Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 07:10 PM EDT

PDB ID	:	4Y4H
Title	:	Crystal structure of the mCD1d/GCK152/iNKTCR ternary complex
Authors	:	Zajonc, D.M.; Yu, E.D.
Deposited on	:	2015-02-10
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

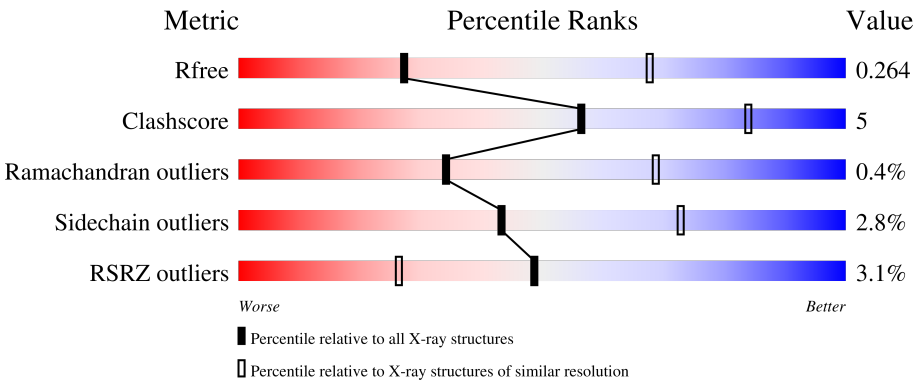
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	285	8%, 80%, 13%, • 6%
1	E	285	5%, 80%, 13%, 6%
2	B	99	2%, 81%, 15%, • •
2	F	99	7%, 81%, 15%, • •
3	C	209	81%, 15%, •

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Mol	Chain	Length	Quality of chain
3	G	209	% 84% 12%
4	D	241	85% 14%
4	H	241	% 84% 15%
5	I	2	100%
5	J	2	100%
5	K	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12468 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 CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2025	1287	339	386	13	0	0	0
1	E	267	2032	1292	340	387	13	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	variant	UNP P11609
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609
E	201	HIS	ASP	variant	UNP P11609
E	280	HIS	-	expression tag	UNP P11609
E	281	HIS	-	expression tag	UNP P11609
E	282	HIS	-	expression tag	UNP P11609
E	283	HIS	-	expression tag	UNP P11609
E	284	HIS	-	expression tag	UNP P11609
E	285	HIS	-	expression tag	UNP P11609

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	96	723	459	122	136	6	0	0	0
2	F	96	744	475	126	137	6	0	0	0

- Molecule 3 is a protein called Chimeric TCR Valpha14/Jalpha18 chain (mouse variable do-

main/ human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	202	1524	942	260	314	8	0	0	0
3	G	202	1514	937	258	311	8	0	0	0

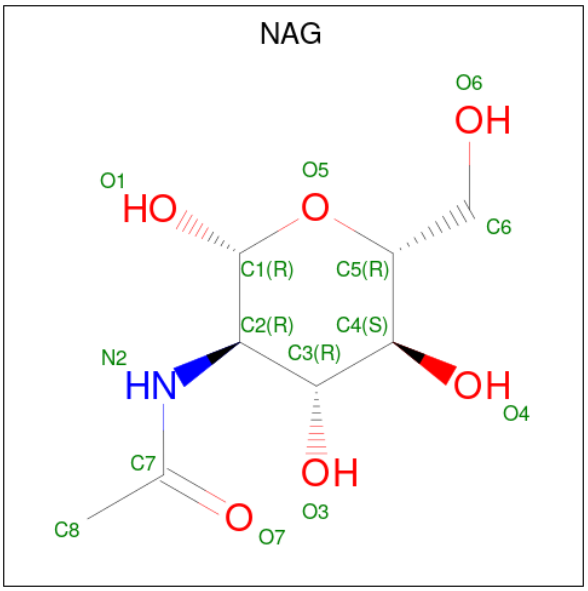
- Molecule 4 is a protein called Chimeric TCR Vbeta8.2 chain (mouse variable domain/ human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	239	1845	1157	328	354	6	0	0	0
4	H	239	1839	1153	325	355	6	0	0	0

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

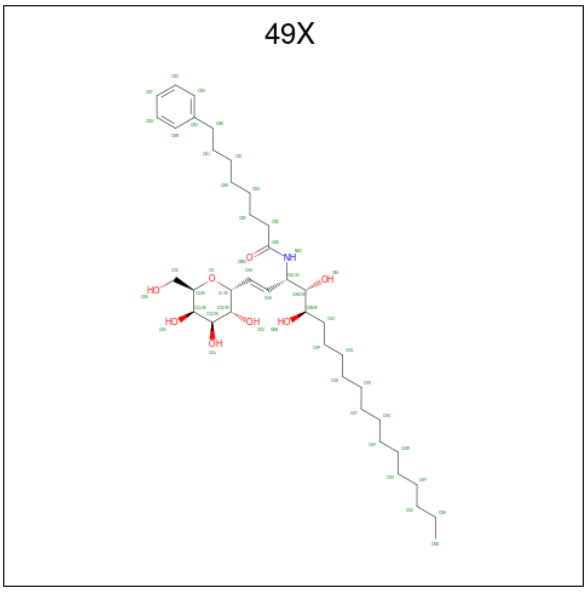
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	2	28	16	2	10	0	0	0
5	J	2	28	16	2	10	0	0	0
5	K	2	28	16	2	10	0	0	0

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



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

- Molecule 7 is (1R)-1,5-anhydro-1-{(1E,3S,4S,5R)-4,5-dihydroxy-3-[(8-phenyloctanoyl)amino]nonadec-1-en-1-yl}-D-galactitol (three-letter code: 49X) (formula: $C_{39}H_{67}NO_8$).



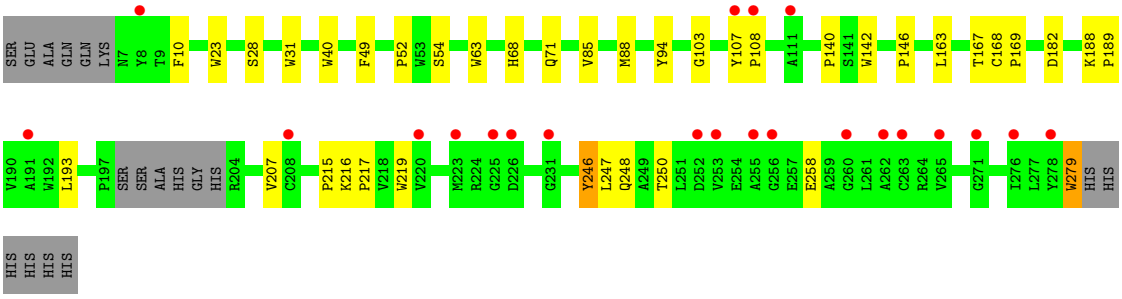
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	48	39	1	8	0	0
			Total	C	N	O		
7	E	1	48	39	1	8	0	0

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.

