



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 06:15 AM EDT

PDB ID : 1SE3
Title : STAPHYLOCOCCAL ENTEROTOXIN B COMPLEXED WITH GM3 TRISACCHARIDE
Authors : Swaminathan, S.; Sax, M.
Deposited on : 1996-10-11
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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

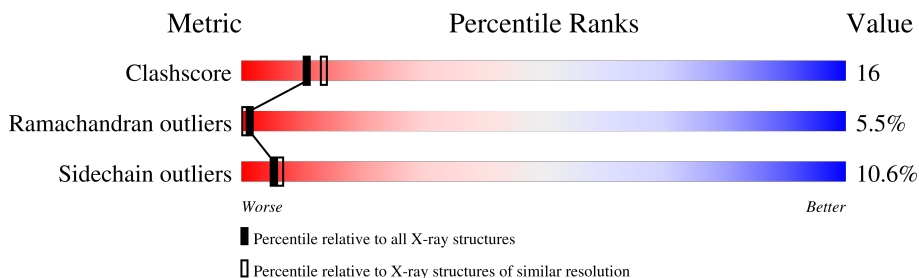
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.


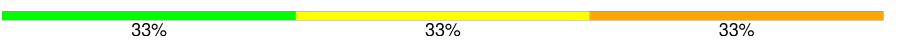
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	239	 65% 26% 8% •
2	B	3	 33% 33% 33%

2 Entry composition [i](#)

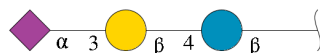
There are 3 unique types of molecules in this entry. The entry contains 2153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STAPHYLOCOCCAL ENTEROTOXIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1975	1262	321	382	10			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total	O	0	0
			135	135		

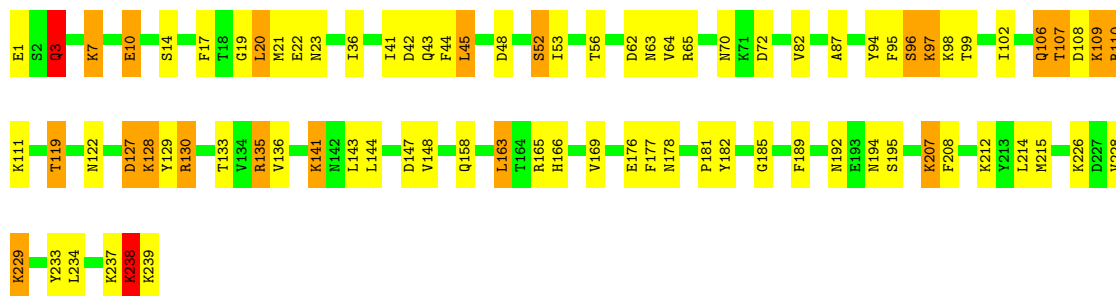
3 Residue-property plots

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: STAPHYLOCOCCAL ENTEROTOXIN B

Chain A: 



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

Chain B: 



4 Data and refinement statistics

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	45.30 Å 71.00 Å 78.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2153	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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, 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	0.58	0/2019	0.84	2/2715 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASP	N-CA-C	-7.98	89.44	111.00
1	A	3	GLN	N-CA-C	-7.64	90.36	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1975	0	1901	64	0
2	B	43	0	37	8	0
3	A	135	0	0	1	0
All	All	2153	0	1938	65	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 16.

