W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Dec 13, 2022 – 12:08 pm GMT

PDB ID	:	7ZIQ
Title	:	BK Polyomavirus VP1 in complex with 6'-Sialyllactose glycomacromolecules (aromatic linker)
Authors	:	Freytag, J.; Mueller, J.C.; Stehle, T.
Deposited on	:	2022-04-08
Resolution	:	1.90 Å(reported)

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

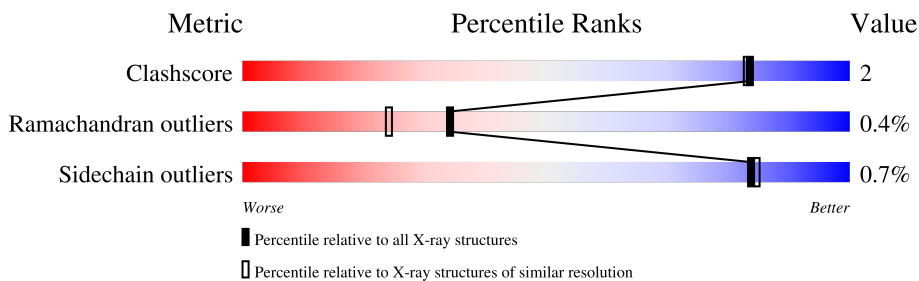|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 1.90 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		2
Ramachandran outliers		0.4%
Sidechain outliers		0.7%

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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	275	89% 5% 5%
1	BBB	275	85% 8% 7%
1	CCC	275	83% 5% 12%
1	DDD	275	90% 7% •
1	EEE	275	86% 8% 5%
2	AaA	3	67% 33%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 10790 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	260	Total 2009	C 1264	N 347	O 385	S 13	0	4	0
1	BBB	255	Total 1970	C 1241	N 343	O 373	S 13	0	3	0
1	CCC	243	Total 1881	C 1181	N 328	O 359	S 13	0	2	0
1	DDD	266	Total 2044	C 1286	N 352	O 392	S 14	0	2	0
1	EEE	260	Total 2030	C 1278	N 351	O 388	S 13	0	6	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	26	GLY	-	expression tag	UNP Q65613
AAA	27	SER	-	expression tag	UNP Q65613
AAA	28	HIS	-	expression tag	UNP Q65613
AAA	29	MET	-	expression tag	UNP Q65613
BBB	26	GLY	-	expression tag	UNP Q65613
BBB	27	SER	-	expression tag	UNP Q65613
BBB	28	HIS	-	expression tag	UNP Q65613
BBB	29	MET	-	expression tag	UNP Q65613
CCC	26	GLY	-	expression tag	UNP Q65613
CCC	27	SER	-	expression tag	UNP Q65613
CCC	28	HIS	-	expression tag	UNP Q65613
CCC	29	MET	-	expression tag	UNP Q65613
DDD	26	GLY	-	expression tag	UNP Q65613
DDD	27	SER	-	expression tag	UNP Q65613
DDD	28	HIS	-	expression tag	UNP Q65613
DDD	29	MET	-	expression tag	UNP Q65613
EEE	26	GLY	-	expression tag	UNP Q65613
EEE	27	SER	-	expression tag	UNP Q65613
EEE	28	HIS	-	expression tag	UNP Q65613

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	29	MET	-	expression tag	UNP Q65613

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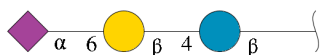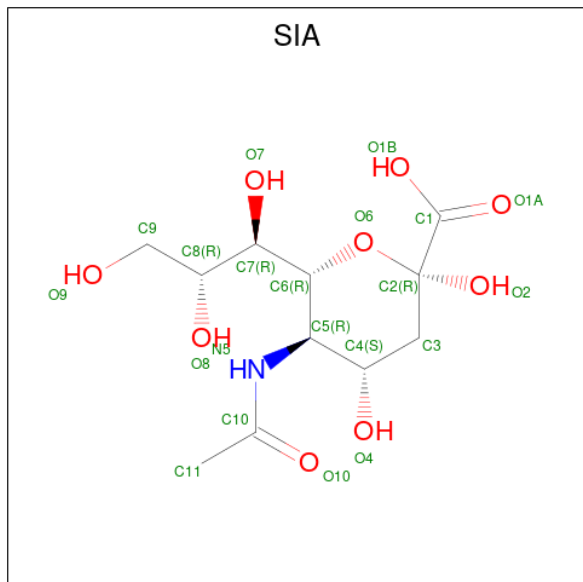

