



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 7ZIL / pdb_00007zil
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

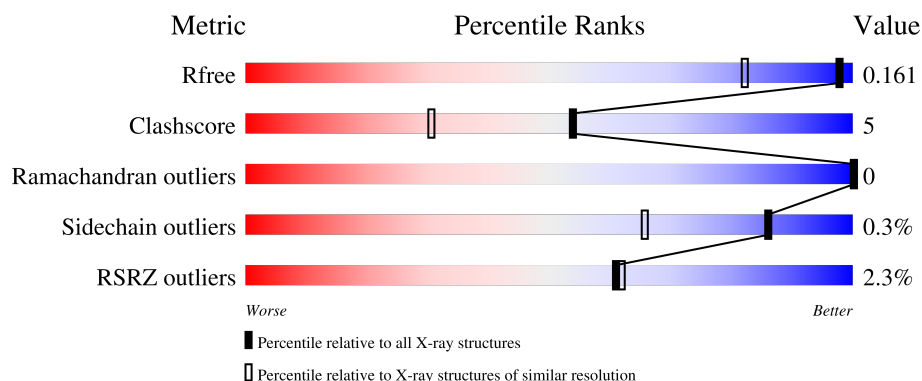
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.24 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))
R_{free}	180053	1630 (1.26-1.22)
Clashscore	190562	1668 (1.26-1.22)
Ramachandran outliers	187476	1635 (1.26-1.22)
Sidechain outliers	187428	1633 (1.26-1.22)
RSRZ outliers	180081	1630 (1.26-1.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	272	3% 89% 7% .
1	BBB	272	2% 86% 8% 5%
1	CCC	272	3% 88% 10% .
1	DDD	272	3% 88% 8% . .
1	EEE	272	0% 88% 6% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	BaB	3	100%
2	CaC	3	33%33%33%
2	DaD	3	33%33%33%

2 Entry composition

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

There are 20 discrepancies between the modelled and reference sequences:

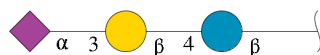
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	18	GLY	-	expression tag	UNP P03089
AAA	19	SER	-	expression tag	UNP P03089
AAA	20	HIS	-	expression tag	UNP P03089
AAA	21	MET	-	expression tag	UNP P03089
BBB	18	GLY	-	expression tag	UNP P03089
BBB	19	SER	-	expression tag	UNP P03089
BBB	20	HIS	-	expression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

Continued on next page...

Continued from previous page...

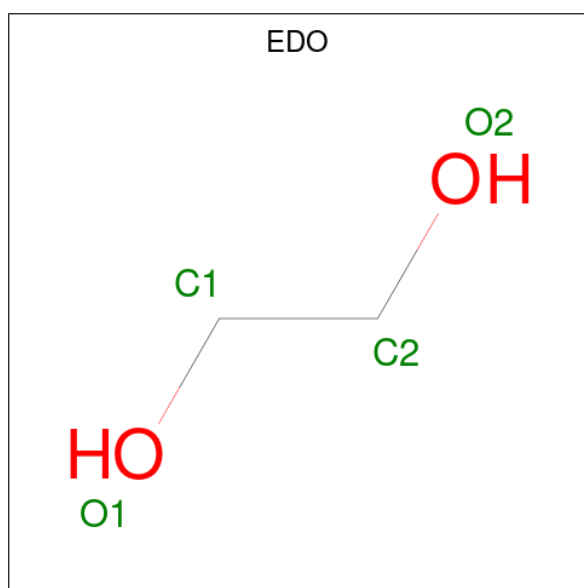
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	21	MET	-	expression tag	UNP P03089

- 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
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 (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

Continued on next page...

Continued from previous page...

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 (CCD ID: 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 (CCD ID: 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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

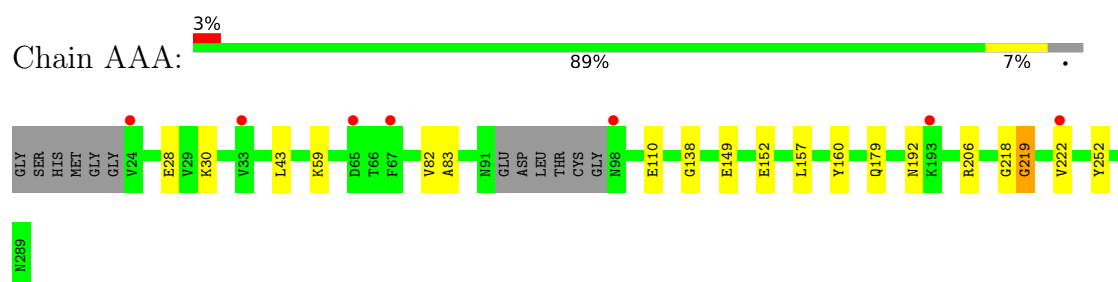
- Molecule 7 is water.