All (65) 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:A:52:SER:HB3	2:B:3:SIA:H112	1.56	0.86
1:A:94:TYR:OH	1:A:97:LYS:HB3	1.76	0.84
1:A:108:ASP:HB2	2:B:3:SIA:H31	1.60	0.83
1:A:207:LYS:HD3	1:A:208:PHE:H	1.45	0.80
1:A:130:ARG:NH1	1:A:226:LYS:HB3	1.99	0.78
1:A:106:GLN:CD	1:A:107:THR:H	1.90	0.75
1:A:238:LYS:HD2	1:A:238:LYS:N	2.05	0.71
1:A:148:VAL:HG13	1:A:163:LEU:HD23	1.74	0.70
1:A:108:ASP:HB2	2:B:3:SIA:C3	2.20	0.70
1:A:130:ARG:CZ	1:A:226:LYS:HB3	2.21	0.70
1:A:185:GLY:HA2	1:A:233:TYR:O	1.98	0.63
1:A:63:ASN:ND2	1:A:107:THR:HG23	2.16	0.61
1:A:95:PHE:CE1	1:A:111:LYS:HB3	2.36	0.61
1:A:44:PHE:CD2	1:A:45:LEU:HD22	2.37	0.59
1:A:45:LEU:HD23	1:A:65:ARG:NH2	2.18	0.59
1:A:23:ASN:ND2	1:A:207:LYS:HE3	2.19	0.58
1:A:165:ARG:O	1:A:169:VAL:HG13	2.03	0.57
1:A:62:ASP:HB3	2:B:3:SIA:O8	2.05	0.57
1:A:106:GLN:CD	1:A:107:THR:N	2.58	0.55
1:A:21:MET:HB3	1:A:176:GLU:O	2.09	0.52
1:A:3:GLN:HB2	1:A:195:SER:O	2.10	0.52
1:A:43:GLN:HG3	1:A:48:ASP:O	2.09	0.52
1:A:87:ALA:H	1:A:158:GLN:HE21	1.58	0.52
1:A:23:ASN:HD22	1:A:207:LYS:HE3	1.75	0.51
1:A:127:ASP:O	1:A:128:LYS:HB2	2.10	0.51
1:A:207:LYS:HD3	1:A:208:PHE:N	2.22	0.51
1:A:237:LYS:O	1:A:239:LYS:N	2.44	0.51
1:A:108:ASP:O	2:B:3:SIA:H31	2.11	0.50
1:A:108:ASP:CB	2:B:3:SIA:H31	2.38	0.49
1:A:96:SER:O	1:A:97:LYS:HG2	2.13	0.49
1:A:185:GLY:HA3	1:A:234:LEU:HD23	1.95	0.48
1:A:94:TYR:OH	1:A:97:LYS:HD2	2.14	0.48
1:A:141:LYS:HB2	1:A:143:LEU:HG	1.96	0.47
1:A:133:THR:HG22	1:A:147:ASP:OD1	2.13	0.47
1:A:96:SER:HB3	1:A:106:GLN:H	1.80	0.47
1:A:135:ARG:HE	1:A:229:LYS:NZ	2.13	0.47
1:A:41:ILE:HD13	1:A:52:SER:OG	2.16	0.46
1:A:1:GLU:HA	1:A:195:SER:HB3	1.99	0.45
1:A:95:PHE:HE1	1:A:111:LYS:HB3	1.79	0.45
1:A:129:TYR:N	1:A:129:TYR:CD1	2.85	0.45
1:A:166:HIS:O	1:A:169:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PHE:CZ	1:A:19:GLY:O	2.70	0.45
1:A:7:LYS:O	1:A:10:GLU:HB2	2.17	0.45
1:A:178:ASN:HB2	3:A:322:HOH:O	2.16	0.45
1:A:20:LEU:HG	1:A:22:GLU:HB3	1.98	0.44
1:A:148:VAL:CG1	1:A:163:LEU:HD23	2.45	0.44
1:A:52:SER:CB	2:B:3:SIA:H112	2.39	0.44
1:A:42:ASP:CG	1:A:106:GLN:HB2	2.38	0.44
1:A:96:SER:HB3	1:A:106:GLN:O	2.17	0.44
1:A:129:TYR:N	1:A:129:TYR:HD1	2.16	0.44
1:A:212:LYS:HD3	1:A:215:MET:HE3	2.00	0.43
1:A:96:SER:O	1:A:97:LYS:CG	2.66	0.43
1:A:181:PRO:HG2	1:A:182:TYR:CD2	2.54	0.43
1:A:182:TYR:O	1:A:237:LYS:HG2	2.19	0.43
1:A:53:ILE:HB	1:A:64:VAL:CG2	2.50	0.42
1:A:70:ASN:OD1	1:A:72:ASP:HB2	2.20	0.42
1:A:82:VAL:HB	1:A:119:THR:O	2.20	0.42
1:A:238:LYS:N	1:A:238:LYS:CD	2.77	0.42
1:A:109:LYS:HG3	1:A:110:ARG:HG3	2.02	0.42
1:A:207:LYS:HZ3	1:A:207:LYS:HA	1.85	0.41
2:B:2:GAL:O3	2:B:3:SIA:H5	2.20	0.41
1:A:127:ASP:O	1:A:128:LYS:CB	2.68	0.41
1:A:189:PHE:O	1:A:195:SER:HA	2.20	0.41
1:A:181:PRO:O	1:A:237:LYS:HB2	2.20	0.41
1:A:189:PHE:CD1	1:A:189:PHE:N	2.89	0.40

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	237/239 (99%)	197 (83%)	27 (11%)	13 (6%)	1 0

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	A	102	ILE
1	A	110	ARG
1	A	20	LEU
1	A	98	LYS
1	A	128	LYS
1	A	238	LYS
1	A	96	SER
1	A	144	LEU
1	A	107	THR
1	A	177	PHE
1	A	192	ASN
1	A	109	LYS

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	217/225 (96%)	194 (89%)	23 (11%)	5 6

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	LYS
1	A	10	GLU
1	A	14	SER
1	A	36	ILE
1	A	45	LEU
1	A	52	SER
1	A	56	THR
1	A	97	LYS
1	A	106	GLN
1	A	119	THR
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	130	ARG
1	A	135	ARG
1	A	136	VAL
1	A	141	LYS
1	A	163	LEU
1	A	194	ASN
1	A	207	LYS
1	A	214	LEU
1	A	228	VAL
1	A	229	LYS
1	A	238	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	HIS
1	A	63	ASN
1	A	158	GLN
1	A	166	HIS

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](#)

