



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2022 – 12:18 pm GMT

PDB ID : 7ZIL
Title : JC Polyomavirus VP1 in complex with 3'-Sialyllactose glycomacromolecules
(aliphatic linker)
Authors : Freytag, J.; Mueller, J.C.; Stehle, T.
Deposited on : 2022-04-08
Resolution : 1.24 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

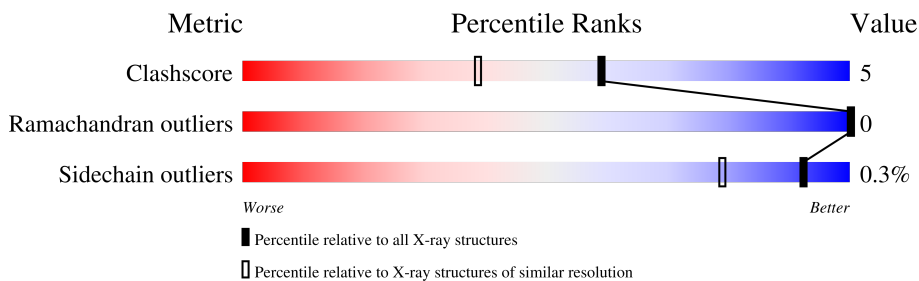
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.24 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))
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	272	
1	BBB	272	
1	CCC	272	
1	DDD	272	
1	EEE	272	
2	BaB	3	
2	CaC	3	
2	DaD	3	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 13339 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	260	2282	1438	387	443	14	0	34	0
1	BBB	259	2224	1405	380	424	15	0	26	0
1	CCC	264	2252	1415	382	440	15	0	28	0
1	DDD	263	2206	1385	377	429	15	0	22	0
1	EEE	257	2223	1399	379	431	14	0	27	0

There are 20 discrepancies between the modelled and reference sequences:

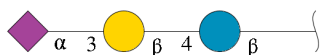
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	GLY	-	expression tag	UNP P03089
AAA	19	SER	-	expression tag	UNP P03089
AAA	20	HIS	-	expression tag	UNP P03089
AAA	21	MET	-	expression tag	UNP P03089
BBB	18	GLY	-	expression tag	UNP P03089
BBB	19	SER	-	expression tag	UNP P03089
BBB	20	HIS	-	expression tag	UNP P03089
BBB	21	MET	-	expression tag	UNP P03089
CCC	18	GLY	-	expression tag	UNP P03089
CCC	19	SER	-	expression tag	UNP P03089
CCC	20	HIS	-	expression tag	UNP P03089
CCC	21	MET	-	expression tag	UNP P03089
DDD	18	GLY	-	expression tag	UNP P03089
DDD	19	SER	-	expression tag	UNP P03089
DDD	20	HIS	-	expression tag	UNP P03089
DDD	21	MET	-	expression tag	UNP P03089
EEE	18	GLY	-	expression tag	UNP P03089
EEE	19	SER	-	expression tag	UNP P03089
EEE	20	HIS	-	expression tag	UNP P03089

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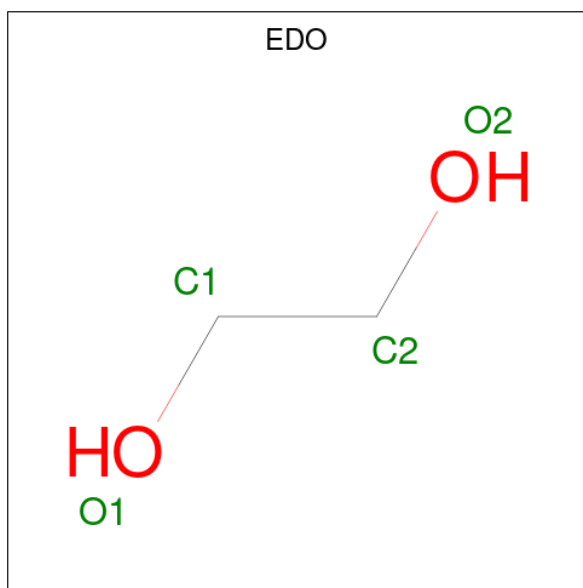
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	21	MET	-	expression tag	UNP P03089

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	BaB	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	CaC	3	Total	C	N	O	0	3	1
			64	34	2	28			
2	DaD	3	Total	C	N	O	0	0	1
			32	17	1	14			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	EEE	1	Total	C	O	0	0
			4	2	2		
3	EEE	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		
4	BBB	1	Total	Cl	0	0
			1	1		
4	EEE	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	2	Total	Na	0	0
			2	2		
5	BBB	2	Total	Na	0	0
			2	2		
5	CCC	2	Total	Na	0	0
			2	2		
5	DDD	2	Total	Na	0	0
			2	2		
5	EEE	2	Total	Na	0	0
			2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	EEE	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	401	Total O 401 401	0	0
7	BBB	379	Total O 379 379	0	0
7	CCC	426	Total O 426 426	0	0
7	DDD	378	Total O 378 378	0	0
7	EEE	381	Total O 381 381	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. 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.