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

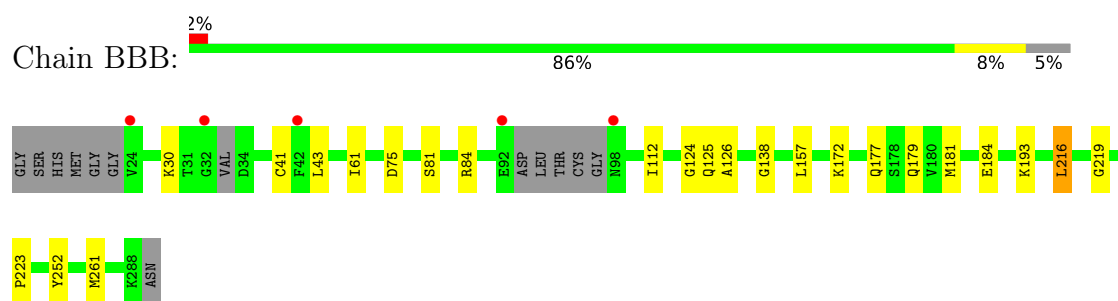
3 Residue-property plots [i](#)

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.

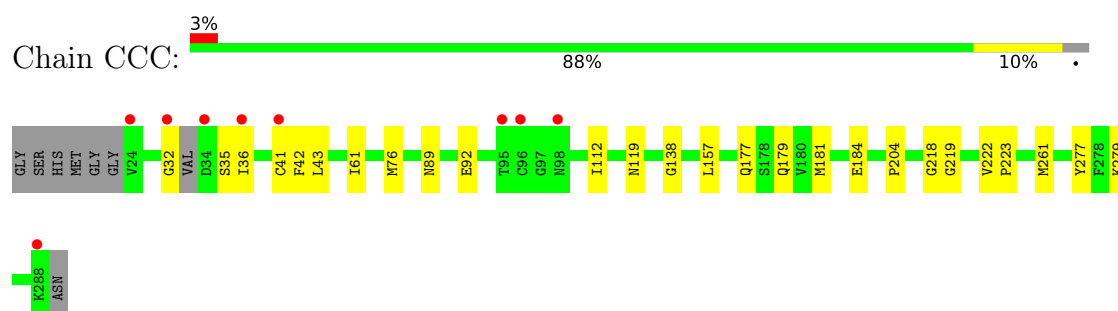
- Molecule 1: Major capsid protein VP1



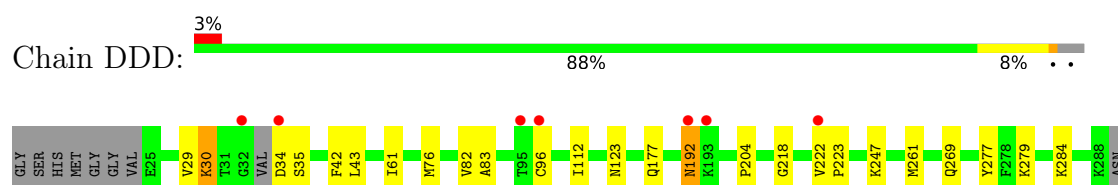
- Molecule 1: Major capsid protein VP1



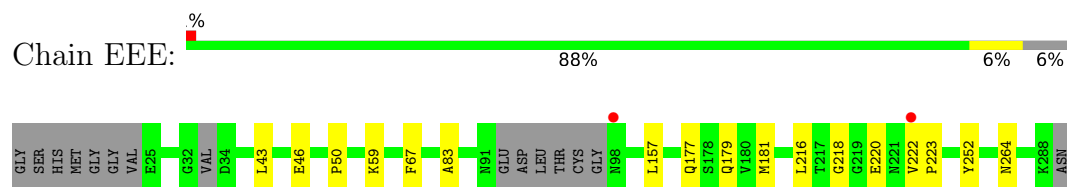
- Molecule 1: Major capsid protein VP1



- Molecule 1: Major capsid protein VP1



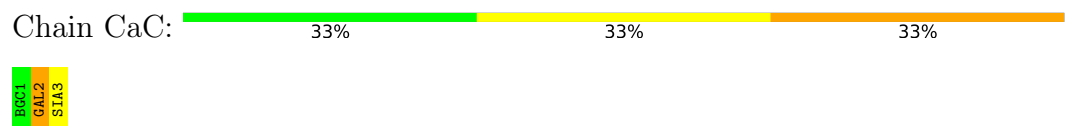
- Molecule 1: Major capsid protein VP1



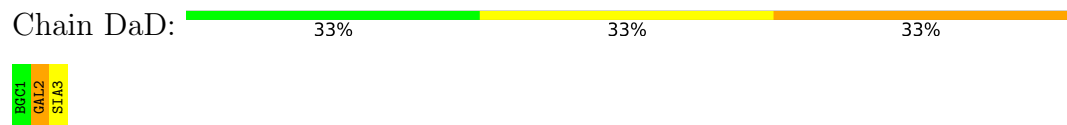
- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



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



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



4 Data and refinement statistics

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 48.01 – 1.24	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.01-1.24) 96.2 (48.01-1.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.138 , 0.155 0.144 , 0.161	Depositor DCC
R_{free} test set	9262 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13339	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage'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: GAL, BGC, PEG, EDO, NA, CL, SIA

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	0.84	0/2346	0.92	1/3190 (0.0%)
1	BBB	0.80	0/2287	0.90	1/3106 (0.0%)
1	CCC	0.82	0/2310	0.91	0/3137
1	DDD	0.82	2/2260 (0.1%)	0.91	0/3067
1	EEE	0.80	0/2270	0.91	0/3084
All	All	0.82	2/11473 (0.0%)	0.91	2/15584 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	30[A]	LYS	C-N	-6.78	1.24	1.33
1	DDD	30[B]	LYS	C-N	-6.78	1.24	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	219	GLY	CA-C-O	-6.07	116.62	121.84
1	BBB	75	ASP	CA-CB-CG	5.06	117.66	112.60