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	AaA	3	43	23	1	19	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).
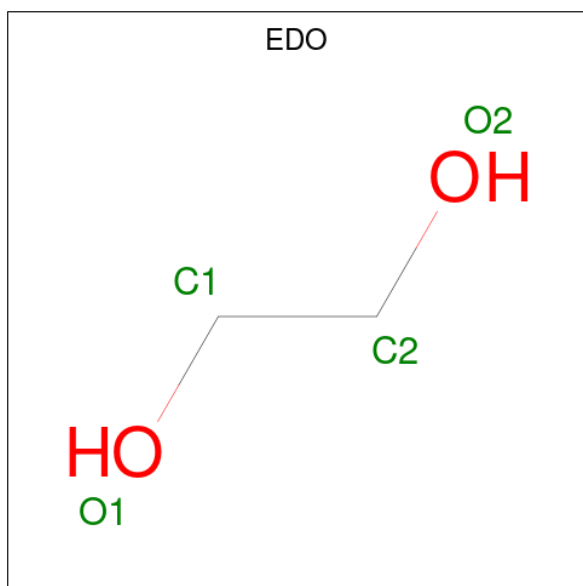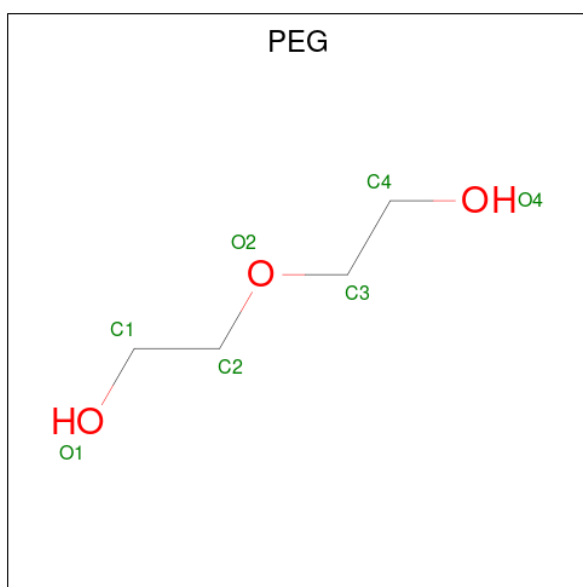

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	BBB	1	4	2	2	0	0
3	CCC	1	4	2	2	0	0
3	EEE	1	4	2	2	0	0
3	EEE	1	4	2	2	0	0

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	BBB	1	Total	C	N	O	0	0
			21	11	1	9		
4	DDD	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	CCC	1	Total 7	C 4	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	145	Total 145	O 145	0	0
6	BBB	150	Total 150	O 150	0	0
6	CCC	133	Total 133	O 133	0	0
6	DDD	158	Total 158	O 158	0	0
6	EEE	162	Total 162	O 162	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.
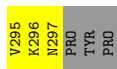
Note EDS failed to run properly.
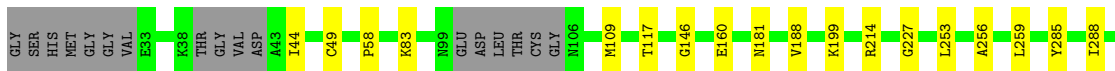
• Molecule 1: Capsid protein VP1

Chain AAA:

• Molecule 1: Capsid protein VP1

Chain BBB:

• Molecule 1: Capsid protein VP1

Chain CCC:
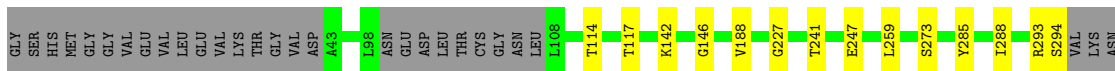
• Molecule 1: Capsid protein VP1

Chain DDD:

• Molecule 1: Capsid protein VP1

Chain EEE:

GLY SER HIS MET GLY GLY V32 G40 VAL ASP ALA I44 C49 P58 R82 K83 L98 D101 LEU THR CYS G105 W110 V113 T114 T117 E137 G146 E160 V188 N201 R214 G227 T241 L245 L259 Y260 V261 S273

