Full wwPDB EM Validation Report ⓘ

Feb 22, 2024 – 03:16 AM JST

PDB ID	:	8K8E
EMDB ID	:	EMD-36948
Title	:	Human gamma-secretase in complex with a substrate mimetic
Authors	:	Shi, Y.G.; Zhou, R.; Wolfe, M.S.
Deposited on	:	2023-07-29
Resolution	:	2.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

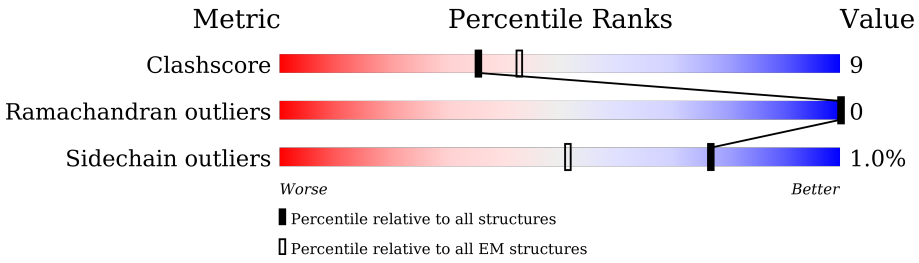
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	709	79% 15% 6%
2	B	467	49% 16% 35%
3	C	265	78% 14% 8%
4	D	101	64% 31% 5%
5	G	18	72% 28%
6	E	2	50% 50%
7	F	3	33% 67%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10716 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	667	5235	3321	890	1003	21	0	0

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	302	2394	1624	362	394	14	0	0

- Molecule 3 is a protein called Gamma-secretase subunit APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	243	1872	1254	299	315	4	0	0

- Molecule 4 is a protein called Gamma-secretase subunit PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	96	814	559	126	128	1	0	0

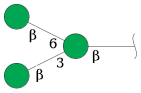
- Molecule 5 is a protein called BOC-VAL-GLY-AIB-VAL-VAL-ILE-AIB-PHE-VAL-AIB-GLY-GLY-GLY-VAL-JUU-LEU-VLM.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	18	133	94	19	20	0	0

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

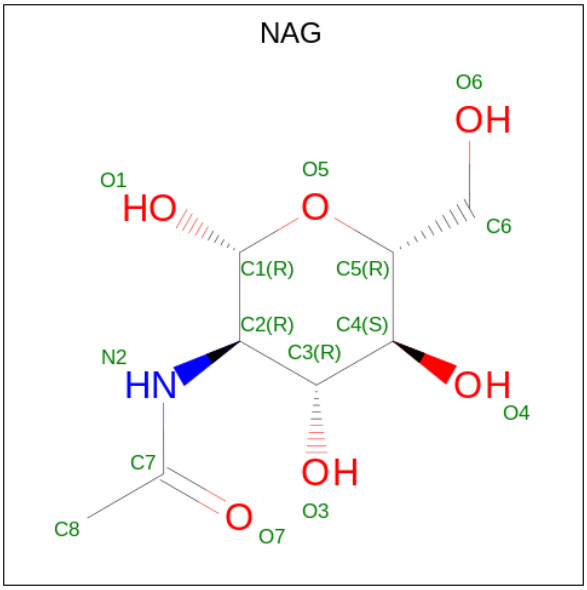
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	3	Total	C	O		0	0
			33	18	15			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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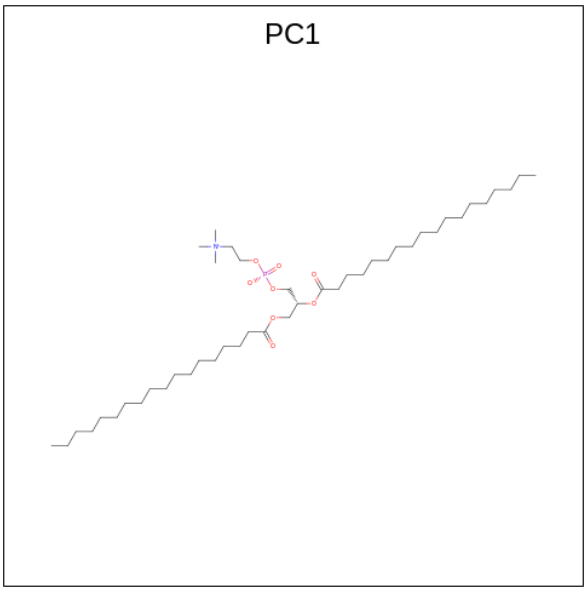
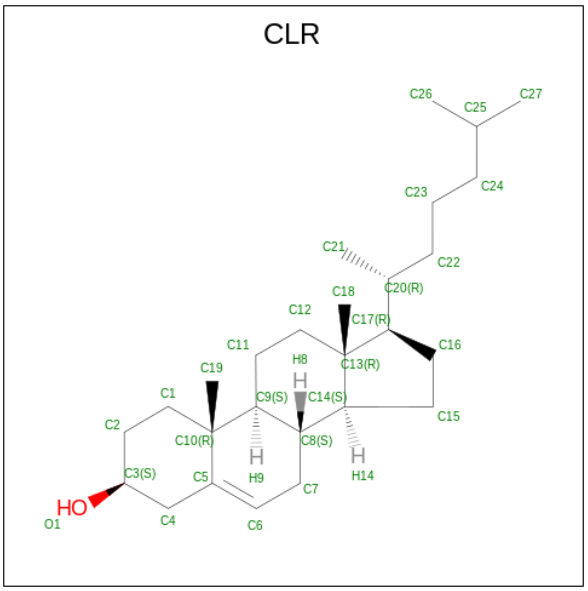
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



