



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:32 PM UTC

PDB ID : 3S6Y / pdb_00003s6y
Title : Structure of reovirus attachment protein sigma1 in complex with alpha-2,6-sialyllactose
Authors : Reiter, D.M.; Dermody, T.S.; Stehle, T.
Deposited on : 2011-05-26
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

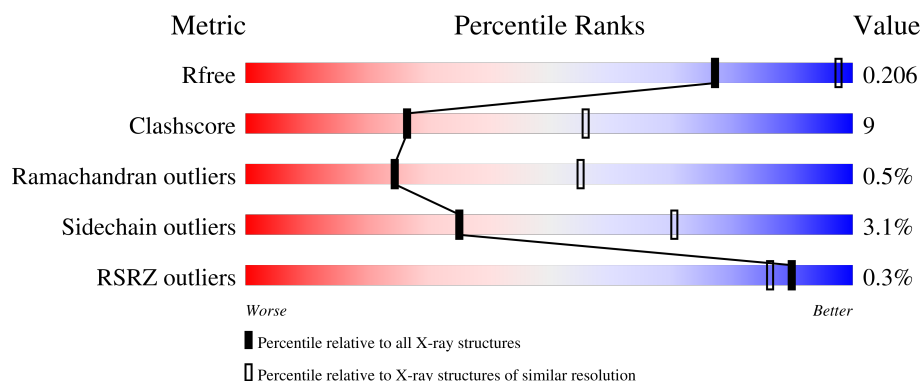
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

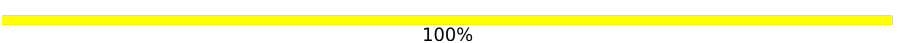
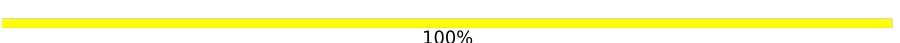
The reported resolution of this entry is 2.79 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	325	 69% 20% 11%
1	B	325	 73% 17% 9%
1	C	325	 70% 19% 10%
2	D	3	 100%
2	E	3	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7215 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2205	1381	386	430	8			
1	B	295	Total	C	N	O	S	0	2	0
			2256	1415	396	437	8			
1	C	291	Total	C	N	O	S	0	1	0
			2218	1392	386	432	8			

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLN	-	expression tag	UNP P03528
A	132	ILE	-	expression tag	UNP P03528
A	133	GLU	-	expression tag	UNP P03528
A	134	ASP	-	expression tag	UNP P03528
A	135	LYS	-	expression tag	UNP P03528
A	136	ILE	-	expression tag	UNP P03528
A	137	GLU	-	expression tag	UNP P03528
A	138	GLU	-	expression tag	UNP P03528
A	139	ILE	-	expression tag	UNP P03528
A	140	LEU	-	expression tag	UNP P03528
A	141	SER	-	expression tag	UNP P03528
A	142	LYS	-	expression tag	UNP P03528
A	143	ILE	-	expression tag	UNP P03528
A	144	TYR	-	expression tag	UNP P03528
A	145	HIS	-	expression tag	UNP P03528
A	146	ILE	-	expression tag	UNP P03528
A	147	GLU	-	expression tag	UNP P03528
A	148	ASN	-	expression tag	UNP P03528
A	149	GLU	-	expression tag	UNP P03528
A	150	ILE	-	expression tag	UNP P03528
A	151	ALA	-	expression tag	UNP P03528
A	152	ARG	-	expression tag	UNP P03528
A	153	ILE	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
A	154	LYS	-	expression tag	UNP P03528
A	155	LYS	-	expression tag	UNP P03528
A	156	LEU	-	expression tag	UNP P03528
A	157	ILE	-	expression tag	UNP P03528
A	158	GLY	-	expression tag	UNP P03528
A	159	GLU	-	expression tag	UNP P03528
A	160	GLY	-	expression tag	UNP P03528
A	161	SER	-	expression tag	UNP P03528
A	162	GLY	-	expression tag	UNP P03528
A	163	ARG	-	expression tag	UNP P03528
A	164	PRO	-	expression tag	UNP P03528
A	165	VAL	-	expression tag	UNP P03528
A	166	LEU	-	expression tag	UNP P03528
A	167	ASN	-	expression tag	UNP P03528
A	168	GLN	-	expression tag	UNP P03528
A	169	GLY	-	expression tag	UNP P03528
A	249	ILE	THR	engineered mutation	UNP P03528
A	408	THR	ALA	conflict	UNP P03528
B	131	GLN	-	expression tag	UNP P03528
B	132	ILE	-	expression tag	UNP P03528
B	133	GLU	-	expression tag	UNP P03528
B	134	ASP	-	expression tag	UNP P03528
B	135	LYS	-	expression tag	UNP P03528
B	136	ILE	-	expression tag	UNP P03528
B	137	GLU	-	expression tag	UNP P03528
B	138	GLU	-	expression tag	UNP P03528
B	139	ILE	-	expression tag	UNP P03528
B	140	LEU	-	expression tag	UNP P03528
B	141	SER	-	expression tag	UNP P03528
B	142	LYS	-	expression tag	UNP P03528
B	143	ILE	-	expression tag	UNP P03528
B	144	TYR	-	expression tag	UNP P03528
B	145	HIS	-	expression tag	UNP P03528
B	146	ILE	-	expression tag	UNP P03528
B	147	GLU	-	expression tag	UNP P03528
B	148	ASN	-	expression tag	UNP P03528
B	149	GLU	-	expression tag	UNP P03528
B	150	ILE	-	expression tag	UNP P03528
B	151	ALA	-	expression tag	UNP P03528
B	152	ARG	-	expression tag	UNP P03528
B	153	ILE	-	expression tag	UNP P03528
B	154	LYS	-	expression tag	UNP P03528

