



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2025 – 01:53 am GMT

PDB ID : 9FXT
Title : L2A5 Fab in complex with STn-Ser
Authors : Laugier, M.E.; Ereno Orbea, J.; Jimenez Barbero, J.; Oyenarte, I.
Deposited on : 2024-07-02
Resolution : 2.30 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:

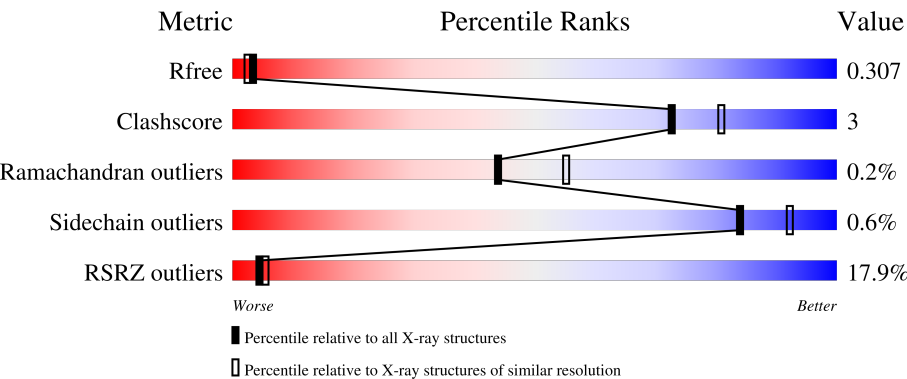
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	H	216	
1	I	216	
2	K	127	
2	V	127	
3	L	215	

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Mol	Chain	Length	Quality of chain
3	M	215	<div><div></div><div>27%</div><div></div><div>84%</div><div></div><div>11%</div><div></div><div>5%</div></div>
4	B	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
4	C	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8110 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 L2A5 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	198	Total	C	N	O	S	0	0	0
			1503	952	251	295	5			
1	I	216	Total	C	N	O	S	0	0	0
			1634	1030	271	327	6			

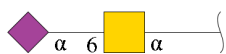
- Molecule 2 is a protein called Anti kappa Variable Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	120	Total	C	N	O	S	0	0	0
			718	438	135	143	2			
2	V	119	Total	C	N	O	S	0	0	0
			712	435	134	141	2			

- Molecule 3 is a protein called L2A5 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1628	1018	269	333	8			
3	M	204	Total	C	N	O	S	0	0	0
			1554	973	259	314	8			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



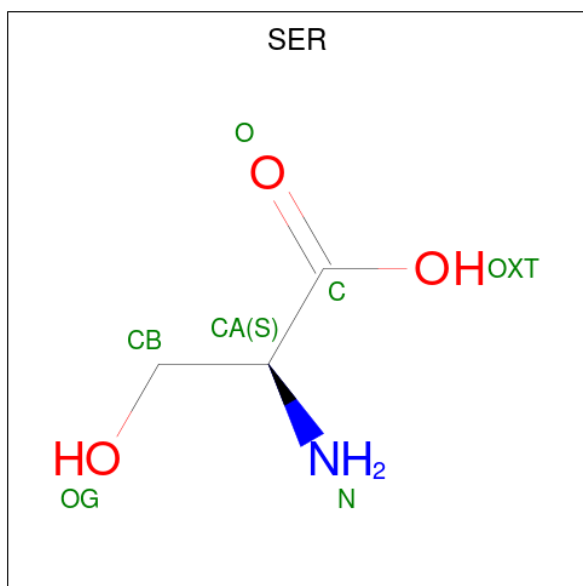
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	2	Total	C	N	O	0	0	0
			34	19	2	13			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			34	19	2	13			

- Molecule 5 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			7	3	1	3		
5	I	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	M	1	Total	C	O	0	0
			6	3	3		
6	V	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



