wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 10:03 AM EDT

PDB ID	:	1PTO
Title	:	THE STRUCTURE OF A PERTUSSIS TOXIN-SUGAR COMPLEX AS A MODEL FOR RECEPTOR BINDING
Authors	:	Stein, P.E.; Read, R.J.
Deposited on	:	1994-03-22
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

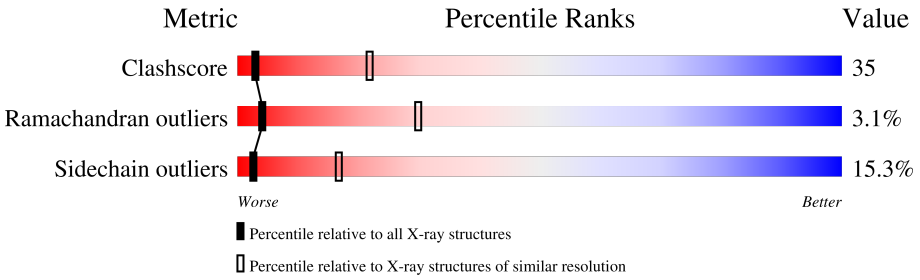
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	244	41% 44% 7% 8%
1	G	244	43% 43% 6% 8%
2	B	196	40% 48% 12%
3	C	196	39% 49% 11% .
3	I	196	37% 51% 12% .
4	D	110	46% 48% 5% .
4	E	110	51% 39% 10%
4	J	110	42% 55% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	K	110	51% 38% 11%
5	F	98	34% 46% 19%
5	L	98	46% 39% 15%
6	H	198	42% 45% 12%
7	M	2	50% 50%
7	N	2	50% 50%
7	O	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14614 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 PERTUSSIS TOXIN (SUBUNIT S1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1769	1095	318	350	6			
1	G	224	Total	C	N	O	S	0	0	0
			1769	1095	318	350	6			

- Molecule 2 is a protein called PERTUSSIS TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1522	961	260	292	9			

- Molecule 3 is a protein called PERTUSSIS TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	0	0	0
			1521	969	258	285	9			
3	I	196	Total	C	N	O	S	0	0	0
			1521	969	258	285	9			

- Molecule 4 is a protein called PERTUSSIS TOXIN (SUBUNIT S4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	E	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	J	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	K	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			

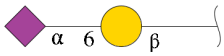
- Molecule 5 is a protein called PERTUSSIS TOXIN (SUBUNIT S5).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			
5	L	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			

- Molecule 6 is a protein called PERTUSSIS TOXIN (SUBUNIT S2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	198	Total	C	N	O	S	7	0	0
			1536	970	262	295	9			

- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	2	Total	C	N	O	0	0	0
			32	17	1	14			
7	N	2	Total	C	N	O	0	0	0
			32	17	1	14			
7	O	2	Total	C	N	O	0	0	0
			32	17	1	14			

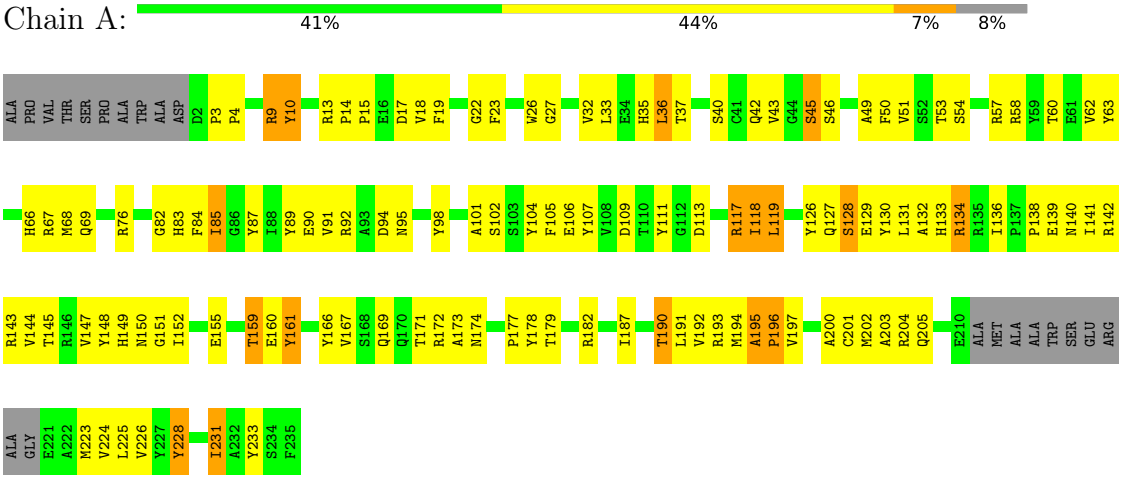
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