Y285 I288 N297 PRO TYR PRO
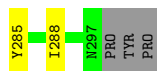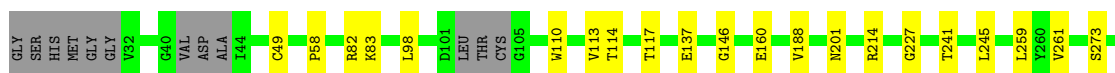
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain AaA:

67%   33%

BGC1 GAL2 SIA3

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.33Å 151.84Å 63.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 1.90	Depositor
% Data completeness (in resolution range)	99.9 (48.50-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.187 , 0.226	Depositor
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.063	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
Total number of atoms	10790	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BGC, GAL, EDO, PEG, 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	AAA	0.65	0/2066	0.82	0/2812
1	BBB	0.66	0/2023	0.81	0/2750
1	CCC	0.64	0/1932	0.82	0/2627
1	DDD	0.66	0/2096	0.82	0/2853
1	EEE	0.68	0/2089	0.83	0/2838
All	All	0.66	0/10206	0.82	0/13880

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	2009	0	1942	7	0
1	BBB	1970	0	1910	14	0
1	CCC	1881	0	1814	6	0
1	DDD	2044	0	1987	12	0
1	EEE	2030	0	1971	10	0
2	AaA	43	0	37	0	0
3	BBB	4	0	6	0	0
3	CCC	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	EEE	8	0	12	0	0
4	BBB	21	0	18	0	0
4	DDD	21	0	18	0	0
5	CCC	7	0	10	0	0
6	AAA	145	0	0	1	0
6	BBB	150	0	0	2	0
6	CCC	133	0	0	0	0
6	DDD	158	0	0	4	0
6	EEE	162	0	0	0	0
All	All	10790	0	9731	48	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 2.

The worst 5 of 48 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:BBB:109:MET:CE	1:BBB:295:VAL:HG11	2.24	0.68
1:BBB:109:MET:HE2	1:BBB:295:VAL:HG11	1.75	0.68
1:BBB:58:PRO:HA	1:BBB:83:LYS:HD2	1.80	0.64
1:BBB:296:LYS:O	1:BBB:297:ASN:HB2	1.97	0.64
1:BBB:44:ILE:C	1:BBB:44:ILE:HD12	2.20	0.62

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	AAA	260/275 (94%)	250 (96%)	9 (4%)	1 (0%)	34	24
1	BBB	252/275 (92%)	239 (95%)	12 (5%)	1 (0%)	34	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	241/275 (88%)	231 (96%)	9 (4%)	1 (0%)	34	24
1	DDD	266/275 (97%)	251 (94%)	14 (5%)	1 (0%)	34	24
1	EEE	260/275 (94%)	248 (95%)	11 (4%)	1 (0%)	34	24
All	All	1279/1375 (93%)	1219 (95%)	55 (4%)	5 (0%)	34	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	188	VAL
1	BBB	188	VAL
1	CCC	188	VAL
1	DDD	188	VAL
1	EEE	188	VAL

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	AAA	220/236 (93%)	219 (100%)	1 (0%)	88	89
1	BBB	215/236 (91%)	212 (99%)	3 (1%)	67	65
1	CCC	206/236 (87%)	204 (99%)	2 (1%)	76	76
1	DDD	225/236 (95%)	224 (100%)	1 (0%)	91	91
1	EEE	223/236 (94%)	221 (99%)	2 (1%)	78	79
All	All	1089/1180 (92%)	1080 (99%)	9 (1%)	84	82

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	137	GLU
1	EEE	273	SER
1	BBB	181	ASN
1	CCC	247	GLU
1	CCC	273	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	AaA	1	2	12,12,12	0.43	0	17,17,17	0.51	0
2	GAL	AaA	2	2	11,11,12	0.26	0	15,15,17	0.60	0
2	SIA	AaA	3	2	20,20,21	0.60	0	24,28,31	1.22	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
2	BGC	AaA	1	2	-	0/2/22/22	0/1/1/1
2	GAL	AaA	2	2	-	0/2/19/22	0/1/1/1
2	SIA	AaA	3	2	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AaA	3	SIA	C6-O6-C2	3.19	118.16	111.34
2	AaA	3	SIA	O1B-C1-C2	2.57	120.38	113.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 AaA