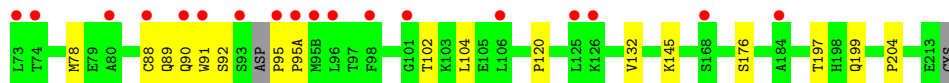
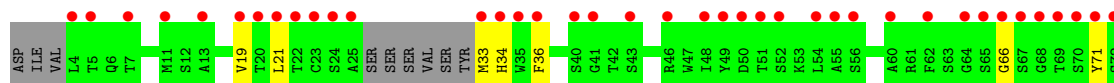
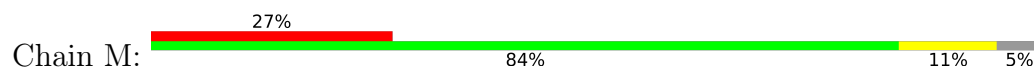
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			7	4	3		
7	I	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	35	Total	O	0	0
			35	35		
8	I	62	Total	O	0	0
			62	62		
8	K	10	Total	O	0	0
			10	10		
8	L	57	Total	O	0	0
			57	57		
8	M	38	Total	O	0	0
			38	38		
8	V	15	Total	O	0	0
			15	15		



• Molecule 3: L2A5 Fab Light Chain



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-alpha-D-galactopyranoside



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-2-acetamido-2-deoxy-alpha-D-galactopyranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.35Å 125.28Å 190.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.69 – 2.30 47.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.69-2.30) 99.7 (47.69-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5109: ???)	Depositor
R, R_{free}	0.261 , 0.312 0.260 , 0.307	Depositor DCC
R_{free} test set	2649 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8110	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: SIA, GOL, PEG, A2G

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	H	0.25	0/1537	0.51	0/2091
1	I	0.26	0/1675	0.53	0/2285
2	K	0.22	0/342	0.53	0/425
2	V	0.22	0/336	0.52	0/417
3	L	0.25	0/1665	0.50	0/2261
3	M	0.26	0/1588	0.52	0/2151
All	All	0.25	0/7143	0.51	0/9630

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	94	ASP	Peptide

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	H	1503	0	1468	9	0
1	I	1634	0	1593	6	0
2	K	718	0	414	5	0
2	V	712	0	410	3	0
3	L	1628	0	1576	10	0
3	M	1554	0	1506	16	0
4	B	34	0	28	1	0
4	C	34	0	28	0	0
5	H	7	0	3	0	0
5	I	7	0	3	0	0
6	H	6	0	8	0	0
6	I	18	0	24	0	0
6	L	12	0	16	2	0
6	M	6	0	8	1	0
6	V	6	0	8	0	0
7	H	7	0	10	1	0
7	I	7	0	10	1	0
8	H	35	0	0	0	0
8	I	62	0	0	1	0
8	K	10	0	0	0	0
8	L	57	0	0	1	0
8	M	38	0	0	0	0
8	V	15	0	0	0	0
All	All	8110	0	7113	47	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 3.