3 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	B	1	2	12,12,12	0.67	0	17,17,17	0.73	0
2	GAL	B	2	2	11,11,12	0.73	0	15,15,17	0.76	0
2	SIA	B	3	2	20,20,21	1.23	4 (20%)	21,28,31	1.04	2 (9%)

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	B	1	2	-	2/2/22/22	0/1/1/1
2	GAL	B	2	2	-	0/2/19/22	0/1/1/1
2	SIA	B	3	2	-	2/18/34/38	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	SIA	C2-C1	2.89	1.55	1.52
2	B	3	SIA	C7-C6	2.39	1.55	1.52
2	B	3	SIA	C4-C5	2.12	1.55	1.53
2	B	3	SIA	O1A-C1	2.00	1.28	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SIA	C8-C7-C6	-2.62	108.12	113.05
2	B	3	SIA	O1B-C1-C2	2.28	118.65	112.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

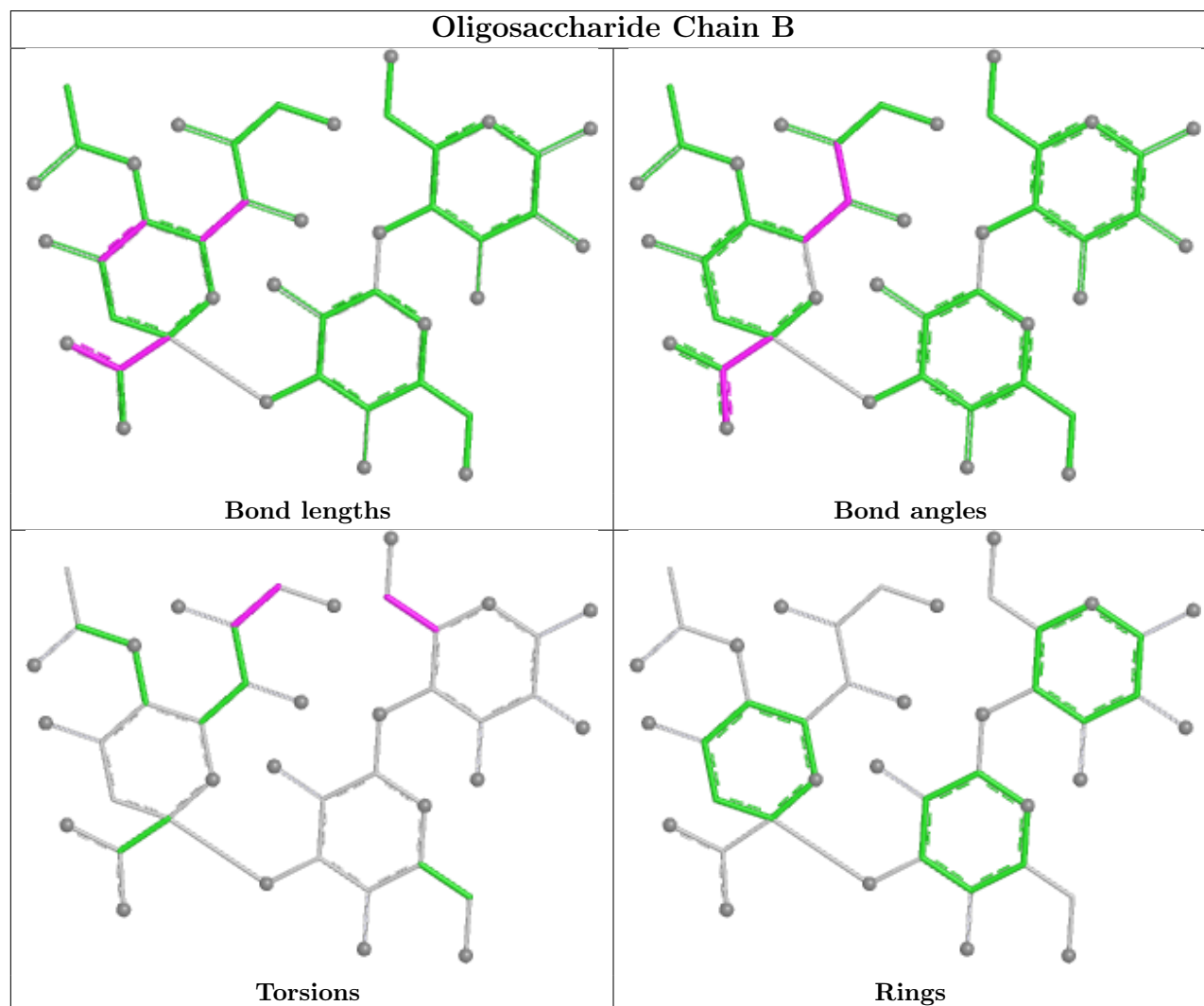
Mol	Chain	Res	Type	Atoms
2	B	3	SIA	O8-C8-C9-O9
2	B	3	SIA	C7-C8-C9-O9
2	B	1	BGC	C4-C5-C6-O6
2	B	1	BGC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GAL	1	0
2	B	3	SIA	8	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](#)

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 ⓘ

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.