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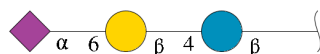
Chain	Residue	Modelled	Actual	Comment	Reference
B	155	LYS	-	expression tag	UNP P03528
B	156	LEU	-	expression tag	UNP P03528
B	157	ILE	-	expression tag	UNP P03528
B	158	GLY	-	expression tag	UNP P03528
B	159	GLU	-	expression tag	UNP P03528
B	160	GLY	-	expression tag	UNP P03528
B	161	SER	-	expression tag	UNP P03528
B	162	GLY	-	expression tag	UNP P03528
B	163	ARG	-	expression tag	UNP P03528
B	164	PRO	-	expression tag	UNP P03528
B	165	VAL	-	expression tag	UNP P03528
B	166	LEU	-	expression tag	UNP P03528
B	167	ASN	-	expression tag	UNP P03528
B	168	GLN	-	expression tag	UNP P03528
B	169	GLY	-	expression tag	UNP P03528
B	249	ILE	THR	engineered mutation	UNP P03528
B	408	THR	ALA	conflict	UNP P03528
C	131	GLN	-	expression tag	UNP P03528
C	132	ILE	-	expression tag	UNP P03528
C	133	GLU	-	expression tag	UNP P03528
C	134	ASP	-	expression tag	UNP P03528
C	135	LYS	-	expression tag	UNP P03528
C	136	ILE	-	expression tag	UNP P03528
C	137	GLU	-	expression tag	UNP P03528
C	138	GLU	-	expression tag	UNP P03528
C	139	ILE	-	expression tag	UNP P03528
C	140	LEU	-	expression tag	UNP P03528
C	141	SER	-	expression tag	UNP P03528
C	142	LYS	-	expression tag	UNP P03528
C	143	ILE	-	expression tag	UNP P03528
C	144	TYR	-	expression tag	UNP P03528
C	145	HIS	-	expression tag	UNP P03528
C	146	ILE	-	expression tag	UNP P03528
C	147	GLU	-	expression tag	UNP P03528
C	148	ASN	-	expression tag	UNP P03528
C	149	GLU	-	expression tag	UNP P03528
C	150	ILE	-	expression tag	UNP P03528
C	151	ALA	-	expression tag	UNP P03528
C	152	ARG	-	expression tag	UNP P03528
C	153	ILE	-	expression tag	UNP P03528
C	154	LYS	-	expression tag	UNP P03528
C	155	LYS	-	expression tag	UNP P03528

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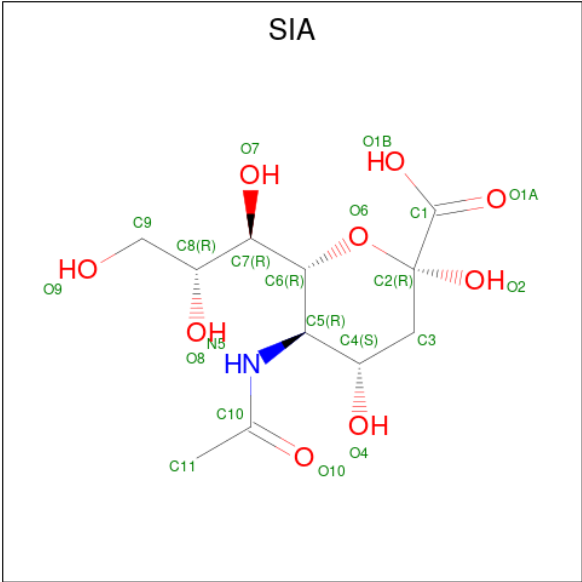
Chain	Residue	Modelled	Actual	Comment	Reference
C	156	LEU	-	expression tag	UNP P03528
C	157	ILE	-	expression tag	UNP P03528
C	158	GLY	-	expression tag	UNP P03528
C	159	GLU	-	expression tag	UNP P03528
C	160	GLY	-	expression tag	UNP P03528
C	161	SER	-	expression tag	UNP P03528
C	162	GLY	-	expression tag	UNP P03528
C	163	ARG	-	expression tag	UNP P03528
C	164	PRO	-	expression tag	UNP P03528
C	165	VAL	-	expression tag	UNP P03528
C	166	LEU	-	expression tag	UNP P03528
C	167	ASN	-	expression tag	UNP P03528
C	168	GLN	-	expression tag	UNP P03528
C	169	GLY	-	expression tag	UNP P03528
C	249	ILE	THR	engineered mutation	UNP P03528
C	408	THR	ALA	conflict	UNP P03528

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	E	3	Total	C	N	O	0	0	0
			43	23	1	19			

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			21	11	1	9		

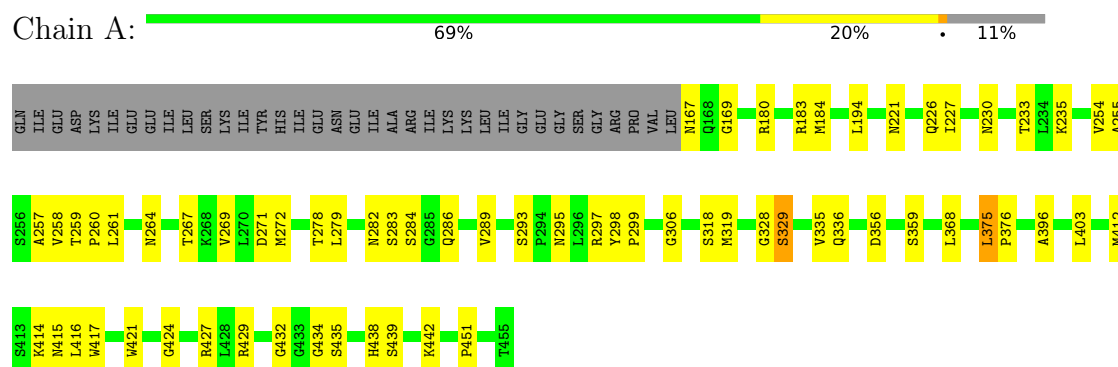
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	135	Total	O	0	0
			135	135		
4	C	139	Total	O	0	0
			139	139		

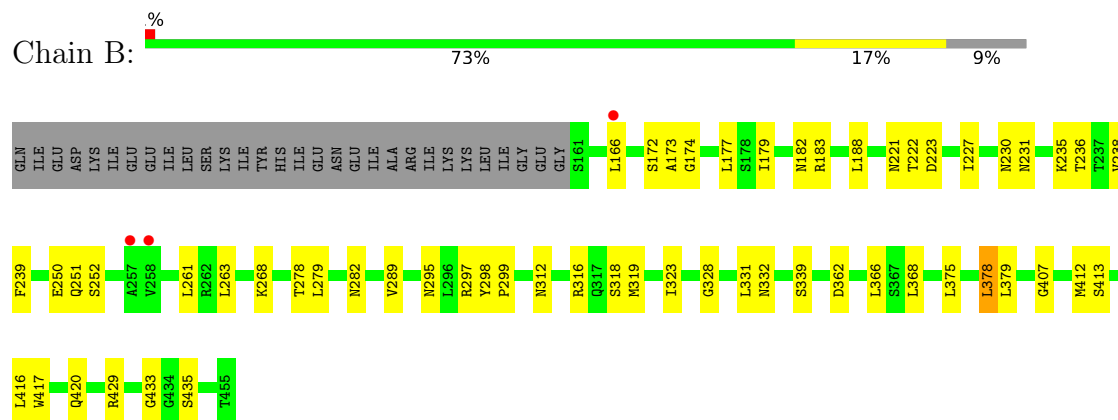
3 Residue-property plots

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.