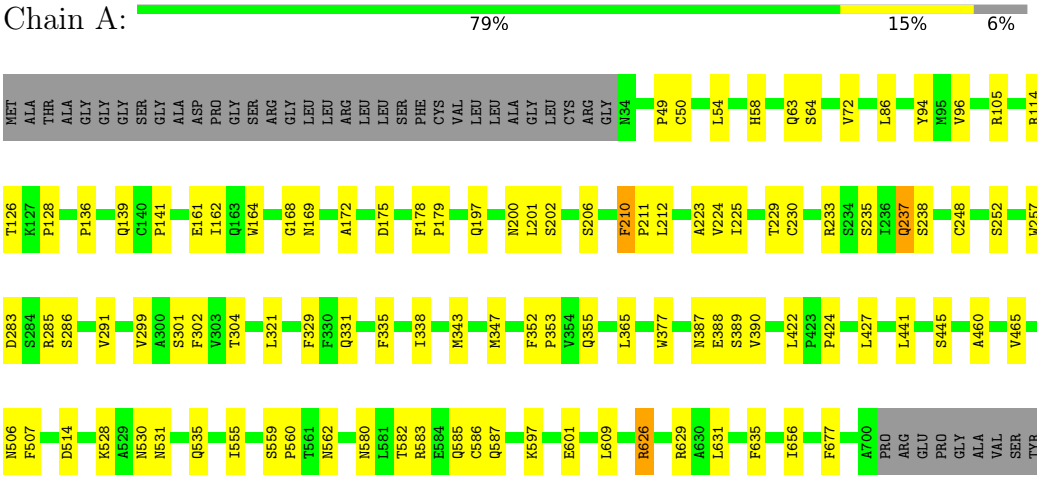
Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			28	27	1	
10	C	1	Total	C	O	0
			28	27	1	
10	C	1	Total	C	O	0
			28	27	1	

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. 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. 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.

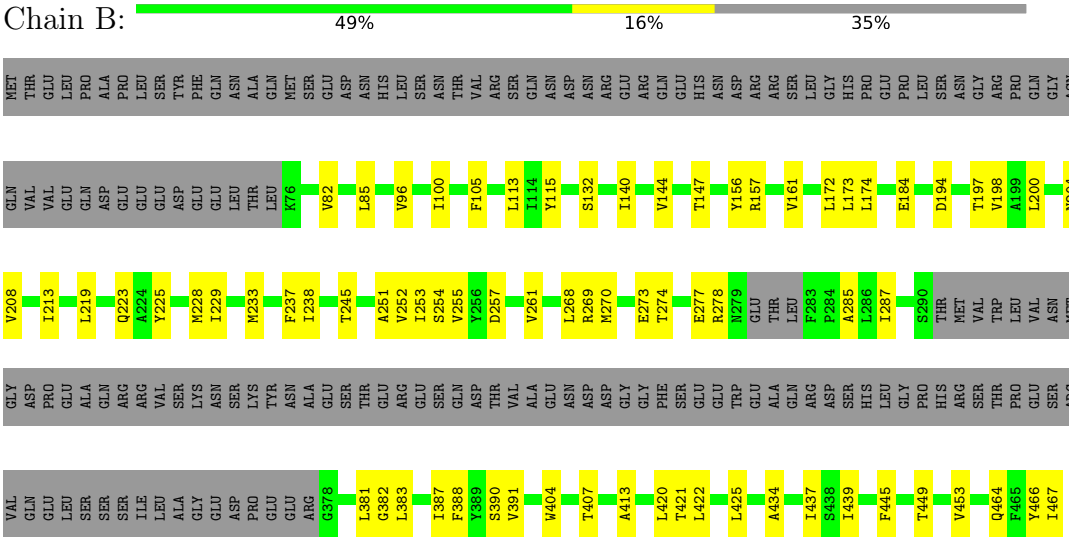
• Molecule 1: Nicastrin

Chain A:



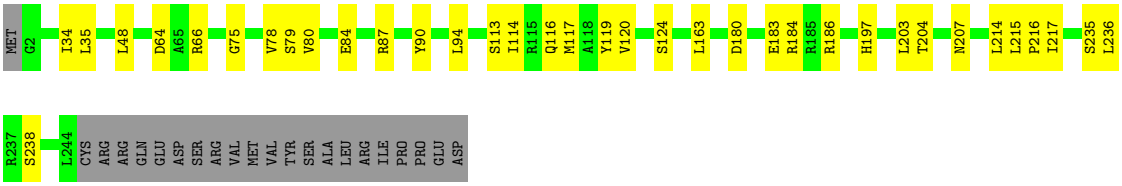
• Molecule 2: Presenilin-1

Chain B:



• Molecule 3: Gamma-secretase subunit APH-1A

Chain C:

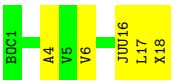


• Molecule 4: Gamma-secretase subunit PEN-2

Chain D:

• Molecule 5: BOC-VAL-GLY-AIB-VAL-VAL-ILE-AIB-PHE-VAL-AIB-GLY-GLY-GLY-VAL-JUU-LEU-VLM

Chain G:



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

Chain E:

• Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	349532	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BOC, AIB, NAG, CLR, BMA, JUU, PC1, VLM

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	0.28	0/5358	0.50	0/7302
2	B	0.26	0/2456	0.45	0/3350
3	C	0.27	0/1924	0.46	0/2624
4	D	0.30	0/847	0.52	0/1157
5	G	0.23	0/77	0.48	0/102
All	All	0.27	0/10662	0.48	0/14535