Note EDS failed to run properly.

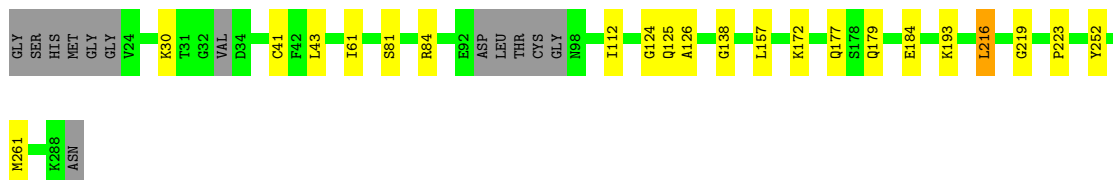
- Molecule 1: Major capsid protein VP1

Chain AAA:  89% 6%



- Molecule 1: Major capsid protein VP1

Chain BBB:  87% 8% 5%



- Molecule 1: Major capsid protein VP1

Chain CCC:  89% 8%



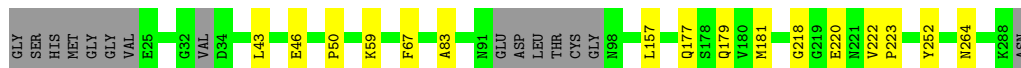
- Molecule 1: Major capsid protein VP1

Chain DDD:  88% 8%



- Molecule 1: Major capsid protein VP1

Chain EEE:  89% 6% 6%




- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain BaB:  100%


BGC1
GAL2
STA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain CaC:  33% 67%

BGC1
GAL2
STA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain DaD:  33% 67%

BGC1
GAL2
STA3

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.10Å 96.02Å 128.06Å 90.00° 110.56° 90.00°	Depositor
Resolution (Å)	48.01 – 1.24	Depositor
% Data completeness (in resolution range)	96.0 (48.01-1.24)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.138 , 0.155	Depositor
Wilson B-factor (Å ²)	14.6	Xtrriage
Anisotropy	0.395	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13339	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: PEG, EDO, SIA, GAL, NA, BGC, CL

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	AAA	0.60	0/2346	0.78	0/3190
1	BBB	0.59	0/2287	0.79	0/3106
1	CCC	0.62	0/2310	0.81	0/3137
1	DDD	0.60	0/2260	0.81	0/3067
1	EEE	0.59	0/2270	0.80	0/3084
All	All	0.60	0/11473	0.80	0/15584