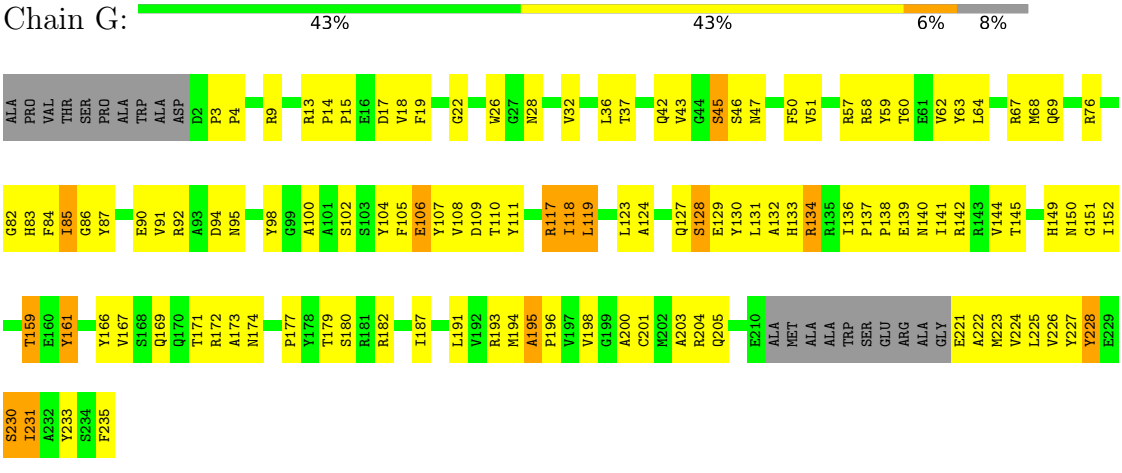
• Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)

Chain A:



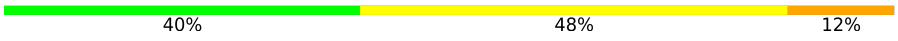
• Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)

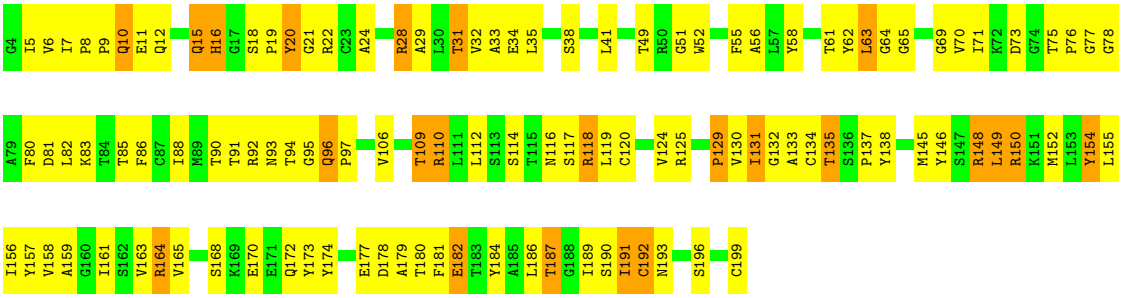
Chain G:



• Molecule 2: PERTUSSIS TOXIN

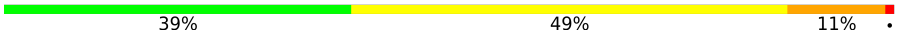
Chain B:

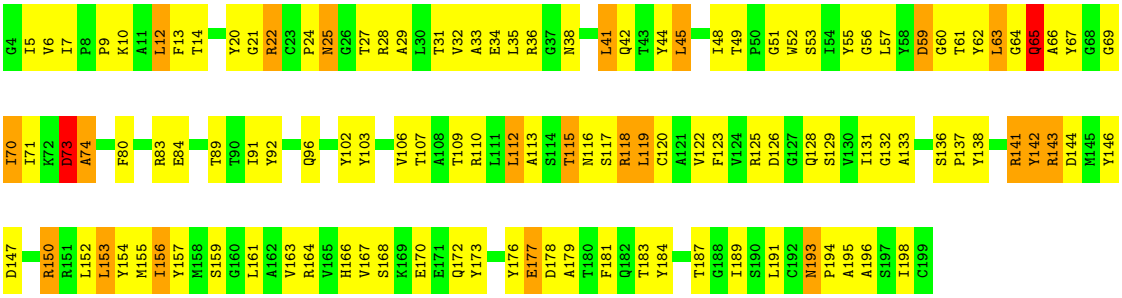




• Molecule 3: PERTUSSIS TOXIN

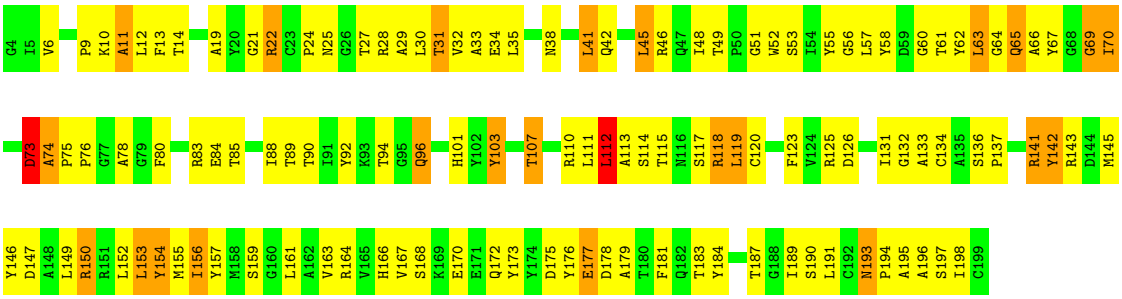
Chain C:





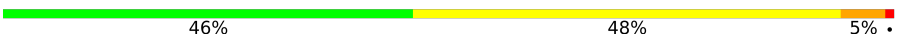
• Molecule 3: PERTUSSIS TOXIN

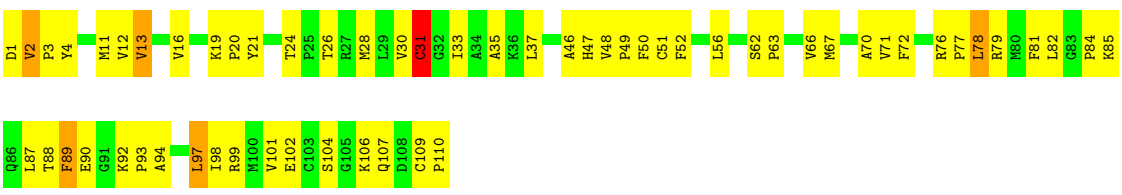
Chain I:



• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain D:



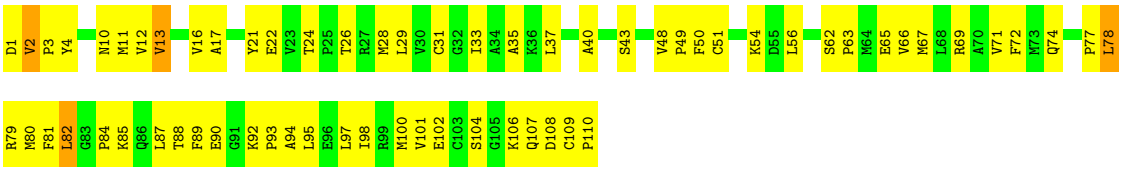


• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain E:

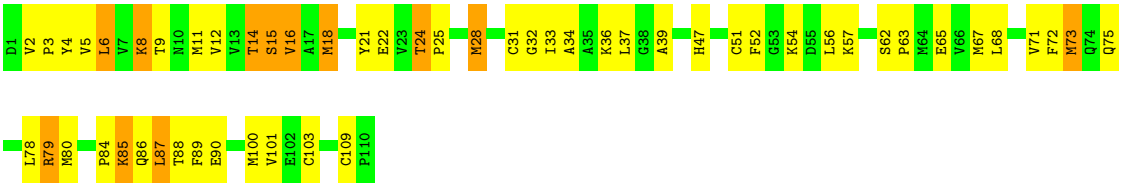
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain J:



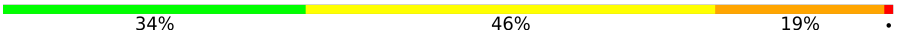
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

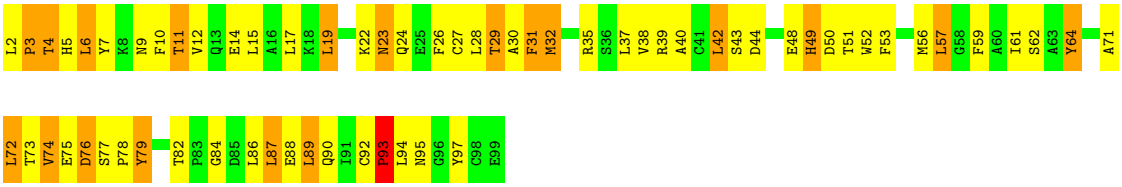
Chain K:



• Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)

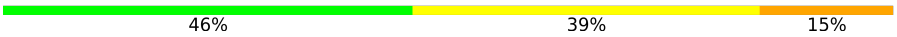
Chain F:

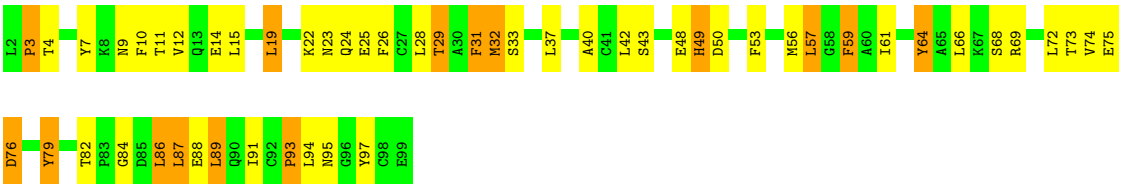




• Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)

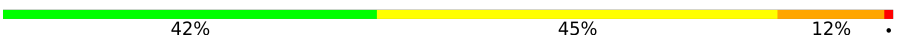
Chain L:

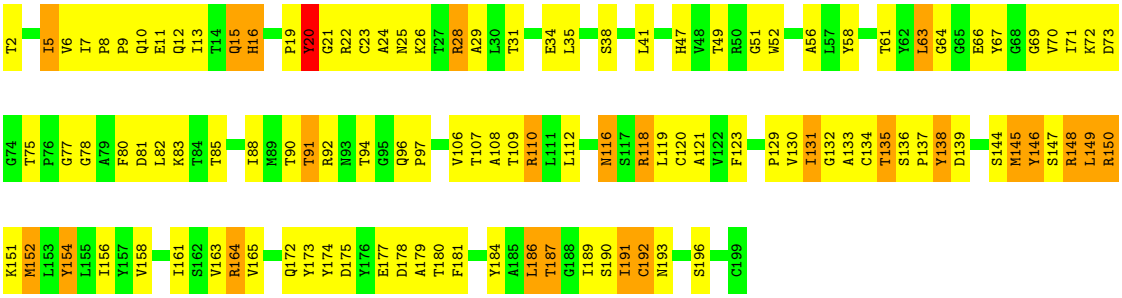




• Molecule 6: PERTUSSIS TOXIN (SUBUNIT S2)

Chain H:





• Molecule 7: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain M:

• Molecule 7: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain N:

• Molecule 7: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain O:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	163.80Å 98.20Å 194.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14614	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, 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	A	0.73	0/1809	0.85	1/2457 (0.0%)
1	G	0.53	0/1809	0.75	0/2457
2	B	0.75	0/1558	0.94	1/2115 (0.0%)
3	C	0.78	0/1557	0.90	1/2115 (0.0%)
3	I	0.69	0/1557	0.89	3/2115 (0.1%)
4	D	0.74	0/856	0.97	1/1155 (0.1%)
4	E	0.79	0/856	0.90	0/1155
4	J	0.67	0/856	0.92	1/1155 (0.1%)
4	K	0.62	0/856	0.87	1/1155 (0.1%)
5	F	0.74	0/782	0.94	1/1059 (0.1%)
5	L	0.62	0/782	0.86	0/1059
6	H	0.67	0/1573	0.92	2/2137 (0.1%)
All	All	0.70	0/14851	0.89	12/20134 (0.1%)

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
1	A	0	1
3	I	0	1
4	D	0	1
5	F	0	1
5	L	0	1
6	H	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	119	LEU	N-CA-C	-6.30	93.98	111.00
6	H	191	ILE	N-CA-C	-5.84	95.22	111.00
3	I	119	LEU	N-CA-C	-5.83	95.27	111.00
3	I	112	LEU	CA-CB-CG	5.63	128.25	115.30
4	D	31	CYS	CA-CB-SG	-5.47	104.16	114.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TYR	Sidechain
4	D	52	PHE	Sidechain
5	F	64	TYR	Sidechain
6	H	146	TYR	Sidechain
3	I	103	TYR	Sidechain

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	A	1769	0	1655	127	0
1	G	1769	0	1655	110	0
2	B	1522	0	1473	125	0
3	C	1521	0	1484	145	0
3	I	1521	0	1484	133	0
4	D	838	0	874	54	0
4	E	838	0	874	58	0
4	J	838	0	874	62	0
4	K	838	0	874	55	0
5	F	764	0	747	60	0
5	L	764	0	747	47	0
6	H	1536	0	1487	114	0
7	M	32	0	28	1	0
7	N	32	0	28	5	0
7	O	32	0	28	7	0
All	All	14614	0	14312	998	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 35.

The worst 5 of 998 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)
6:H:28:ARG:HH21	6:H:177:GLU:HA	1.22	1.01
2:B:28:ARG:HH21	2:B:177:GLU:HA	1.26	0.99
3:I:60:GLY:HA2	3:I:74:ALA:HB3	1.46	0.97
1:G:51:VAL:HB	1:G:132:ALA:HB3	1.51	0.93
2:B:163:VAL:HG21	2:B:189:ILE:HG22	1.52	0.91

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	220/244 (90%)	198 (90%)	17 (8%)	5 (2%)	6 36
1	G	220/244 (90%)	193 (88%)	21 (10%)	6 (3%)	5 33
2	B	194/196 (99%)	154 (79%)	30 (16%)	10 (5%)	2 18
3	C	194/196 (99%)	171 (88%)	17 (9%)	6 (3%)	4 30
3	I	194/196 (99%)	170 (88%)	19 (10%)	5 (3%)	5 33
4	D	108/110 (98%)	96 (89%)	10 (9%)	2 (2%)	8 40
4	E	108/110 (98%)	91 (84%)	15 (14%)	2 (2%)	8 40
4	J	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17 56
4	K	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	8 40
5	F	96/98 (98%)	84 (88%)	8 (8%)	4 (4%)	3 23
5	L	96/98 (98%)	84 (88%)	8 (8%)	4 (4%)	3 23
6	H	196/198 (99%)	159 (81%)	26 (13%)	11 (6%)	2 17
All	All	1842/1910 (96%)	1592 (86%)	192 (10%)	58 (3%)	4 30

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	ILE
2	B	94	THR
3	C	73	ASP
4	E	22	GLU
5	F	50	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/197 (94%)	166 (90%)	19 (10%)	7 32
1	G	185/197 (94%)	168 (91%)	17 (9%)	9 36
2	B	163/163 (100%)	136 (83%)	27 (17%)	2 13
3	C	155/155 (100%)	129 (83%)	26 (17%)	2 12
3	I	155/155 (100%)	129 (83%)	26 (17%)	2 12
4	D	94/94 (100%)	83 (88%)	11 (12%)	5 26
4	E	94/94 (100%)	81 (86%)	13 (14%)	3 20
4	J	94/94 (100%)	83 (88%)	11 (12%)	5 26
4	K	94/94 (100%)	81 (86%)	13 (14%)	3 20
5	F	83/83 (100%)	63 (76%)	20 (24%)	0 4
5	L	83/83 (100%)	62 (75%)	21 (25%)	0 3
6	H	165/165 (100%)	132 (80%)	33 (20%)	1 7
All	All	1550/1574 (98%)	1313 (85%)	237 (15%)	2 17