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	18	0
1	BBB	2224	0	2148	22	0
1	CCC	2252	0	2148	30	0
1	DDD	2206	0	2120	31	0
1	EEE	2223	0	2127	24	0
2	BaB	43	0	37	0	0
2	CaC	64	0	52	1	0
2	DaD	32	0	26	1	0
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	7	0
7	CCC	426	0	0	7	0
7	DDD	378	0	0	8	0
7	EEE	381	0	0	4	0
All	All	13339	0	10912	110	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 (110) 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:76[B]:MET:HE1	7:DDD:789:HOH:O	1.51	1.10
1:DDD:261[B]:MET:HG2	1:DDD:269:GLN:HB3	1.28	1.06
1:CCC:76[B]:MET:HE1	7:CCC:612:HOH:O	1.56	1.03
1:CCC:36[B]:ILE:HG23	7:CCC:598:HOH:O	1.64	0.96
1:BBB:124:GLY:C	1:BBB:125[C]:GLN:CA	2.39	0.94
1:CCC:184[B]:GLU:HG2	7:CCC:680:HOH:O	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:61[B]:ILE:HD12	1:BBB:261[B]:MET:HE1	1.54	0.86
1:BBB:61[B]:ILE:CD1	1:BBB:261[B]:MET:HE1	2.06	0.84
1:AAA:160:TYR:H	1:AAA:179:GLN:HE21	1.22	0.83
1:CCC:61[B]:ILE:HD12	1:CCC:261[B]:MET:HE1	1.62	0.82
1:BBB:177[B]:GLN:CD	7:BBB:601:HOH:O	2.27	0.77
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:CCC:76[B]:MET:CE	7:CCC:612:HOH:O	2.23	0.73
1:DDD:76[B]:MET:CE	7:DDD:789:HOH:O	2.23	0.71
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: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:BBB:181[B]:MET:HE2	7:BBB:952:HOH:O	2.00	0.62
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:172:LYS:NZ	7:BBB:602:HOH:O	2.24	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:DDD:112:ILE:HG21	1:EEE:181[B]:MET:HE1	1.87	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	0.54
1:CCC:61[B]:ILE:CD1	1:CCC:261[B]:MET:HE1	2.36	0.54
1:DDD:247:LYS:NZ	7:DDD:606:HOH:O	2.41	0.54
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:216[B]:LEU:C	1:BBB:216[B]:LEU:HD13	2.34	0.52
1:BBB:84[B]:ARG:CZ	7:BBB:631:HOH:O	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:177[B]:GLN:HG3	7:CCC:467:HOH:O	2.11	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
2:CaC:2[A]:GAL:O6	2:CaC:2[A]:GAL:O4	2.24	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: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: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:CCC:32:GLY:O	1:CCC:35:SER:OG	2.31	0.46
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:BBB:261[B]:MET:HB3	1:BBB:261[B]:MET:HE2	1.45	0.44
1:CCC:42[B]:PHE:HE2	1:CCC:112[B]:ILE:HG13	1.83	0.44
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:28:GLU:OE2	1:AAA:30:LYS:NZ	2.48	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
7:DDD:867:HOH:O	2:DaD:2:GAL:H3	2.18	0.42
1:EEE:43[B]:LEU:HD21	1:EEE:83:ALA:CB	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CCC:119:ASN:OD1	1:CCC:119:ASN:C	2.63	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:CCC:157:LEU:O	1:CCC:179:GLN:HA	2.21	0.41
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: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:EEE:216[B]:LEU:HD13	1:EEE:216[B]:LEU:C	2.46	0.40
1:DDD:261[B]:MET:HB2	1:DDD:261[B]:MET:HE2	1.78	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	73	44
1	CCC	249/237 (105%)	249 (100%)	0	100	100
1	DDD	245/237 (103%)	244 (100%)	1 (0%)	84	63
1	EEE	246/237 (104%)	245 (100%)	1 (0%)	84	63
All	All	1246/1185 (105%)	1242 (100%)	4 (0%)	86	66

