wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 21, 2024 – 02:06 am BST

PDB ID : 6I3K
Title : Bilirubin oxidase from Myrothecium verrucaria, mutant W396A in complex with ferricyanide
Authors : Koval, T.; Svecova, L.; Skalova, T.; Kolenko, P.; Duskova, J.; Ostergaard, L.H.; Dohnalek, J.
Deposited on : 2018-11-06
Resolution : 1.60 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 ⓘ 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:

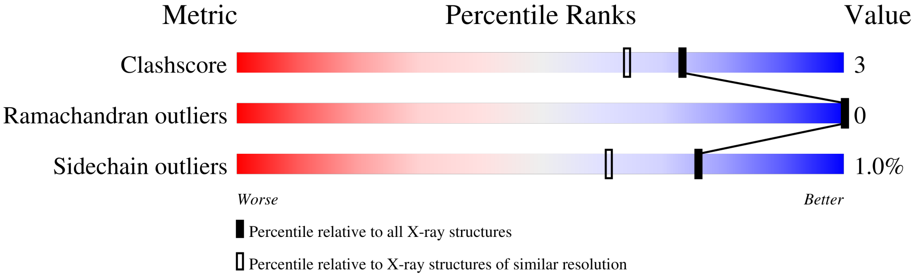
MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : FAILED
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 1.60 Å.

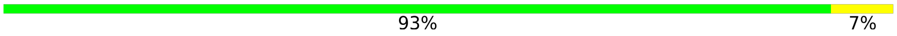
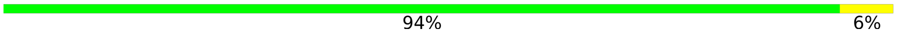
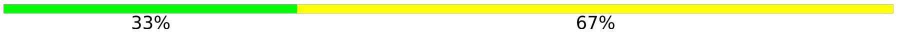
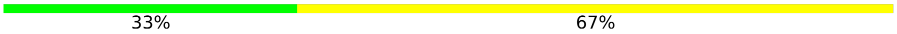
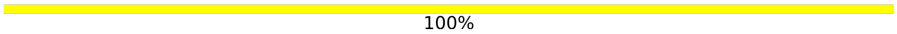
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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	A	534	
1	B	534	
2	C	3	
2	D	3	
2	E	3	
3	F	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SIN	B	615	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11063 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.

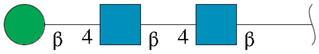
- Molecule 1 is a protein called Bilirubin oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total 4555	C 2911	N 766	O 860	S 18	0	50	0
1	B	534	Total 4429	C 2838	N 739	O 835	S 17	0	34	0

There are 2 discrepancies between the modelled and reference sequences:

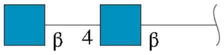
Chain	Residue	Modelled	Actual	Comment	Reference
A	396	ALA	TRP	engineered mutation	UNP Q12737
B	396	ALA	TRP	engineered mutation	UNP Q12737

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total 39	C 22	N 2	O 15	0	0	0
2	D	3	Total 39	C 22	N 2	O 15	0	0	0
2	E	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

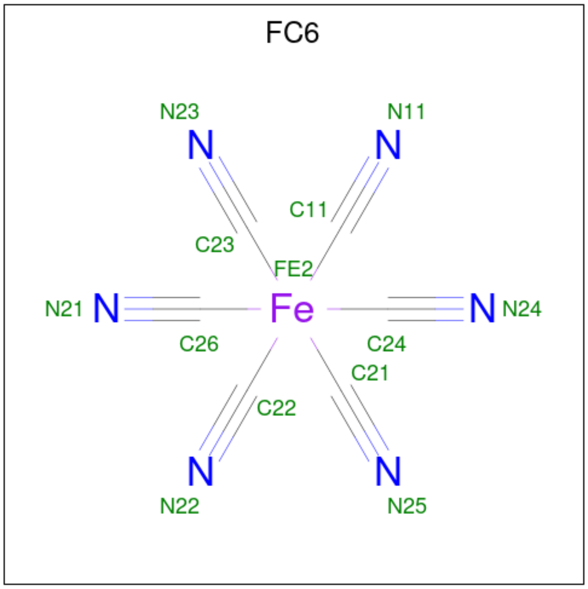


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	2	Total C N O 30 17 2 11	0	1	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