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

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	5235	0	5129	88	0
2	B	2394	0	2513	56	0
3	C	1872	0	1911	27	0
4	D	814	0	804	23	0
5	G	133	0	126	7	0
6	E	28	0	25	1	0
7	F	33	0	28	0	0
8	A	84	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	39	0	52	0	0
10	C	84	0	138	0	0
All	All	10716	0	10804	186	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 (186) 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:283:ASP:HB3	1:A:331:GLN:NE2	1.67	1.09
1:A:224:VAL:HG22	1:A:230:CYS:HB2	1.33	1.07
1:A:283:ASP:HB3	1:A:331:GLN:HE22	1.15	1.05
1:A:387:ASN:HD22	1:A:390:VAL:HG23	1.23	1.03
1:A:285:ARG:HD3	1:A:335:PHE:HZ	1.31	0.95
1:A:224:VAL:CG2	1:A:230:CYS:HB2	1.97	0.93
1:A:387:ASN:HD22	1:A:390:VAL:CG2	1.84	0.91
2:B:172:LEU:HD21	5:G:6:VAL:HB	1.51	0.91
1:A:387:ASN:ND2	1:A:390:VAL:HG23	1.88	0.87
1:A:285:ARG:HD3	1:A:335:PHE:CZ	2.13	0.84
2:B:467:ILE:HD11	3:C:79:SER:HB3	1.63	0.80
4:D:61:ALA:O	4:D:65:LEU:HD13	1.84	0.77
1:A:283:ASP:CB	1:A:331:GLN:HE22	1.97	0.75
2:B:204:ASN:HD21	4:D:27:PRO:HD2	1.52	0.74
1:A:224:VAL:HG22	1:A:230:CYS:CB	2.14	0.72
1:A:235:SER:HA	1:A:238:SER:OG	1.89	0.72
1:A:224:VAL:HG21	1:A:229:THR:C	2.10	0.72
2:B:261:VAL:HG12	2:B:268:LEU:HD11	1.74	0.69
3:C:203:LEU:HD21	3:C:216:PRO:HB2	1.74	0.69
1:A:285:ARG:HG2	1:A:286:SER:H	1.57	0.68
4:D:9:GLU:N	4:D:9:GLU:OE2	2.24	0.67
1:A:63:GLN:NE2	1:A:64:SER:O	2.28	0.67
1:A:559:SER:HB2	1:A:629:ARG:HH12	1.58	0.67
2:B:464:GLN:O	3:C:207:ASN:ND2	2.22	0.67
4:D:39:ARG:HG3	4:D:43:LEU:HD12	1.77	0.66
2:B:225:TYR:HA	2:B:228:MET:HE2	1.78	0.66
1:A:86:LEU:HD12	1:A:114:ARG:HD3	1.78	0.66
3:C:180:ASP:OD1	3:C:184:ARG:NH2	2.29	0.66
1:A:283:ASP:CB	1:A:331:GLN:NE2	2.52	0.66
1:A:528:LYS:O	1:A:531:ASN:ND2	2.28	0.65
1:A:506:ASN:OD1	1:A:507:PHE:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:VAL:CG2	1:A:230:CYS:CB	2.75	0.64
1:A:285:ARG:HG2	1:A:286:SER:N	2.12	0.64
2:B:82:VAL:HG22	2:B:422:LEU:HD13	1.80	0.63
2:B:261:VAL:HG12	2:B:268:LEU:CD1	2.28	0.63
4:D:44:VAL:O	4:D:50:GLN:NE2	2.32	0.63
2:B:233:MET:HB3	2:B:387:ILE:HD12	1.80	0.63
1:A:387:ASN:HB3	1:A:390:VAL:HB	1.81	0.62
1:A:601:GLU:OE2	1:A:626:ARG:NH1	2.33	0.62
2:B:274:THR:HA	2:B:277:GLU:HG2	1.81	0.62
1:A:347:MET:O	1:A:355:GLN:NE2	2.32	0.62
1:A:580:ASN:OD1	1:A:580:ASN:N	2.33	0.61
1:A:120:GLY:H	1:A:178:PHE:HB2	1.66	0.60
4:D:26:LEU:HB3	4:D:29:LEU:HB2	1.82	0.60
1:A:530:ASN:OD1	1:A:535:GLN:NE2	2.34	0.59
1:A:224:VAL:HG21	1:A:230:CYS:N	2.17	0.59
3:C:34:ILE:HD11	3:C:120:VAL:HB	1.85	0.59
2:B:268:LEU:HD13	5:G:16:JUU:C78	2.33	0.59
1:A:237:GLN:O	1:A:237:GLN:HG3	2.03	0.59
2:B:261:VAL:CG1	2:B:268:LEU:HD11	2.32	0.58
4:D:52:GLN:N	4:D:52:GLN:OE1	2.37	0.58
1:A:224:VAL:HG21	1:A:230:CYS:CA	2.33	0.58
2:B:268:LEU:HD13	5:G:16:JUU:C79	2.34	0.57
1:A:477:LEU:HD11	1:A:531:ASN:HB3	1.86	0.56
3:C:180:ASP:OD1	3:C:184:ARG:CZ	2.53	0.56
1:A:285:ARG:CG	1:A:286:SER:H	2.20	0.55
2:B:270:MET:HA	2:B:273:GLU:HB2	1.88	0.55
2:B:173:LEU:HD13	2:B:229:ILE:HG23	1.88	0.55
1:A:235:SER:O	1:A:238:SER:OG	2.24	0.55
3:C:64:ASP:OD1	3:C:66:ARG:N	2.39	0.55
1:A:105:ARG:NH1	1:A:169:ASN:O	2.40	0.54
2:B:277:GLU:HG3	2:B:278:ARG:HD3	1.89	0.54
3:C:184:ARG:HE	3:C:186:ARG:NH2	2.05	0.54
1:A:126:THR:HG22	1:A:128:PRO:HD2	1.88	0.54
2:B:156:TYR:HD2	2:B:157:ARG:HG3	1.73	0.54
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.90	0.54
2:B:420:LEU:HD12	2:B:437:ILE:HD11	1.91	0.53
2:B:194:ASP:HB2	2:B:197:THR:H	1.72	0.53
4:D:27:PRO:HG3	4:D:67:TRP:CG	2.43	0.53
3:C:113:SER:OG	3:C:116:GLN:OE1	2.22	0.52
1:A:161:GLU:HG2	1:A:162:ILE:HG23	1.92	0.52
2:B:269:ARG:NH1	2:B:273:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:VAL:CG2	1:A:230:CYS:CA	2.87	0.52
4:D:48:THR:OG1	4:D:49:GLU:N	2.41	0.52
2:B:381:LEU:HD13	5:G:17:LEU:HD12	1.90	0.52
1:A:58:HIS:HB2	6:E:1:NAG:H5	1.92	0.52
1:A:49:PRO:HG3	1:A:656:ILE:HG21	1.92	0.51
2:B:198:VAL:HG21	4:D:94:PHE:CD2	2.45	0.51
4:D:12:LEU:HA	4:D:53:ILE:HD11	1.91	0.51
1:A:64:SER:HB3	1:A:179:PRO:HG3	1.92	0.51
4:D:58:TRP:O	4:D:62:VAL:HG13	2.10	0.51
4:D:10:GLU:OE2	4:D:10:GLU:HA	2.10	0.51
1:A:331:GLN:HE21	1:A:555:ILE:HB	1.76	0.51
2:B:157:ARG:HD3	2:B:161:VAL:CG2	2.41	0.51
2:B:132:SER:HA	2:B:245:THR:HG22	1.93	0.51
1:A:197:GLN:HA	1:A:201:LEU:HD21	1.93	0.50
2:B:225:TYR:O	2:B:229:ILE:HD13	2.12	0.50
2:B:383:LEU:O	2:B:387:ILE:HG12	2.12	0.50
1:A:235:SER:CA	1:A:238:SER:OG	2.59	0.49