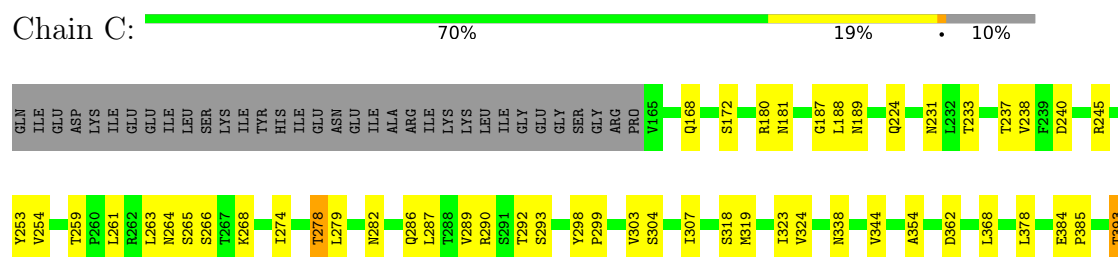
• Molecule 1: Outer capsid protein sigma-1

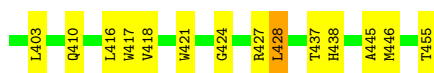


• Molecule 1: Outer capsid protein sigma-1



• Molecule 1: Outer capsid protein sigma-1





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:  100%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain E:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.15Å 333.18Å 58.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.79 48.06 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.06-2.79) 99.0 (48.06-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.13 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.158 , 0.208 0.156 , 0.206	Depositor DCC
R_{free} test set	2188 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7215	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, BGC

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	0.47	0/2249	0.84	1/3062 (0.0%)
1	B	0.48	0/2304	0.85	2/3136 (0.1%)
1	C	0.47	0/2265	0.86	2/3084 (0.1%)
All	All	0.48	0/6818	0.85	5/9282 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ILE	CB-CA-C	-5.46	105.33	111.23
1	C	323	ILE	N-CA-C	5.46	115.97	107.99
1	B	420	GLN	N-CA-C	5.18	116.28	108.46
1	B	323	ILE	N-CA-C	5.07	115.39	107.99
1	A	283	SER	N-CA-C	-5.02	106.42	112.54

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	2205	0	2161	57	0
1	B	2256	0	2229	42	0
1	C	2218	0	2186	49	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	37	1	0
2	E	43	0	37	0	0
3	B	21	0	18	2	0
4	A	155	0	0	5	1
4	B	135	0	0	3	3
4	C	139	0	0	4	3
All	All	7215	0	6668	125	4