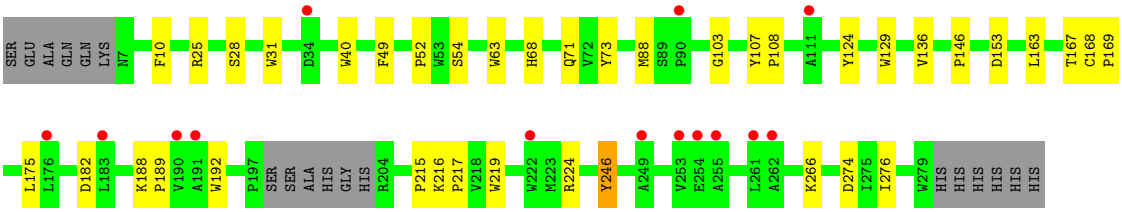
• Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain A:



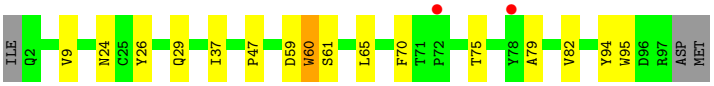
• Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain E:



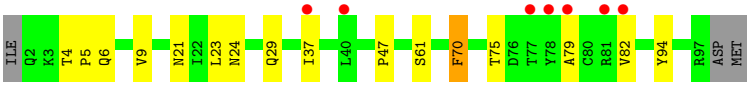
• Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin

Chain F:

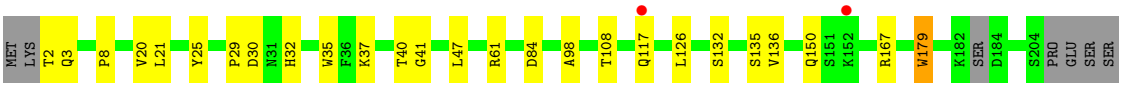


• Molecule 3: Chimeric TCR Valpha14/Jalpha18 chain (mouse variable domain/ human constant domain)

Chain C:

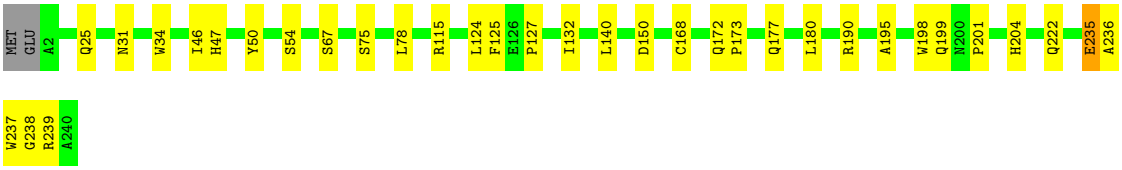
• Molecule 3: Chimeric TCR Valpha14/Jalpha18 chain (mouse variable domain/ human constant domain)

Chain G:



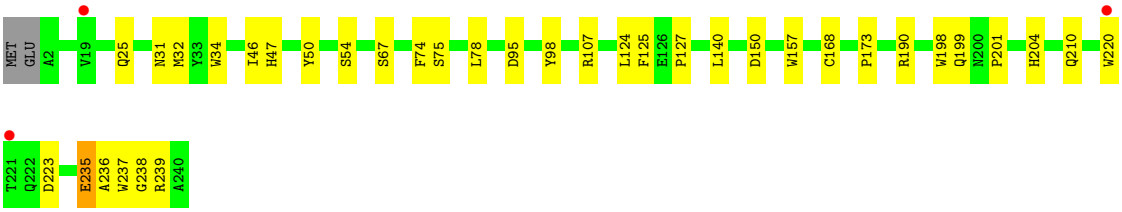
• Molecule 4: Chimeric TCR Vbeta8.2 chain (mouse variable domain/ human constant domain)

Chain D:



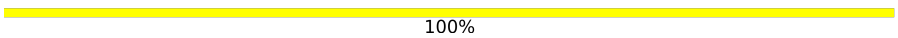
• Molecule 4: Chimeric TCR Vbeta8.2 chain (mouse variable domain/ human constant domain)

Chain H:



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

Chain I:



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

Chain J: 100%

NAG1
NAG2

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

Chain K: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.42Å 150.38Å 102.49Å 90.00° 96.38° 90.00°	Depositor
Resolution (Å)	38.17 – 3.10 38.17 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.17-3.10) 98.7 (38.17-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.242 , 0.287 0.212 , 0.264	Depositor DCC
R_{free} test set	1334 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å^2)	83.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12468	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, 49X

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	0.71	6/2085 (0.3%)	0.62	0/2854
1	E	0.69	5/2092 (0.2%)	0.61	0/2861
2	B	0.65	2/749 (0.3%)	0.61	0/1031
2	F	0.60	0/770	0.58	0/1058
3	C	0.60	2/1551 (0.1%)	0.65	0/2115
3	G	0.60	2/1541 (0.1%)	0.64	0/2103
4	D	0.64	2/1896 (0.1%)	0.63	0/2593
4	H	0.66	4/1890 (0.2%)	0.63	0/2585
All	All	0.65	23/12574 (0.2%)	0.62	0/17200

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	40	TRP	CD2-CE2	5.68	1.48	1.41
4	H	220	TRP	CD2-CE2	5.67	1.48	1.41
4	D	237	TRP	CD2-CE2	5.61	1.48	1.41
3	C	179	TRP	CD2-CE2	5.57	1.48	1.41
4	H	157	TRP	CD2-CE2	5.57	1.48	1.41
4	H	237	TRP	CD2-CE2	5.57	1.48	1.41
2	B	60	TRP	CD2-CE2	5.56	1.48	1.41
1	E	63	TRP	CD2-CE2	5.49	1.48	1.41
3	G	35	TRP	CD2-CE2	5.49	1.48	1.41
4	H	34	TRP	CD2-CE2	5.44	1.47	1.41
3	G	179	TRP	CD2-CE2	5.40	1.47	1.41
4	D	34	TRP	CD2-CE2	5.36	1.47	1.41
1	A	40	TRP	CD2-CE2	5.34	1.47	1.41
1	A	31	TRP	CD2-CE2	5.26	1.47	1.41
1	E	129	TRP	CD2-CE2	5.23	1.47	1.41
1	A	63	TRP	CD2-CE2	5.23	1.47	1.41
1	A	279	TRP	CD2-CE2	5.22	1.47	1.41
1	E	192	TRP	CD2-CE2	5.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	TRP	CD2-CE2	5.21	1.47	1.41
3	C	35	TRP	CD2-CE2	5.20	1.47	1.41
1	A	219	TRP	CD2-CE2	5.19	1.47	1.41
2	B	95	TRP	CD2-CE2	5.18	1.47	1.41
1	E	31	TRP	CD2-CE2	5.11	1.47	1.41