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	93	PRO
5	L	23	ASN
6	H	81	ASP
5	L	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	93	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	25	ASN
3	I	96	GLN
5	L	49	HIS
3	C	96	GLN
2	B	105	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
7	GAL	M	1	7	12,12,12	0.70	0	17,17,17	0.56	0
7	SIA	M	2	7	20,20,21	1.22	1 (5%)	24,28,31	1.12	2 (8%)
7	GAL	N	1	7	12,12,12	0.71	0	17,17,17	0.62	0
7	SIA	N	2	7	20,20,21	1.49	1 (5%)	24,28,31	1.25	5 (20%)
7	GAL	O	1	7	12,12,12	0.62	0	17,17,17	0.79	0
7	SIA	O	2	7	20,20,21	1.81	3 (15%)	24,28,31	1.30	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GAL	M	1	7	-	0/2/22/22	0/1/1/1
7	SIA	M	2	7	-	4/18/34/38	0/1/1/1
7	GAL	N	1	7	-	2/2/22/22	0/1/1/1
7	SIA	N	2	7	-	4/18/34/38	0/1/1/1
7	GAL	O	1	7	-	0/2/22/22	0/1/1/1
7	SIA	O	2	7	-	5/18/34/38	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	2	SIA	C2-C1	5.97	1.57	1.52
7	N	2	SIA	C2-C1	5.83	1.57	1.52
7	M	2	SIA	C2-C1	3.96	1.55	1.52
7	O	2	SIA	C4-C5	3.51	1.56	1.53
7	O	2	SIA	C7-C6	-2.12	1.50	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	2	SIA	C8-C7-C6	-4.35	104.78	113.03
7	M	2	SIA	C8-C7-C6	-3.75	105.91	113.03
7	N	2	SIA	C8-C7-C6	-2.61	108.08	113.03
7	N	2	SIA	C4-C3-C2	2.42	114.14	109.81
7	N	2	SIA	O6-C2-C3	-2.21	107.42	110.46

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	2	SIA	C7-C8-C9-O9
7	M	2	SIA	O8-C8-C9-O9
7	N	1	GAL	C4-C5-C6-O6
7	N	1	GAL	O5-C5-C6-O6
7	O	2	SIA	C6-C7-C8-C9