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 (125) 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:C:427:ARG:NH2	4:C:729:HOH:O	1.93	1.01
1:A:415:ASN:HD21	1:C:445:ALA:H	1.12	0.97
1:A:435:SER:OG	4:A:608:HOH:O	1.92	0.87
1:B:316[A]:ARG:NH1	4:B:504:HOH:O	2.08	0.86
1:A:221:ASN:HB2	1:C:233:THR:HG22	1.58	0.85
1:B:319:MET:HB3	1:B:375:LEU:HD22	1.61	0.82
1:A:415:ASN:ND2	1:C:445:ALA:H	1.79	0.80
1:A:289:VAL:HG22	1:B:278:THR:HB	1.62	0.79
1:A:255:ALA:O	1:B:252:SER:OG	2.02	0.77
1:A:435:SER:N	4:A:519:HOH:O	2.09	0.71
1:A:415:ASN:HD21	1:C:445:ALA:N	1.87	0.68
1:A:375:LEU:HD13	1:A:376:PRO:HD2	1.77	0.66
1:A:403:LEU:HD12	1:A:412:MET:HG3	1.77	0.66
1:B:332:ASN:HB2	4:B:508:HOH:O	1.96	0.65
1:C:237:THR:HA	1:C:240:ASP:CG	2.23	0.63
1:B:268:LYS:HD3	1:C:253:TYR:CE2	2.35	0.61
1:B:174:GLY:O	1:B:177:LEU:HB2	2.02	0.59
1:A:282:ASN:HB2	1:A:286:GLN:H	1.69	0.57
1:B:238:VAL:HG13	1:B:239:PHE:CD1	2.39	0.57
1:A:167:ASN:C	1:A:169:GLY:H	2.10	0.57
1:A:278:THR:HB	1:C:289:VAL:HG22	1.86	0.57
1:B:279:LEU:HD23	1:B:289:VAL:HA	1.85	0.57
1:C:224:GLN:HA	1:C:238:VAL:CG2	2.36	0.55
1:C:403:LEU:HD13	1:C:438:HIS:CE1	2.42	0.55
1:C:362:ASP:OD2	4:C:573:HOH:O	2.18	0.54
1:C:282:ASN:OD1	1:C:286:GLN:N	2.40	0.54
1:C:231:ASN:O	1:C:233:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:843:HOH:O	1:C:233:THR:HG21	2.07	0.54
1:B:312:ASN:HB3	1:B:316[B]:ARG:HH12	1.72	0.53
1:C:279:LEU:HD23	1:C:289:VAL:HA	1.90	0.53
2:D:1:BGC:O3	2:D:2:GAL:O5	2.26	0.53
1:A:414:LYS:HE2	1:A:432:GLY:O	2.08	0.53
1:B:416:LEU:HD23	1:B:417:TRP:N	2.23	0.52
1:A:254:VAL:HG22	1:C:263:LEU:HD13	1.92	0.52
1:C:427:ARG:HD3	4:C:519:HOH:O	2.08	0.52
1:A:258:VAL:O	1:A:261:LEU:HB2	2.10	0.51
1:B:263:LEU:HD13	1:C:254:VAL:HG22	1.92	0.51
1:A:328:GLY:O	1:A:329:SER:C	2.53	0.51
1:C:319:MET:HE2	1:C:338:ASN:HB2	1.92	0.51
1:A:298:TYR:CG	1:A:299:PRO:HA	2.46	0.50
1:A:272:MET:HE2	1:C:287:LEU:HD22	1.93	0.50
1:A:356:ASP:OD1	1:A:442:LYS:HG3	2.11	0.50
1:C:264:ASN:C	1:C:266:SER:H	2.18	0.50
1:C:290:ARG:O	1:C:292:THR:HG23	2.12	0.50
1:B:235:LYS:O	1:B:238:VAL:HG12	2.12	0.49
1:B:298:TYR:CG	1:B:299:PRO:HA	2.47	0.49
1:B:250:GLU:OE2	1:C:245:ARG:HD2	2.12	0.49
1:B:368:LEU:HD12	1:B:368:LEU:N	2.27	0.49
1:A:227:ILE:CG2	1:A:230:ASN:HA	2.42	0.49
1:C:416:LEU:C	1:C:416:LEU:HD23	2.37	0.49
1:C:318:SER:HB3	1:C:378:LEU:HD22	1.93	0.49
1:B:183:ARG:HG3	1:C:172:SER:OG	2.13	0.49
1:A:318:SER:OG	1:A:319:MET:N	2.45	0.49
1:A:421:TRP:CZ2	1:A:424:GLY:HA2	2.48	0.48
1:B:413:SER:O	1:B:433:GLY:HA3	2.12	0.48
1:A:230:ASN:ND2	3:B:1:SIA:H111	2.27	0.48
1:B:221:ASN:OD1	1:B:223:ASP:HB2	2.12	0.48
1:A:278:THR:CG2	1:C:289:VAL:HG22	2.44	0.48
1:B:318:SER:CB	1:B:378:LEU:HD22	2.44	0.48
1:B:318:SER:HB3	1:B:378:LEU:HD22	1.96	0.47
1:A:282:ASN:HB2	1:A:286:GLN:N	2.29	0.47
1:A:279:LEU:HD23	1:A:289:VAL:HA	1.95	0.47
1:A:416:LEU:C	1:A:416:LEU:HD23	2.39	0.47
1:C:421:TRP:CZ2	1:C:424:GLY:HA2	2.50	0.47
1:A:226:GLN:HB3	1:A:235:LYS:HD3	1.94	0.47
1:C:393:THR:HG23	1:C:417:TRP:CE2	2.50	0.47
1:A:264:ASN:HB3	1:A:267:THR:OG1	2.15	0.46
1:A:282:ASN:ND2	1:A:286:GLN:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD12	1:A:368:LEU:N	2.31	0.46
1:C:237:THR:HG22	1:C:240:ASP:OD2	2.16	0.46
1:A:396:ALA:HA	1:A:417:TRP:HB3	1.98	0.46
1:C:187:GLY:O	1:C:188:LEU:HD23	2.16	0.46
1:A:278:THR:CB	1:C:289:VAL:HG22	2.46	0.45
1:A:282:ASN:HB3	1:A:284:SER:H	1.81	0.45
1:A:427:ARG:HG3	4:A:515:HOH:O	2.17	0.45
1:A:295:ASN:HD21	1:A:297:ARG:HH22	1.65	0.45
1:C:318:SER:CB	1:C:378:LEU:HD22	2.46	0.45
1:A:306:GLY:HA3	1:B:297:ARG:HD3	1.99	0.45
1:C:298:TYR:CG	1:C:299:PRO:HA	2.51	0.45
1:A:359:SER:OG	1:A:439:SER:HA	2.17	0.44
1:C:224:GLN:HA	1:C:238:VAL:HG22	1.97	0.44
1:B:416:LEU:HD23	1:B:416:LEU:C	2.43	0.44
1:A:412:MET:HE2	1:A:434:GLY:O	2.17	0.44
1:B:362:ASP:OD1	1:B:435:SER:HB3	2.18	0.44
1:B:179:ILE:HA	1:B:183:ARG:O	2.17	0.44
1:C:259:THR:HA	1:C:261:LEU:N	2.33	0.44
1:A:255:ALA:HB3	1:C:268:LYS:HB3	2.00	0.43
1:B:227:ILE:CG2	1:B:230:ASN:HA	2.48	0.43
1:C:274:ILE:C	1:C:274:ILE:HD12	2.43	0.43
1:B:289:VAL:HG22	1:C:278:THR:CB	2.48	0.43
1:B:412:MET:HE3	1:B:412:MET:HB3	1.91	0.43
1:B:251:GLN:HG3	1:B:252:SER:H	1.83	0.43
1:B:328:GLY:O	1:B:331:LEU:HB2	2.18	0.43
1:B:182:ASN:N	4:B:475:HOH:O	2.39	0.43
1:B:366:LEU:HD12	1:B:366:LEU:HA	1.85	0.43
1:B:227:ILE:HA	1:B:231:ASN:O	2.19	0.42
1:B:416:LEU:HA	1:B:429:ARG:O	2.20	0.42
1:A:278:THR:HB	1:C:289:VAL:HG13	2.00	0.42
1:C:418:VAL:HA	1:C:428:LEU:HD12	2.01	0.42
1:A:298:TYR:CD2	1:A:299:PRO:HA	2.53	0.42
1:A:375:LEU:HD13	1:A:376:PRO:CD	2.47	0.42
1:B:289:VAL:HG22	1:C:278:THR:OG1	2.20	0.42
1:A:295:ASN:ND2	1:A:297:ARG:HH22	2.16	0.42
1:A:416:LEU:HA	1:A:429:ARG:O	2.19	0.42
1:C:303:VAL:O	1:C:304:SER:C	2.63	0.42
1:A:167:ASN:C	1:A:169:GLY:N	2.76	0.42
1:A:403:LEU:HD22	1:A:438:HIS:CD2	2.54	0.41
1:C:180:ARG:O	1:C:181:ASN:C	2.64	0.41
1:A:259:THR:HA	1:A:260:PRO:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:THR:O	1:A:269:VAL:HG23	2.20	0.41
1:B:331:LEU:HA	1:B:331:LEU:HD23	1.76	0.41
1:C:410:GLN:HE21	1:C:410:GLN:HB2	1.68	0.41
1:A:257:ALA:HB1	1:A:261:LEU:HB3	2.02	0.41
1:B:417:TRP:CZ2	1:B:429:ARG:HG2	2.55	0.41
1:C:446:MET:HE3	1:C:446:MET:HB2	1.79	0.41
1:A:271:ASP:HA	1:B:261:LEU:HD12	2.03	0.41
1:A:435:SER:CA	4:A:519:HOH:O	2.61	0.41
1:A:183:ARG:HA	1:B:172:SER:O	2.21	0.41
1:A:451:PRO:HB3	1:C:344:VAL:HG21	2.03	0.40
1:B:319:MET:HG3	1:B:339:SER:O	2.22	0.40
1:B:368:LEU:N	1:B:368:LEU:CD1	2.83	0.40
1:C:384:GLU:HA	1:C:385:PRO:HD3	1.96	0.40
1:C:437:THR:HA	4:C:473:HOH:O	2.22	0.40
1:A:184:MET:O	1:B:173:ALA:HA	2.21	0.40
1:A:230:ASN:HD21	3:B:1:SIA:H111	1.87	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:464:HOH:O	4:C:931:HOH:O[2_455]	2.08	0.12
4:B:495:HOH:O	4:C:469:HOH:O[3_456]	2.09	0.11
1:C:354:ALA:O	4:C:497:HOH:O[3_446]	2.16	0.04
4:A:464:HOH:O	4:B:484:HOH:O[4_545]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	288/325 (89%)	270 (94%)	17 (6%)	1 (0%)	36 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	295/325 (91%)	277 (94%)	16 (5%)	2 (1%)	18	47
1	C	290/325 (89%)	270 (93%)	19 (7%)	1 (0%)	36	66
All	All	873/975 (90%)	817 (94%)	52 (6%)	4 (0%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	SER
1	B	407	GLY
1	C	265	SER
1	B	282	ASN

