W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 04:23 PM BST

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

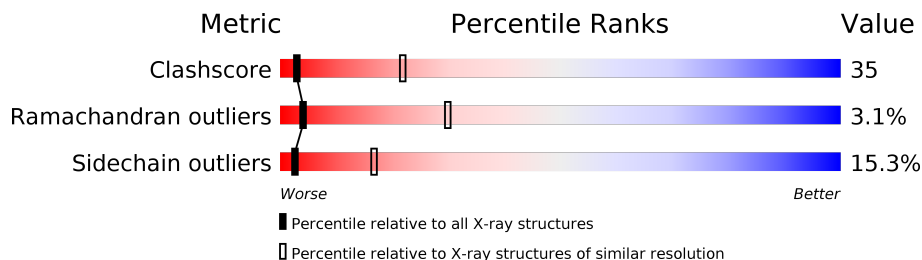|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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	Percentile Ranks	Value
Clashscore		35
Ramachandran outliers		3.1%
Sidechain outliers		15.3%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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)
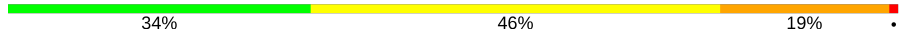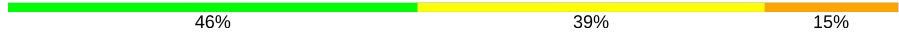
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% / •

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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 1769	C 1095	N 318	O 350	S 6	0	0	0
1	G	224	Total 1769	C 1095	N 318	O 350	S 6	0	0	0

- Molecule 2 is a protein called PERTUSSIS TOXIN.

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

- Molecule 3 is a protein called PERTUSSIS TOXIN.

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

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

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

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

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

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

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

- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose.
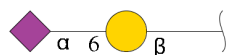
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	2	Total 32	C 17	N 1	O 14	0	0	0
7	N	2	Total 32	C 17	N 1	O 14	0	0	0
7	O	2	Total 32	C 17	N 1	O 14	0	0	0

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. 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)
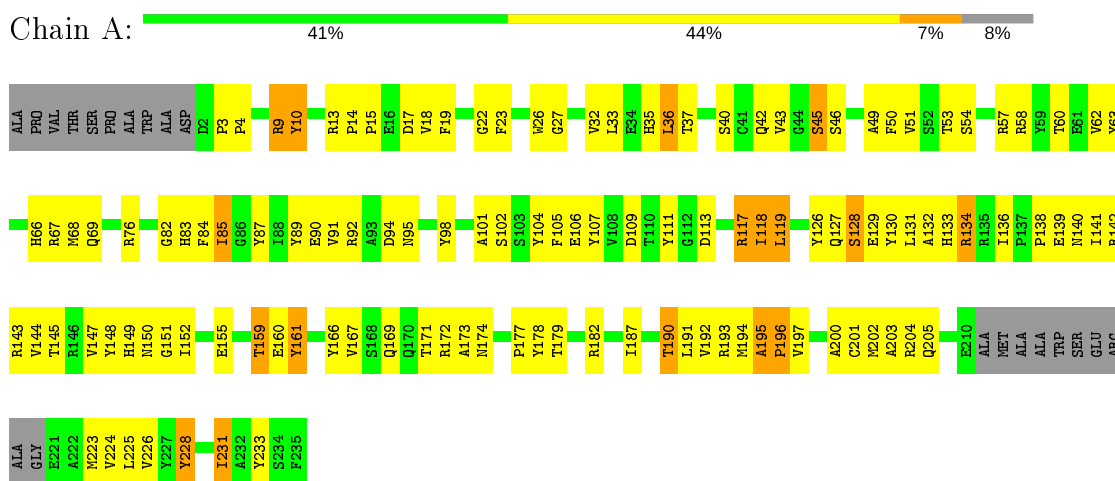
- Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)

- Molecule 2: PERTUSSIS TOXIN

G4 I5 V6 I7 P8 P9 Q10 E11 Q12 Q15 H16 G17 S18 P19 Y20 G21 R22 C23 A24 R28 A29 L30 T31 V32 A33 E34 L35 S38 L41 T49 B50 G51 W52 F55 A56 L57 Y58 T61 Y62 L63 G64 G65 G69 V70 I71 K72 D73 G74 T75 P76 G77 G78