All (47) 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)
3:L:142:ARG:HH12	6:L:302:GOL:H32	1.61	0.65
3:M:36:PHE:HE1	3:M:89:GLN:HB3	1.61	0.65
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.82	0.61
1:I:81:LYS:NZ	8:I:404:HOH:O	2.35	0.60
1:I:82(B):SER:O	1:I:82(B):SER:OG	2.17	0.59
3:M:78:MET:HE1	3:M:104:LEU:HD21	1.85	0.58
1:H:59:TYR:HH	1:H:69:ILE:N	2.03	0.55
1:H:52:ASN:O	1:H:71:ARG:NH1	2.39	0.55
3:L:210:ASN:ND2	8:L:401:HOH:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:21:LEU:HD22	3:L:102:THR:HG21	1.90	0.54
1:I:87:THR:HG22	7:I:305:PEG:H32	1.90	0.53
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.91	0.52
3:L:66:GLY:HA3	3:L:71:TYR:HA	1.91	0.51
3:L:142:ARG:NH1	6:L:302:GOL:H32	2.22	0.51
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.92	0.51
3:M:78:MET:HE1	3:M:104:LEU:HD11	1.92	0.51
2:K:13:UNK:HA	2:K:120:THR:HG23	1.93	0.50
1:I:35(A):ASN:OD1	4:B:2:SIA:H111	2.13	0.49
3:M:145:LYS:HB3	3:M:197:THR:OG1	2.13	0.48
3:M:120:PRO:HD3	3:M:132:VAL:HG22	1.95	0.48
1:H:7:SER:OG	1:H:21:THR:OG1	2.32	0.48
2:K:41:GLN:HB2	2:K:47:ARG:HG2	1.96	0.48
1:H:197:ASN:ND2	1:H:208:ASP:OD1	2.39	0.47
3:M:66:GLY:HA3	3:M:71:TYR:HA	1.97	0.47
3:M:90:GLN:HG2	3:M:91:TRP:N	2.29	0.47
1:H:87:THR:HG23	1:H:110:THR:HA	1.98	0.46
3:M:21:LEU:HD23	3:M:102:THR:HB	1.97	0.46
3:L:106:LEU:O	3:L:166:GLN:NE2	2.45	0.46
1:H:51:ILE:HD13	1:H:71:ARG:HB3	1.98	0.46
2:K:9:SER:HA	2:K:117:THR:HG21	1.96	0.45
2:K:93:UNK:HA	2:K:119:VAL:O	2.16	0.45
3:L:123:GLU:O	3:L:126:LYS:HG2	2.17	0.45
1:H:114:ALA:HA	7:H:303:PEG:H22	1.98	0.45
1:I:65:ASP:OD2	1:I:66:ARG:HG2	2.18	0.44
3:M:33:MET:HB2	3:M:71:TYR:CD2	2.53	0.44
1:H:81:LYS:HE3	1:H:81:LYS:HB3	1.88	0.44
2:K:108:UNK:CB	3:M:199:GLN:HA	2.49	0.43
3:M:197:THR:HG22	3:M:204:PRO:HG3	2.03	0.41
3:M:90:GLN:NE2	3:M:92:SER:OG	2.54	0.41
3:M:176:SER:OG	6:M:301:GOL:H11	2.21	0.41
3:M:34:HIS:O	3:M:88:CYS:HA	2.21	0.41
3:M:19:VAL:HG21	3:M:78:MET:HE3	2.03	0.41
2:V:14:VAL:HB	2:V:121:VAL:HG22	2.03	0.41
3:L:125:LEU:O	3:L:183:LYS:HD3	2.21	0.40
3:M:95:PRO:HA	3:M:95(A):PRO:HD2	1.92	0.40
2:V:93:UNK:HA	2:V:119:VAL:O	2.21	0.40
3:L:199:GLN:HA	2:V:108:UNK:CB	2.51	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	H	186/216 (86%)	180 (97%)	6 (3%)	0	100	100
1	I	214/216 (99%)	207 (97%)	6 (3%)	1 (0%)	25	32
2	K	47/127 (37%)	46 (98%)	1 (2%)	0	100	100
2	V	46/127 (36%)	45 (98%)	1 (2%)	0	100	100
3	L	212/215 (99%)	205 (97%)	6 (3%)	1 (0%)	25	32
3	M	198/215 (92%)	192 (97%)	6 (3%)	0	100	100
All	All	903/1116 (81%)	875 (97%)	26 (3%)	2 (0%)	44	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	95	PRO
1	I	95	GLY

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	H	173/189 (92%)	170 (98%)	3 (2%)	56	72
1	I	189/189 (100%)	188 (100%)	1 (0%)	86	93
2	K	38/45 (84%)	38 (100%)	0	100	100
2	V	37/45 (82%)	37 (100%)	0	100	100
3	L	185/186 (100%)	184 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	175/186 (94%)	175 (100%)	0	100	100
All	All	797/840 (95%)	792 (99%)	5 (1%)	84	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	29	ILE
1	H	44	LYS
1	H	65	ASP
1	I	82(B)	SER
3	L	145	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	82(A)	ASN
1	H	105	GLN
1	I	5	GLN
1	I	105	GLN
3	M	34	HIS
3	M	90	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 ⓘ

4 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	$\# Z > 2$
4	A2G	B	1	4,5	14,14,15	0.38	0	17,19,21	0.40	0
4	SIA	B	2	4	20,20,21	0.83	1 (5%)	24,28,31	1.08	3 (12%)
4	A2G	C	1	4,5	14,14,15	0.34	0	17,19,21	0.44	0
4	SIA	C	2	4	20,20,21	0.78	1 (5%)	24,28,31	1.03	3 (12%)