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	A	246/278 (88%)	239 (97%)	7 (3%)	38	73
1	B	253/278 (91%)	246 (97%)	7 (3%)	38	73
1	C	249/278 (90%)	240 (96%)	9 (4%)	31	66
All	All	748/834 (90%)	725 (97%)	23 (3%)	35	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	ARG
1	A	194	LEU
1	A	233	THR
1	A	293	SER
1	A	335	VAL
1	A	336	GLN
1	A	375	LEU
1	B	166	LEU
1	B	188	LEU
1	B	222	THR

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Mol	Chain	Res	Type
1	B	236	THR
1	B	295	ASN
1	B	378	LEU
1	B	379	LEU
1	C	168	GLN
1	C	189	ASN
1	C	278	THR
1	C	293	SER
1	C	324	VAL
1	C	368	LEU
1	C	393	THR
1	C	428	LEU
1	C	455	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	182	ASN
1	A	213	ASN
1	A	226	GLN
1	A	243	ASN
1	A	282	ASN
1	A	295	ASN
1	A	336	GLN
1	A	415	ASN
1	B	167	ASN
1	B	168	GLN
1	B	182	ASN
1	B	197	ASN
1	B	198	ASN
1	B	210	ASN
1	B	213	ASN
1	B	295	ASN
1	C	189	ASN
1	C	226	GLN
1	C	286	GLN
1	C	317	GLN
1	C	410	GLN

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 ⓘ

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	D	1	2	12,12,12	0.51	0	17,17,17	0.64	0
2	GAL	D	2	2	11,11,12	0.73	0	15,15,17	0.71	0
2	SIA	D	3	2	20,20,21	0.64	0	21,28,31	1.28	2 (9%)
2	BGC	E	1	2	12,12,12	0.58	0	17,17,17	1.18	2 (11%)
2	GAL	E	2	2	11,11,12	0.62	0	15,15,17	1.06	1 (6%)
2	SIA	E	3	2	20,20,21	0.60	0	21,28,31	1.04	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	D	1	2	-	2/2/22/22	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	SIA	E	3	2	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	SIA	C8-C7-C6	-3.11	107.22	113.05
2	E	2	GAL	C2-C3-C4	-3.01	105.57	110.86
2	D	3	SIA	O6-C2-C3	2.97	114.55	110.56
2	E	3	SIA	C8-C7-C6	-2.63	108.11	113.05
2	E	1	BGC	C1-O5-C5	-2.45	108.90	113.65
2	E	1	BGC	C3-C4-C5	2.45	114.67	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

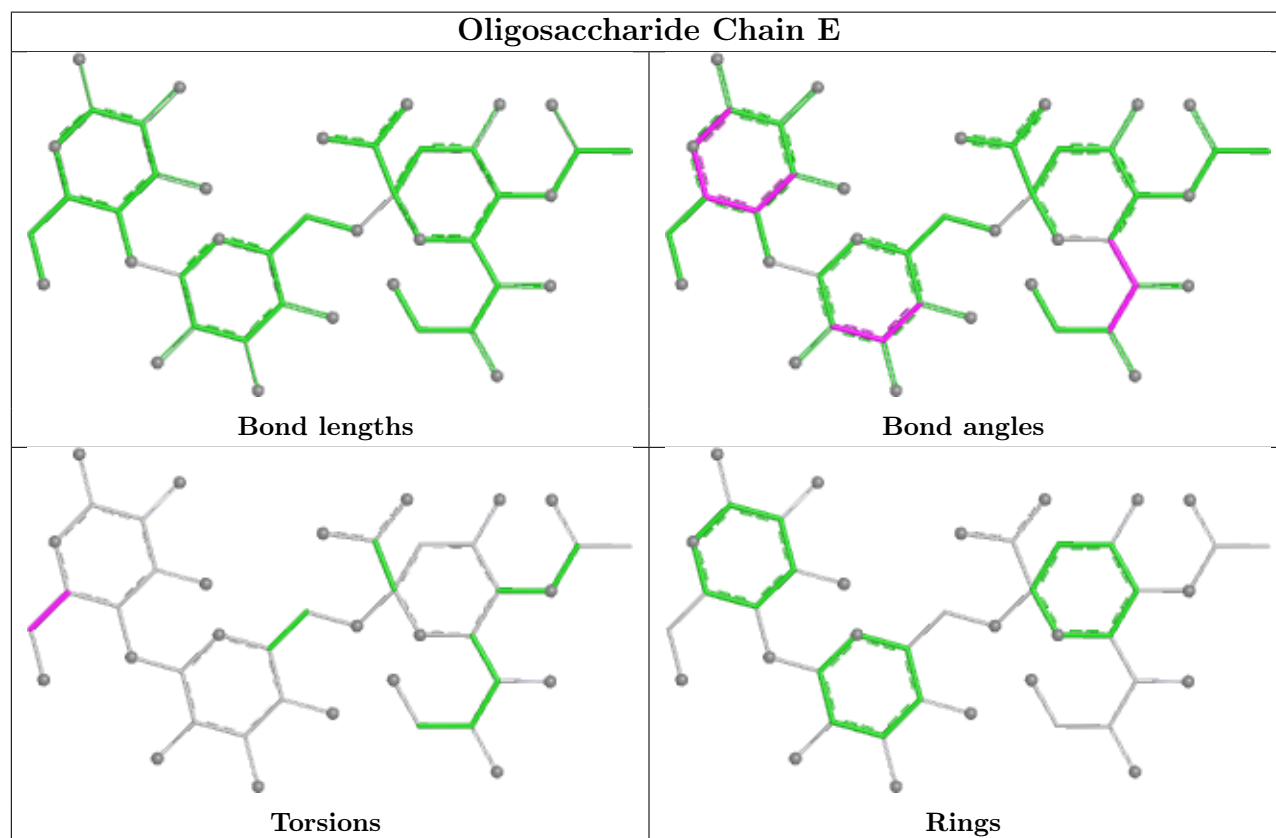
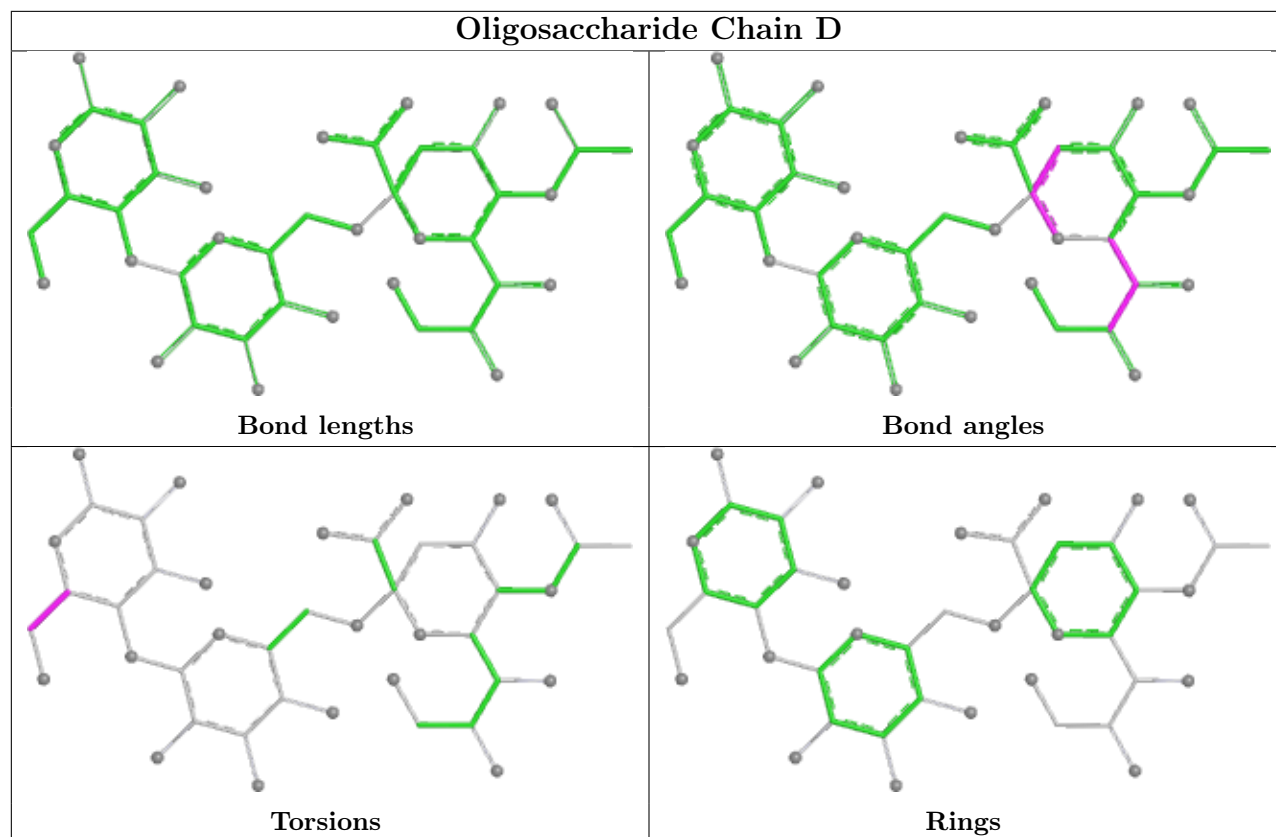
Mol	Chain	Res	Type	Atoms
2	D	1	BGC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	BGC	1	0
2	D	2	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.