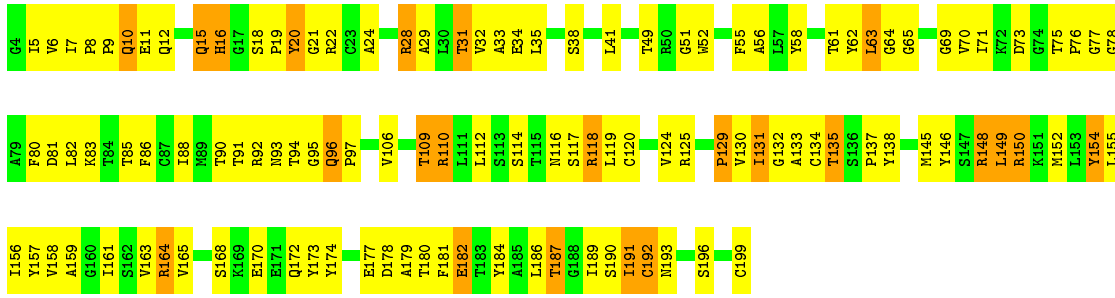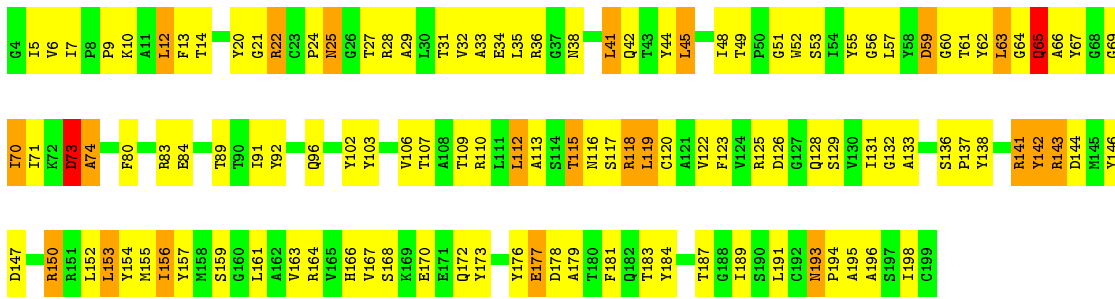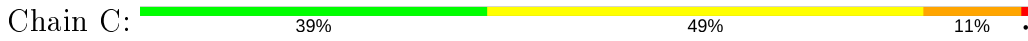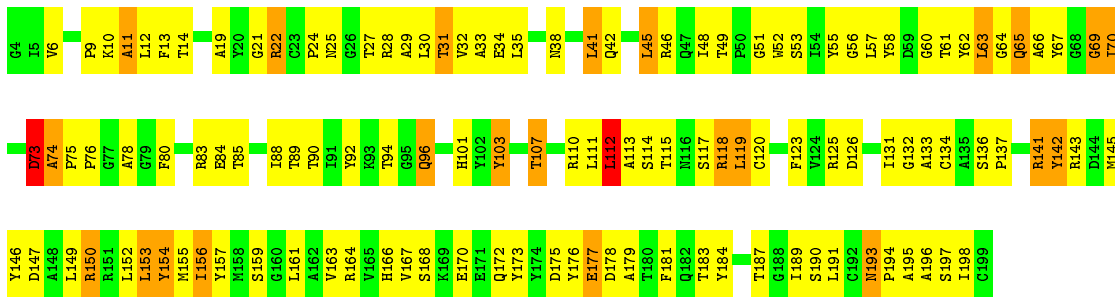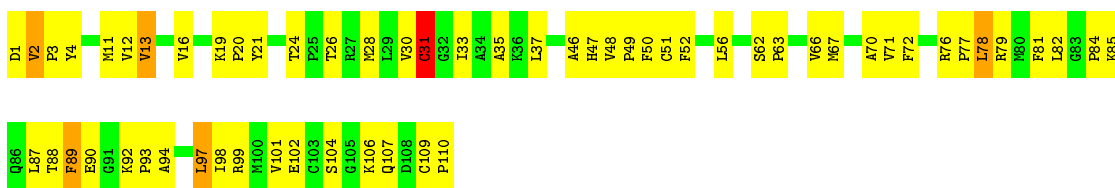A79 F80 D81 L82 K83 T84 T85 F86 C87 I88 M89 T90 T91 R92 N93 T94 G95 Q96 P97 V106 T109 R110 L111 L112 S113 S114 T115 N116 S117 R118 L119 C120 V124 R125 P129 V130 I131 G132 A133 C134 T135 S136 P137 Y138 M445 Y146 S147 R148 L149 R150 K151 M152 L153 Y154 L155