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
4	A2G	B	1	4,5	-	1/6/23/26	0/1/1/1
4	SIA	B	2	4	-	0/18/34/38	0/1/1/1
4	A2G	C	1	4,5	-	2/6/23/26	0/1/1/1
4	SIA	C	2	4	-	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)
4	B	2	SIA	C2-C1	2.62	1.54	1.52
4	C	2	SIA	C2-C1	2.54	1.54	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	SIA	O1A-C1-C2	-2.90	115.73	122.57
4	C	2	SIA	O1A-C1-C2	-2.82	115.91	122.57
4	C	2	SIA	C6-O6-C2	2.66	117.02	111.34
4	B	2	SIA	C6-O6-C2	2.60	116.90	111.34
4	B	2	SIA	C3-C4-C5	-2.39	108.57	111.46
4	C	2	SIA	C3-C4-C5	-2.26	108.73	111.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	A2G	C4-C5-C6-O6
4	B	1	A2G	C4-C5-C6-O6

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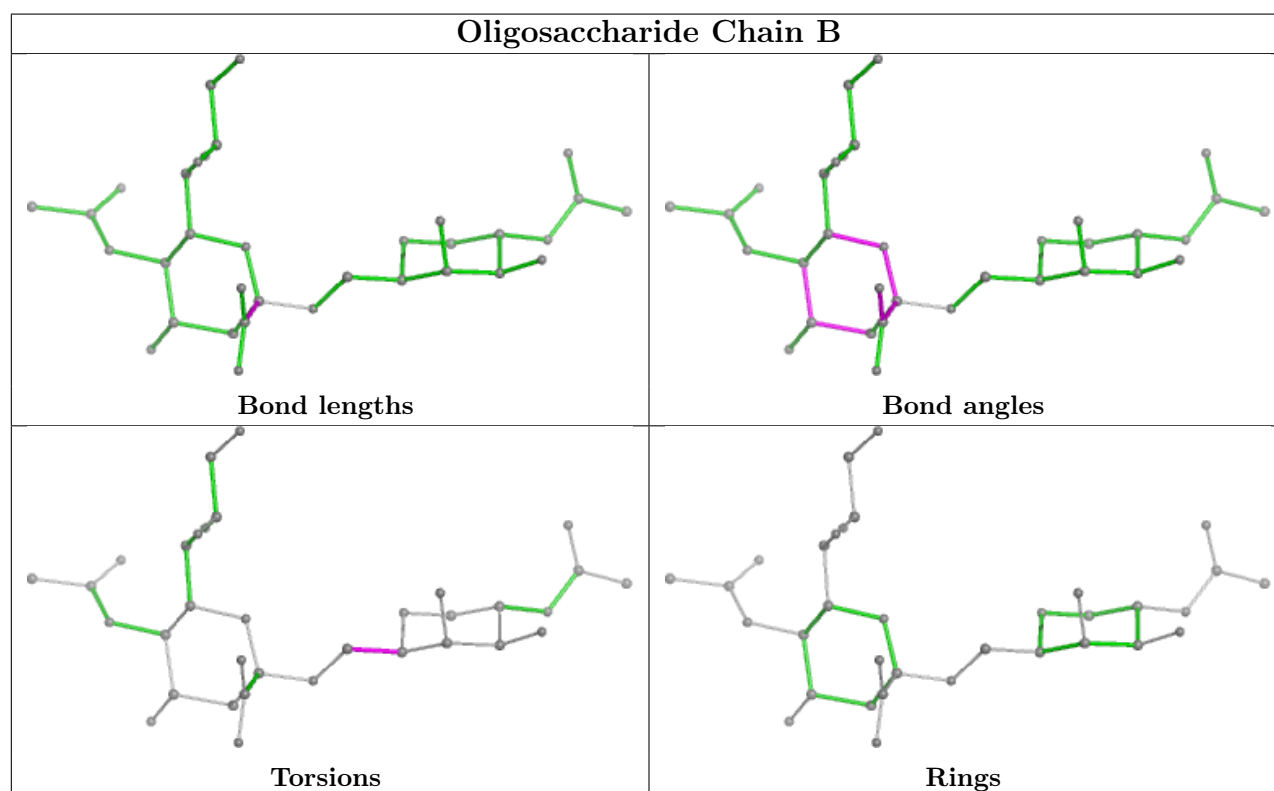
Mol	Chain	Res	Type	Atoms
4	C	1	A2G	O5-C5-C6-O6