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	2025	0	1794	22	0
1	E	2032	0	1812	22	0
2	B	723	0	612	6	0
2	F	744	0	663	8	0
3	C	1524	0	1414	16	0
3	G	1514	0	1397	16	0
4	D	1845	0	1713	15	0
4	H	1839	0	1700	16	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
6	A	14	0	13	0	0
6	E	28	0	26	1	0
7	A	48	0	67	3	0
7	E	48	0	67	5	0
All	All	12468	0	11353	118	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 (118) 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:204:HIS:NE2	4:H:235:GLU:HG3	1.88	0.86
4:D:204:HIS:NE2	4:D:235:GLU:HG3	1.90	0.86
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.67	0.75
1:E:49:PHE:CD1	1:E:54:SER:HB2	2.24	0.73
1:A:49:PHE:HD1	1:A:54:SER:CB	2.02	0.72
3:G:8:PRO:O	3:G:108:THR:HG23	1.89	0.72
1:E:219:TRP:HB3	1:E:266:LYS:HB2	1.71	0.71
1:A:49:PHE:CD1	1:A:54:SER:HB2	2.26	0.70
3:C:61:ARG:NH2	3:C:84:ASP:OD2	2.23	0.69
1:E:49:PHE:HD1	1:E:54:SER:CB	2.09	0.66
1:E:168:CYS:HB3	1:E:169:PRO:HD3	1.76	0.66
1:A:258:GLU:HB3	1:A:279:TRP:CD1	2.32	0.65
3:G:61:ARG:NH2	3:G:84:ASP:OD2	2.28	0.64
3:C:8:PRO:O	3:C:108:THR:HG23	1.96	0.64
1:A:49:PHE:HD1	1:A:54:SER:HB2	1.61	0.63
3:C:2:THR:O	3:C:2:THR:HG23	1.99	0.62
1:E:49:PHE:HD1	1:E:54:SER:HB2	1.63	0.62
1:E:219:TRP:CE3	1:E:266:LYS:HG3	2.35	0.62
1:A:68:HIS:HA	1:A:71:GLN:OE1	1.99	0.61
4:H:201:PRO:HA	4:H:238:GLY:O	2.02	0.60
4:D:235:GLU:HG2	4:D:236:ALA:N	2.17	0.60
1:A:49:PHE:HD1	1:A:54:SER:HB3	1.68	0.59
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.85	0.58
4:D:201:PRO:HA	4:D:238:GLY:O	2.03	0.58
2:F:29:GLN:HA	2:F:61:SER:HB2	1.86	0.58
3:G:2:THR:O	3:G:2:THR:HG23	2.04	0.58
3:G:20:VAL:C	3:G:21:LEU:HD12	2.25	0.57
1:E:68:HIS:HA	1:E:71:GLN:OE1	2.04	0.56
1:A:215:PRO:HB2	1:A:217:PRO:HD2	1.88	0.56
3:C:20:VAL:C	3:C:21:LEU:HD12	2.26	0.55
4:D:127:PRO:HD2	4:D:198:TRP:CZ2	2.41	0.55
3:C:126:LEU:O	3:C:135:SER:HB2	2.06	0.55
4:D:115:ARG:HB2	4:D:222:GLN:NE2	2.22	0.55
1:A:49:PHE:CD1	1:A:54:SER:CB	2.86	0.55
4:H:235:GLU:HG2	4:H:236:ALA:N	2.21	0.55
1:E:107:TYR:HB3	1:E:108:PRO:HD2	1.90	0.54
3:G:37:LYS:HB2	3:G:47:LEU:HD11	1.89	0.54
7:A:306:49X:H40	3:C:29:PRO:HB3	1.90	0.53
4:H:124:LEU:HD11	4:H:140:LEU:HD23	1.90	0.53
4:H:199:GLN:HA	4:H:239:ARG:O	2.08	0.53
3:G:126:LEU:O	3:G:135:SER:HB2	2.09	0.52
2:B:29:GLN:HA	2:B:61:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:LEU:HD12	4:D:78:LEU:N	2.25	0.51
7:E:305:49X:NBC	7:E:305:49X:H30	2.26	0.51
1:E:88:MET:HE3	1:E:146:PRO:HD3	1.93	0.50
3:C:117:GLN:HE21	3:C:117:GLN:HA	1.76	0.50
1:A:246:TYR:C	1:A:246:TYR:CD2	2.86	0.49
4:H:204:HIS:NE2	4:H:235:GLU:CG	2.68	0.49
4:D:199:GLN:HA	4:D:239:ARG:O	2.12	0.49
2:F:37:ILE:HG12	2:F:82:VAL:HG22	1.95	0.49
2:F:9:VAL:HA	2:F:24:ASN:O	2.13	0.49
2:B:37:ILE:HG12	2:B:82:VAL:HG22	1.95	0.48
3:G:117:GLN:HE21	3:G:117:GLN:HA	1.78	0.48
4:H:31:ASN:OD1	4:H:50:TYR:HD1	1.97	0.47
4:H:78:LEU:HD12	4:H:78:LEU:N	2.29	0.47
2:B:26:TYR:HB2	2:B:65:LEU:CD1	2.44	0.47
3:G:32:HIS:CE1	4:H:98:TYR:CD1	3.03	0.47
4:D:177:GLN:HB3	4:D:180:LEU:HG	1.96	0.47
4:D:115:ARG:HB2	4:D:222:GLN:HE22	1.80	0.47
4:D:31:ASN:OD1	4:D:50:TYR:HD1	1.98	0.46
3:C:24:ASN:OD1	3:C:72:HIS:ND1	2.49	0.46
4:H:127:PRO:HD2	4:H:198:TRP:CZ2	2.50	0.46
1:A:88:MET:HE3	1:A:146:PRO:HD3	1.96	0.46
2:B:9:VAL:HA	2:B:24:ASN:O	2.15	0.46
3:G:98:ALA:HB2	4:H:95:ASP:O	2.15	0.46
1:E:153:ASP:OD2	7:E:305:49X:OG3	2.31	0.45
4:H:46:ILE:HG22	4:H:47:HIS:CD2	2.51	0.45
1:E:49:PHE:HD1	1:E:54:SER:HB3	1.78	0.45
1:A:85:VAL:HG11	1:A:94:TYR:CE1	2.52	0.45
7:E:305:49X:H40	3:G:29:PRO:CB	2.47	0.45
7:E:305:49X:H40	3:G:29:PRO:HB3	1.98	0.45
4:D:124:LEU:HD11	4:D:140:LEU:HD23	1.99	0.45
3:C:37:LYS:HB2	3:C:47:LEU:HD11	1.97	0.45
1:E:216:LYS:N	1:E:217:PRO:CD	2.80	0.45
2:F:21:ASN:HB3	2:F:70:PHE:CE2	2.52	0.45
3:C:136:VAL:HG12	3:C:179:TRP:HB3	2.00	0.44
1:E:215:PRO:HB2	1:E:217:PRO:HD2	1.98	0.44
1:A:207:VAL:HG22	1:A:250:THR:HG22	1.99	0.44
1:E:246:TYR:CD2	1:E:246:TYR:C	2.91	0.44
1:A:140:PRO:HB2	1:A:142:TRP:CD1	2.53	0.43
7:A:306:49X:H40	3:C:29:PRO:CB	2.47	0.43
1:E:49:PHE:CD1	1:E:54:SER:CB	2.90	0.43
4:D:46:ILE:HG22	4:D:47:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HA	1:A:167:THR:HB	2.01	0.43
1:A:10:PHE:O	1:A:103:GLY:HA3	2.19	0.43
1:E:163:LEU:HA	1:E:167:THR:HB	1.99	0.42
7:A:306:49X:H1	3:C:95:ARG:HD3	2.01	0.42
3:G:136:VAL:HG12	3:G:179:TRP:HB3	2.01	0.42
2:B:79:ALA:HB2	2:B:94:TYR:CD2	2.54	0.42
1:E:73:TYR:CD1	7:E:305:49X:H56	2.54	0.42
1:E:188:LYS:HA	1:E:189:PRO:HD2	1.90	0.42
2:F:9:VAL:HG12	2:F:23:LEU:HD11	2.01	0.42
3:C:133:ASP:OD1	3:C:134:LYS:N	2.53	0.42
4:H:125:PHE:CD1	4:H:125:PHE:N	2.87	0.42
4:H:150:ASP:HB2	4:H:173:PRO:HG2	2.02	0.42
2:B:59:ASP:O	2:B:60:TRP:HB2	2.20	0.41
2:F:6:GLN:OE1	2:F:6:GLN:HA	2.21	0.41
2:F:79:ALA:HB2	2:F:94:TYR:CD2	2.55	0.41
4:D:125:PHE:CD1	4:D:125:PHE:N	2.89	0.41
1:E:124:TYR:CZ	1:E:136:VAL:HG11	2.56	0.41
1:A:188:LYS:HA	1:A:189:PRO:HD2	1.88	0.41
1:A:247:LEU:HD12	1:A:248:GLN:H	1.86	0.41
1:A:52:PRO:HB3	1:E:52:PRO:O	2.21	0.41
3:C:63:SER:O	3:C:75:LEU:HD12	2.21	0.41
1:E:25:ARG:HB3	6:E:302:NAG:H82	2.02	0.41
3:G:3:GLN:O	3:G:25:TYR:HA	2.21	0.41
3:G:21:LEU:HD12	3:G:21:LEU:N	2.36	0.41
3:G:41:GLY:CA	4:H:107:ARG:HH22	2.34	0.41
1:A:216:LYS:N	1:A:217:PRO:CD	2.84	0.41
4:H:32:MET:SD	4:H:74:PHE:HB2	2.61	0.41
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.46	0.40
3:C:3:GLN:O	3:C:25:TYR:HA	2.20	0.40
1:E:10:PHE:O	1:E:103:GLY:HA3	2.21	0.40
3:C:121:PRO:HB2	3:C:200:THR:HG23	2.03	0.40
2:F:4:THR:HA	2:F:5:PRO:HD3	1.90	0.40
4:D:132:ILE:HG23	4:D:195:ALA:HB1	2.02	0.40
3:G:30:ASP:N	3:G:30:ASP:OD1	2.55	0.40
4:D:150:ASP:HB2	4:D:173:PRO:HG2	2.03	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	263/285 (92%)	248 (94%)	15 (6%)	0	100	100
1	E	263/285 (92%)	249 (95%)	14 (5%)	0	100	100
2	B	94/99 (95%)	91 (97%)	2 (2%)	1 (1%)	14	46
2	F	94/99 (95%)	91 (97%)	2 (2%)	1 (1%)	14	46
3	C	198/209 (95%)	183 (92%)	12 (6%)	3 (2%)	10	39
3	G	198/209 (95%)	181 (91%)	15 (8%)	2 (1%)	15	49
4	D	237/241 (98%)	230 (97%)	7 (3%)	0	100	100
4	H	237/241 (98%)	229 (97%)	8 (3%)	0	100	100
All	All	1584/1668 (95%)	1502 (95%)	75 (5%)	7 (0%)	34	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	150	GLN
3	C	42	LYS
3	C	150	GLN
2	B	47	PRO
2	F	47	PRO
3	G	132	SER
3	C	27	VAL

