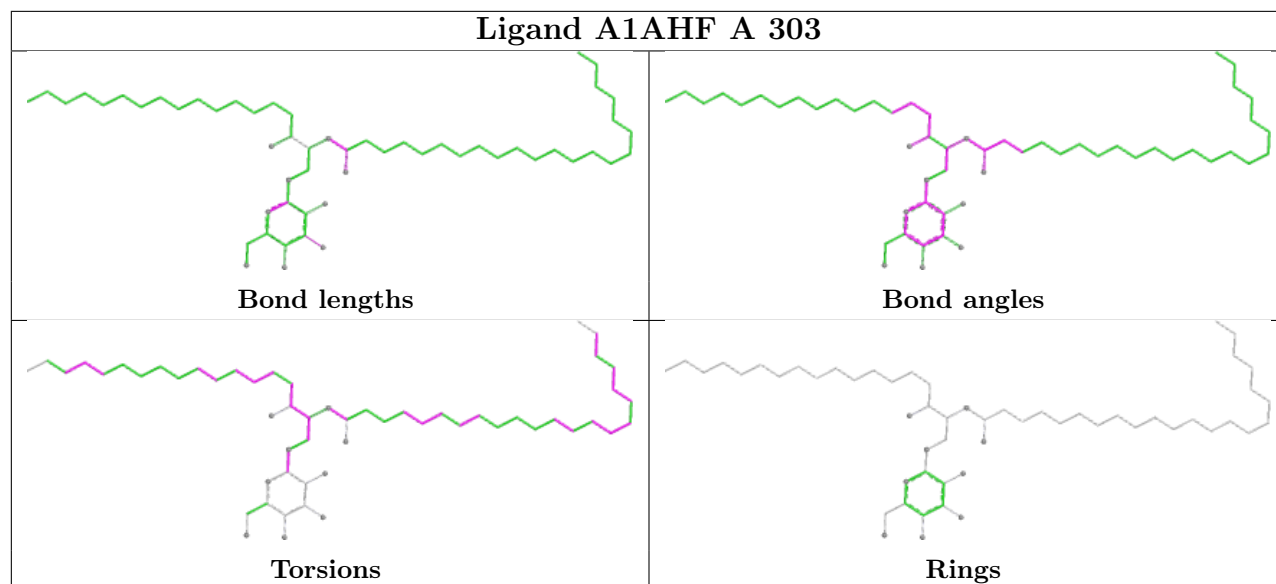
Mol	Chain	Res	Type	Atoms
9	A	303	A1AHF	O-C17-N-C18
9	A	303	A1AHF	C21-C20-O1-C19
7	A	301	NAG	O5-C5-C6-O6
7	A	301	NAG	C4-C5-C6-O6
9	A	303	A1AHF	C72-C-C1-C2
9	A	303	A1AHF	C64-C65-C66-C67
9	A	303	A1AHF	C9-C10-C11-C12
9	A	303	A1AHF	C11-C12-C13-C14
9	A	303	A1AHF	C55-C56-C57-C58
9	A	303	A1AHF	C73-C70-C71-C72
9	A	303	A1AHF	C58-C59-C60-C61
9	A	303	A1AHF	C1-C-C72-C71
9	A	303	A1AHF	N-C18-C54-O28
9	A	303	A1AHF	C56-C57-C58-C59
9	A	303	A1AHF	C12-C13-C14-C15
9	A	303	A1AHF	C1-C2-C3-C4
9	A	303	A1AHF	C4-C5-C6-C7
9	A	303	A1AHF	C65-C66-C67-C68
9	A	303	A1AHF	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	303	A1AHF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	271/274 (98%)	0.05	10 (3%) 45 40	35, 49, 92, 108	0
2	B	98/100 (98%)	-0.36	0 100 100	34, 42, 64, 82	0
3	C	203/207 (98%)	-0.03	9 (4%) 39 34	30, 45, 74, 87	0
4	D	236/243 (97%)	0.14	7 (2%) 52 48	30, 53, 77, 88	0
All	All	808/824 (98%)	0.01	26 (3%) 50 46	30, 48, 79, 108	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	PRO	4.1
4	D	81	THR	3.5
1	A	109	ALA	3.5
1	A	202	LEU	3.4
1	A	253	ALA	3.4
3	C	129	SER	3.2
4	D	80	VAL	3.1
3	C	130	SER	3.0
3	C	97	THR	2.9
1	A	108	ASN	2.8
1	A	255	GLU	2.8
1	A	252	VAL	2.7
3	C	204	GLU	2.7
4	D	54	VAL	2.5
4	D	226	ASP	2.5
1	A	201	ARG	2.4
4	D	183	LEU	2.3
4	D	57	PHE	2.3
3	C	98	TYR	2.3
1	A	200	GLY	2.3
3	C	2	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	192	SER	2.2
3	C	131	ASP	2.2
3	C	152	SER	2.1
4	D	58	GLN	2.1
1	A	6	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