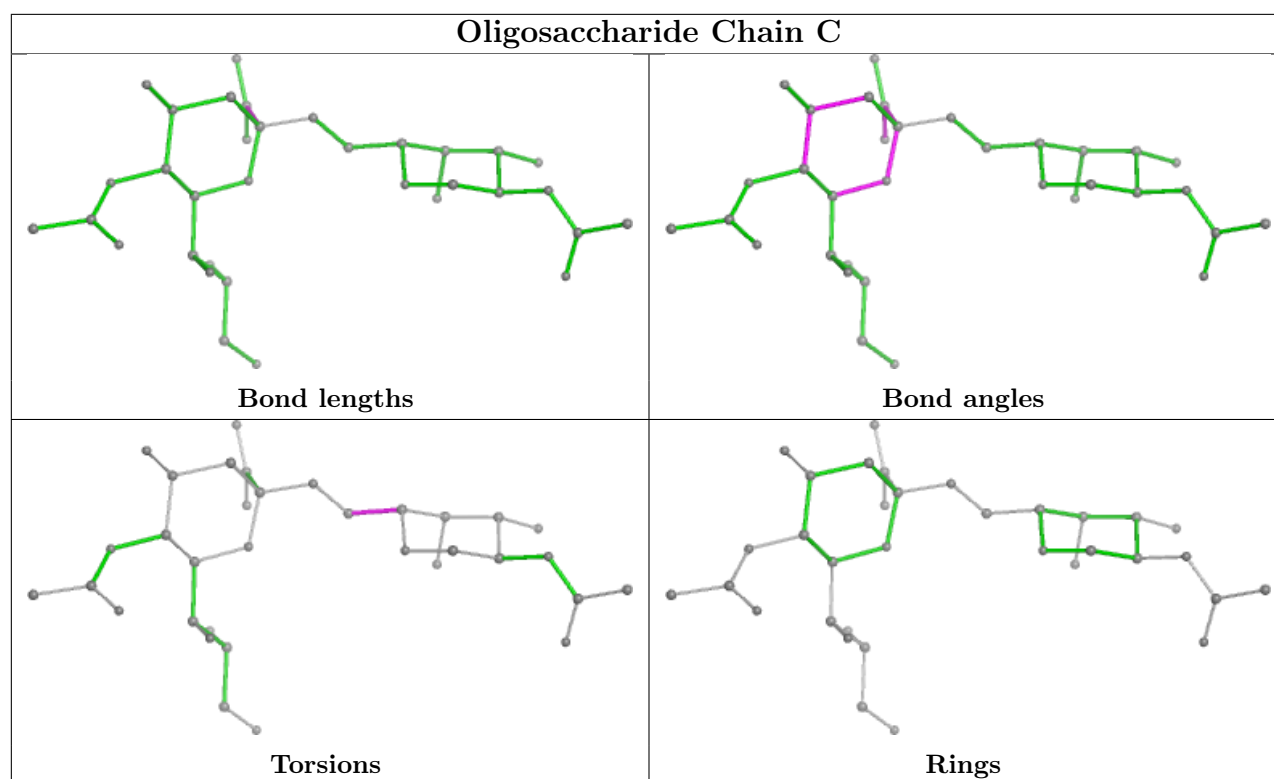
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	SIA	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 [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PEG	I	305	-	6,6,6	0.24	0	5,5,5	0.26	0
6	GOL	M	301	-	5,5,5	0.33	0	5,5,5	0.40	0
6	GOL	H	302	-	5,5,5	0.33	0	5,5,5	0.38	0
5	SER	H	301	4	5,6,6	0.94	0	5,7,7	1.17	0
7	PEG	H	303	-	6,6,6	0.25	0	5,5,5	0.27	0
6	GOL	L	301	-	5,5,5	0.35	0	5,5,5	0.43	0
6	GOL	I	304	-	5,5,5	0.36	0	5,5,5	0.38	0
5	SER	I	301	4	5,6,6	0.95	0	5,7,7	1.15	0
6	GOL	L	302	-	5,5,5	0.35	0	5,5,5	0.40	0
6	GOL	V	201	-	5,5,5	0.35	0	5,5,5	0.37	0
6	GOL	I	302	-	5,5,5	0.35	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	I	303	-	5,5,5	0.36	0	5,5,5	0.38	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
7	PEG	I	305	-	-	3/4/4/4	-
6	GOL	M	301	-	-	0/4/4/4	-
6	GOL	H	302	-	-	0/4/4/4	-
5	SER	H	301	4	-	2/6/6/6	-
7	PEG	H	303	-	-	2/4/4/4	-
6	GOL	L	301	-	-	0/4/4/4	-
6	GOL	I	304	-	-	2/4/4/4	-
5	SER	I	301	4	-	2/6/6/6	-
6	GOL	L	302	-	-	0/4/4/4	-
6	GOL	V	201	-	-	0/4/4/4	-
6	GOL	I	302	-	-	0/4/4/4	-
6	GOL	I	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	303	GOL	C1-C2-C3-O3
6	I	304	GOL	O1-C1-C2-C3
7	I	305	PEG	O1-C1-C2-O2
7	I	305	PEG	O2-C3-C4-O4
6	I	303	GOL	O2-C2-C3-O3
6	I	304	GOL	O1-C1-C2-O2
5	H	301	SER	O-C-CA-N
5	I	301	SER	O-C-CA-N
7	I	305	PEG	C4-C3-O2-C2
7	H	303	PEG	O1-C1-C2-O2
7	H	303	PEG	C1-C2-O2-C3
5	H	301	SER	OXT-C-CA-N
5	I	301	SER	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	305	PEG	1	0
6	M	301	GOL	1	0
7	H	303	PEG	1	0
6	L	302	GOL	2	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