Bond lengths   Bond angles

Torsions   Rings
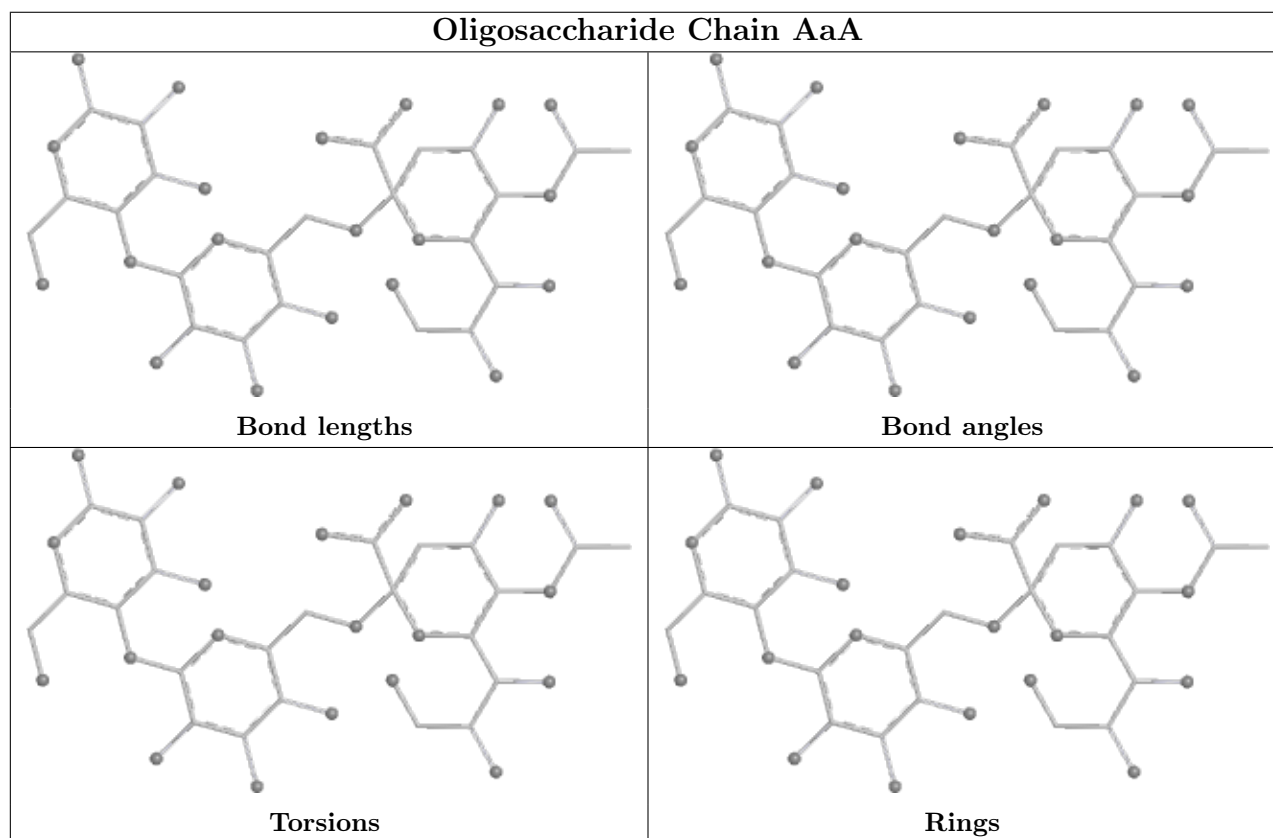
5.6   Ligand geometry ⓘ