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	AAA	2282	0	2202	17	0
1	BBB	2224	0	2148	22	0
1	CCC	2252	0	2148	28	0
1	DDD	2206	0	2120	30	0
1	EEE	2223	0	2127	23	0
2	BaB	43	0	37	0	0
2	CaC	64	0	52	0	0
2	DaD	32	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	12	0	18	0	0
3	BBB	4	0	6	0	0
3	DDD	4	0	6	0	0
3	EEE	8	0	12	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	EEE	1	0	0	0	0
5	AAA	2	0	0	0	0
5	BBB	2	0	0	0	0
5	CCC	2	0	0	0	0
5	DDD	2	0	0	0	0
5	EEE	2	0	0	0	0
6	EEE	7	0	10	1	0
7	AAA	401	0	0	3	0
7	BBB	379	0	0	6	0
7	CCC	426	0	0	8	0
7	DDD	378	0	0	6	0
7	EEE	381	0	0	4	0
All	All	13339	0	10912	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:218[B]:GLY:O	1:AAA:222[B]:VAL:HG21	1.35	1.20
1:AAA:218[B]:GLY:O	1:AAA:222[B]:VAL:CG2	1.96	1.13
1:DDD:261[B]:MET:HG2	1:DDD:269:GLN:HB3	1.28	1.06
1:DDD:76[B]:MET:HE1	7:DDD:789:HOH:O	1.62	0.98
1:CCC:36[B]:ILE:HG23	7:CCC:598:HOH:O	1.64	0.96
1:CCC:76[B]:MET:HE1	7:CCC:612:HOH:O	1.70	0.92
1:BBB:124:GLY:C	1:BBB:125[C]:GLN:CA	2.39	0.90
1:CCC:184[B]:GLU:HG2	7:CCC:680:HOH:O	1.73	0.88
1:CCC:76[B]:MET:CE	7:CCC:612:HOH:O	2.23	0.84
1:AAA:160:TYR:H	1:AAA:179:GLN:HE21	1.22	0.83
1:DDD:76[B]:MET:CE	7:DDD:789:HOH:O	2.23	0.81
1:AAA:218[A]:GLY:O	1:EEE:223[A]:PRO:HB2	1.85	0.76
1:BBB:125[C]:GLN:CA	1:BBB:126:ALA:N	2.48	0.76
1:AAA:218[A]:GLY:O	1:EEE:223[A]:PRO:CB	2.35	0.73
1:BBB:177[B]:GLN:CD	7:BBB:601:HOH:O	2.27	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:172:LYS:NZ	7:BBB:602:HOH:O	2.24	0.70
1:CCC:218[B]:GLY:O	1:CCC:222:VAL:HG21	1.91	0.70
1:CCC:177[B]:GLN:HG2	1:CCC:181[B]:MET:O	1.92	0.69
1:BBB:41[B]:CYS:SG	1:BBB:43[B]:LEU:HD12	2.34	0.68
1:DDD:218[A]:GLY:O	1:DDD:222:VAL:HG11	1.93	0.68
1:EEE:252[B]:TYR:HE2	7:EEE:584:HOH:O	1.80	0.65
1:CCC:61[B]:ILE:HD12	1:CCC:261[B]:MET:HE1	1.79	0.65
1:DDD:123:ASN:HD22	1:EEE:67:PHE:H	1.45	0.65
1:CCC:36[B]:ILE:HD11	7:CCC:807:HOH:O	1.97	0.64
1:BBB:223[B]:PRO:HB3	1:CCC:218[B]:GLY:O	1.98	0.63
1:EEE:177[B]:GLN:HG2	1:EEE:181[B]:MET:O	2.01	0.61
1:DDD:42:PHE:CE1	1:EEE:181[B]:MET:HG2	2.35	0.61
1:CCC:177[A]:GLN:HG2	7:CCC:697:HOH:O	2.01	0.61
1:AAA:110[A]:GLU:HB2	7:AAA:566:HOH:O	2.00	0.60
1:AAA:252[B]:TYR:HE2	7:AAA:586:HOH:O	1.85	0.60
1:BBB:61[B]:ILE:CD1	1:BBB:261[B]:MET:HE3	2.32	0.59
1:AAA:218[B]:GLY:O	1:AAA:222[B]:VAL:HG23	1.97	0.58
1:DDD:261[B]:MET:CG	1:DDD:269:GLN:HB3	2.19	0.58
1:BBB:30:LYS:CG	7:BBB:856:HOH:O	2.51	0.57
1:CCC:41:CYS:SG	1:CCC:43:LEU:HD12	2.45	0.57
1:EEE:43[B]:LEU:HD21	1:EEE:83:ALA:HB2	1.87	0.56
1:DDD:177[A]:GLN:HG2	7:DDD:870:HOH:O	2.05	0.56
1:CCC:89[A]:ASN:ND2	1:CCC:92:GLU:HG2	2.22	0.55
1:AAA:82:VAL:O	1:AAA:192[B]:ASN:ND2	2.40	0.55
1:CCC:61[B]:ILE:HD12	1:CCC:261[B]:MET:CE	2.36	0.55
1:BBB:112[B]:ILE:HD11	1:CCC:204:PRO:HG3	1.90	0.53
1:DDD:96:CYS:SG	7:DDD:892:HOH:O	2.59	0.53
1:BBB:84[B]:ARG:CZ	7:BBB:631:HOH:O	2.58	0.51
1:CCC:177[B]:GLN:HG3	7:CCC:467:HOH:O	2.11	0.50
1:BBB:61[B]:ILE:HD11	1:BBB:261[B]:MET:HE3	1.94	0.50
1:AAA:138:GLY:HA2	1:AAA:219:GLY:O	2.12	0.49
7:DDD:722:HOH:O	1:EEE:218[A]:GLY:HA3	2.11	0.48
1:CCC:112[B]:ILE:CD1	1:DDD:204:PRO:HG3	2.44	0.48
1:BBB:184[B]:GLU:HG3	7:BBB:706:HOH:O	2.13	0.48
1:CCC:138:GLY:HA2	1:CCC:219:GLY:O	2.14	0.48
1:DDD:218[A]:GLY:O	1:DDD:222:VAL:CG1	2.62	0.48
1:DDD:112:ILE:HG21	1:EEE:181[B]:MET:HE1	1.96	0.47