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1.73	5 (29%)
2	GAL	BaB	2	2	11,11,12	0.64	0	15,15,17	0.96	1 (6%)
2	SIA	BaB	3	2	20,20,21	0.84	1 (5%)	21,28,31	1.04	2 (9%)
2	GAL	CaC	2[A]	2	11,11,12	1.16	1 (9%)	15,15,17	2.16	6 (40%)
2	GAL	CaC	2[B]	2	11,11,12	0.73	0	15,15,17	1.54	4 (26%)
2	SIA	CaC	3[A]	2	20,20,21	0.78	0	21,28,31	1.21	2 (9%)
2	SIA	CaC	3[B]	2	20,20,21	0.66	0	21,28,31	1.08	2 (9%)
2	GAL	DaD	2	2	11,11,12	0.81	0	15,15,17	2.31	7 (46%)
2	SIA	DaD	3	2	20,20,21	0.65	0	21,28,31	1.05	1 (4%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.98	1.50	1.43
2	BaB	3	SIA	C2-C1	2.21	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DaD	2	GAL	C1-O5-C5	5.58	119.67	112.19
2	CaC	2[A]	GAL	O3-C3-C2	4.21	118.66	110.05
2	DaD	2	GAL	C3-C4-C5	3.80	117.12	110.23
2	CaC	2[B]	GAL	C1-O5-C5	3.55	116.94	112.19
2	CaC	2[A]	GAL	C3-C4-C5	3.42	116.44	110.23
2	CaC	2[A]	GAL	C2-C3-C4	3.29	116.65	110.86
2	BaB	1	BGC	O5-C1-C2	-3.12	104.81	110.30
2	BaB	1	BGC	O1-C1-C2	3.06	117.87	108.98
2	BaB	1	BGC	O1-C1-O5	-3.04	101.39	110.41
2	CaC	2[A]	GAL	O2-C2-C3	-3.03	103.88	110.15
2	CaC	3[A]	SIA	O6-C2-C3	-2.96	106.57	110.56
2	BaB	2	GAL	O3-C3-C2	-2.82	104.30	110.05
2	DaD	2	GAL	O5-C5-C6	-2.75	102.31	107.66
2	BaB	3	SIA	O1A-C1-C2	-2.65	117.13	122.85
2	DaD	2	GAL	O5-C5-C4	2.62	117.20	110.83
2	CaC	3[B]	SIA	O1B-C1-C2	2.59	119.43	112.71
2	DaD	3	SIA	O1B-C1-C2	2.52	119.27	112.71
2	CaC	3[B]	SIA	O6-C2-C3	-2.50	107.20	110.56
2	CaC	3[A]	SIA	O1B-C1-C2	2.49	119.20	112.71
2	BaB	3	SIA	O1B-C1-C2	2.46	119.11	112.71
2	CaC	2[A]	GAL	O2-C2-C1	-2.38	103.77	109.22
2	CaC	2[B]	GAL	C3-C4-C5	2.36	114.52	110.23
2	CaC	2[B]	GAL	O2-C2-C3	2.34	114.99	110.15
2	CaC	2[B]	GAL	O3-C3-C4	-2.29	104.99	110.38
2	DaD	2	GAL	C2-C3-C4	-2.25	106.90	110.86
2	BaB	1	BGC	O4-C4-C3	-2.22	105.15	110.38
2	DaD	2	GAL	C1-C2-C3	2.18	112.82	109.64
2	CaC	2[A]	GAL	C1-C2-C3	2.17	112.81	109.64
2	DaD	2	GAL	O3-C3-C2	-2.15	105.66	110.05
2	BaB	1	BGC	O2-C2-C3	-2.05	105.56	110.38

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

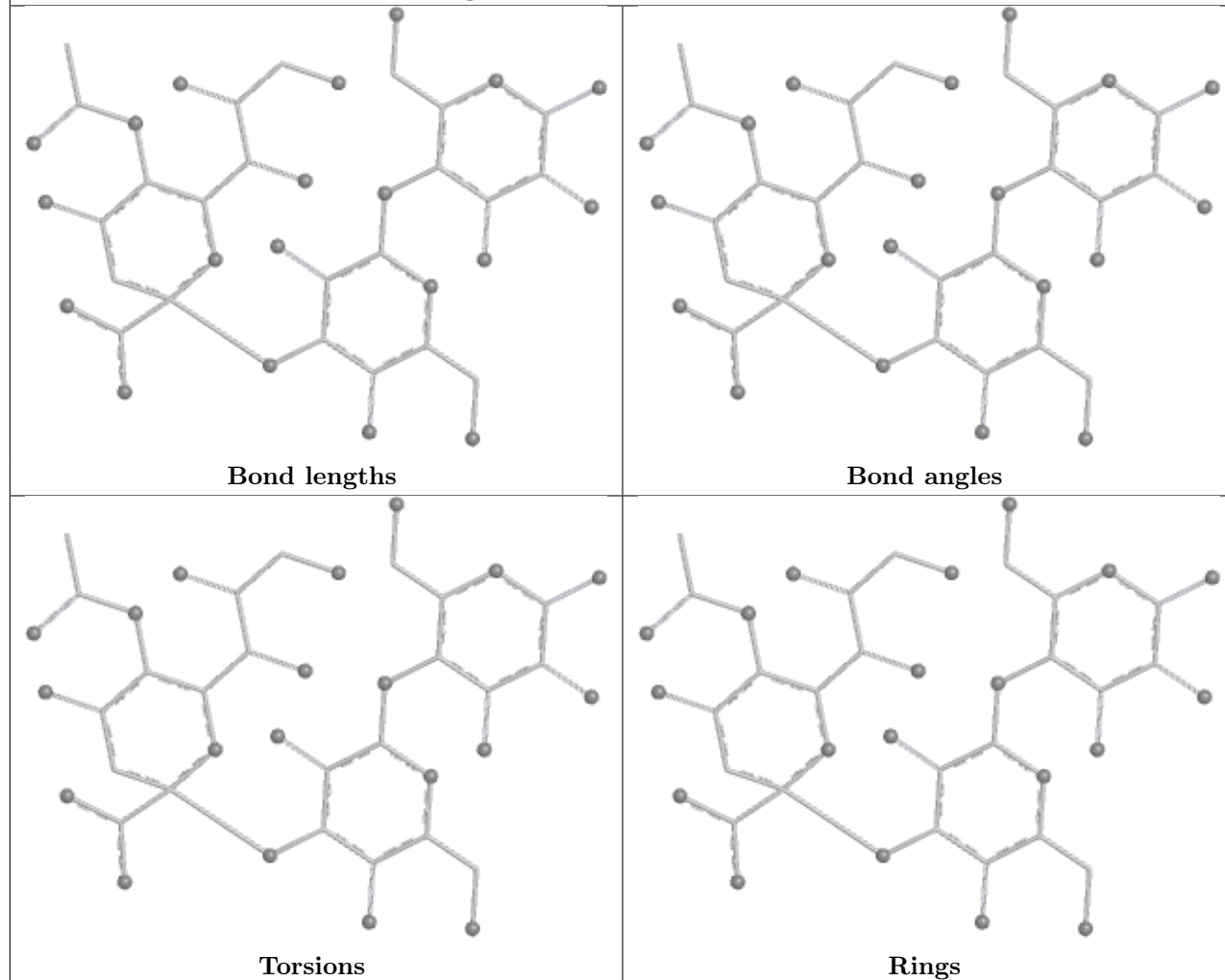
There are no ring outliers.