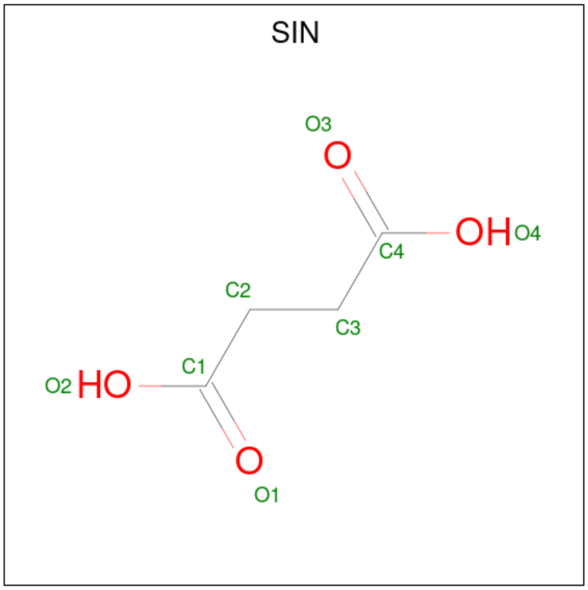
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cu 4 4	0	0
4	B	4	Total Cu 4 4	0	0

- Molecule 5 is HEXACYANOFERRATE(3-) (three-letter code: FC6) (formula: C_6FeN_6) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Fe N 13 6 1 6	0	0
5	A	1	Total C Fe N 13 6 1 6	0	0
5	B	1	Total C Fe N 13 6 1 6	0	0
5	B	1	Total C Fe N 13 6 1 6	0	0

- Molecule 6 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 8 4 4	0	0
6	A	1	Total C O 8 4 4	0	0
6	A	1	Total C O 8 4 4	0	0
6	B	1	Total C O 8 4 4	0	0
6	B	1	Total C O 8 4 4	0	0
6	B	1	Total C O 8 4 4	0	0
6	B	1	Total C O 8 4 4	0	0

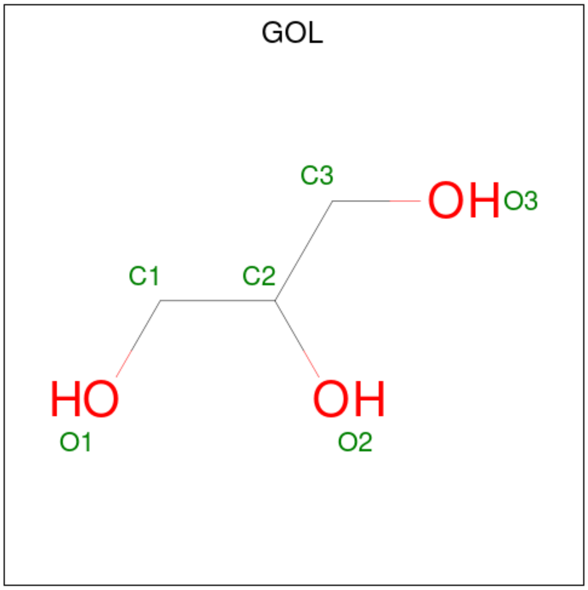
- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	0
8	B	1	Total K 1 1	0	0

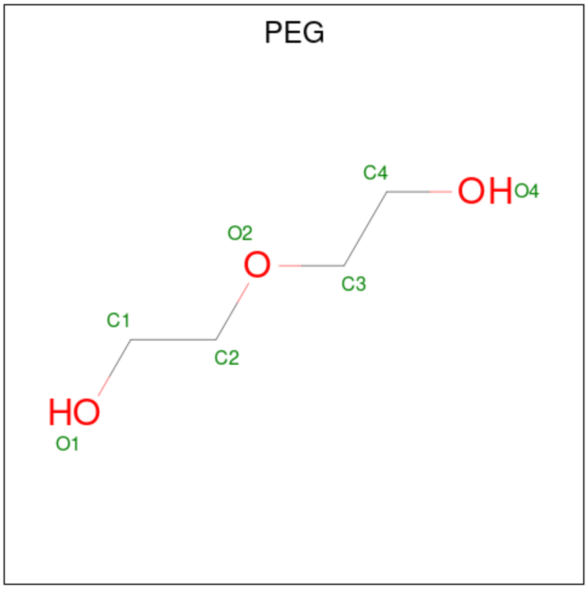
- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 12 6 6	0	1
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 12 6 6	0	1
9	A	1	Total C O 12 6 6	0	1
9	B	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:

$C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 7 4 3	0	0
10	B	1	Total C O 7 4 3	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	870	Total O 900 900	0	30
11	B	800	Total O 826 826	0	26