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	H	198/216 (91%)	1.47	61 (30%) 1 1	32, 57, 92, 101	0
1	I	216/216 (100%)	0.58	12 (5%) 31 33	32, 41, 55, 76	0
2	K	48/127 (37%)	1.32	9 (18%) 4 5	38, 53, 72, 77	0
2	V	47/127 (37%)	1.35	11 (23%) 2 3	39, 53, 70, 78	0
3	L	214/215 (99%)	0.67	16 (7%) 22 23	28, 44, 61, 81	0
3	M	204/215 (94%)	1.23	57 (27%) 2 2	31, 52, 85, 92	0
All	All	927/1116 (83%)	1.01	166 (17%) 4 5	28, 47, 82, 101	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	95	GLY	7.1
1	H	30	THR	5.5
3	M	95	PRO	4.9
1	H	78	PHE	4.8
1	H	76	ASN	4.8
1	H	35	TRP	4.8
1	H	24	VAL	4.7
3	M	69	THR	4.5
1	H	29	ILE	4.4
3	M	91	TRP	4.4
1	H	63	LEU	4.4
1	H	93	ALA	4.2
1	H	2	VAL	4.2
1	H	69	ILE	4.0
1	H	34	TYR	3.9
3	M	7	THR	3.9
1	H	64	LYS	3.8
2	V	14	VAL	3.8
1	H	61	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	52	ASN	3.8
1	H	28	SER	3.7
3	L	94	ASP	3.7
3	M	96	LEU	3.7
1	H	26	GLY	3.6
1	H	79	PHE	3.6
3	M	4	LEU	3.6
3	M	25	ALA	3.6
1	H	128	SER	3.4
3	L	95	PRO	3.4
1	H	105	GLN	3.4
1	I	215	SER	3.4
1	H	4	LEU	3.4
1	H	36	TRP	3.4
3	M	36	PHE	3.3
1	H	96	GLY	3.3
1	I	133	GLY	3.3
1	H	94	ARG	3.2
1	H	191	THR	3.2
1	H	27	TYR	3.2
2	V	4	VAL	3.2
3	M	93	SER	3.2
1	H	35(A)	ASN	3.1
3	L	1	ASP	3.1
1	H	51	ILE	3.1
3	M	68	GLY	3.1
3	M	95(A)	PRO	3.1
1	H	73	THR	3.1
2	V	20	LEU	3.0
1	H	62	SER	3.0
1	H	22	CYS	3.0
3	M	71	TYR	3.0
3	L	75	ILE	3.0
1	H	187	SER	3.0
1	H	77	GLN	3.0
1	H	70	THR	2.9
2	K	15	GLN	2.9
3	M	56	SER	2.9
3	M	72	SER	2.9
3	M	19	VAL	2.9
3	M	101	GLY	2.9
1	H	82	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	M	106	LEU	2.9
3	M	55	ALA	2.9
3	M	98	PHE	2.8
3	M	54	LEU	2.8
1	H	23	SER	2.8
3	L	154	LEU	2.8
1	H	47	TRP	2.8
2	K	120	THR	2.8
3	M	35	TRP	2.8
3	M	51	THR	2.8
2	K	5	GLN	2.8
2	V	19	SER	2.7
1	I	1	GLU	2.7
3	M	95(B)	MET	2.7
2	V	43	PRO	2.7
3	M	88	CYS	2.7
3	L	24	SER	2.7
3	M	34	HIS	2.7
3	M	90	GLN	2.7
3	M	33	MET	2.7
1	H	49	GLY	2.7
1	H	21	THR	2.7
1	H	82(A)	ASN	2.6
1	H	102	TYR	2.6
2	K	122	SER	2.6
3	M	5	THR	2.6