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	204/249 (82%)	200 (98%)	4 (2%)	55	80
1	E	206/249 (83%)	199 (97%)	7 (3%)	37	69
2	B	72/93 (77%)	70 (97%)	2 (3%)	43	73
2	F	78/93 (84%)	76 (97%)	2 (3%)	46	74
3	C	171/188 (91%)	169 (99%)	2 (1%)	71	88
3	G	168/188 (89%)	166 (99%)	2 (1%)	71	88
4	D	195/208 (94%)	187 (96%)	8 (4%)	30	64
4	H	194/208 (93%)	185 (95%)	9 (5%)	27	59
All	All	1288/1476 (87%)	1252 (97%)	36 (3%)	43	73

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	182	ASP
1	A	193	LEU
1	A	246	TYR
2	B	70	PHE
2	B	75	THR
3	C	11	LEU
3	C	167	ARG
4	D	25	GLN
4	D	54	SER
4	D	67	SER
4	D	75	SER
4	D	168	CYS
4	D	172	GLN
4	D	190	ARG
4	D	235	GLU
1	E	28	SER
1	E	175	LEU
1	E	182	ASP
1	E	224	ARG
1	E	246	TYR
1	E	274	ASP
1	E	276	ILE
2	F	70	PHE
2	F	75	THR
3	G	40	THR
3	G	167	ARG

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Mol	Chain	Res	Type
4	H	25	GLN
4	H	54	SER
4	H	67	SER
4	H	75	SER
4	H	168	CYS
4	H	190	ARG
4	H	210	GLN
4	H	223	ASP
4	H	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
2	B	13	HIS
3	C	31	ASN
3	C	117	GLN
4	D	24	ASN
4	D	222	GLN
4	D	230	GLN
1	E	117	HIS
2	F	13	HIS
3	G	31	ASN
3	G	117	GLN
4	H	24	ASN
4	H	230	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)

6 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	I	1	5,1	14,14,15	0.51	0	17,19,21	2.05	1 (5%)
5	NAG	I	2	5	14,14,15	0.69	0	17,19,21	1.05	1 (5%)
5	NAG	J	1	5,1	14,14,15	0.72	0	17,19,21	2.01	6 (35%)
5	NAG	J	2	5	14,14,15	0.58	0	17,19,21	1.69	3 (17%)
5	NAG	K	1	5,1	14,14,15	0.43	0	17,19,21	1.38	4 (23%)
5	NAG	K	2	5	14,14,15	0.61	0	17,19,21	1.23	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
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1	NAG	C1-O5-C5	7.28	122.06	112.19
5	J	1	NAG	C6-C5-C4	4.60	123.77	113.00
5	J	2	NAG	O5-C5-C6	3.84	113.23	107.20
5	J	1	NAG	C2-N2-C7	3.59	128.02	122.90
5	J	1	NAG	C3-C4-C5	-3.51	103.97	110.24
5	J	2	NAG	C4-C3-C2	3.48	116.11	111.02
5	K	1	NAG	C1-O5-C5	3.07	116.35	112.19
5	I	2	NAG	C4-C3-C2	3.04	115.47	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	2	NAG	O5-C1-C2	-2.94	106.65	111.29
5	K	2	NAG	O5-C5-C6	2.58	111.25	107.20
5	K	1	NAG	C4-C3-C2	2.55	114.75	111.02
5	J	1	NAG	C4-C3-C2	2.42	114.56	111.02
5	J	1	NAG	C1-C2-N2	2.35	114.50	110.49
5	K	1	NAG	O5-C1-C2	-2.31	107.64	111.29
5	J	1	NAG	O7-C7-C8	-2.15	118.06	122.06
5	K	1	NAG	O5-C5-C6	2.07	110.45	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

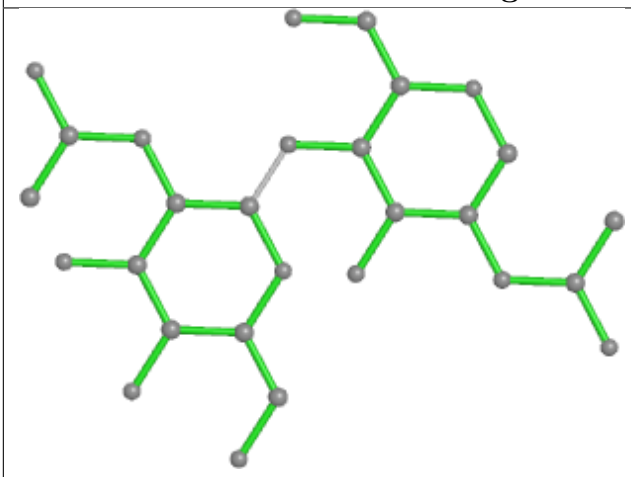
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6

There are no ring outliers.

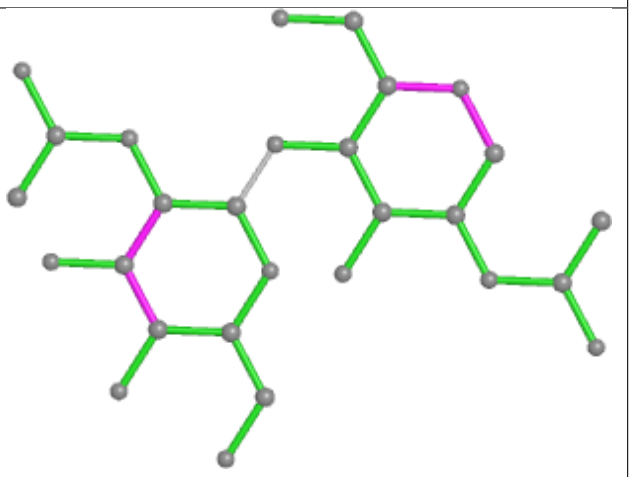
No monomer is involved in short contacts.