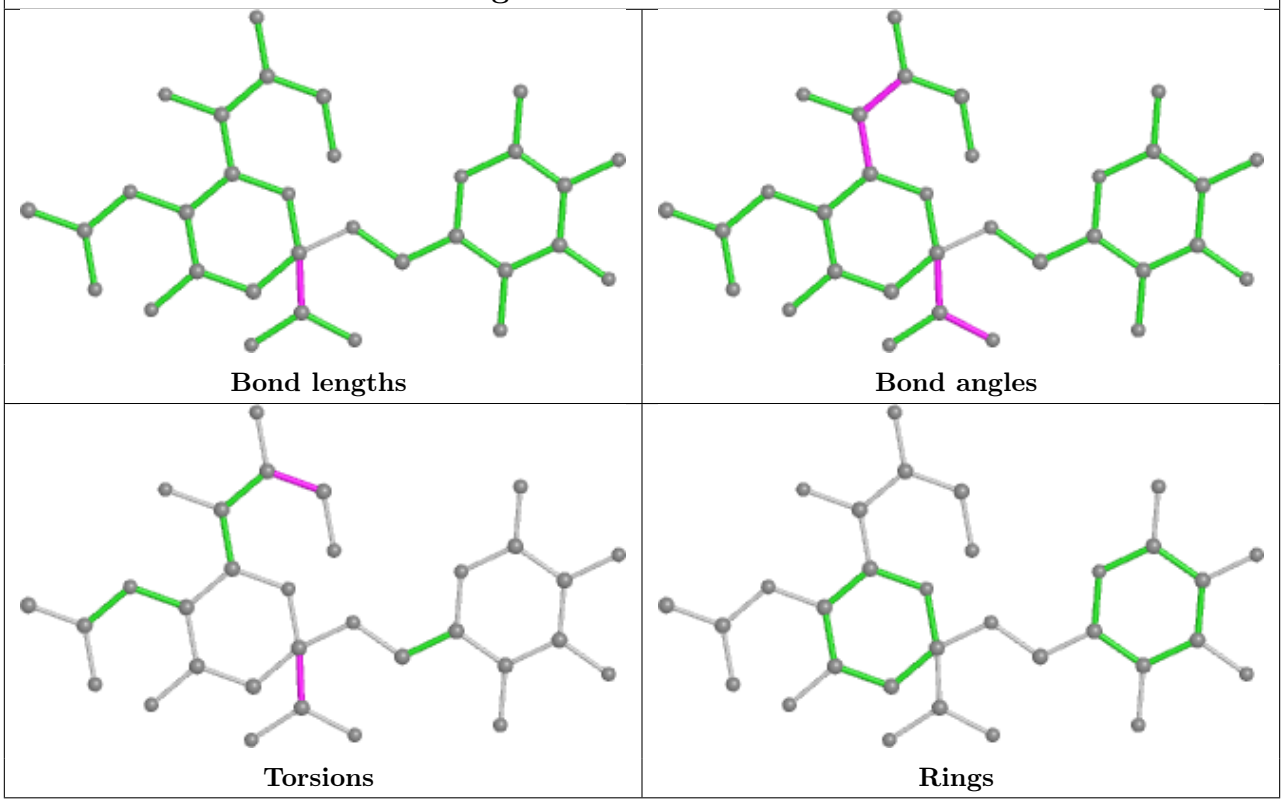
There are no ring outliers.

4 monomers are involved in 13 short contacts:

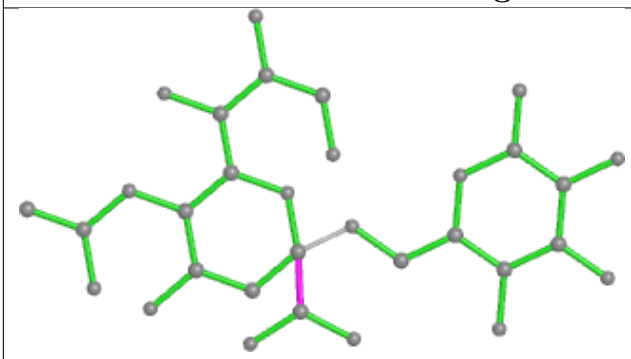
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	O	2	SIA	7	0
7	N	2	SIA	5	0
7	N	1	GAL	2	0
7	M	2	SIA	1	0