5.6 Ligand geometry

1 ligand is 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$
3	SIA	B	1	-	21,21,21	1.07	1 (4%)	24,31,31	1.76	4 (16%)

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
3	SIA	B	1	-	-	9/20/38/38	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	SIA	O2-C2	2.97	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	SIA	O6-C6-C5	4.69	114.14	109.84
3	B	1	SIA	O6-C6-C7	4.19	113.20	106.65
3	B	1	SIA	C3-C2-C1	-4.16	105.12	112.84
3	B	1	SIA	O1A-C1-C2	-2.30	120.01	123.85

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	SIA	C6-C7-C8-C9
3	B	1	SIA	C6-C7-C8-O8
3	B	1	SIA	O7-C7-C8-C9

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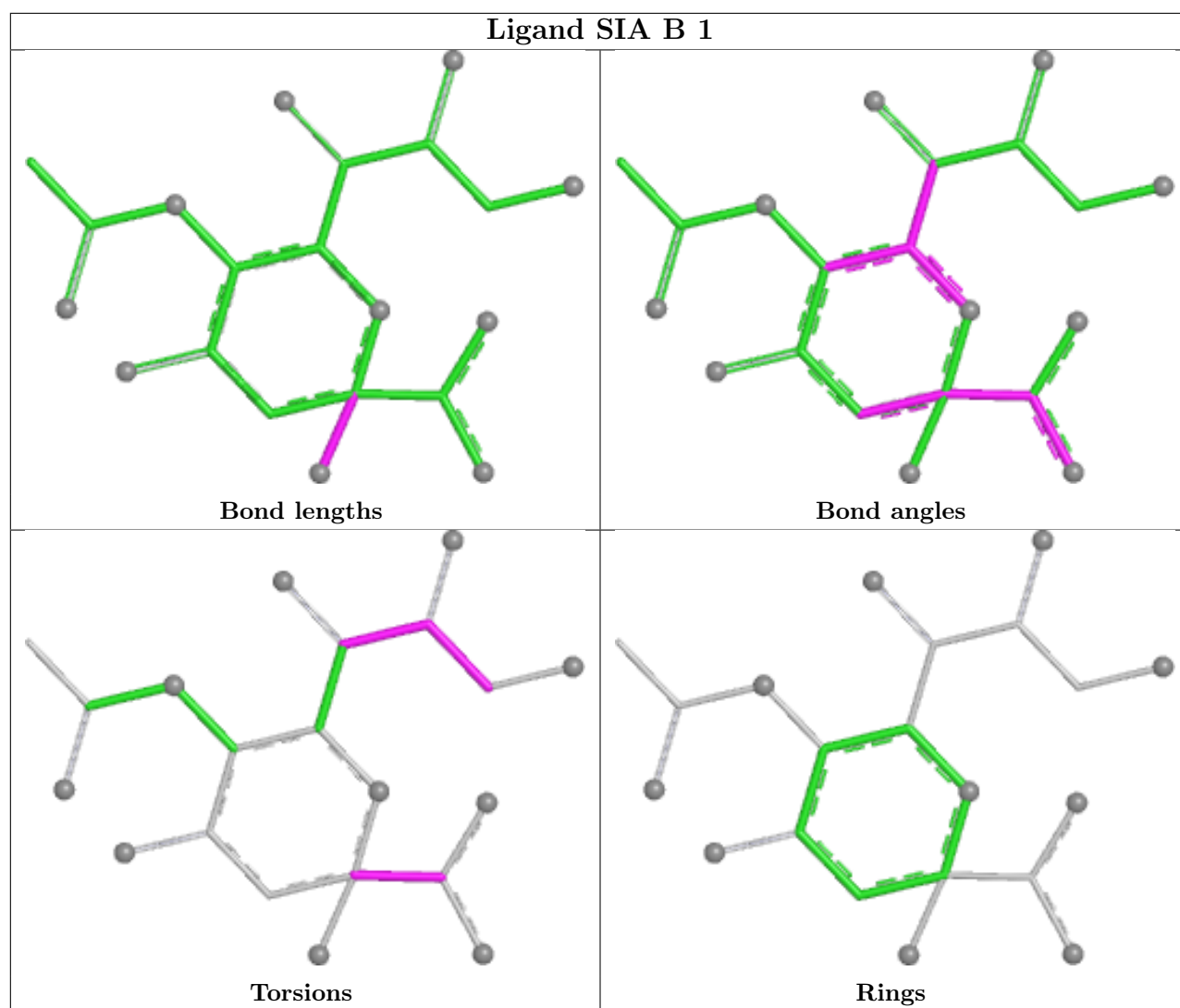
Mol	Chain	Res	Type	Atoms
3	B	1	SIA	O7-C7-C8-O8
3	B	1	SIA	C7-C8-C9-O9
3	B	1	SIA	O1A-C1-C2-O2
3	B	1	SIA	O8-C8-C9-O9
3	B	1	SIA	O1A-C1-C2-C3
3	B	1	SIA	O1B-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	SIA	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/325 (88%)	-0.54	0 100 100	16, 43, 119, 145	1 (0%)
1	B	295/325 (90%)	-0.47	3 (1%) 79 72	14, 45, 119, 144	2 (0%)
1	C	291/325 (89%)	-0.56	0 100 100	21, 46, 123, 143	1 (0%)
All	All	875/975 (89%)	-0.52	3 (0%) 90 86	14, 45, 121, 145	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	LEU	3.0
1	B	257	ALA	2.4
1	B	258	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