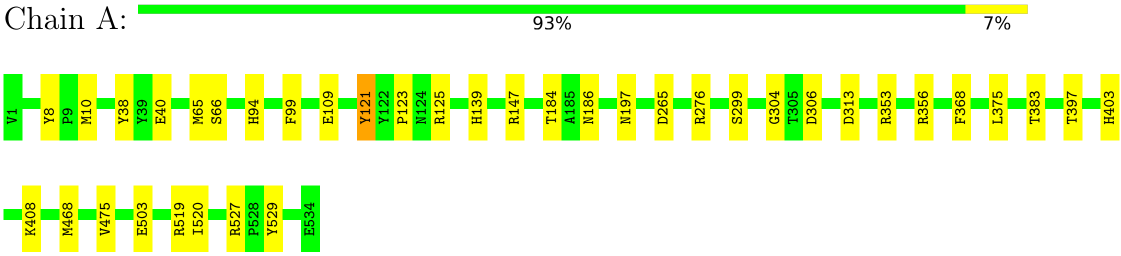
3 Residue-property plots ⓘ

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.

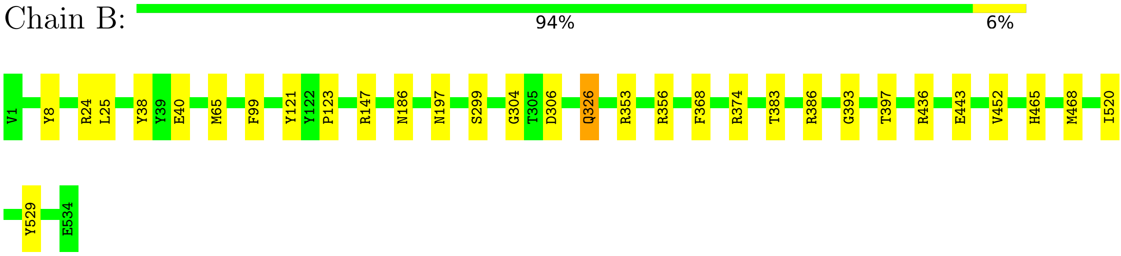
- Molecule 1: Bilirubin oxidase

Chain A:



- Molecule 1: Bilirubin oxidase

Chain B:



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

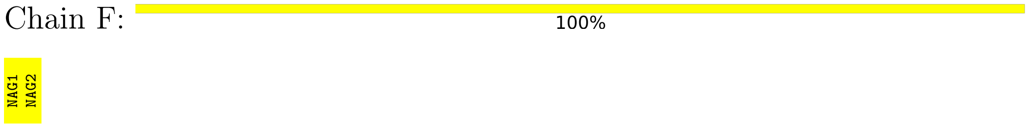
Chain D:

- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	136.91Å 201.80Å 217.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 1.60	Depositor
% Data completeness (in resolution range)	99.5 (47.93-1.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.131 , 0.154	Depositor
Wilson B-factor (Å^2)	14.2	Xtriage
Anisotropy	0.048	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11063	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FC6, SIN, BMA, K, GOL, CU, PEG, NA, NAG

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	0.75	0/4778	0.87	4/6523 (0.1%)
1	B	0.75	0/4647	0.85	2/6347 (0.0%)
All	All	0.75	0/9425	0.86	6/12870 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	121	TYR	CB-CG-CD1	6.45	124.87	121.00
1	B	147	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	8	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	B	8	TYR	CB-CG-CD1	-5.58	117.65	121.00

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	4555	0	4398	30	0
1	B	4429	0	4284	28	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	39	0	34	0	0
3	F	30	0	20	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	26	0	0	0	0
5	B	26	0	0	3	0
6	A	24	0	12	1	0
6	B	32	0	16	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	54	0	72	1	0
9	B	18	0	24	0	0
10	A	7	0	10	1	0
10	B	7	0	10	2	0
11	A	900	0	0	20	0
11	B	826	0	0	16	0
All	All	11063	0	8948	60	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.