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

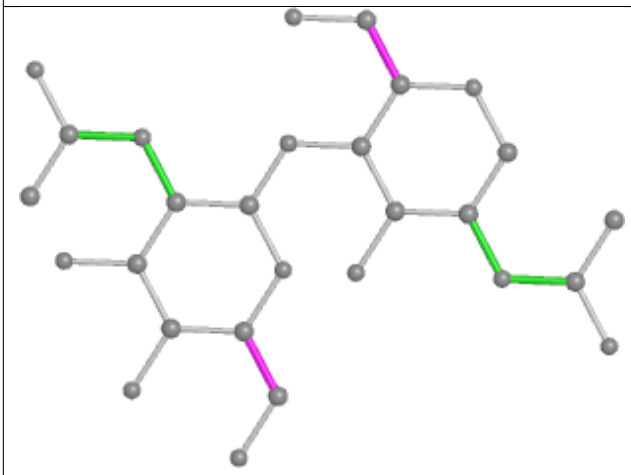
Oligosaccharide Chain I



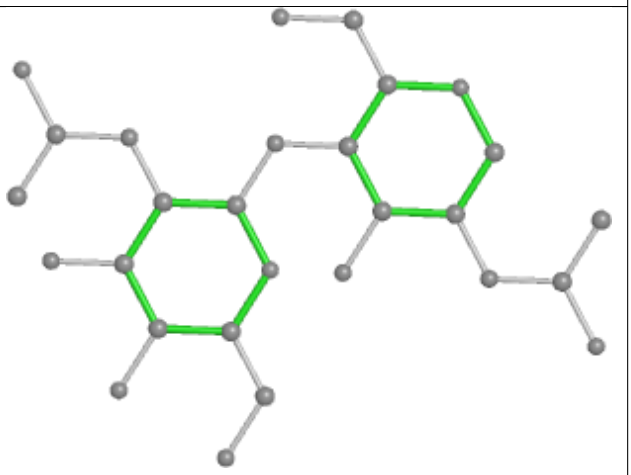
Bond lengths



Bond angles

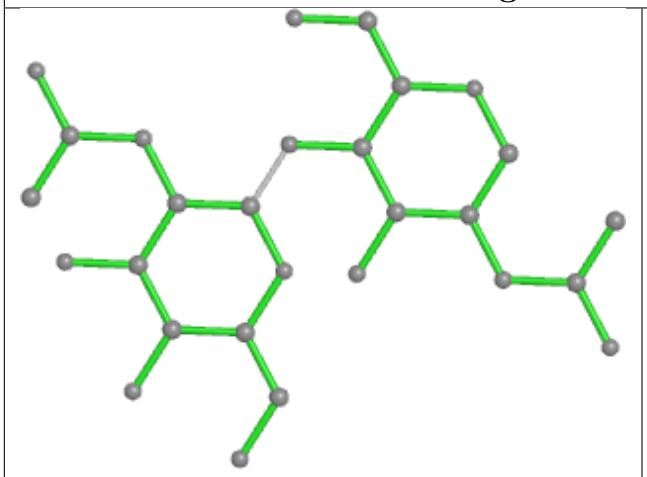


Torsions

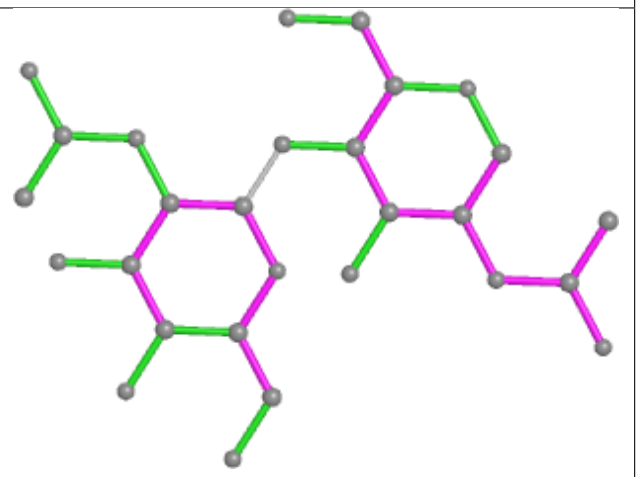


Rings

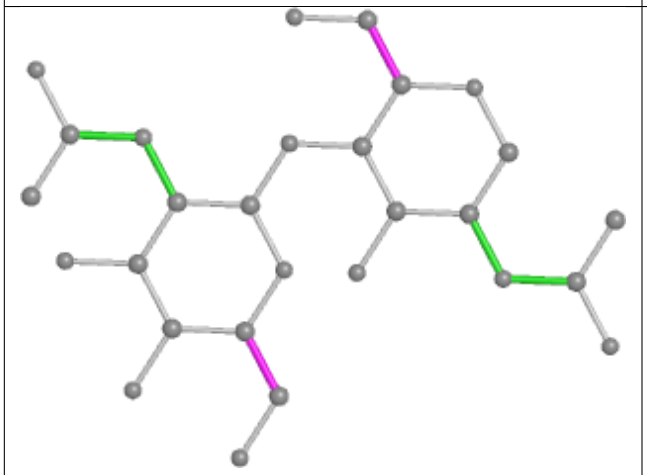
Oligosaccharide Chain J



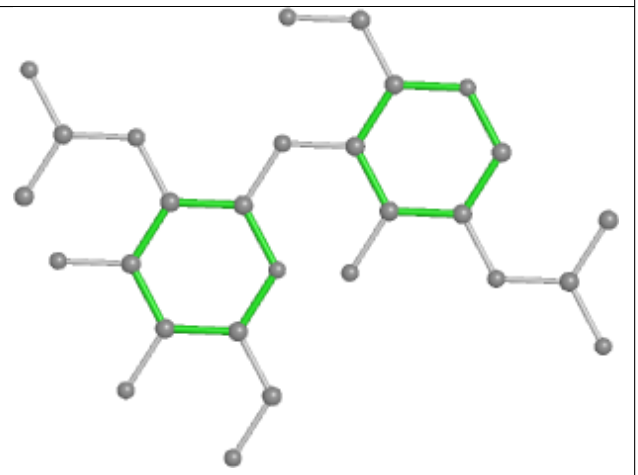
Bond lengths



Bond angles

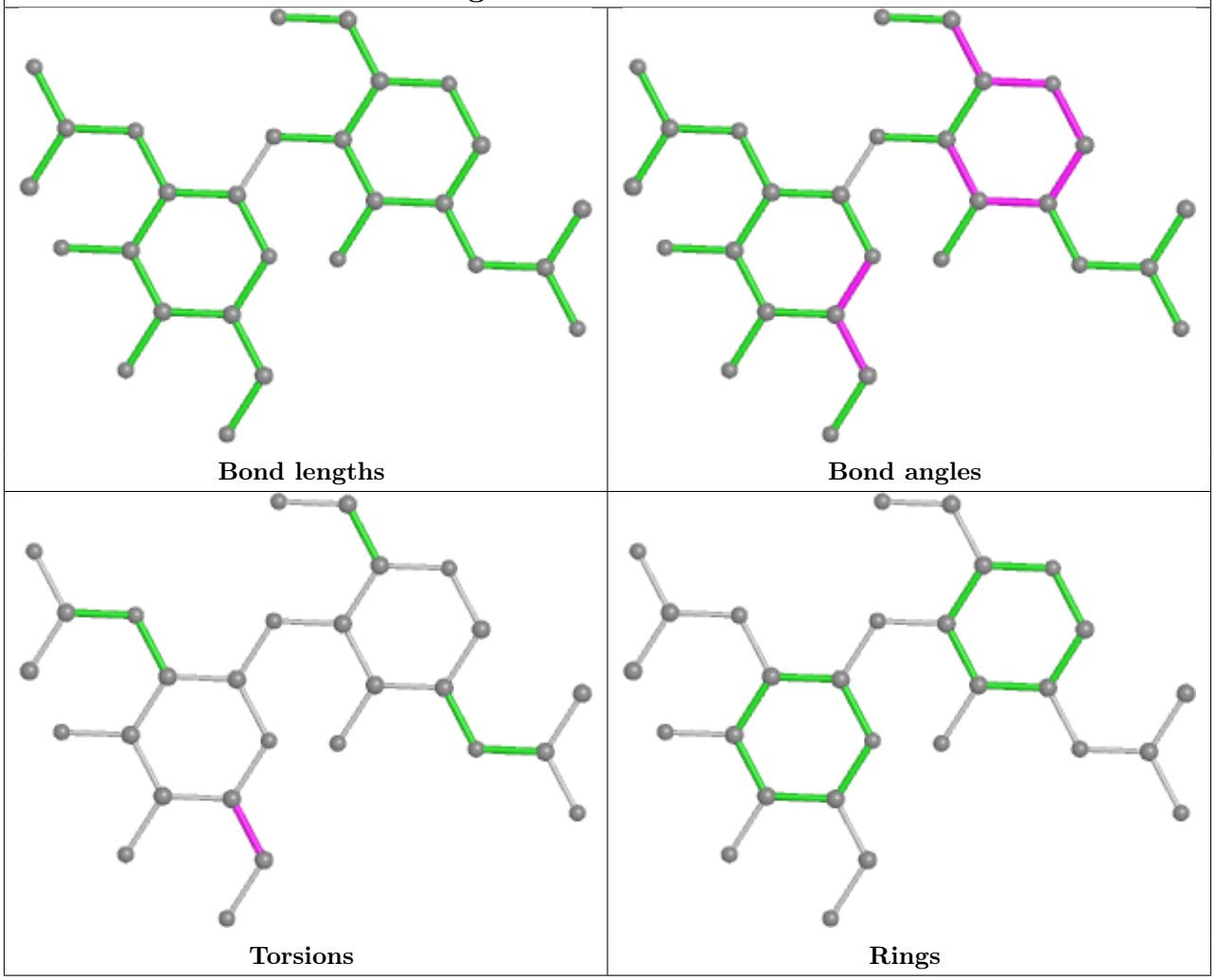


Torsions



Rings

Oligosaccharide Chain K



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	$\#\|Z\| > 2$
6	NAG	E	302	1	14,14,15	0.52	0	17,19,21	1.81	3 (17%)
6	NAG	E	301	1	14,14,15	0.70	0	17,19,21	1.20	2 (11%)
7	49X	E	305	-	49,49,49	0.87	2 (4%)	52,60,60	0.98	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	49X	A	306	-	49,49,49	0.92	3 (6%)	52,60,60	1.21	4 (7%)
6	NAG	A	301	1	14,14,15	0.50	0	17,19,21	1.44	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
6	NAG	E	302	1	-	2/6/23/26	0/1/1/1
6	NAG	E	301	1	-	0/6/23/26	0/1/1/1
7	49X	E	305	-	-	25/43/63/63	0/2/2/2
7	49X	A	306	-	-	20/43/63/63	0/2/2/2
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	306	49X	CAH-CAK	2.87	1.40	1.32
7	E	305	49X	C1-CAH	-2.86	1.40	1.50
7	E	305	49X	CAH-CAK	2.63	1.40	1.32
7	A	306	49X	C1-CAH	-2.61	1.41	1.50
7	A	306	49X	CAL-CAK	2.22	1.55	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	306	49X	CAP-CAO-CAN	-4.90	106.12	114.18
6	A	301	NAG	O5-C5-C6	4.75	114.65	107.20
6	E	302	NAG	C1-O5-C5	4.54	118.34	112.19
7	A	306	49X	OBL-CAM-CAN	-3.51	100.33	108.81
6	E	302	NAG	C3-C4-C5	-3.27	104.40	110.24
7	A	306	49X	CG-OG-C1	-2.92	107.62	112.81
6	E	301	NAG	C4-C3-C2	2.81	115.14	111.02
6	E	302	NAG	C4-C3-C2	-2.52	107.32	111.02
7	E	305	49X	CG5-CG-CG4	2.39	118.61	113.00