1:CCC:218[B]:GLY:O	1:CCC:222:VAL:CG2	2.61	0.47
1:DDD:43[B]:LEU:HD21	1:DDD:83:ALA:CB	2.44	0.47
1:DDD:42:PHE:CE1	1:EEE:181[B]:MET:CG	2.98	0.47
1:BBB:216[B]:LEU:C	1:BBB:216[B]:LEU:HD13	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:59[A]:LYS:NZ	7:AAA:503:HOH:O	2.35	0.47
1:BBB:252[B]:TYR:HE2	7:BBB:688:HOH:O	1.96	0.47
7:DDD:722:HOH:O	1:EEE:218[B]:GLY:HA3	2.14	0.47
1:EEE:264[B]:ASN:ND2	7:EEE:511:HOH:O	2.47	0.47
1:CCC:277:TYR:OH	1:CCC:279:LYS:HE2	2.14	0.47
1:BBB:41[B]:CYS:SG	1:BBB:43[B]:LEU:CD1	3.02	0.47
1:DDD:112:ILE:HG21	1:EEE:181[B]:MET:CE	2.46	0.46
1:CCC:61[B]:ILE:HA	1:CCC:76[B]:MET:SD	2.56	0.46
1:BBB:43[A]:LEU:HG	1:BBB:81:SER:HB3	1.98	0.46
1:DDD:42:PHE:CZ	1:EEE:181[B]:MET:HG2	2.51	0.45
1:CCC:112[B]:ILE:HD11	1:DDD:204:PRO:HG3	1.99	0.45
1:CCC:223:PRO:CB	1:DDD:218[B]:GLY:O	2.65	0.44
1:DDD:61[B]:ILE:HA	1:DDD:76[B]:MET:SD	2.57	0.44
6:EEE:401:PEG:H12	7:EEE:773:HOH:O	2.17	0.44
1:DDD:43[B]:LEU:HD21	1:DDD:83:ALA:HB2	1.98	0.44
1:CCC:42[B]:PHE:HE2	1:CCC:112[B]:ILE:HG13	1.83	0.44
1:CCC:76[B]:MET:HE3	7:CCC:612:HOH:O	2.04	0.43
1:AAA:160:TYR:N	1:AAA:179:GLN:HE21	2.03	0.43
1:DDD:223:PRO:HB2	1:EEE:218[A]:GLY:O	2.19	0.43
1:DDD:123:ASN:HD22	1:EEE:67:PHE:N	2.15	0.43
1:BBB:138:GLY:HA2	1:BBB:219:GLY:O	2.19	0.43
1:DDD:29:VAL:HG12	1:DDD:30[B]:LYS:O	2.17	0.43
1:AAA:152:GLU:HB3	1:AAA:206[B]:ARG:CZ	2.49	0.43
1:AAA:157:LEU:O	1:AAA:179:GLN:HA	2.19	0.42
1:CCC:42[B]:PHE:CE2	1:CCC:112[B]:ILE:HG13	2.55	0.42
1:DDD:34:ASP:O	1:DDD:284:LYS:HE3	2.19	0.42
1:BBB:61[B]:ILE:HD12	1:BBB:261[B]:MET:CE	2.50	0.42
1:EEE:43[B]:LEU:HD21	1:EEE:83:ALA:CB	2.47	0.42
1:BBB:193[B]:LYS:O	1:BBB:193[B]:LYS:HG3	2.19	0.42
1:AAA:43[B]:LEU:HD21	1:AAA:83:ALA:HB2	2.02	0.42
1:EEE:218[A]:GLY:O	1:EEE:222[A]:VAL:HG11	2.20	0.42
1:DDD:42:PHE:CD1	1:EEE:181[B]:MET:HG2	2.55	0.41
1:EEE:50:PRO:HB3	1:EEE:59[B]:LYS:HB2	2.01	0.41
1:BBB:112[B]:ILE:CD1	1:CCC:204:PRO:HG3	2.51	0.41
1:BBB:157:LEU:O	1:BBB:179:GLN:HA	2.20	0.41
1:CCC:61[B]:ILE:CD1	1:CCC:261[B]:MET:SD	3.08	0.41
1:DDD:277:TYR:OH	1:DDD:279:LYS:HE3	2.20	0.41
1:EEE:157:LEU:O	1:EEE:179:GLN:HA	2.20	0.41
1:AAA:82:VAL:HG13	1:AAA:192[B]:ASN:OD1	2.20	0.41
1:BBB:61[B]:ILE:CD1	1:BBB:261[B]:MET:CE	2.99	0.41
1:CCC:157:LEU:O	1:CCC:179:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:42:PHE:CZ	1:EEE:181[B]:MET:CG	3.03	0.41
1:DDD:30[A]:LYS:O	1:DDD:35:SER:HB2	2.21	0.41
1:DDD:76[B]:MET:HE2	1:DDD:76[B]:MET:HB2	1.91	0.40
1:DDD:82:VAL:O	1:DDD:192:ASN:OD1	2.39	0.40
1:EEE:46:GLU:HG3	7:EEE:542:HOH:O	2.20	0.40
1:AAA:149:GLU:HA	1:AAA:252[B]:TYR:CE2	2.57	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	AAA	291/272 (107%)	279 (96%)	12 (4%)	0	100	100
1	BBB	282/272 (104%)	272 (96%)	10 (4%)	0	100	100
1	CCC	289/272 (106%)	279 (96%)	10 (4%)	0	100	100
1	DDD	283/272 (104%)	274 (97%)	9 (3%)	0	100	100
1	EEE	281/272 (103%)	270 (96%)	11 (4%)	0	100	100
All	All	1426/1360 (105%)	1374 (96%)	52 (4%)	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 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	AAA	257/237 (108%)	257 (100%)	0	100	100
1	BBB	249/237 (105%)	247 (99%)	2 (1%)	81	55
1	CCC	249/237 (105%)	249 (100%)	0	100	100
1	DDD	245/237 (103%)	244 (100%)	1 (0%)	91	77
1	EEE	246/237 (104%)	245 (100%)	1 (0%)	91	77
All	All	1246/1185 (105%)	1242 (100%)	4 (0%)	92	79