2 monomers are involved in 2 short contacts:

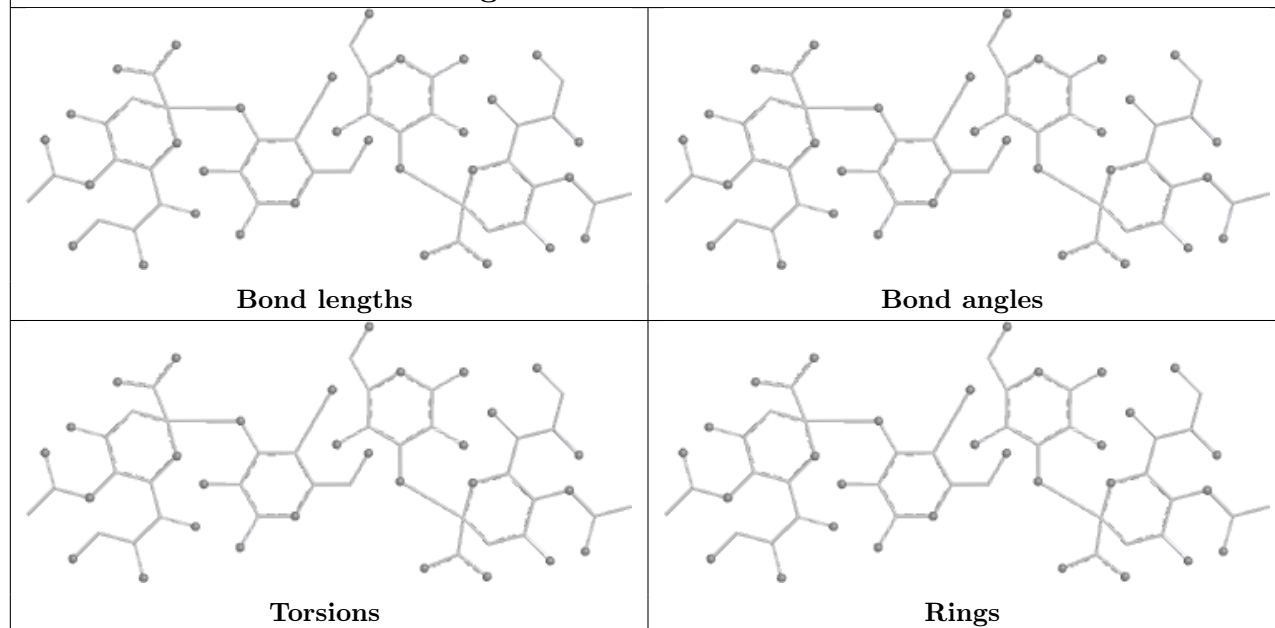
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DaD	2	GAL	1	0
2	CaC	2[A]	GAL	1	0