I156 Y157 V158 A159 G160 I161 S162 V163 R164 V165 S168 K169 E170 E171 Q172 Y173 Y174 E177 D178 A179 T180 F181 E182 T183 Y184 A185 L186 T187 G188 I189 S190 I191 C192 N193 S196 C199

● Molecule 3: PERTUSSIS TOXIN

Chain C:

| 39% | 49% | 11% | . |

G4 I5 V6 I7 P8 P9 K10 A11 L12 F13 T14 Y20 G21 R22 C23 P24 N25 G26 T27 R28 A29 L30 T31 V32 A33 E34 L35 R36 G37 N38 L41 Q42 T43 Y44 L45 I48 T49 P50 G51 W52 S53 I54 Y55 G56 L57 Y58 D59 G60 T61 Y62 L63 G64 Q65 A66 Y67 G68 G69

I70 I71 K72 D73 A74 F80 R83 E84 T89 T90 I91 Y92 Q96 Y102 Y103 V106 T107 A108 T109 R110 L111 L112 A113 S114 T115 N116 S117 R118 L119 C120 A121 V122 F123 V124 R125 D126 G127 Q128 S129 V130 I131 G132 A133 S136 P137 Y138 R141 Y142 R143 D144 M145 Y146

D147 R150 R151 L152 L153 Y154 M155 I156 Y157 M158 S159 G160 L161 A162 V163 R164 V165 H166 V167 S168 K169 E170 E171 Q172 Y173 Y176 E177 D178 A179 T180 F181 Q182 T183 Y184 T187 G188 I189 S190 L191 C192 N193 P194 A195 A196 S197 I198 C199

● Molecule 3: PERTUSSIS TOXIN

Chain I:

| 37% | 51% | 12% | . |

G4 I5 V6 P9 K10 A11 L12 F13 T14 A19 Y20 G21 R22 C23 P24 N25 G26 T27 R28 A29 L30 T31 V32 A33 E34 L35 N38 L41 Q42 L45 R46 Q47 I48 T49 P50 G51 W52 S53 I54 Y55 G56 L57 Y58 D59 G60 T61 Y62 L63 G64 Q65 A66 Y67 G68 G69 I70

D73 A74 P75 P76 G77 A78 G79 F80 R83 E84 T85 I88 T89 T90 I91 Y92 K93 T94 G95 Q96 H101 Y102 Y103 T107 R110 L111 I112 A113 S114 T115 N116 R118 L119 C120 F123 V124 R125 D126 I131 G132 A133 C134 A135 S136 P137 R141 Y142 R143 D144 M145

Y146 D147 A148 L149 R150 R151 L152 L153 Y154 M155 I156 Y157 M158 S159 G160 L161 A162 V163 R164 V165 H166 V167 S168 K169 E170 E171 Q172 Y173 Y174 D175 Y176 E177 D178 A179 T180 F181 Q182 T183 Y184 T187 G188 I189 S190 L191 C192 N193 P194 A195 A196 S197 I198 C199

● Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain D:

| 46% | 48% | 5% | . |

D1 V2 P3 Y4 M11 V12 V13 V16 K19 P20 Y21 T24 P25 T26 R27 M28 L29 V30 C31 G32 A34 A35 K36 L37 A46 H47 V48 P49 F50 C51 F52 L56 S62 P63 V66 M67 A70 V71 F72 R76 P77 L78 R79 M80 F81 L82 G83 P84 K85

Q86 L87 T88 F89 E90 G91 K92 P93 A94 L97 I98 R99 M100 V101 E102 C103 S104 G105 K106 Q107 D108 C109 P110

● Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)
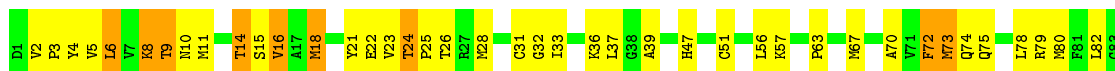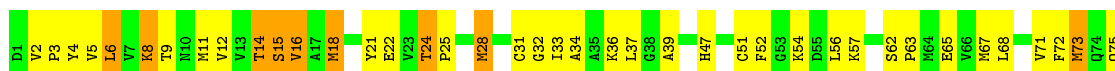
Chain E:

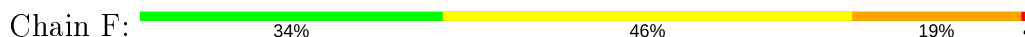| 51% | 39% | 10% |

• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain J:

• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain K:

• Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)
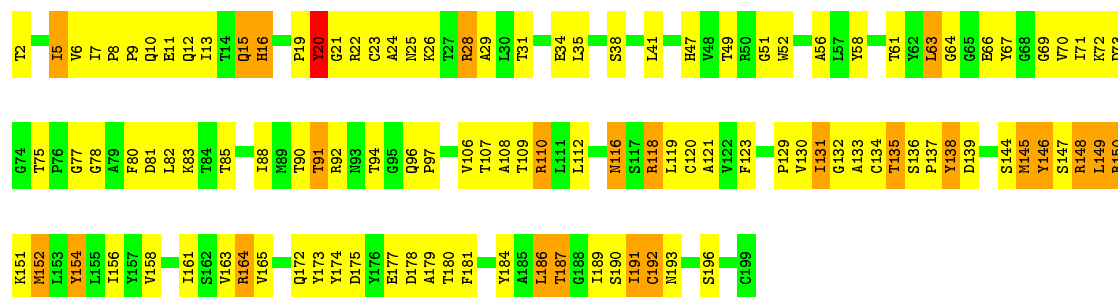
Chain F:

• 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: SIA, GAL

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:

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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 ⓘ

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	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	57	LEU
1	G	231	ILE
5	L	19	LEU
5	F	74	VAL

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Mol	Chain	Res	Type
1	G	106	GLU

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

Mol	Chain	Res	Type
3	C	182	GLN
1	G	28	ASN
3	I	172	GLN
3	C	193	ASN
4	E	86	GLN

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	17,20,21	0.80	0	21,28,31	1.03	1 (4%)
7	GAL	N	1	7	12,12,12	0.71	0	17,17,17	0.62	0
7	SIA	N	2	7	17,20,21	0.61	0	21,28,31	1.16	4 (19%)
7	GAL	O	1	7	12,12,12	0.62	0	17,17,17	0.79	0
7	SIA	O	2	7	17,20,21	1.21	2 (11%)	21,28,31	1.25	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
7	GAL	M	1	7	-	0/2/22/22	0/1/1/1
7	SIA	M	2	7	-	2/14/34/38	0/1/1/1
7	GAL	N	1	7	-	2/2/22/22	0/1/1/1
7	SIA	N	2	7	-	3/14/34/38	0/1/1/1
7	GAL	O	1	7	-	0/2/22/22	0/1/1/1
7	SIA	O	2	7	-	5/14/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C3-C4-C5	2.05	113.94	111.46

There are no chirality outliers.

5 of 12 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	1	GAL	2	0
7	N	2	SIA	5	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