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

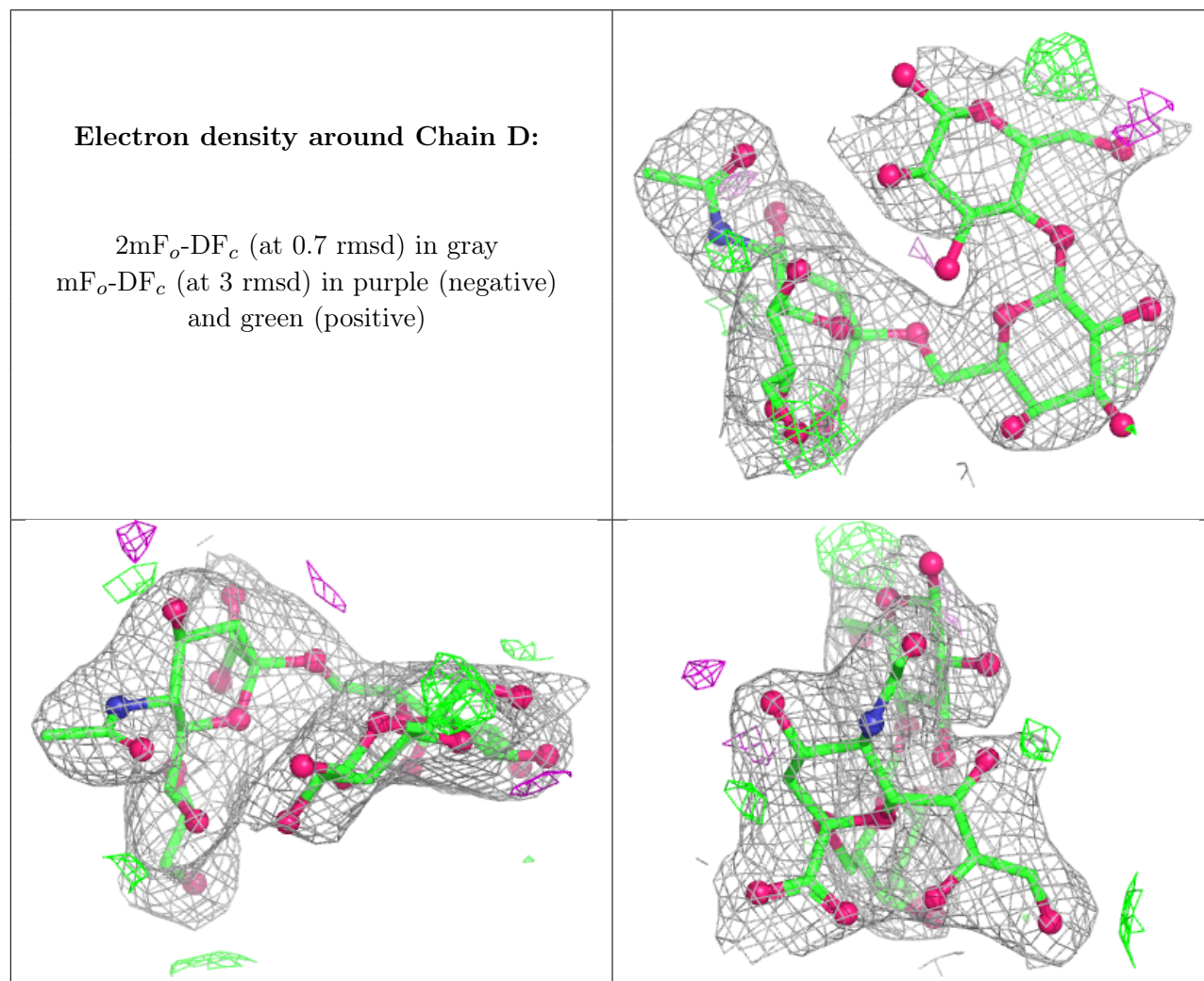
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	D	1	12/12	0.80	0.15	98,116,122,125	0
2	GAL	D	2	11/12	0.92	0.09	65,79,84,86	4
2	BGC	E	1	12/12	0.94	0.06	63,75,91,93	0
2	SIA	E	3	20/21	0.95	0.07	30,57,65,65	0
2	GAL	E	2	11/12	0.96	0.06	38,48,52,53	3