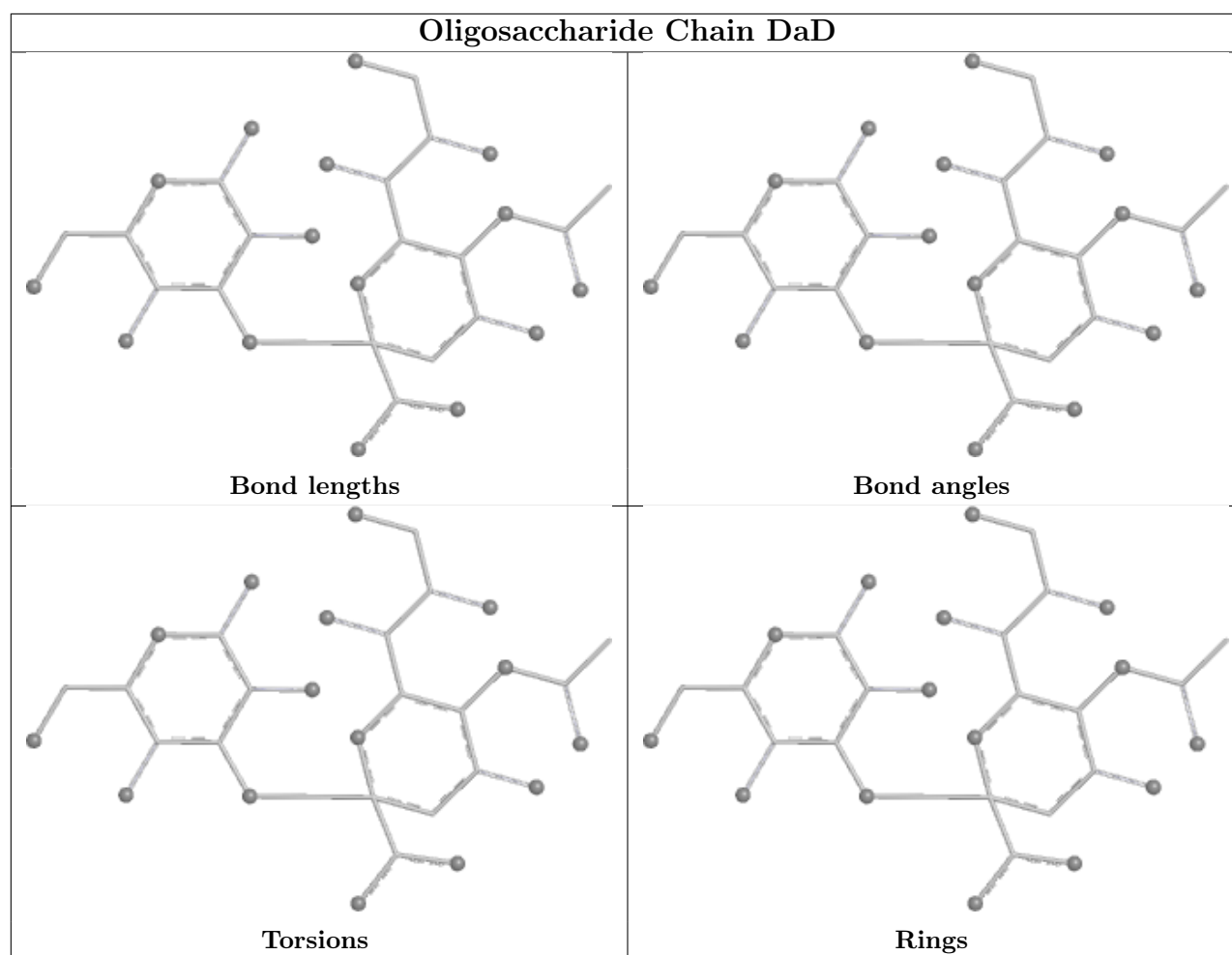
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain BaB



Oligosaccharide Chain CaC





5.6 Ligand geometry [i](#)

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	AAA	401	-	3,3,3	0.11	0	2,2,2	0.17	0
3	EDO	EEE	403	-	3,3,3	0.21	0	2,2,2	0.29	0
3	EDO	EEE	402	-	3,3,3	0.09	0	2,2,2	0.18	0
3	EDO	AAA	403	-	3,3,3	0.04	0	2,2,2	0.04	0
3	EDO	BBB	501	-	3,3,3	0.15	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	DDD	501	-	3,3,3	0.16	0	2,2,2	0.25	0
3	EDO	AAA	402	-	3,3,3	0.15	0	2,2,2	0.07	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	AAA	401	-	-	1/1/1/1	-
3	EDO	EEE	403	-	-	0/1/1/1	-
3	EDO	EEE	402	-	-	1/1/1/1	-
3	EDO	AAA	403	-	-	0/1/1/1	-
3	EDO	BBB	501	-	-	1/1/1/1	-
3	EDO	DDD	501	-	-	1/1/1/1	-
3	EDO	AAA	402	-	-	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	DDD	501	EDO	O1-C1-C2-O2
6	EEE	401	PEG	C4-C3-O2-C2
3	AAA	401	EDO	O1-C1-C2-O2

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	260/272 (95%)	-0.22	7 (2%) 56 57	5, 13, 27, 53	34 (13%)
1	BBB	259/272 (95%)	-0.20	5 (1%) 66 66	5, 14, 30, 51	26 (10%)
1	CCC	264/272 (97%)	-0.16	9 (3%) 48 48	5, 13, 27, 52	28 (10%)
1	DDD	263/272 (96%)	-0.22	7 (2%) 56 57	5, 13, 24, 48	22 (8%)
1	EEE	257/272 (94%)	-0.27	2 (0%) 82 83	4, 13, 26, 43	27 (10%)
All	All	1303/1360 (95%)	-0.21	30 (2%) 61 62	4, 13, 27, 53	137 (10%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	41	CYS	5.2
1	AAA	24	VAL	4.6
1	BBB	24	VAL	4.1
1	CCC	32	GLY	3.7
1	DDD	96	CYS	3.7
1	DDD	32	GLY	3.4
1	CCC	96	CYS	3.4
1	BBB	32	GLY	3.3
1	CCC	24	VAL	3.3
1	DDD	34	ASP	3.2
1	AAA	33	VAL	3.2
1	CCC	95	THR	3.2
1	EEE	222[A]	VAL	3.1
1	BBB	92	GLU	3.0
1	AAA	193	LYS	2.9
1	CCC	98	ASN	2.7
1	CCC	288	LYS	2.4
1	CCC	34	ASP	2.4
1	BBB	42[A]	PHE	2.4
1	CCC	36[A]	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	EEE	98	ASN	2.4
1	AAA	98	ASN	2.3
1	DDD	95	THR	2.3
1	DDD	192	ASN	2.3
1	AAA	65[A]	ASP	2.3
1	AAA	222[A]	VAL	2.3
1	BBB	98	ASN	2.2
1	DDD	222	VAL	2.1
1	AAA	67[A]	PHE	2.1
1	DDD	193[A]	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