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	216[A]	LEU
1	BBB	216[B]	LEU
1	DDD	192	ASN
1	EEE	220	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 12 monosaccharides modelled in this entry, 9 were used for Mogul analysis.

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
2	BGC	BaB	1	2	12,12,12	0.82	0	17,17,17	1.74	5 (29%)
2	GAL	BaB	2	2	11,11,12	0.65	0	15,15,17	1.03	1 (6%)
2	SIA	BaB	3	2	20,20,21	0.94	1 (5%)	24,28,31	0.97	2 (8%)
2	GAL	CaC	2[A]	2	11,11,12	1.20	1 (9%)	15,15,17	2.28	6 (40%)
2	GAL	CaC	2[B]	2	11,11,12	0.74	0	15,15,17	1.57	4 (26%)
2	SIA	CaC	3[A]	2	20,20,21	0.83	0	24,28,31	1.29	4 (16%)
2	SIA	CaC	3[B]	2	20,20,21	0.69	0	24,28,31	1.10	2 (8%)
2	GAL	DaD	2	2	11,11,12	0.83	0	15,15,17	2.38	7 (46%)
2	SIA	DaD	3	2	20,20,21	0.66	0	24,28,31	1.08	2 (8%)

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
2	BGC	BaB	1	2	-	0/2/22/22	0/1/1/1
2	GAL	BaB	2	2	-	0/2/19/22	0/1/1/1
2	SIA	BaB	3	2	-	0/18/34/38	0/1/1/1
2	GAL	CaC	2[A]	2	-	2/2/19/22	0/1/1/1
2	GAL	CaC	2[B]	2	-	1/2/19/22	0/1/1/1
2	SIA	CaC	3[A]	2	-	0/18/34/38	0/1/1/1
2	SIA	CaC	3[B]	2	-	0/18/34/38	0/1/1/1
2	GAL	DaD	2	2	-	2/2/19/22	0/1/1/1
2	SIA	DaD	3	2	-	0/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CaC	2[A]	GAL	O3-C3	3.12	1.50	1.43
2	BaB	3	SIA	C2-C1	2.84	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DaD	2	GAL	C1-O5-C5	5.52	119.67	112.19
2	CaC	2[A]	GAL	O3-C3-C2	4.52	118.66	109.99
2	DaD	2	GAL	C3-C4-C5	3.86	117.12	110.24
2	CaC	2[B]	GAL	C1-O5-C5	3.51	116.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CaC	2[A]	GAL	C3-C4-C5	3.47	116.44	110.24
2	CaC	2[A]	GAL	C2-C3-C4	3.33	116.65	110.89
2	BaB	1	BGC	O1-C1-C2	3.14	117.87	109.03
2	CaC	2[A]	GAL	O2-C2-C3	-3.12	103.88	110.14
2	DaD	2	GAL	O5-C5-C6	-3.12	102.31	107.20
2	BaB	1	BGC	O5-C1-C2	-3.07	104.81	110.28
2	BaB	1	BGC	O1-C1-O5	-2.99	101.39	110.38
2	BaB	2	GAL	O3-C3-C2	-2.97	104.30	109.99
2	CaC	3[A]	SIA	O6-C2-C3	-2.83	106.57	110.46
2	CaC	2[A]	GAL	O2-C2-C1	-2.63	103.77	109.15
2	DaD	2	GAL	O5-C5-C4	2.62	117.20	110.83
2	DaD	2	GAL	C1-C2-C3	2.57	112.82	109.67
2	CaC	2[A]	GAL	C1-C2-C3	2.56	112.81	109.67
2	CaC	2[B]	GAL	O2-C2-C3	2.42	114.99	110.14
2	CaC	2[B]	GAL	C3-C4-C5	2.40	114.52	110.24
2	CaC	3[B]	SIA	O6-C2-C3	-2.37	107.20	110.46
2	CaC	2[B]	GAL	O3-C3-C4	-2.32	104.99	110.35
2	DaD	2	GAL	C2-C3-C4	-2.31	106.90	110.89
2	BaB	3	SIA	O1A-C1-C2	-2.30	117.13	122.57
2	CaC	3[A]	SIA	C4-C3-C2	2.30	113.93	109.81
2	DaD	2	GAL	O3-C3-C2	-2.26	105.66	109.99
2	BaB	1	BGC	O4-C4-C3	-2.25	105.15	110.35
2	CaC	3[B]	SIA	O1B-C1-C2	2.24	119.43	113.03
2	DaD	3	SIA	C6-O6-C2	2.20	116.04	111.34
2	DaD	3	SIA	O1B-C1-C2	2.19	119.27	113.03
2	CaC	3[A]	SIA	O1B-C1-C2	2.16	119.20	113.03
2	BaB	3	SIA	O1B-C1-C2	2.13	119.11	113.03
2	BaB	1	BGC	O2-C2-C3	-2.07	105.56	110.35
2	CaC	3[A]	SIA	C6-O6-C2	2.05	115.72	111.34