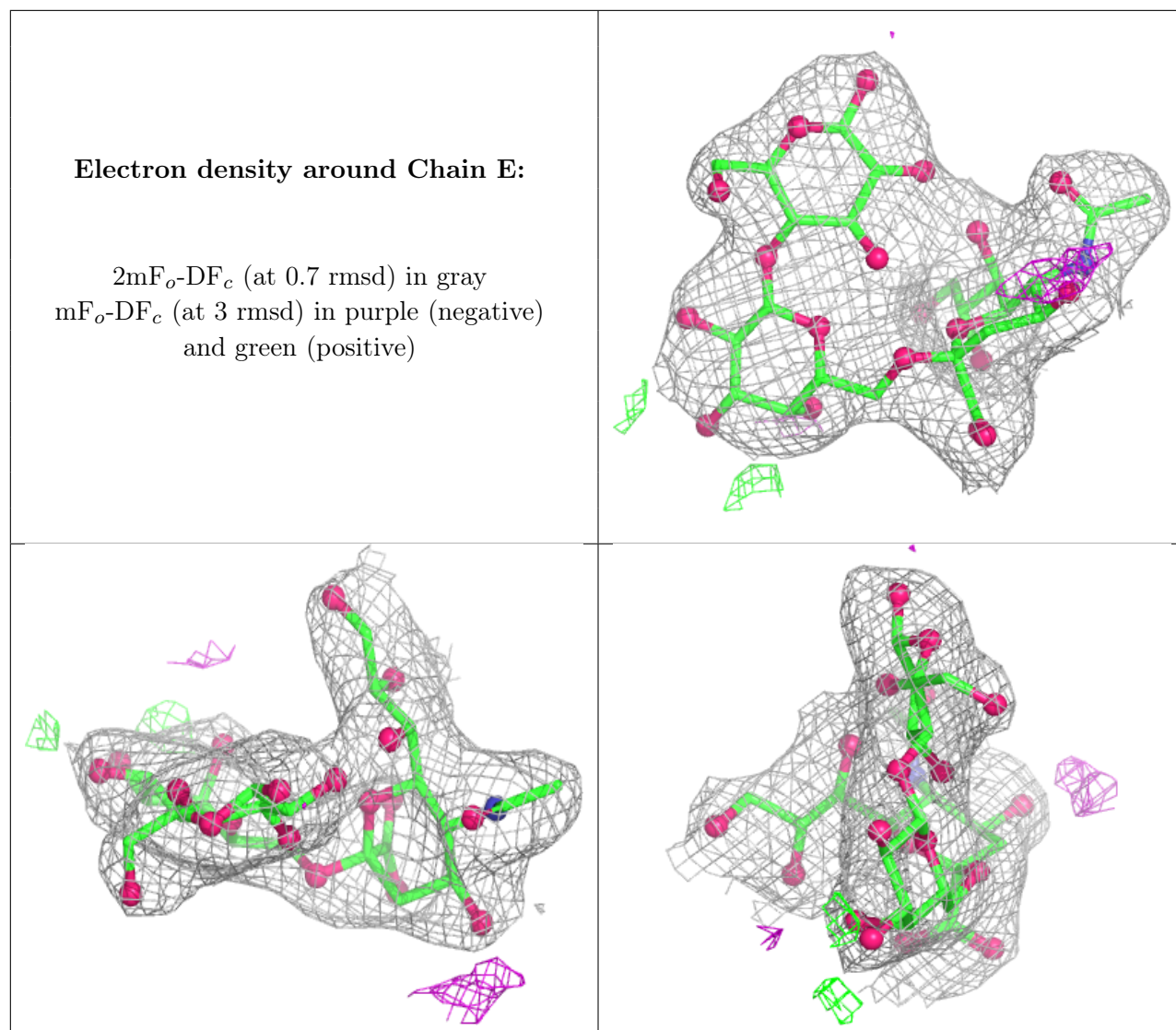
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SIA	D	3	20/21	0.97	0.05	30,48,61,67	0

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.





6.4 Ligands ⓘ

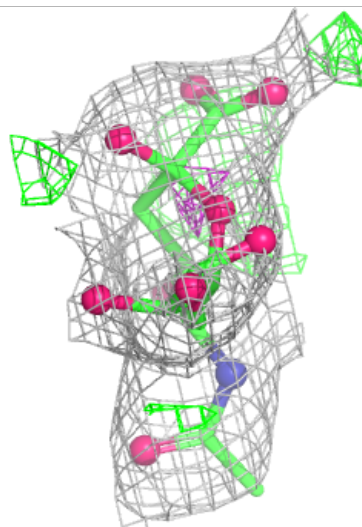
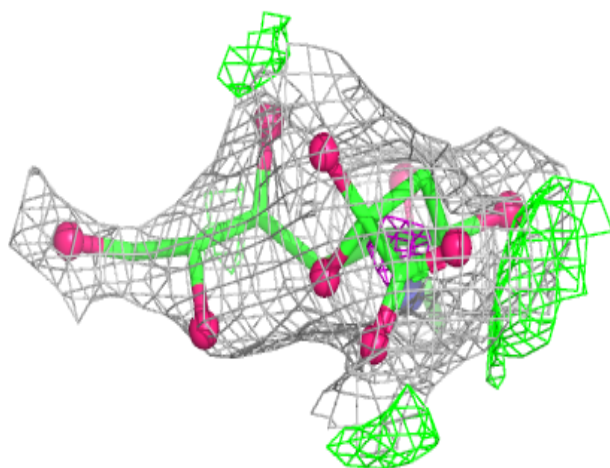
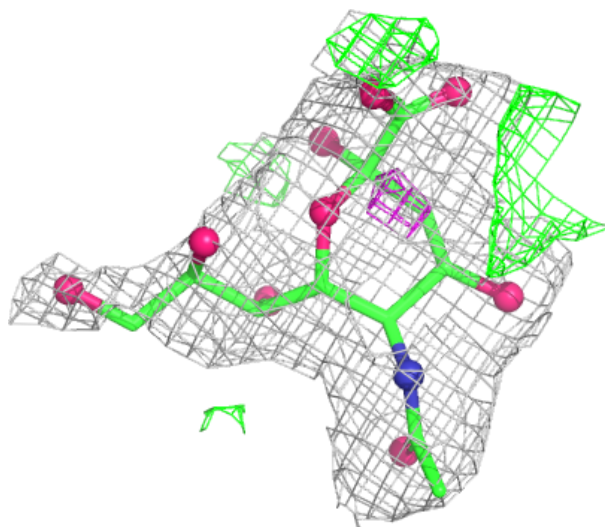
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	SIA	B	1	21/21	0.86	0.13	60,92,99,100	0

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

Electron density around SIA B 1:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.