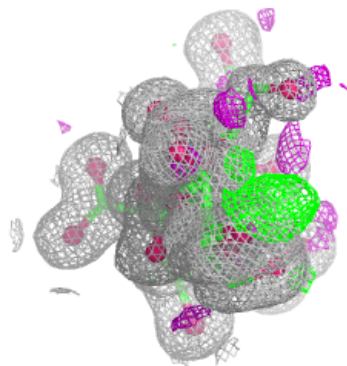
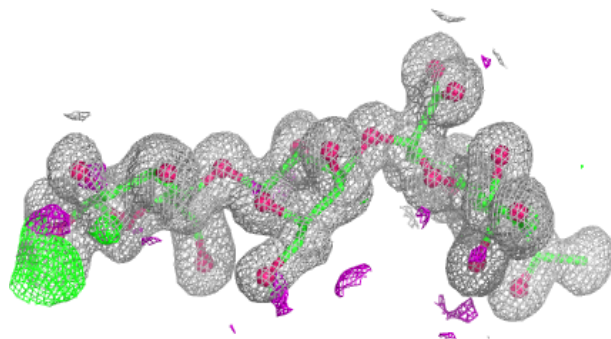
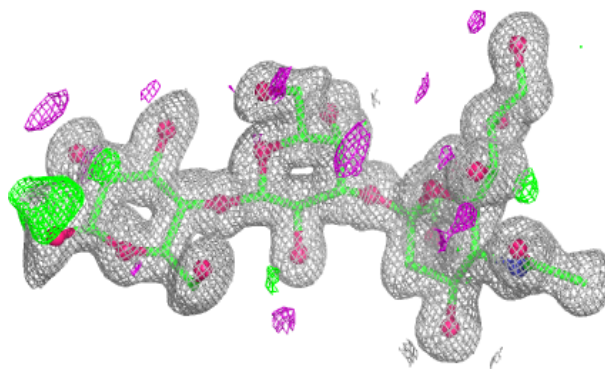
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	BaB	1	12/12	-	-	18,26,36,43	0
2	GAL	BaB	2	11/12	-	-	13,16,23,29	0
2	SIA	BaB	3	20/21	-	-	11,12,14,15	0
2	BGC	CaC	1[A]	1/12	-	-	42,42,42,42	1
2	BGC	CaC	1[B]	1/12	-	-	37,37,37,37	1
2	GAL	CaC	2[A]	11/12	-	-	18,31,42,52	11
2	GAL	CaC	2[B]	11/12	-	-	17,29,45,58	11
2	SIA	CaC	3[A]	20/21	-	-	12,14,16,16	20
2	SIA	CaC	3[B]	20/21	-	-	12,14,16,16	20
2	BGC	DaD	1	1/12	-	-	51,51,51,51	0
2	GAL	DaD	2	11/12	-	-	20,37,56,60	0
2	SIA	DaD	3	20/21	-	-	13,14,16,18	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.

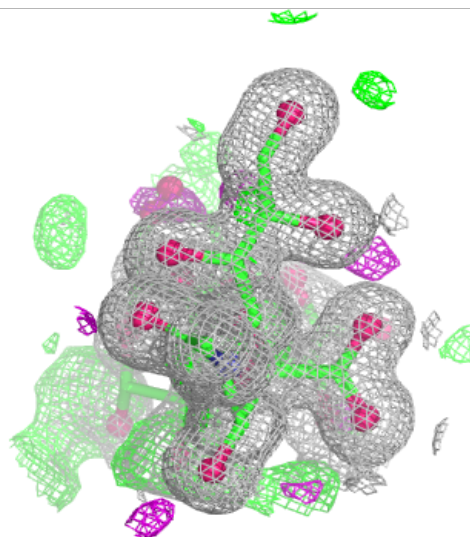
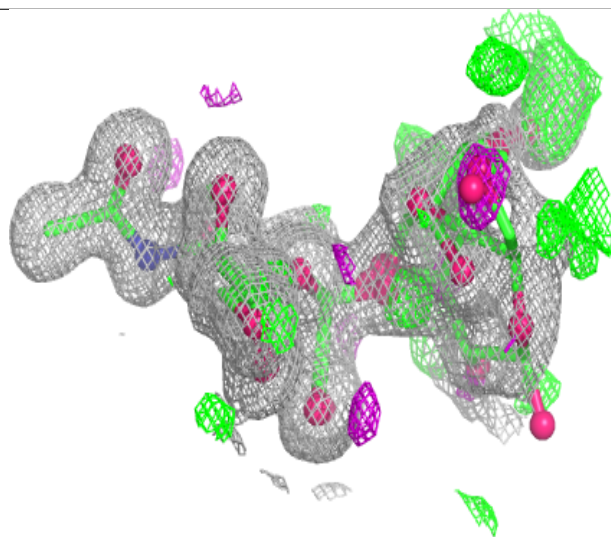
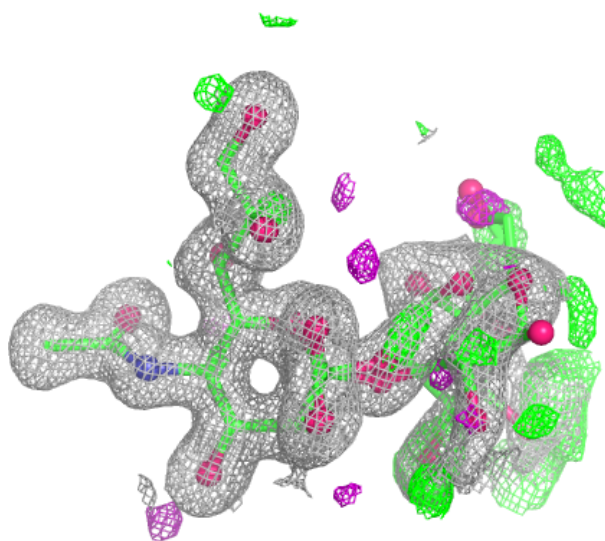
Electron density around Chain BaB:

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



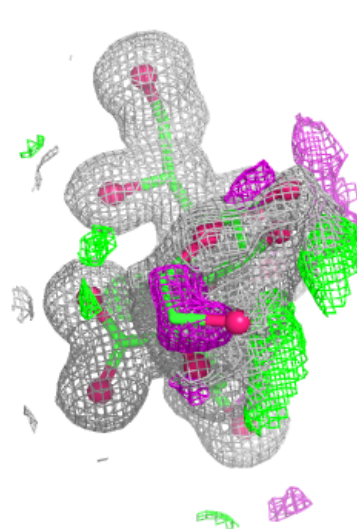
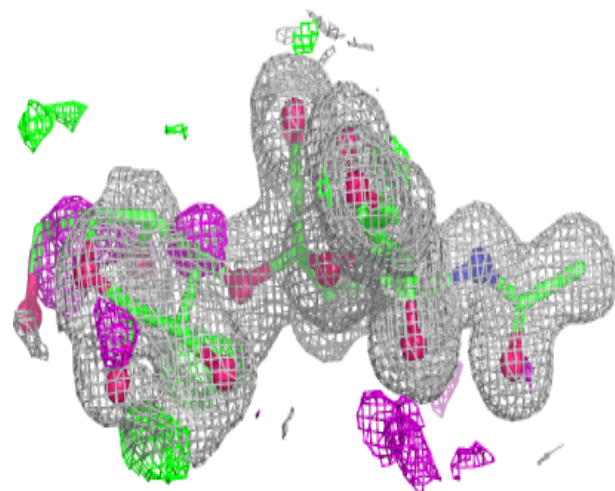
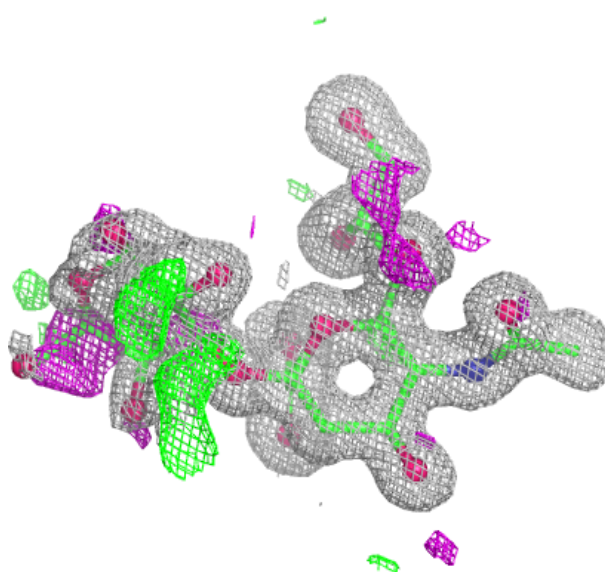
Electron density around Chain CaC:

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



Electron density around Chain DaD:

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

**6.4 Ligands** ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	AAA	403	4/4	0.72	0.20	50,52,54,56	0
3	EDO	AAA	402	4/4	0.76	0.18	46,48,49,53	0
3	EDO	BBB	501	4/4	0.87	0.15	54,55,62,62	0
6	PEG	EEE	401	7/7	0.87	0.17	30,45,60,69	0
3	EDO	EEE	402	4/4	0.88	0.13	41,43,51,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	DDD	501	4/4	0.89	0.13	31,39,42,51	0
3	EDO	AAA	401	4/4	0.91	0.11	37,46,47,50	0
4	CL	BBB	502	1/1	0.92	0.15	66,66,66,66	0
4	CL	AAA	404	1/1	0.95	0.12	41,41,41,41	0
4	CL	EEE	404	1/1	0.97	0.07	41,41,41,41	0
5	NA	BBB	503	1/1	0.97	0.11	26,26,26,26	0
3	EDO	EEE	403	4/4	0.97	0.11	14,30,35,35	0
5	NA	DDD	503	1/1	0.98	0.06	24,24,24,24	0
5	NA	CCC	302	1/1	0.98	0.05	26,26,26,26	0
5	NA	DDD	502	1/1	0.99	0.11	25,25,25,25	0
5	NA	CCC	301	1/1	0.99	0.09	24,24,24,24	0
5	NA	EEE	405	1/1	0.99	0.05	25,25,25,25	0
5	NA	EEE	406	1/1	0.99	0.03	22,22,22,22	0
5	NA	AAA	405	1/1	0.99	0.06	24,24,24,24	0
5	NA	BBB	504	1/1	1.00	0.03	23,23,23,23	0
5	NA	AAA	406	1/1	1.00	0.03	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.