The worst 5 of 60 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:B:356[A]:ARG:CZ	11:B:714:HOH:O	1.68	1.31
1:A:383[A]:THR:HG21	11:A:870:HOH:O	1.07	1.24
1:B:186:ASN:OD1	11:B:713:HOH:O	1.53	1.20
1:B:383[A]:THR:HG21	11:B:817:HOH:O	1.03	1.20
1:B:197[B]:ASN:OD1	11:B:714:HOH:O	1.60	1.18

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	582/534 (109%)	558 (96%)	24 (4%)	0	100	100
1	B	566/534 (106%)	543 (96%)	23 (4%)	0	100	100
All	All	1148/1068 (108%)	1101 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	500/452 (111%)	494 (99%)	6 (1%)	71	54
1	B	486/452 (108%)	481 (99%)	5 (1%)	76	61
All	All	986/904 (109%)	975 (99%)	11 (1%)	76	57

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	TYR
1	B	306	ASP
1	B	326[B]	GLN
1	B	326[A]	GLN
1	A	375[A]	LEU

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 ⓘ

12 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	NAG	C	1	2,1	14,14,15	1.31	2 (14%)	17,19,21	1.50	2 (11%)
2	NAG	C	2	2	14,14,15	1.14	2 (14%)	17,19,21	1.04	1 (5%)
2	BMA	C	3	2	11,11,12	0.62	0	15,15,17	1.06	0
2	NAG	D	1	2,1	14,14,15	0.79	0	17,19,21	1.15	1 (5%)
2	NAG	D	2	2	14,14,15	1.48	2 (14%)	17,19,21	1.77	5 (29%)
2	BMA	D	3	2	11,11,12	0.38	0	15,15,17	0.78	0
2	NAG	E	1	2,1	14,14,15	1.28	2 (14%)	17,19,21	0.89	1 (5%)
2	NAG	E	2	2	14,14,15	0.85	0	17,19,21	1.06	0
2	BMA	E	3	2	11,11,12	0.60	0	15,15,17	1.25	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.93	1 (7%)	17,19,21	0.79	0
3	NAG	F	2[A]	-	14,14,15	0.82	1 (7%)	17,19,21	1.94	5 (29%)
3	NAG	F	2[B]	-	14,14,15	0.81	1 (7%)	17,19,21	1.98	6 (35%)

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	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2[A]	-	-	2/6/23/26	0/1/1/1
3	NAG	F	2[B]	-	-	1/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C1	-3.74	1.37	1.43
2	C	1	NAG	O5-C1	-3.36	1.38	1.43
2	C	1	NAG	C2-N2	-2.72	1.41	1.46
2	E	1	NAG	O5-C1	-2.58	1.39	1.43
3	F	1	NAG	C1-C2	2.43	1.56	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	C1-O5-C5	-4.47	106.14	112.19
3	F	2[A]	NAG	C1-O5-C5	-4.06	106.69	112.19
3	F	2[B]	NAG	C1-O5-C5	-4.06	106.69	112.19
2	C	1	NAG	O7-C7-C8	3.64	128.81	122.06
3	F	2[A]	NAG	O4-C4-C3	-3.61	102.00	110.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