6	E	301	NAG	O5-C5-C6	2.35	110.89	107.20
7	E	305	49X	OG6-CG5-CG	-2.34	103.28	111.29
7	E	305	49X	CAL-NBC-CBD	-2.23	120.74	123.13
7	E	305	49X	CAP-CAO-CAN	-2.22	110.52	114.18
7	A	306	49X	OG-CG-CG5	2.19	111.87	106.44

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	306	49X	OG-C1-CAH-CAK
7	A	306	49X	CG2-C1-CAH-CAK
7	A	306	49X	CAH-CAK-CAL-CAM
7	A	306	49X	CAH-CAK-CAL-NBC
7	E	305	49X	OG-C1-CAH-CAK
7	E	305	49X	CG2-C1-CAH-CAK
7	E	305	49X	OBN-CAN-CAO-CAP
7	E	305	49X	NBC-CAL-CAM-OBL
7	E	305	49X	CAH-CAK-CAL-CAM
7	E	305	49X	CAH-CAK-CAL-NBC
6	A	301	NAG	O5-C5-C6-O6
6	E	302	NAG	O5-C5-C6-O6
7	E	305	49X	CBD-CBE-CBF-CBG
7	A	306	49X	OG-CG-CG5-OG6
7	E	305	49X	OG-CG-CG5-OG6
6	A	301	NAG	C4-C5-C6-O6
7	E	305	49X	CG4-CG-CG5-OG6
7	A	306	49X	CAR-CAS-CAT-CAU
7	A	306	49X	CBD-CBE-CBF-CBG
7	E	305	49X	CBI-CBJ-CBK-CBO
7	A	306	49X	CBI-CBJ-CBK-CBO
7	A	306	49X	CG4-CG-CG5-OG6
7	A	306	49X	CAT-CAU-CAV-CAW
6	E	302	NAG	C4-C5-C6-O6
7	A	306	49X	CBF-CBG-CBH-CBI
7	E	305	49X	CAT-CAU-CAV-CAW
7	A	306	49X	CBE-CBF-CBG-CBH
7	E	305	49X	CAV-CAW-CAX-CAY
7	E	305	49X	CAX-CAY-CAZ-CBA
7	E	305	49X	CBE-CBF-CBG-CBH
7	E	305	49X	CBF-CBG-CBH-CBI
7	E	305	49X	CAO-CAP-CAQ-CAR
7	A	306	49X	CAW-CAX-CAY-CAZ
7	E	305	49X	CAU-CAV-CAW-CAX
7	E	305	49X	CAK-CAL-CAM-OBL
7	E	305	49X	CAP-CAQ-CAR-CAS
7	E	305	49X	CBH-CBI-CBJ-CBK
7	A	306	49X	CBH-CBI-CBJ-CBK
7	A	306	49X	CAQ-CAR-CAS-CAT
7	E	305	49X	CAM-CAN-CAO-CAP

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Mol	Chain	Res	Type	Atoms
7	A	306	49X	CAV-CAW-CAX-CAY
7	A	306	49X	CAU-CAV-CAW-CAX
7	A	306	49X	CAY-CAZ-CBA-CBB
7	E	305	49X	CBJ-CBK-CBO-CBR
7	E	305	49X	CBJ-CBK-CBO-CBV
7	E	305	49X	CAR-CAS-CAT-CAU
7	A	306	49X	CBJ-CBK-CBO-CBR
7	A	306	49X	CBJ-CBK-CBO-CBV
7	E	305	49X	CAK-CAL-CAM-CAN

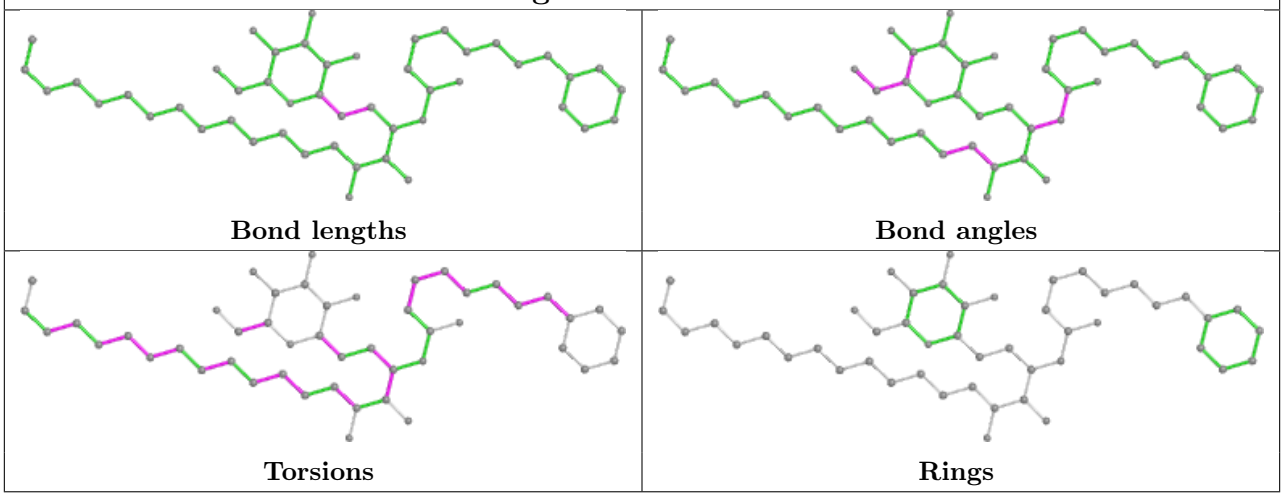
There are no ring outliers.