1:A:200:ASN:ND2	1:A:212:LEU:HB3	2.27	0.49
1:A:388:GLU:HG2	1:A:389:SER:N	2.28	0.49
1:A:224:VAL:HG12	1:A:233:ARG:NH1	2.28	0.49
1:A:225:ILE:H	1:A:225:ILE:HD12	1.78	0.49
1:A:365:LEU:HD11	1:A:494:LEU:HD22	1.95	0.49
1:A:210:PHE:O	1:A:212:LEU:N	2.46	0.48
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.93	0.48
3:C:34:ILE:O	3:C:90:TYR:OH	2.26	0.48
1:A:224:VAL:HG21	1:A:229:THR:O	2.12	0.48
2:B:157:ARG:HD3	2:B:161:VAL:HG21	1.96	0.48
3:C:84:GLU:OE1	3:C:87:ARG:NH1	2.43	0.48
1:A:559:SER:OG	1:A:560:PRO:HD3	2.13	0.48
2:B:140:ILE:HG12	2:B:252:VAL:HG12	1.94	0.48
4:D:55:GLY:O	4:D:59:ARG:HG3	2.13	0.47
4:D:61:ALA:O	4:D:65:LEU:CD1	2.60	0.47
2:B:413:ALA:HB2	2:B:445:PHE:HD2	1.79	0.47
3:C:80:VAL:HG13	3:C:197:HIS:CD2	2.49	0.47
1:A:175:ASP:OD1	1:A:175:ASP:N	2.47	0.47
2:B:105:PHE:CD2	2:B:184:GLU:HG3	2.50	0.47
3:C:94:LEU:HD13	3:C:117:MET:HG2	1.96	0.47
1:A:136:PRO:HB2	1:A:172:ALA:HB2	1.96	0.47
2:B:287:ILE:HG13	2:B:382:GLY:HA2	1.96	0.47
2:B:425:LEU:HD13	5:G:17:LEU:HD23	1.96	0.46
1:A:261:LYS:NZ	1:A:321:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ILE:HG21	2:B:285:ALA:HB2	1.96	0.46
3:C:114:ILE:HG13	3:C:117:MET:HE3	1.96	0.46
3:C:203:LEU:HB3	3:C:217:ILE:HD11	1.98	0.46
2:B:207:VAL:CG1	4:D:26:LEU:HD11	2.46	0.46
2:B:404:TRP:HA	2:B:407:THR:HG22	1.97	0.46
1:A:285:ARG:CD	1:A:335:PHE:HZ	2.15	0.46
2:B:466:TYR:CE2	3:C:163:LEU:HB3	2.50	0.46
1:A:343:MET:O	1:A:347:MET:HG3	2.16	0.45
3:C:204:THR:O	3:C:207:ASN:HB2	2.15	0.45
1:A:162:ILE:HD11	1:A:164:TRP:CH2	2.51	0.45
2:B:100:ILE:HD11	2:B:238:ILE:HD13	1.98	0.45
1:A:352:PHE:CD1	1:A:353:PRO:HD2	2.52	0.45
1:A:54:LEU:HD11	1:A:223:ALA:HB1	1.99	0.45
1:A:460:ALA:HB1	1:A:465:VAL:HB	1.97	0.45
2:B:85:LEU:HD22	2:B:422:LEU:HD11	1.98	0.45
1:A:141:PRO:HG2	1:A:424:PRO:HG3	1.98	0.44
3:C:235:SER:N	3:C:238:SER:OG	2.49	0.44
1:A:299:VAL:HA	1:A:302:PHE:CE2	2.52	0.44
1:A:64:SER:CB	1:A:179:PRO:HG3	2.47	0.44
2:B:208:VAL:HG21	4:D:28:PHE:CD2	2.52	0.44
4:D:92:LEU:HD12	4:D:92:LEU:O	2.18	0.44
2:B:268:LEU:O	2:B:268:LEU:HD12	2.18	0.44
2:B:449:THR:HA	2:B:453:VAL:HB	1.99	0.44
3:C:215:LEU:HB2	3:C:216:PRO:HD3	2.00	0.44
1:A:210:PHE:N	1:A:211:PRO:HD2	2.33	0.44
2:B:251:ALA:O	2:B:255:VAL:HG23	2.18	0.44
3:C:35:LEU:HG	3:C:124:SER:HB2	2.00	0.44
1:A:583:ARG:O	1:A:587:GLN:HG2	2.18	0.44
3:C:163:LEU:HD13	3:C:214:LEU:HD13	2.00	0.44
4:D:73:SER:O	4:D:77:ILE:HG13	2.18	0.44
1:A:202:SER:HB2	1:A:206:SER:O	2.18	0.43
2:B:421:THR:HG21	2:B:434:ALA:HA	2.00	0.43
1:A:365:LEU:HD23	1:A:441:LEU:HB2	2.00	0.43
1:A:377:TRP:CE2	1:A:445:SER:HB3	2.53	0.43
1:A:286:SER:OG	1:A:291:VAL:O	2.28	0.43
2:B:113:LEU:HB2	5:G:4:AIB:HB11	1.99	0.43
1:A:224:VAL:HG21	1:A:230:CYS:HA	2.00	0.43
1:A:559:SER:HB2	1:A:629:ARG:NH1	2.30	0.43
3:C:75:GLY:HA2	3:C:78:VAL:HG12	2.00	0.43
1:A:631:LEU:HD21	1:A:635:PHE:HB2	2.01	0.42
1:A:72:VAL:HG13	1:A:94:TYR:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:HB3	1:A:631:LEU:HD12	2.01	0.42
1:A:514:ASP:OD1	1:A:514:ASP:N	2.51	0.42
3:C:180:ASP:OD1	3:C:184:ARG:NH1	2.52	0.42
1:A:609:LEU:HD12	1:A:609:LEU:HA	1.84	0.42
3:C:114:ILE:HD13	3:C:183:GLU:OE1	2.20	0.42
4:D:78:PHE:CZ	4:D:82:ARG:HG3	2.53	0.42
4:D:82:ARG:HB3	4:D:83:PRO:HD3	2.01	0.42
1:A:285:ARG:CD	1:A:335:PHE:CZ	2.95	0.42
2:B:254:SER:OG	2:B:439:ILE:HG21	2.20	0.42
2:B:268:LEU:CD1	5:G:16:JUU:C79	2.98	0.42
1:A:139:GLN:NE2	1:A:168:GLY:O	2.49	0.41
1:A:422:LEU:HD21	1:A:427:LEU:HD23	2.02	0.41
2:B:253:ILE:HD13	2:B:388:PHE:CZ	2.56	0.41
1:A:285:ARG:CG	1:A:286:SER:N	2.75	0.41
2:B:144:VAL:HA	2:B:147:THR:HG22	2.02	0.41
3:C:235:SER:OG	3:C:236:LEU:N	2.53	0.41
4:D:22:GLY:HA2	4:D:26:LEU:HB2	2.01	0.41
1:A:335:PHE:O	1:A:338:ILE:HG13	2.20	0.41
2:B:113:LEU:HG	2:B:115:TYR:H	1.85	0.41
2:B:413:ALA:HB2	2:B:445:PHE:CD2	2.56	0.41
1:A:331:GLN:HG3	1:A:555:ILE:HD12	2.03	0.41
1:A:301:SER:O	1:A:304:THR:OG1	2.35	0.41
2:B:174:LEU:CD1	2:B:229:ILE:HD11	2.51	0.41
3:C:116:GLN:HA	3:C:119:TYR:HB3	2.02	0.41
1:A:96:VAL:HG23	1:A:121:LEU:HB2	2.02	0.41
2:B:156:TYR:CD2	2:B:157:ARG:HG3	2.54	0.40
3:C:48:LEU:HD12	3:C:48:LEU:HA	1.89	0.40
1:A:597:LYS:HB3	1:A:597:LYS:HE3	1.66	0.40
2:B:200:LEU:HD22	4:D:71:LEU:HD11	2.03	0.40
1:A:582:THR:HG23	1:A:585:GLN:H	1.85	0.40
2:B:219:LEU:O	2:B:223:GLN:HG3	2.21	0.40
2:B:238:ILE:HD11	2:B:391:VAL:HA	2.04	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 PDB entries followed by that with respect to all EM