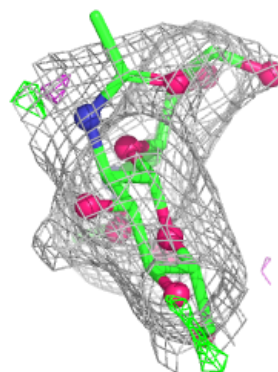
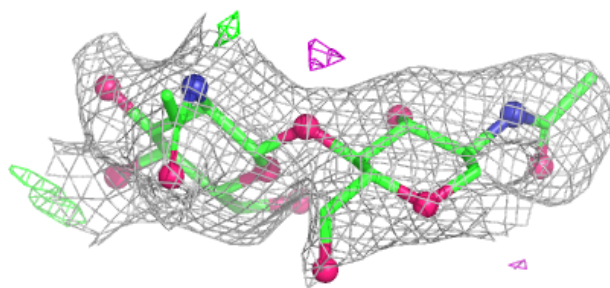
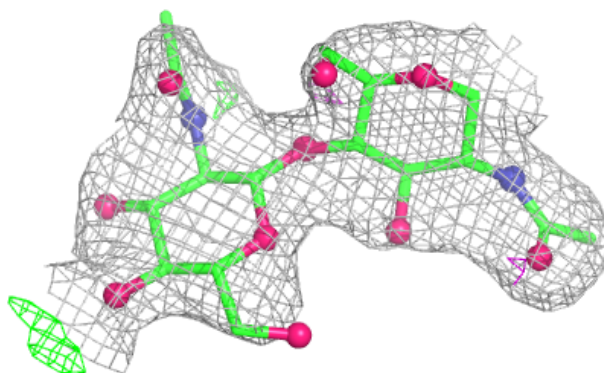
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	F	3	11/12	0.64	0.17	63,69,75,76	0
5	NAG	E	2	14/15	0.76	0.13	82,89,91,92	0
6	NAG	F	2	14/15	0.87	0.10	41,56,64,68	0
5	NAG	E	1	14/15	0.92	0.10	53,59,73,80	0
6	NAG	F	1	14/15	0.93	0.08	39,50,55,57	0

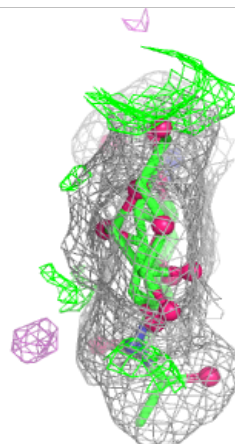
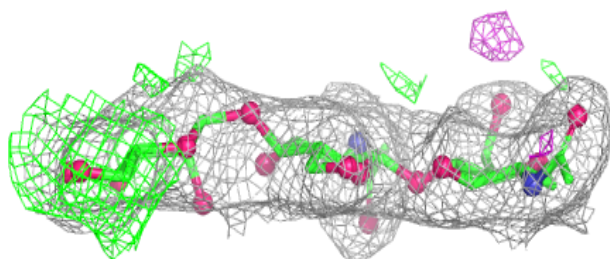
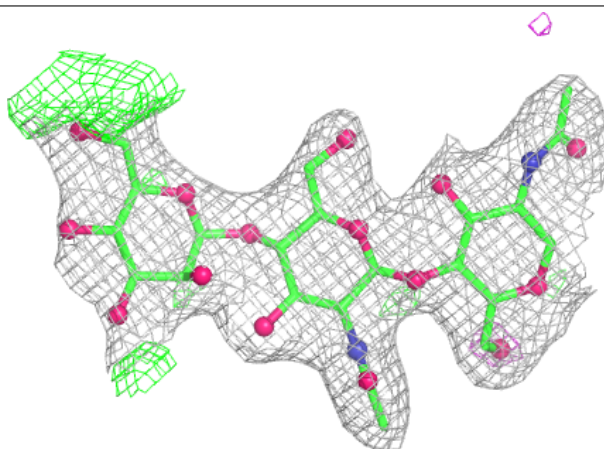
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain 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 ⓘ

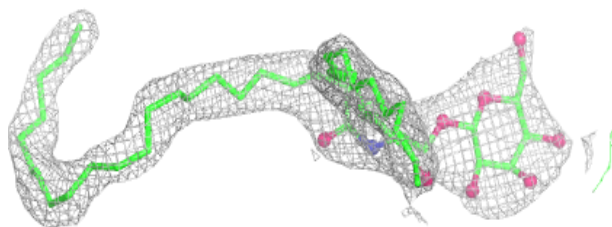
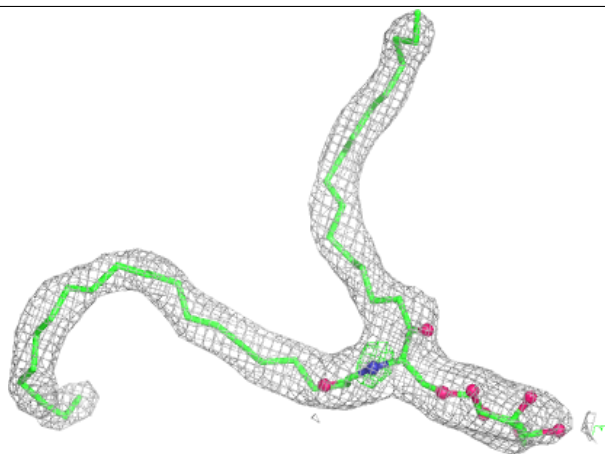
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	NAG	A	301	14/15	0.80	0.11	65,73,78,80	0
10	SO4	A	304	5/5	0.84	0.12	87,87,87,94	0
10	SO4	B	101	5/5	0.90	0.11	91,91,92,93	0
8	GOL	A	302	6/6	0.91	0.14	52,54,59,60	0
9	A1AHF	A	303	55/55	0.93	0.11	40,49,73,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1AHF A 303:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.