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

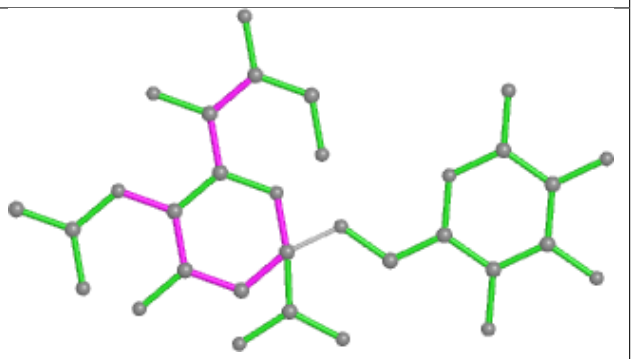
Oligosaccharide Chain M



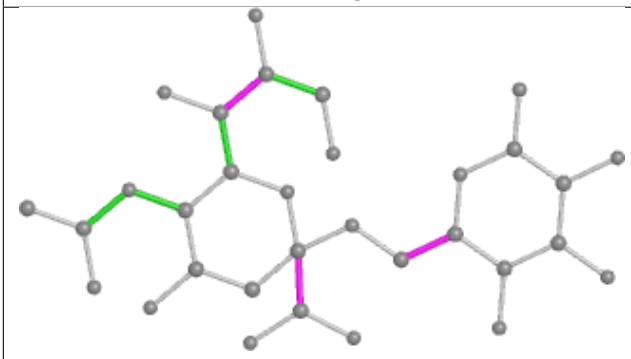
Oligosaccharide Chain N



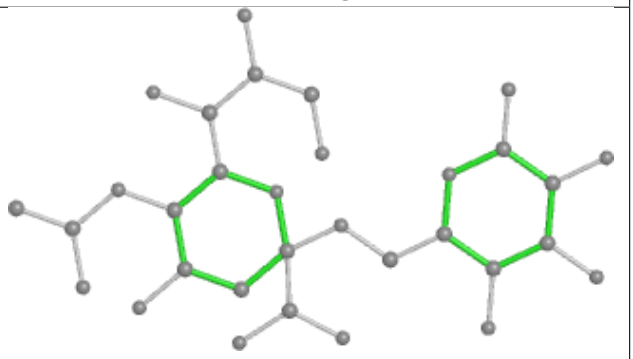
Bond lengths



Bond angles

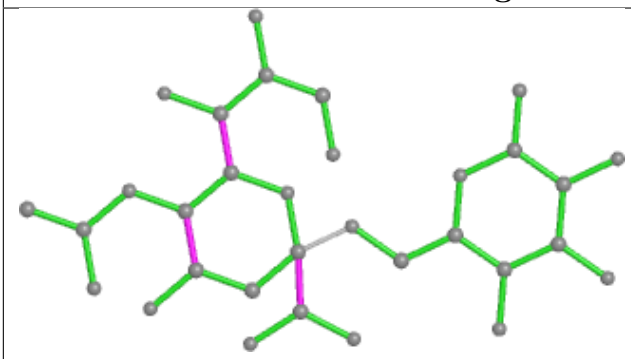


Torsions

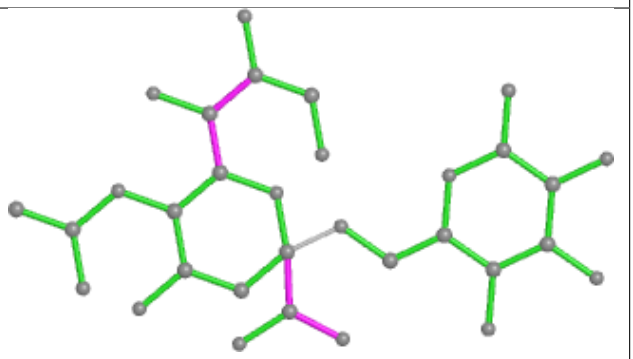


Rings

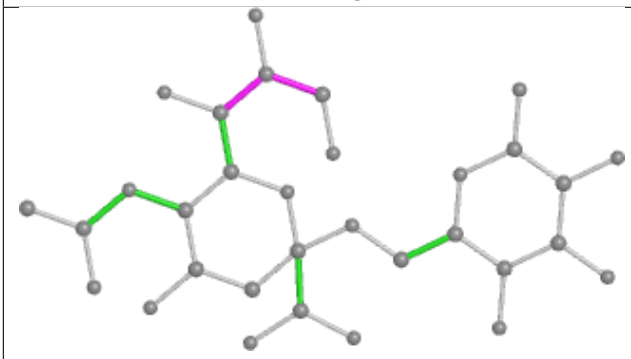
Oligosaccharide Chain O



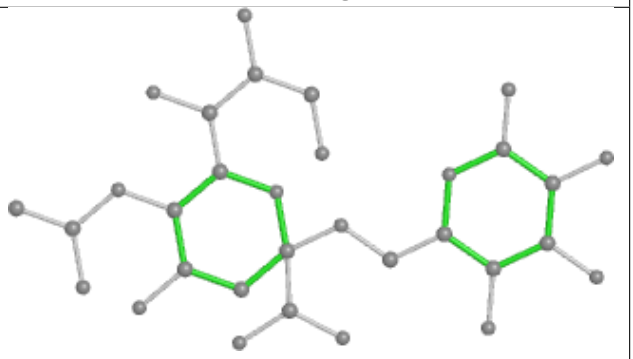
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.