entries.

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	665/709 (94%)	612 (92%)	53 (8%)	0	100	100
2	B	296/467 (63%)	286 (97%)	10 (3%)	0	100	100
3	C	241/265 (91%)	235 (98%)	6 (2%)	0	100	100
4	D	94/101 (93%)	89 (95%)	5 (5%)	0	100	100
5	G	10/18 (56%)	9 (90%)	1 (10%)	0	100	100
All	All	1306/1560 (84%)	1231 (94%)	75 (6%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	584/612 (95%)	575 (98%)	9 (2%)	65	83
2	B	260/408 (64%)	258 (99%)	2 (1%)	81	92
3	C	193/214 (90%)	193 (100%)	0	100	100
4	D	84/89 (94%)	84 (100%)	0	100	100
5	G	8/8 (100%)	8 (100%)	0	100	100
All	All	1129/1331 (85%)	1118 (99%)	11 (1%)	77	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	210	PHE
1	A	237	GLN
1	A	248	CYS
1	A	257	TRP
1	A	562	ASN

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Mol	Chain	Res	Type
1	A	586	CYS
1	A	626	ARG
1	A	677	PHE
2	B	237	PHE
2	B	257	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	GLN
1	A	387	ASN
2	B	204	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	AIB	G	8	5	1,5,6	1.19	0	2,7,9	0.99	0
5	AIB	G	11	5	1,5,6	1.16	0	2,7,9	1.07	0
5	AIB	G	4	5	1,5,6	1.11	0	2,7,9	1.03	0
5	VLM	G	18	5	6,7,7	2.33	2 (33%)	7,9,9	1.01	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	AIB	G	8	5	-	1/2/3/6	-
5	AIB	G	11	5	-	2/2/3/6	-
5	AIB	G	4	5	-	0/2/3/6	-
5	VLM	G	18	5	-	0/7/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	18	VLM	C-NT	5.02	1.45	1.32
5	G	18	VLM	O-C	-2.63	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	11	AIB	O-C-CA-CB2
5	G	11	AIB	O-C-CA-CB1
5	G	8	AIB	O-C-CA-CB2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	4	AIB	1	0