7 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	#$|Z|>2$
3	EDO	EEE	502	-	3,3,3	0.17	0	2,2,2	0.06	0
5	PEG	CCC	402	-	6,6,6	0.16	0	5,5,5	0.09	0
3	EDO	BBB	501	-	3,3,3	0.14	0	2,2,2	0.33	0
4	SIA	BBB	502	-	21,21,21	1.57	3 (14%)	25,31,31	1.29	1 (4%)
3	EDO	CCC	401	-	3,3,3	0.09	0	2,2,2	0.09	0
3	EDO	EEE	501	-	3,3,3	0.20	0	2,2,2	0.45	0
4	SIA	DDD	501	-	21,21,21	1.56	3 (14%)	25,31,31	1.62	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	EDO	EEE	502	-	-	0/1/1/1	-
5	PEG	CCC	402	-	-	2/4/4/4	-
3	EDO	BBB	501	-	-	1/1/1/1	-
4	SIA	BBB	502	-	-	0/20/38/38	0/1/1/1
3	EDO	CCC	401	-	-	0/1/1/1	-
3	EDO	EEE	501	-	-	0/1/1/1	-
4	SIA	DDD	501	-	-	3/20/38/38	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	502	SIA	O2-C2	4.57	1.45	1.39
4	DDD	501	SIA	O2-C2	4.45	1.45	1.39
4	BBB	502	SIA	O6-C2	3.28	1.46	1.43
4	BBB	502	SIA	C3-C2	3.02	1.55	1.51
4	DDD	501	SIA	C3-C2	2.67	1.55	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	DDD	501	SIA	O1A-C1-C2	-5.22	115.68	123.59
4	BBB	502	SIA	O1A-C1-C2	-3.93	117.64	123.59
4	DDD	501	SIA	O6-C6-C5	2.60	112.32	109.78
4	DDD	501	SIA	C11-C10-N5	2.21	119.85	116.10
4	DDD	501	SIA	C3-C4-C5	2.21	113.37	109.98

There are no chirality outliers.
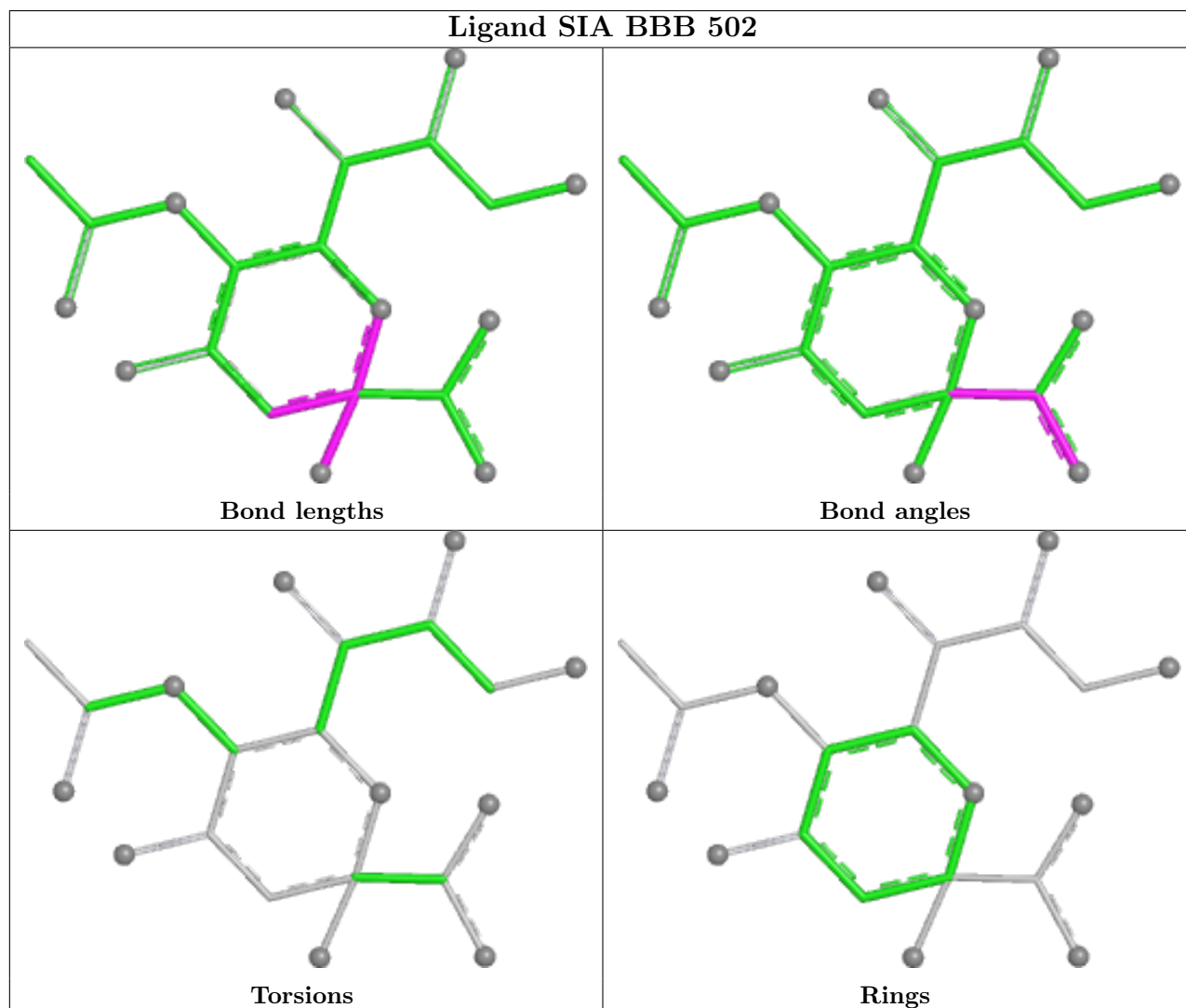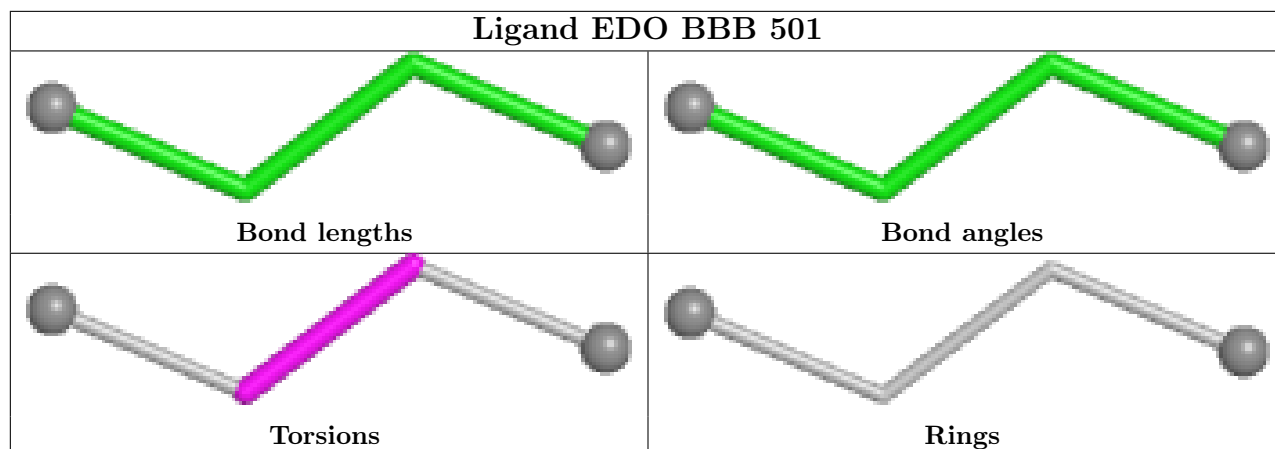
5 of 6 torsion outliers are listed below:

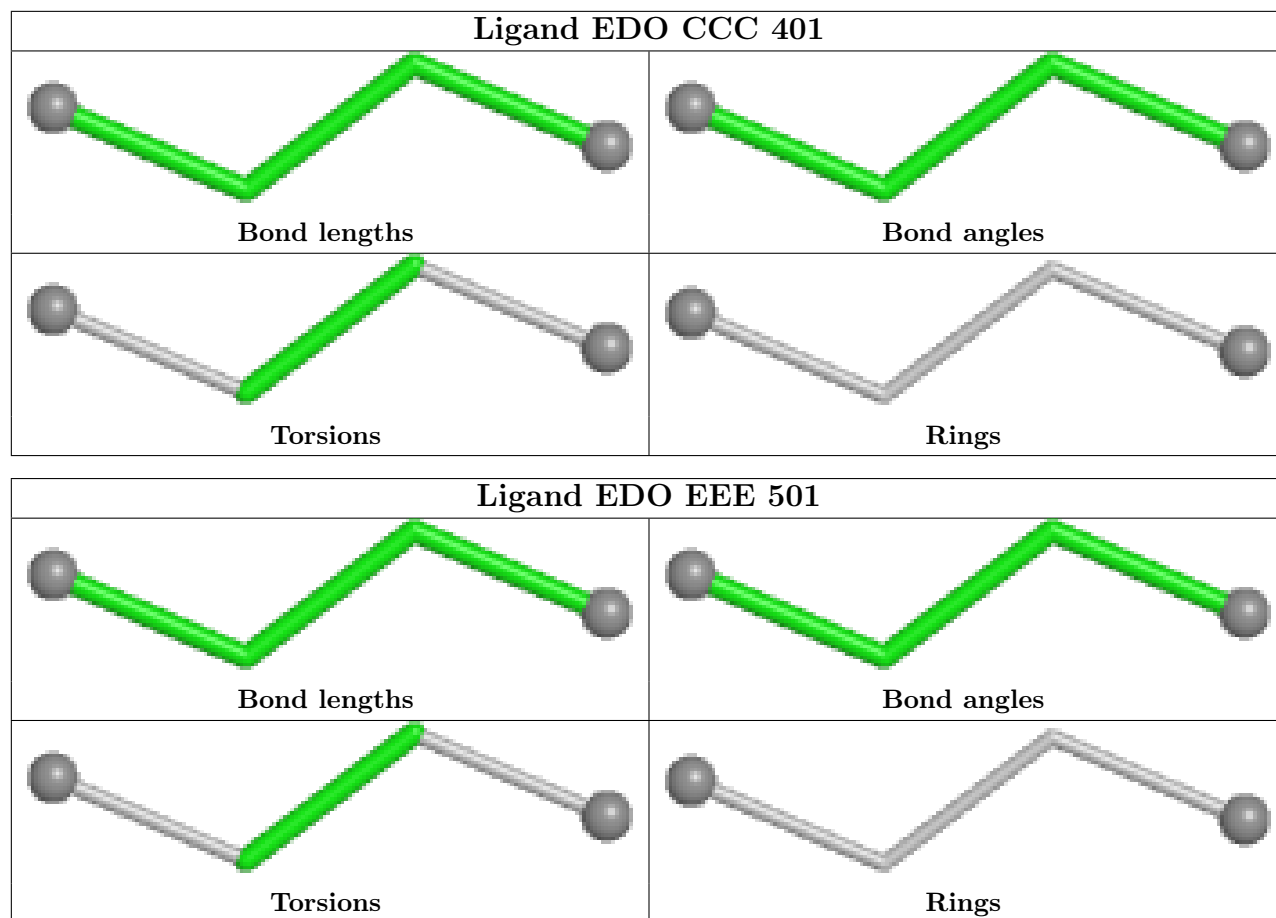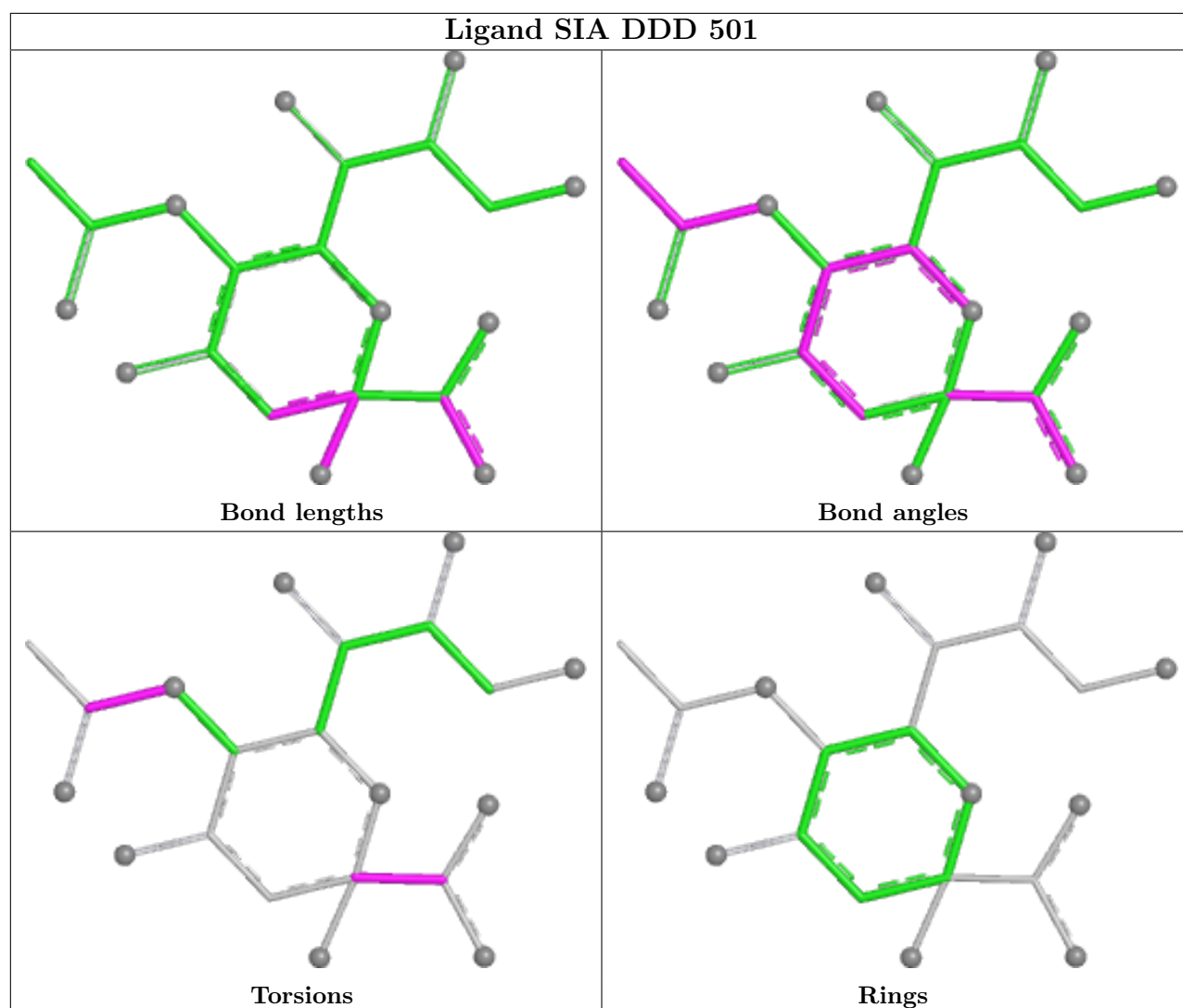| Mol	Chain	Res	Type	Atoms
4	DDD	501	SIA	C11-C10-N5-C5
4	DDD	501	SIA	O10-C10-N5-C5
3	BBB	501	EDO	O1-C1-C2-O2
5	CCC	402	PEG	O1-C1-C2-O2
5	CCC	402	PEG	O2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand EDO EEE 502