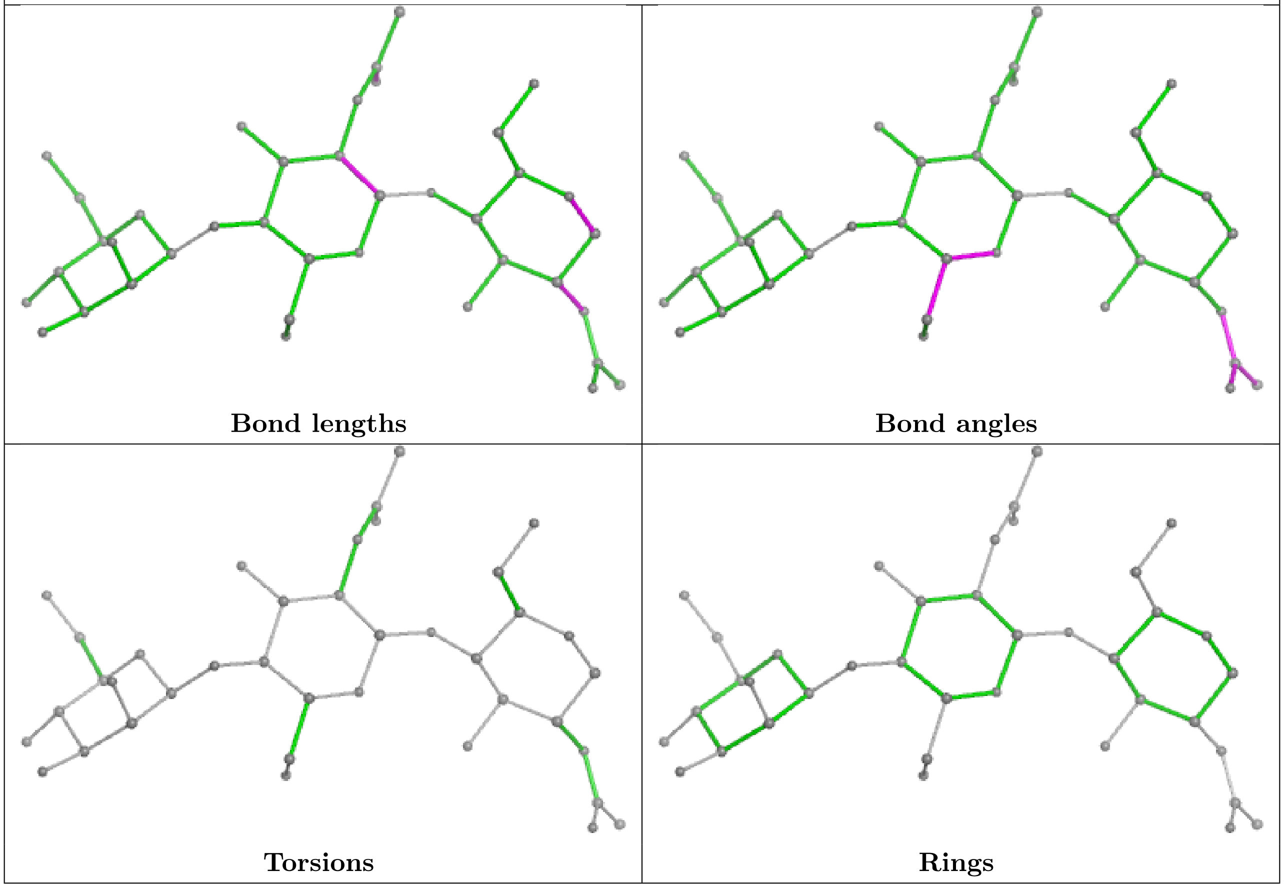
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
3	F	2[A]	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	F	2[A]	NAG	C4-C5-C6-O6
3	F	2[B]	NAG	C4-C5-C6-O6

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 C



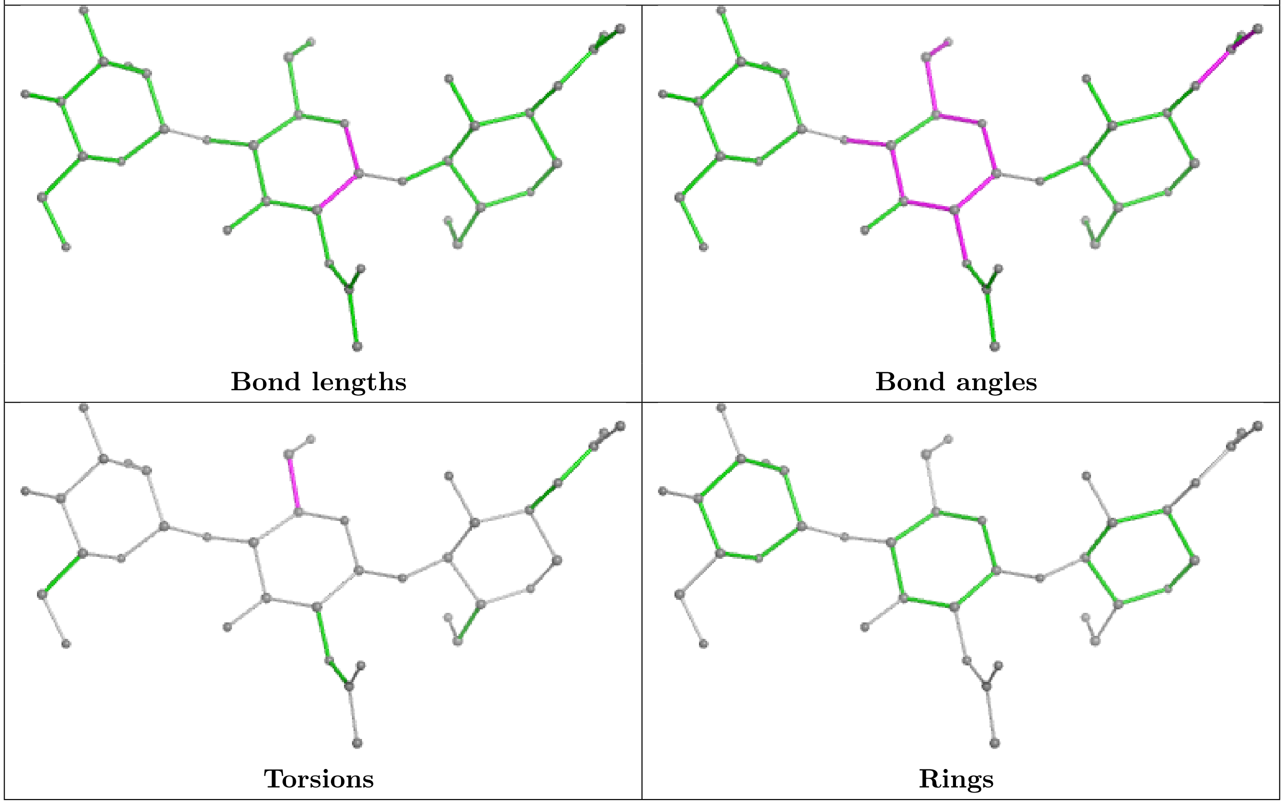
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D