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	$\#\|Z\| > 2$
6	NAG	E	1	6,1	14,14,15	0.29	0	17,19,21	0.46	0
6	NAG	E	2	6	14,14,15	0.24	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	F	1	7	11,11,12	0.53	0	15,15,17	1.18	1 (6%)
7	BMA	F	2	7	11,11,12	0.61	0	15,15,17	0.67	0
7	BMA	F	3	7	11,11,12	0.81	0	15,15,17	1.14	1 (6%)

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	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
7	BMA	F	1	7	-	0/2/19/22	0/1/1/1
7	BMA	F	2	7	-	1/2/19/22	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	3	BMA	C1-O5-C5	3.43	116.84	112.19
7	F	1	BMA	C1-C2-C3	2.54	112.78	109.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	2	NAG	O5-C5-C6-O6
6	E	1	NAG	C8-C7-N2-C2
6	E	1	NAG	O7-C7-N2-C2
6	E	2	NAG	C4-C5-C6-O6
7	F	2	BMA	O5-C5-C6-O6
6	E	1	NAG	C4-C5-C6-O6
6	E	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

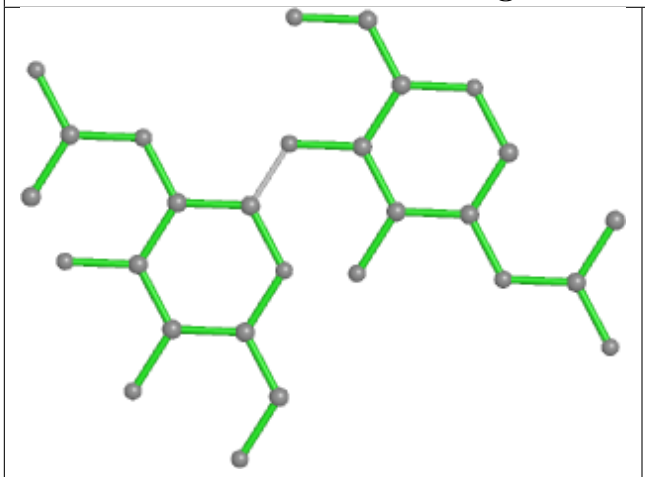
Mol	Chain	Res	Type	Atoms
7	F	3	BMA	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

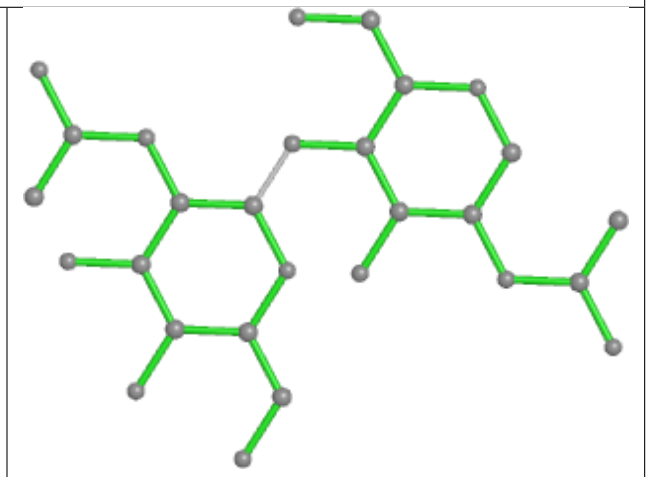
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1	NAG	1	0