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings
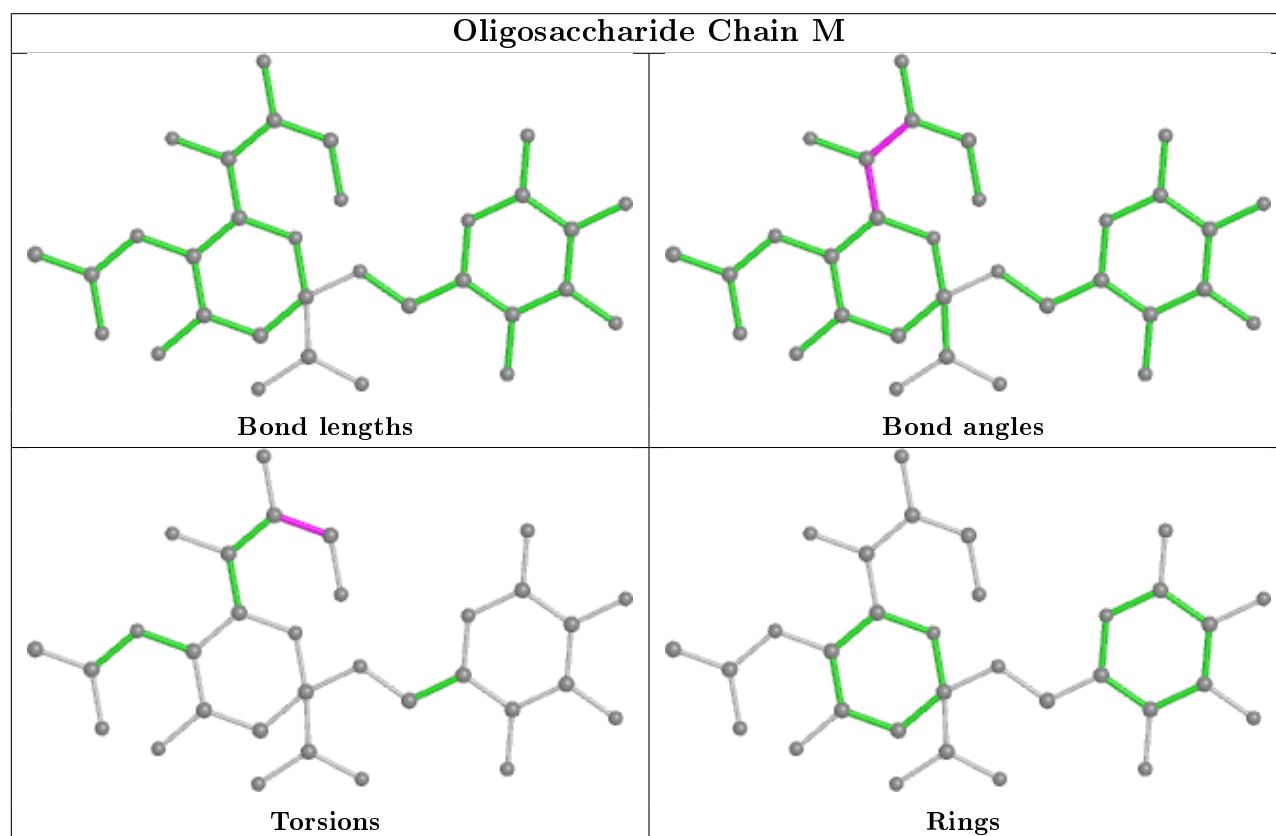