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO BBB 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA BBB 502

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO CCC 401

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO EEE 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA DDD 501

Bond lengths

Bond angles

Torsions

Rings
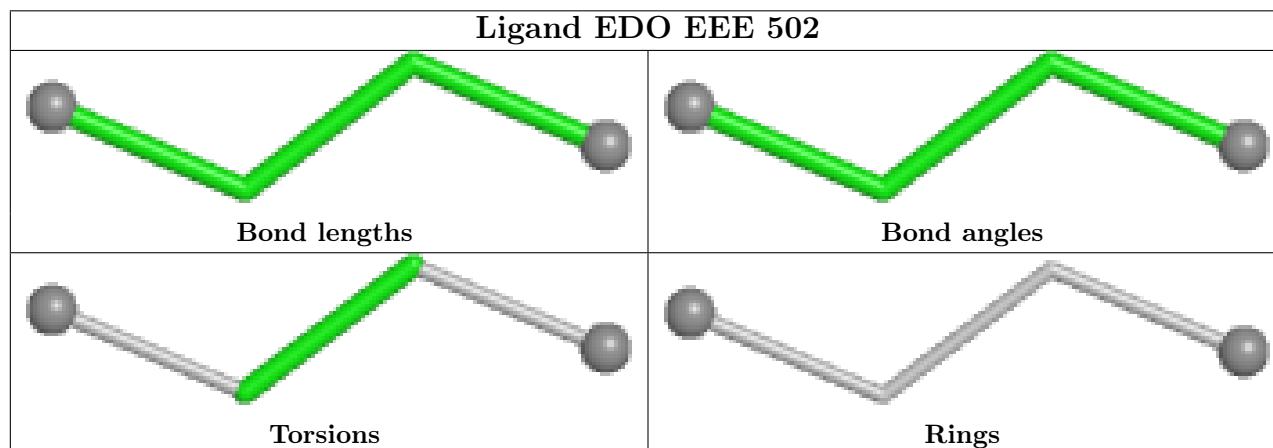
5.7 Other polymers ⓘ

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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.