3	M	20	THR	2.6
1	I	65	ASP	2.6
1	H	59	TYR	2.5
3	L	188	LYS	2.5
2	V	6	LEU	2.5
1	H	214	LYS	2.5
3	M	60	ALA	2.5
3	M	49	TYR	2.5
3	M	50	ASP	2.5
3	M	64	GLY	2.5
3	M	73	LEU	2.5
3	M	46	ARG	2.5
1	H	67	ILE	2.4
3	M	48	ILE	2.4
1	H	48	MET	2.4
1	I	28	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	M	24	SER	2.4
3	M	70	SER	2.4
1	H	7	SER	2.4
2	K	20	LEU	2.3
2	K	14	VAL	2.3
3	M	23	CYS	2.3
1	I	206	LYS	2.3
1	H	15	SER	2.3
3	M	43	SER	2.3
3	M	126	LYS	2.3
3	M	65	SER	2.3
1	H	162	GLY	2.3
1	I	82	LEU	2.3
1	H	189	LEU	2.2
3	M	62	PHE	2.2
1	H	92	CYS	2.2
1	I	216	CYS	2.2
1	H	72	ASP	2.2
3	L	56	SER	2.2
1	H	9	PRO	2.2
3	M	13	ALA	2.2
2	K	119	VAL	2.2
1	H	82(B)	SER	2.2
2	V	48	GLU	2.2
3	L	76	SER	2.1
1	H	190	GLY	2.1
3	L	2	ILE	2.1
3	M	66	GLY	2.1
2	V	5	GLN	2.1
1	H	75	LYS	2.1
3	M	74	THR	2.1
3	L	58	VAL	2.1
1	H	65	ASP	2.1
1	I	49	GLY	2.1
2	V	17	GLY	2.1
1	I	195	ILE	2.1
1	H	16	GLN	2.1
3	L	65	SER	2.1
3	L	77	SER	2.1
3	M	40	SER	2.1
3	M	22	THR	2.1
3	M	184	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	90	TYR	2.1
3	M	67	SER	2.1
3	M	11	MET	2.1
1	H	133	GLY	2.0
2	K	44	GLY	2.0
3	L	212	GLY	2.0
3	M	41	GLY	2.0
3	L	93	SER	2.0
3	M	52	SER	2.0
2	K	43	PRO	2.0
3	M	21	LEU	2.0
3	M	125	LEU	2.0
3	L	5	THR	2.0
3	M	80	ALA	2.0
1	H	19	SER	2.0
1	I	62	SER	2.0
1	I	132	SER	2.0
3	M	168	SER	2.0
1	H	3	GLN	2.0
2	V	15	GLN	2.0
2	V	88	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SER	H	301	7/7	0.39	0.20	86,87,88,91	0
6	GOL	H	302	6/6	0.55	0.22	72,73,77,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	L	301	6/6	0.58	0.27	47,51,59,63	0
6	GOL	I	303	6/6	0.71	0.24	47,49,54,61	0
7	PEG	I	305	7/7	0.72	0.28	40,42,53,54	0
5	SER	I	301	7/7	0.75	0.13	52,54,56,60	0
6	GOL	L	302	6/6	0.76	0.20	43,48,49,55	0
7	PEG	H	303	7/7	0.82	0.15	48,48,56,61	0
6	GOL	M	301	6/6	0.83	0.22	33,39,40,42	0
6	GOL	I	304	6/6	0.84	0.13	44,47,54,55	0
6	GOL	I	302	6/6	0.85	0.16	36,45,49,53	0
6	GOL	V	201	6/6	0.85	0.18	51,56,62,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.