3 monomers are involved in 9 short contacts:

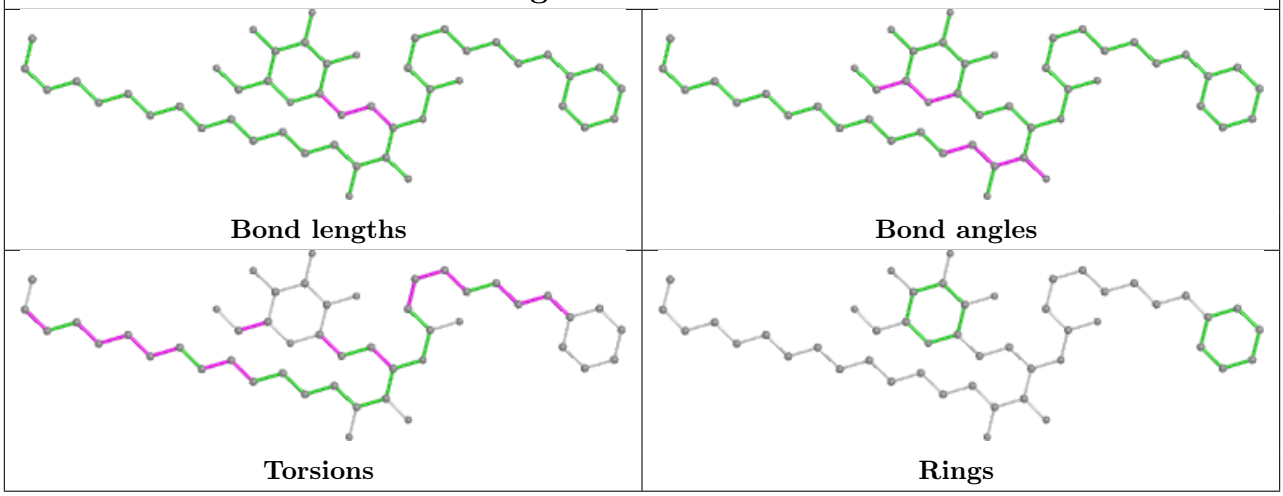
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	302	NAG	1	0
7	E	305	49X	5	0
7	A	306	49X	3	0

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 then 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.

Ligand 49X E 305



Ligand 49X A 306



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	267/285 (93%)	0.30	22 (8%) 11 4	39, 79, 170, 204	0
1	E	267/285 (93%)	0.00	14 (5%) 27 12	40, 76, 136, 169	0
2	B	96/99 (96%)	-0.15	2 (2%) 63 43	47, 81, 111, 125	0
2	F	96/99 (96%)	0.33	7 (7%) 15 6	59, 95, 118, 127	0
3	C	202/209 (96%)	-0.24	0 100 100	36, 57, 114, 148	0
3	G	202/209 (96%)	-0.30	2 (0%) 82 67	34, 57, 112, 153	0
4	D	239/241 (99%)	-0.28	0 100 100	40, 60, 108, 123	0
4	H	239/241 (99%)	-0.34	3 (1%) 77 59	36, 60, 97, 123	0
All	All	1608/1668 (96%)	-0.10	50 (3%) 49 26	34, 67, 128, 204	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	VAL	7.3
1	E	262	ALA	6.3
1	A	191	ALA	6.2
2	F	79	ALA	6.2
1	A	256	GLY	5.9
1	E	90	PRO	4.8
1	A	223	MET	4.7
1	A	271	GLY	4.0
1	A	263	CYS	4.0
1	A	276	ILE	3.9
2	F	77	THR	3.7
1	E	222	TRP	3.6
1	A	255	ALA	3.6
1	A	220	VAL	3.4
1	E	253	VAL	3.3
1	A	111	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	261	LEU	3.2
4	H	221	THR	3.1
1	E	254	GLU	3.1
1	E	34	ASP	3.1
1	E	191	ALA	3.1
1	A	107	TYR	3.1
2	F	40	LEU	2.9
1	A	260	GLY	2.9
2	F	78	TYR	2.8
1	A	265	VAL	2.8
1	A	108	PRO	2.8
1	A	231	GLY	2.7
2	F	37	ILE	2.6
1	E	255	ALA	2.6
1	A	225	GLY	2.5
1	A	226	ASP	2.5
1	E	249	ALA	2.5
1	A	262	ALA	2.4
1	A	278	TYR	2.4
1	A	208	CYS	2.4
1	E	183	LEU	2.3
4	H	220	TRP	2.3
1	A	252	ASP	2.3
1	E	111	ALA	2.2
4	H	19	VAL	2.2
3	G	152	LYS	2.2
1	E	190	VAL	2.2
2	B	72	PRO	2.2
3	G	117	GLN	2.2
2	F	82	VAL	2.1
1	E	176	LEU	2.1
2	F	81	ARG	2.1
1	A	8	TYR	2.1
2	B	78	TYR	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)

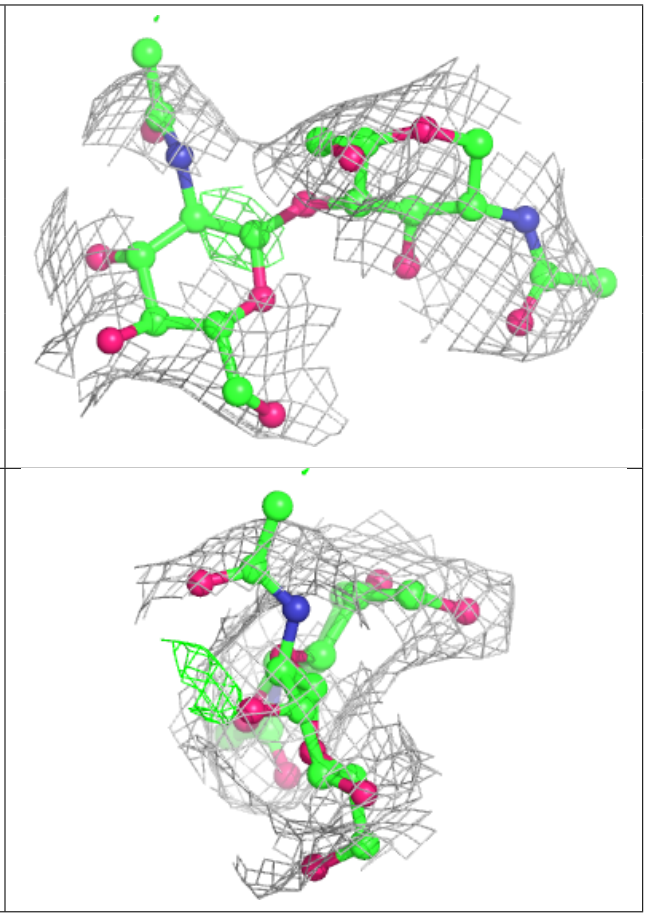
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	I	2	14/15	0.86	0.26	99,111,125,126	0
5	NAG	K	2	14/15	0.87	0.17	76,87,94,95	0
5	NAG	J	1	14/15	0.90	0.16	51,63,70,71	0
5	NAG	I	1	14/15	0.92	0.25	64,69,75,90	0
5	NAG	J	2	14/15	0.93	0.23	74,86,93,94	0
5	NAG	K	1	14/15	0.94	0.19	57,62,71,72	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.