There are no chirality outliers.

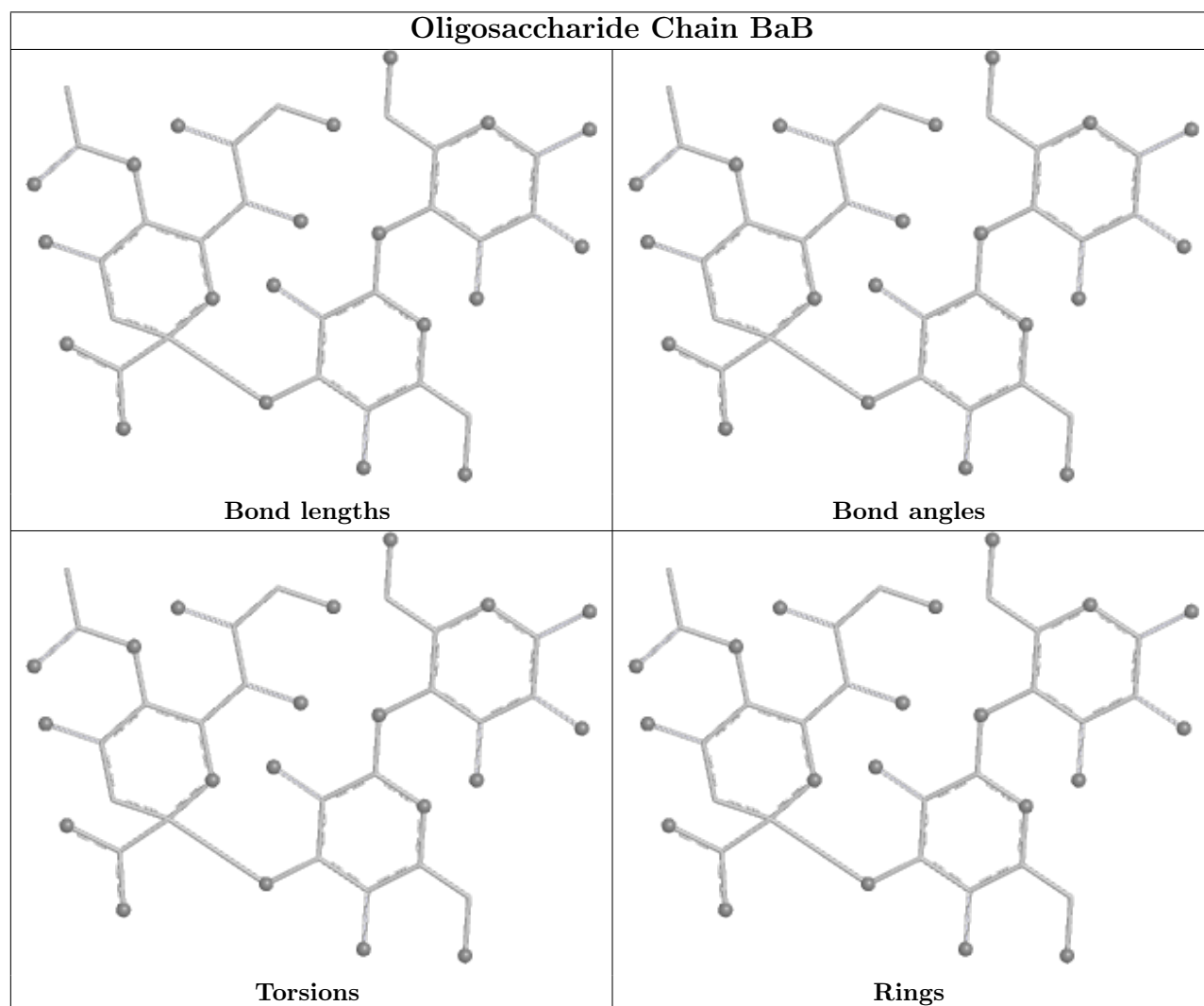
All (5) torsion outliers are listed below:

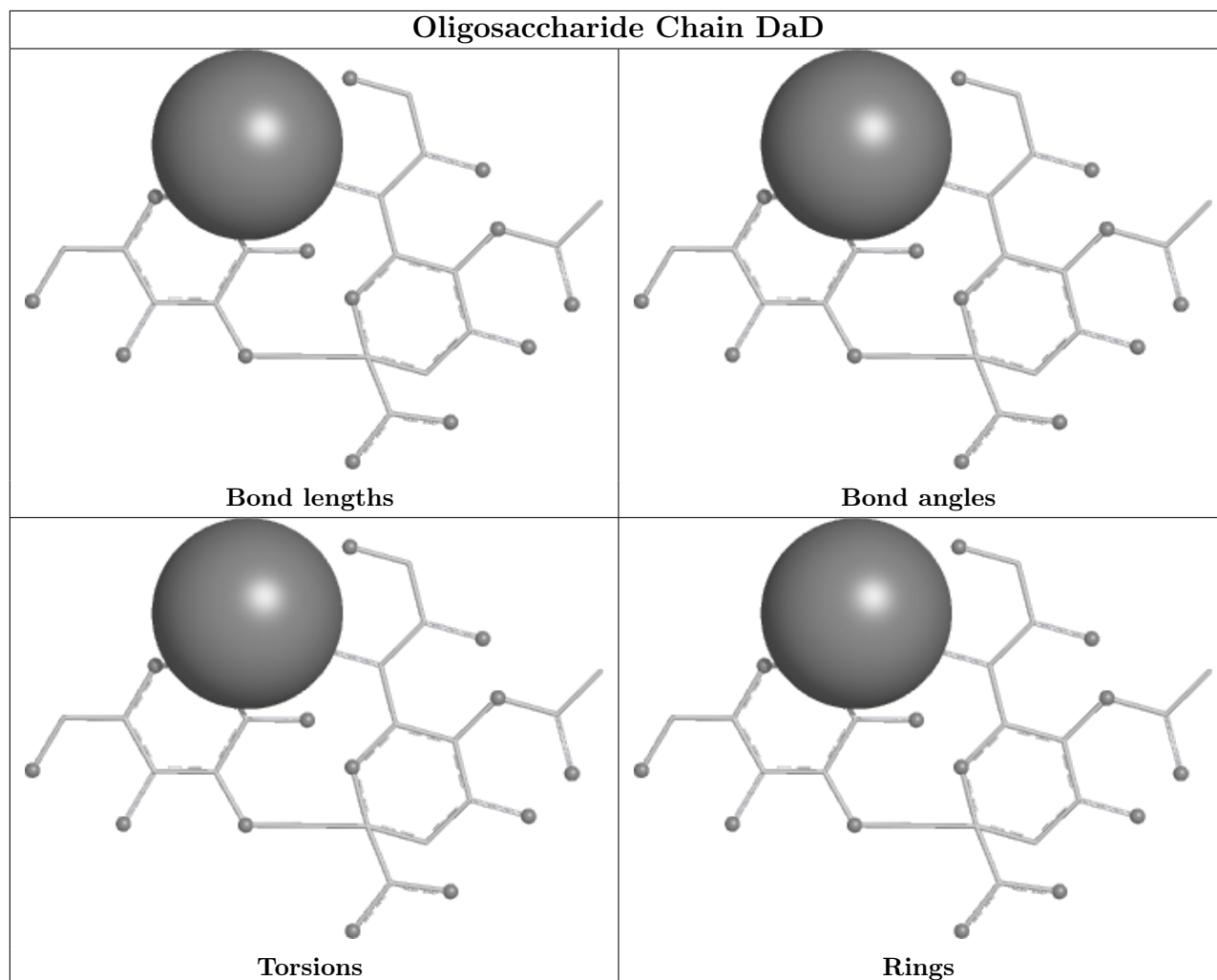
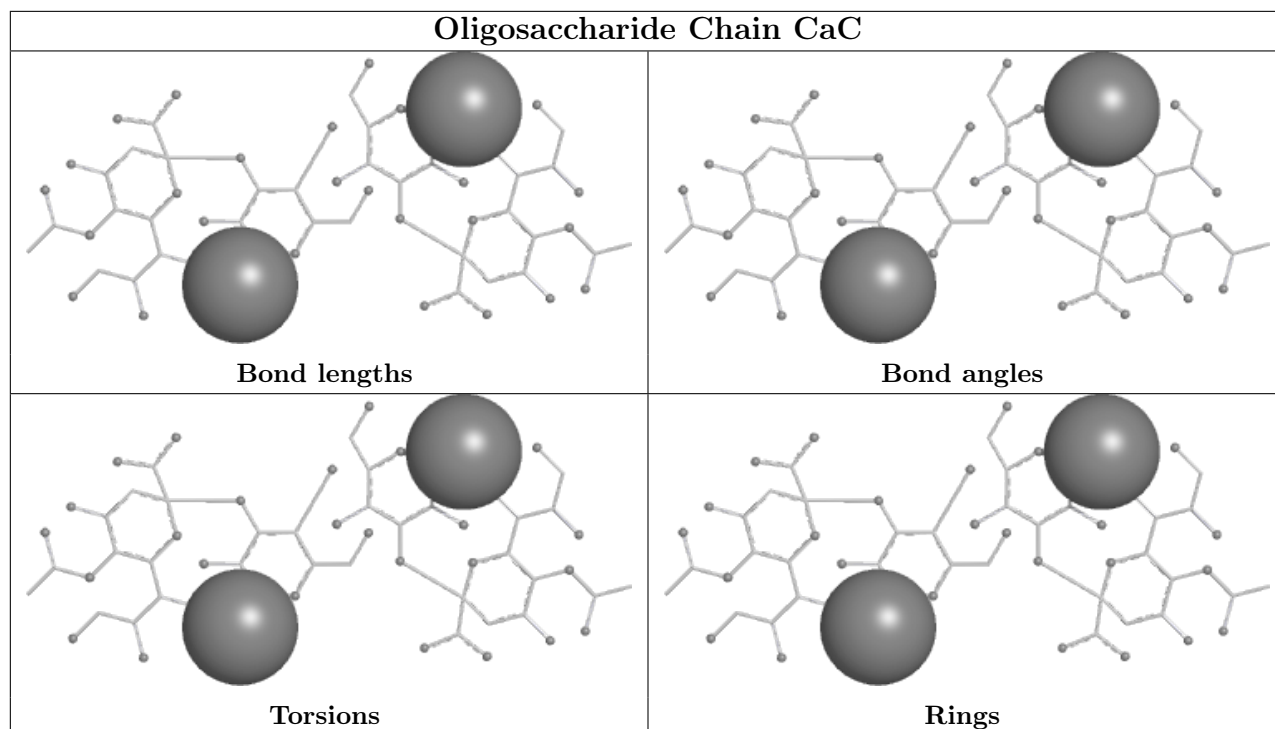
Mol	Chain	Res	Type	Atoms
2	CaC	2[A]	GAL	O5-C5-C6-O6
2	CaC	2[B]	GAL	O5-C5-C6-O6
2	DaD	2	GAL	C4-C5-C6-O6
2	CaC	2[A]	GAL	C4-C5-C6-O6
2	DaD	2	GAL	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry

Of 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 for Mogul analysis.

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	PEG	EEE	401	-	6,6,6	0.23	0	5,5,5	0.23	0
3	EDO	EEE	402	-	3,3,3	0.09	0	2,2,2	0.24	0
3	EDO	AAA	403	-	3,3,3	0.04	0	2,2,2	0.09	0
3	EDO	AAA	402	-	3,3,3	0.15	0	2,2,2	0.14	0
3	EDO	BBB	501	-	3,3,3	0.15	0	2,2,2	0.38	0
3	EDO	EEE	403	-	3,3,3	0.21	0	2,2,2	0.36	0
3	EDO	AAA	401	-	3,3,3	0.12	0	2,2,2	0.22	0
3	EDO	DDD	501	-	3,3,3	0.16	0	2,2,2	0.31	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
6	PEG	EEE	401	-	-	1/4/4/4	-
3	EDO	EEE	402	-	-	1/1/1/1	-
3	EDO	AAA	403	-	-	0/1/1/1	-
3	EDO	AAA	402	-	-	1/1/1/1	-
3	EDO	BBB	501	-	-	1/1/1/1	-
3	EDO	EEE	403	-	-	0/1/1/1	-
3	EDO	AAA	401	-	-	1/1/1/1	-
3	EDO	DDD	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	402	EDO	O1-C1-C2-O2
3	BBB	501	EDO	O1-C1-C2-O2
3	EEE	402	EDO	O1-C1-C2-O2
3	AAA	401	EDO	O1-C1-C2-O2
3	DDD	501	EDO	O1-C1-C2-O2
6	EEE	401	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	EEE	401	PEG	1	0

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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.