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

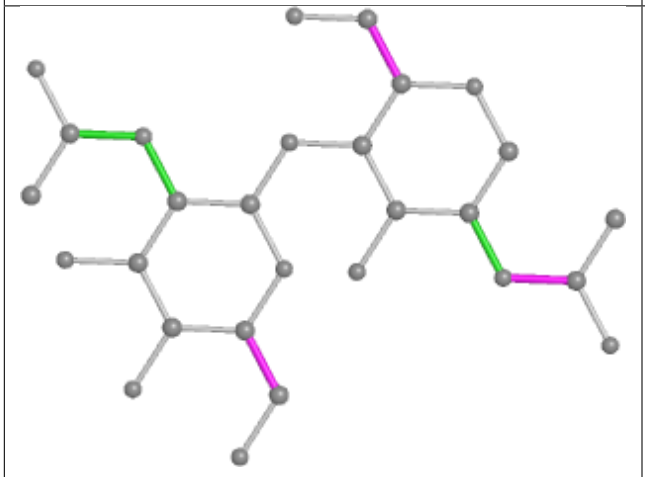
Oligosaccharide Chain E



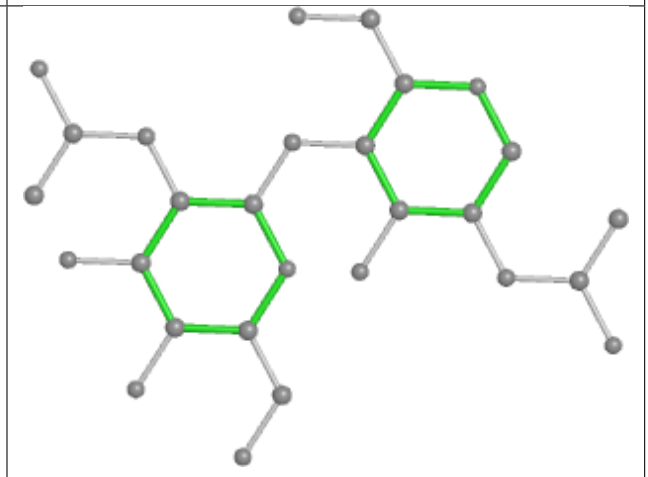
Bond lengths



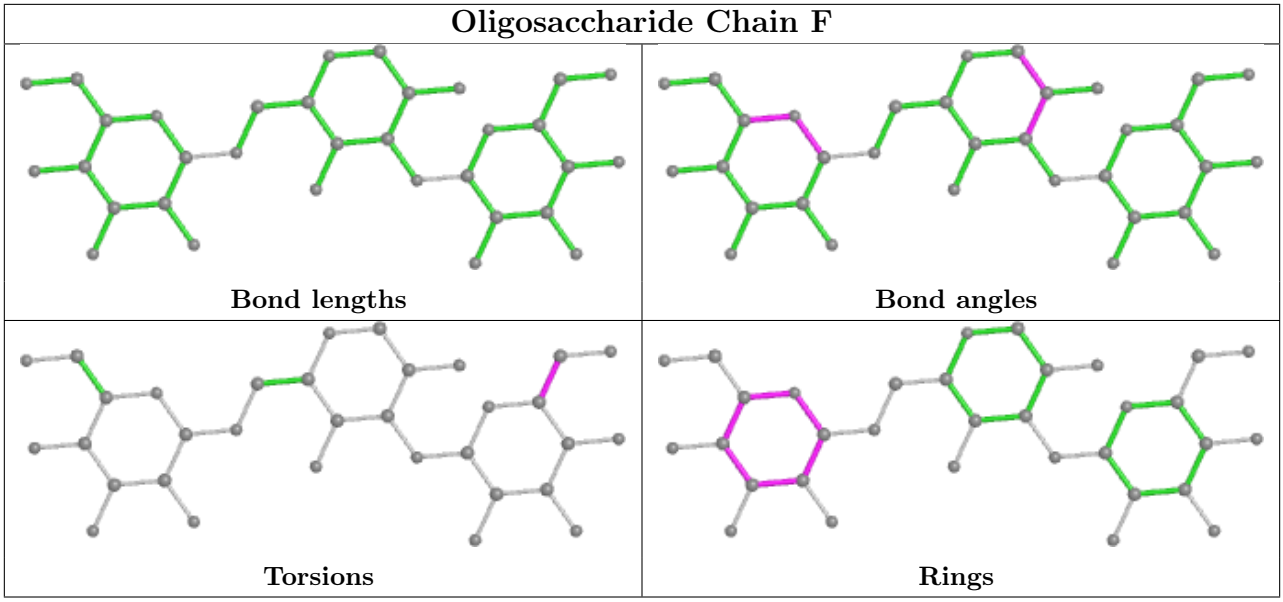
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
8	NAG	A	801	1	14,14,15	0.40	0	17,19,21	0.40	0
8	NAG	A	806	1	14,14,15	0.19	0	17,19,21	0.41	0
10	CLR	C	303	-	31,31,31	0.30	0	48,48,48	0.41	0
10	CLR	C	301	-	31,31,31	0.30	0	48,48,48	0.43	0
8	NAG	A	803	1	14,14,15	0.55	0	17,19,21	0.51	0
8	NAG	A	802	1	14,14,15	0.36	0	17,19,21	0.51	0
8	NAG	A	805	1	14,14,15	0.32	0	17,19,21	0.33	0
8	NAG	A	804	1	14,14,15	0.30	0	17,19,21	0.39	0
9	PC1	B	501	-	38,38,53	0.30	0	44,46,61	0.38	0
10	CLR	C	302	-	31,31,31	0.29	0	48,48,48	0.40	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
8	NAG	A	801	1	-	2/6/23/26	0/1/1/1
8	NAG	A	806	1	-	1/6/23/26	0/1/1/1
10	CLR	C	303	-	-	2/10/68/68	0/4/4/4
10	CLR	C	301	-	-	2/10/68/68	0/4/4/4
8	NAG	A	803	1	-	2/6/23/26	0/1/1/1
8	NAG	A	802	1	-	3/6/23/26	0/1/1/1
8	NAG	A	805	1	-	0/6/23/26	0/1/1/1
8	NAG	A	804	1	-	2/6/23/26	0/1/1/1
9	PC1	B	501	-	-	2/42/42/57	-
10	CLR	C	302	-	-	0/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	PC1	C1-O11-P-O14
8	A	801	NAG	O5-C5-C6-O6
8	A	801	NAG	C4-C5-C6-O6
8	A	804	NAG	O5-C5-C6-O6
8	A	804	NAG	C4-C5-C6-O6
10	C	301	CLR	C17-C20-C22-C23
10	C	303	CLR	C22-C23-C24-C25
8	A	802	NAG	C4-C5-C6-O6
8	A	806	NAG	O5-C5-C6-O6
10	C	301	CLR	C21-C20-C22-C23
8	A	803	NAG	C4-C5-C6-O6
8	A	802	NAG	O5-C5-C6-O6
8	A	803	NAG	O5-C5-C6-O6
9	B	501	PC1	C1-O11-P-O13
8	A	802	NAG	C3-C2-N2-C7
10	C	303	CLR	C20-C22-C23-C24