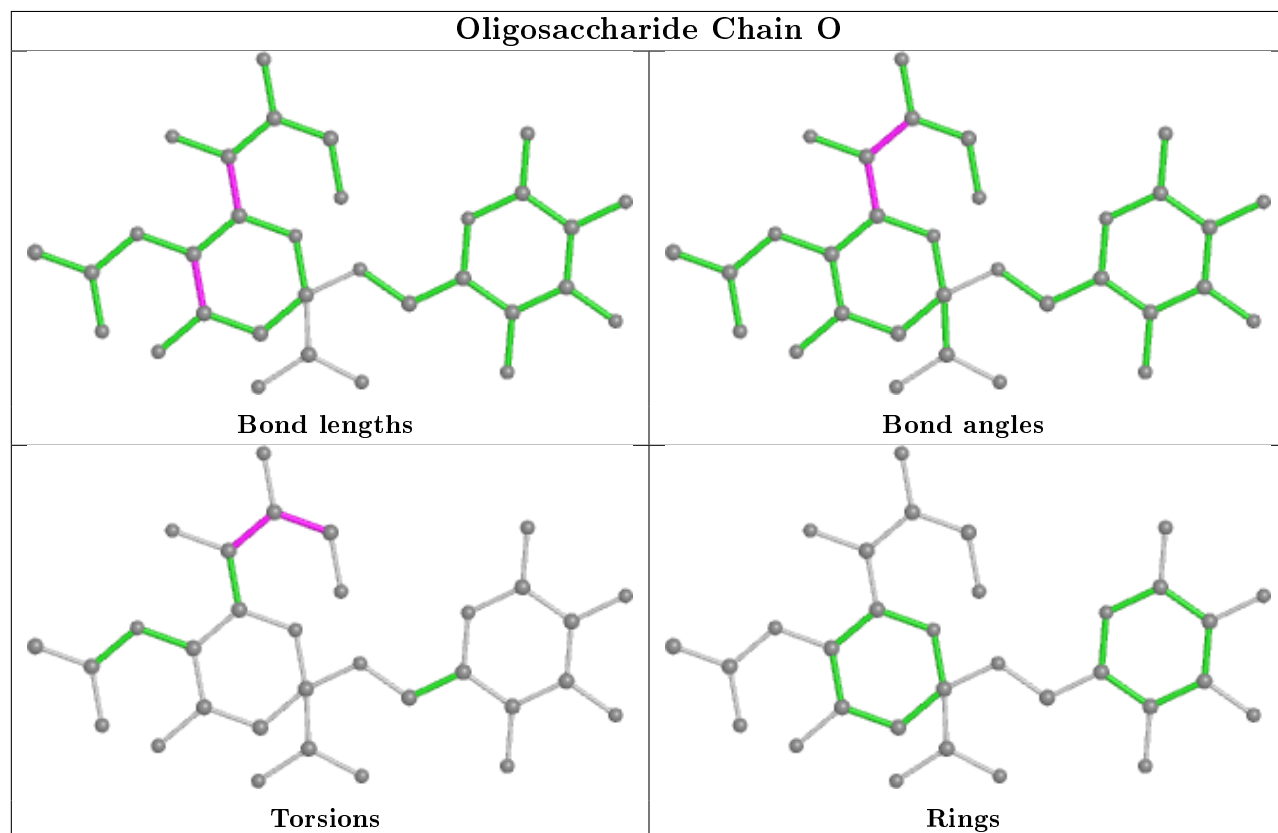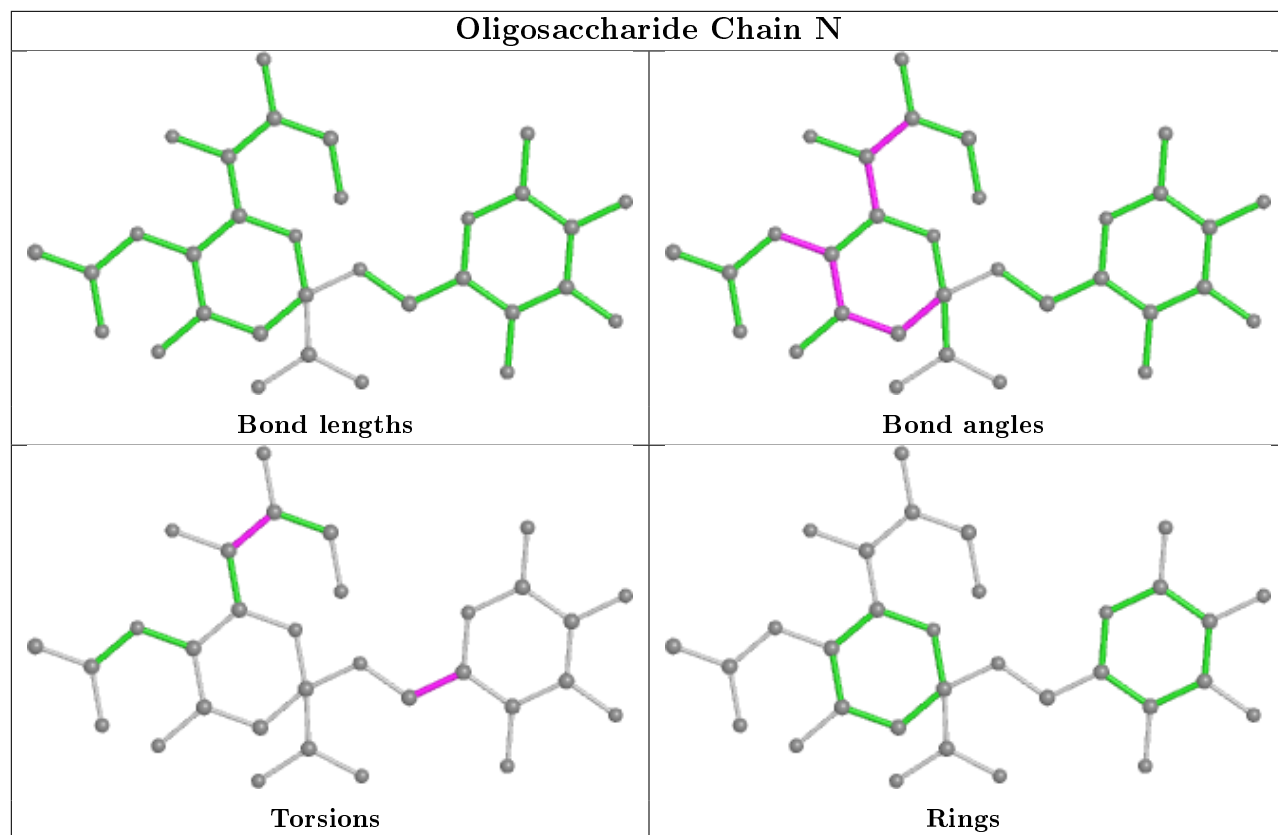
5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.