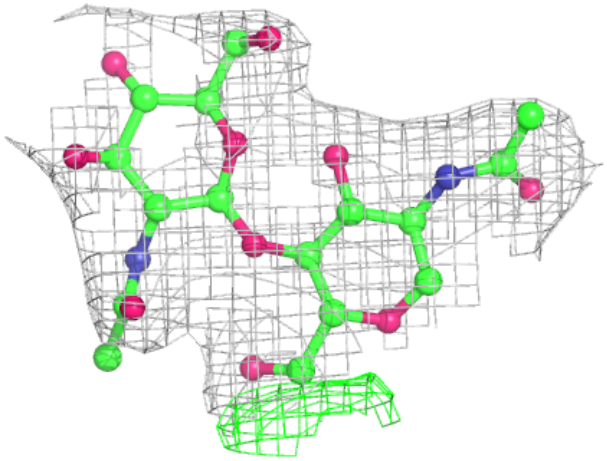
Electron density around Chain I:

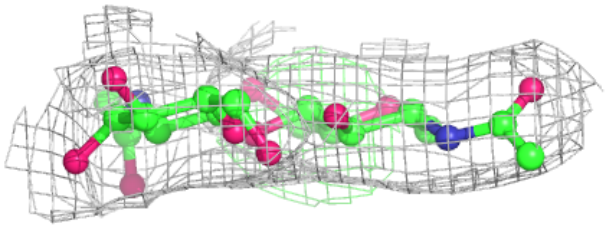
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

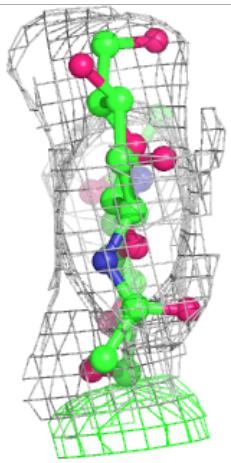


Electron density around Chain J:

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

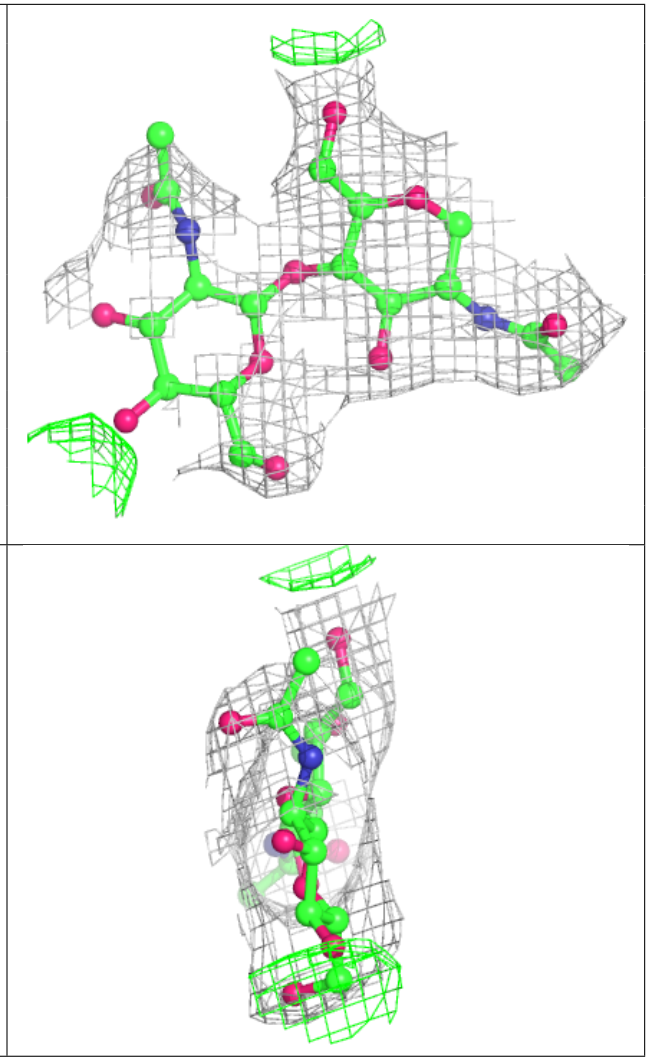






Electron density around Chain K:

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



6.4 Ligands (i)

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

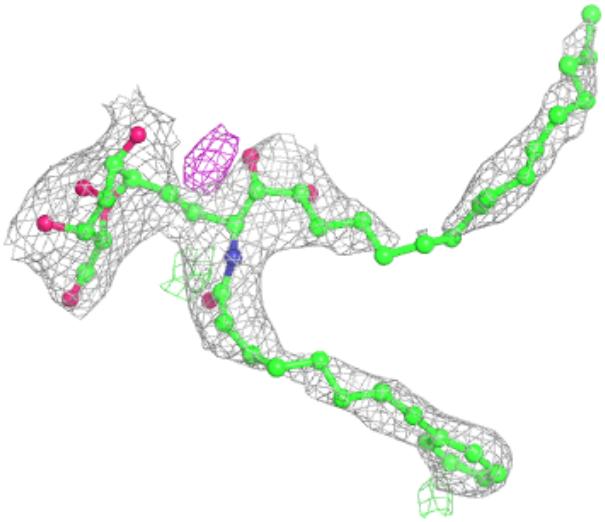
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	301	14/15	0.88	0.21	90,97,106,109	0
6	NAG	E	301	14/15	0.89	0.23	82,100,106,112	0
6	NAG	E	302	14/15	0.89	0.27	69,70,74,79	0
7	49X	A	306	48/48	0.95	0.30	46,57,75,77	0
7	49X	E	305	48/48	0.95	0.30	42,53,64,68	0

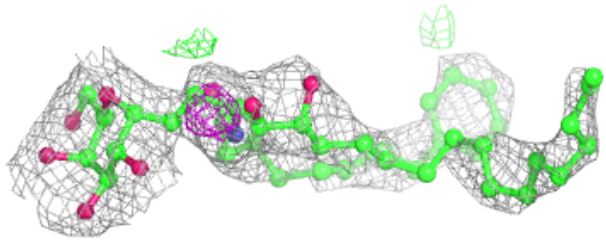
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

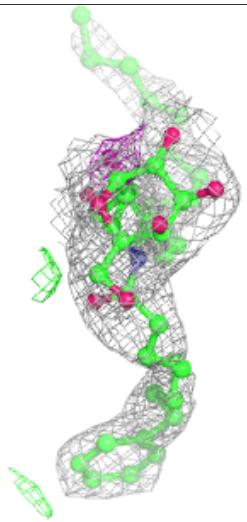
orientation to approximate a three-dimensional view.

Electron density around 49X A 306:

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

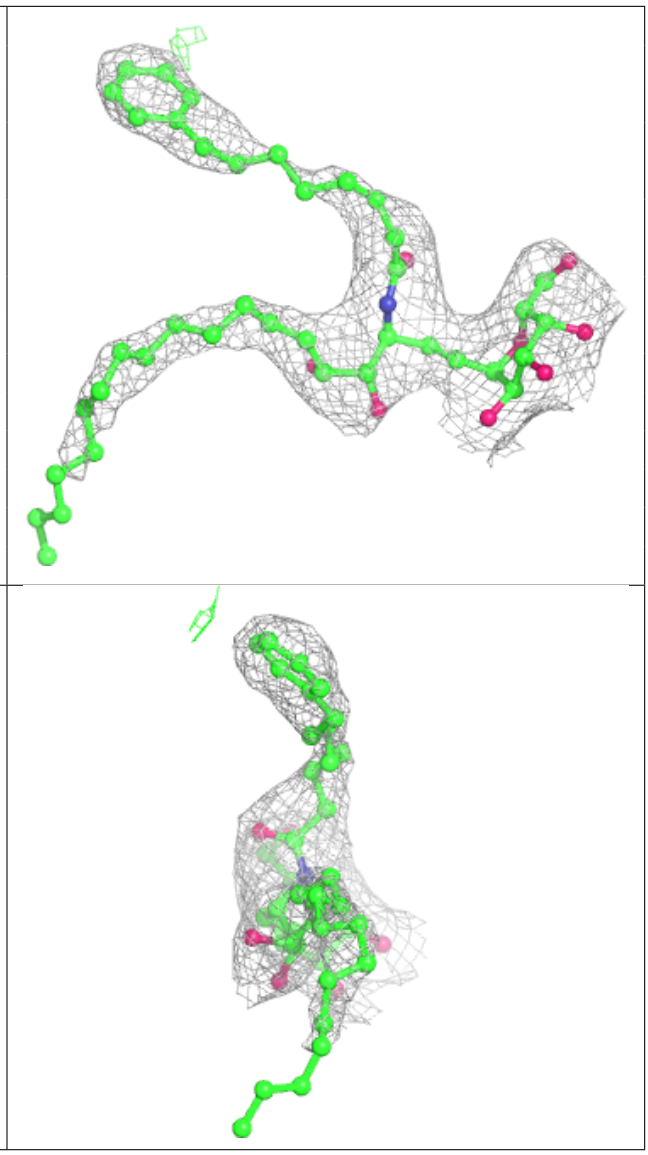






Electron density around 49X E 305:

$2mF_o$-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.