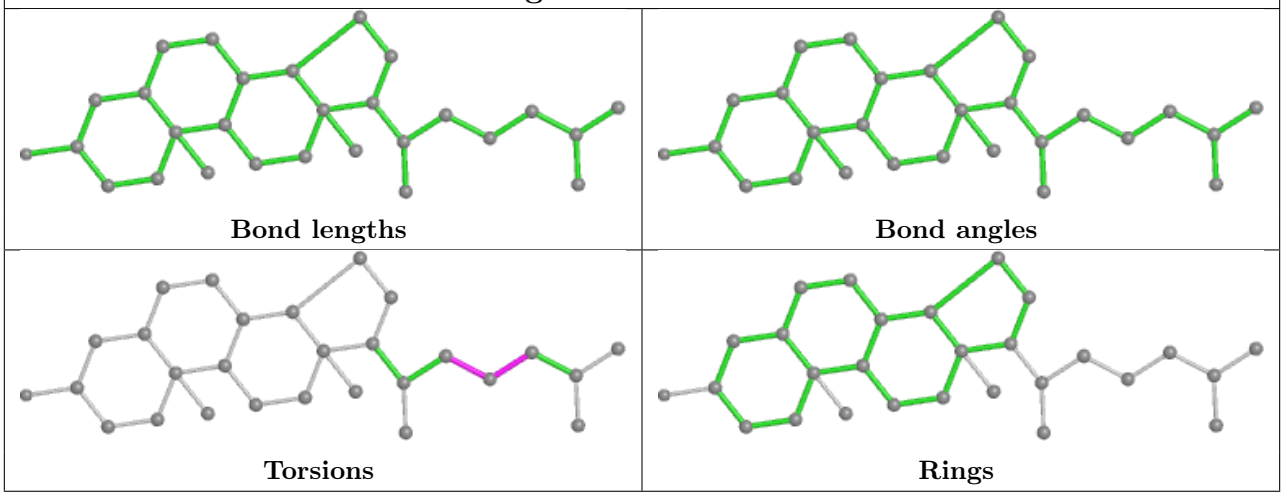
There are no ring outliers.

No monomer is involved in short contacts.

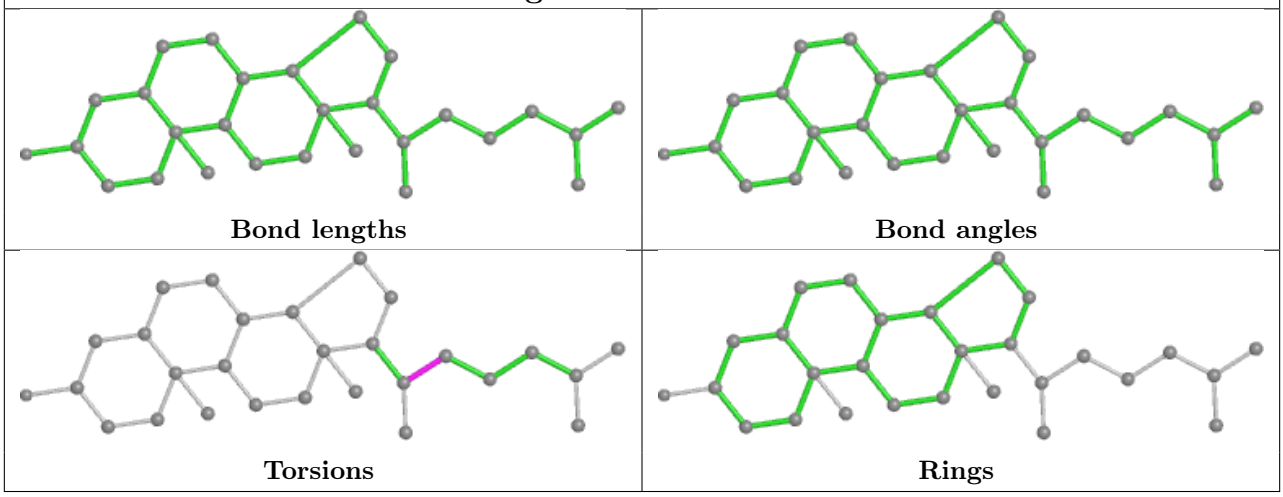
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

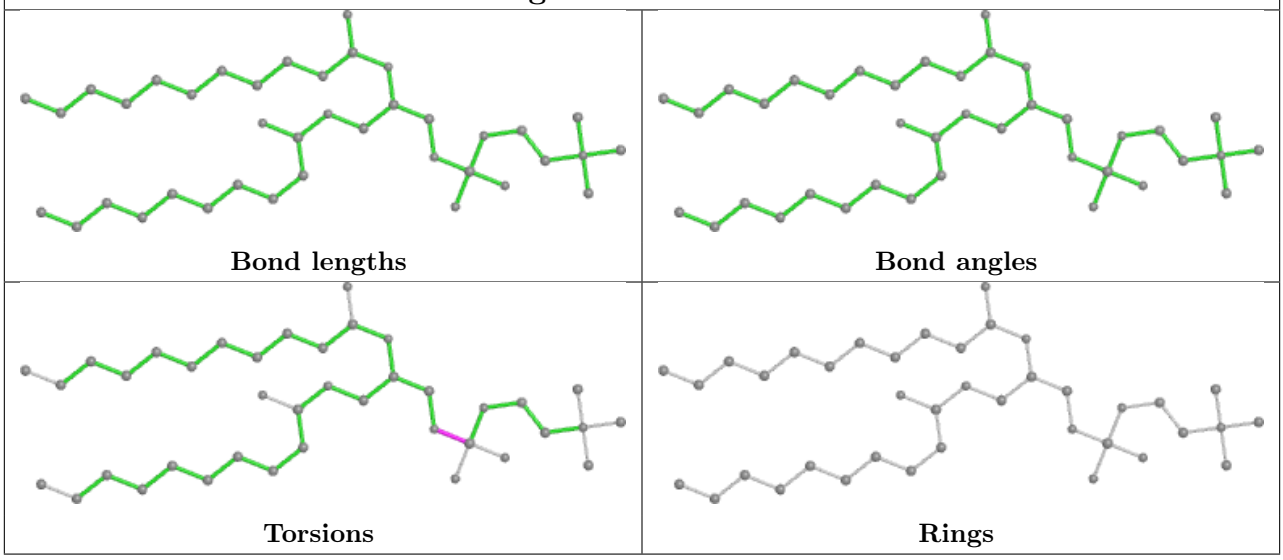
Ligand CLR C 303



Ligand CLR C 301



Ligand PC1 B 501



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.