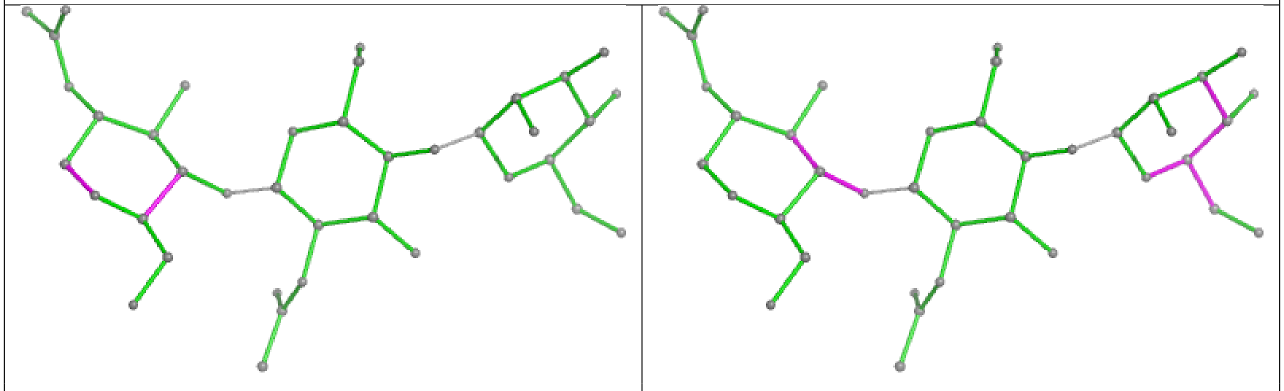
Bond lengths

Bond angles

Torsions

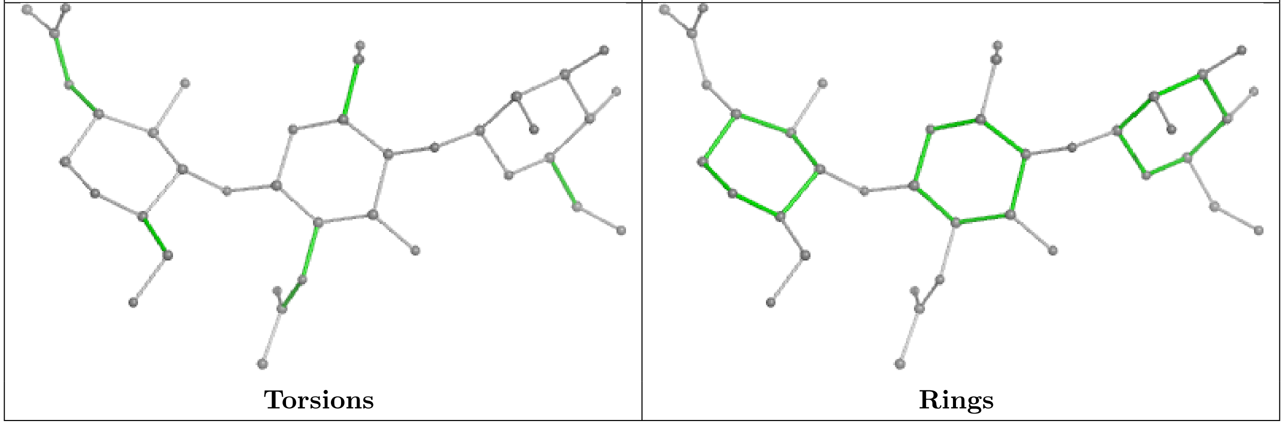
Rings

Oligosaccharide Chain E



Bond lengths

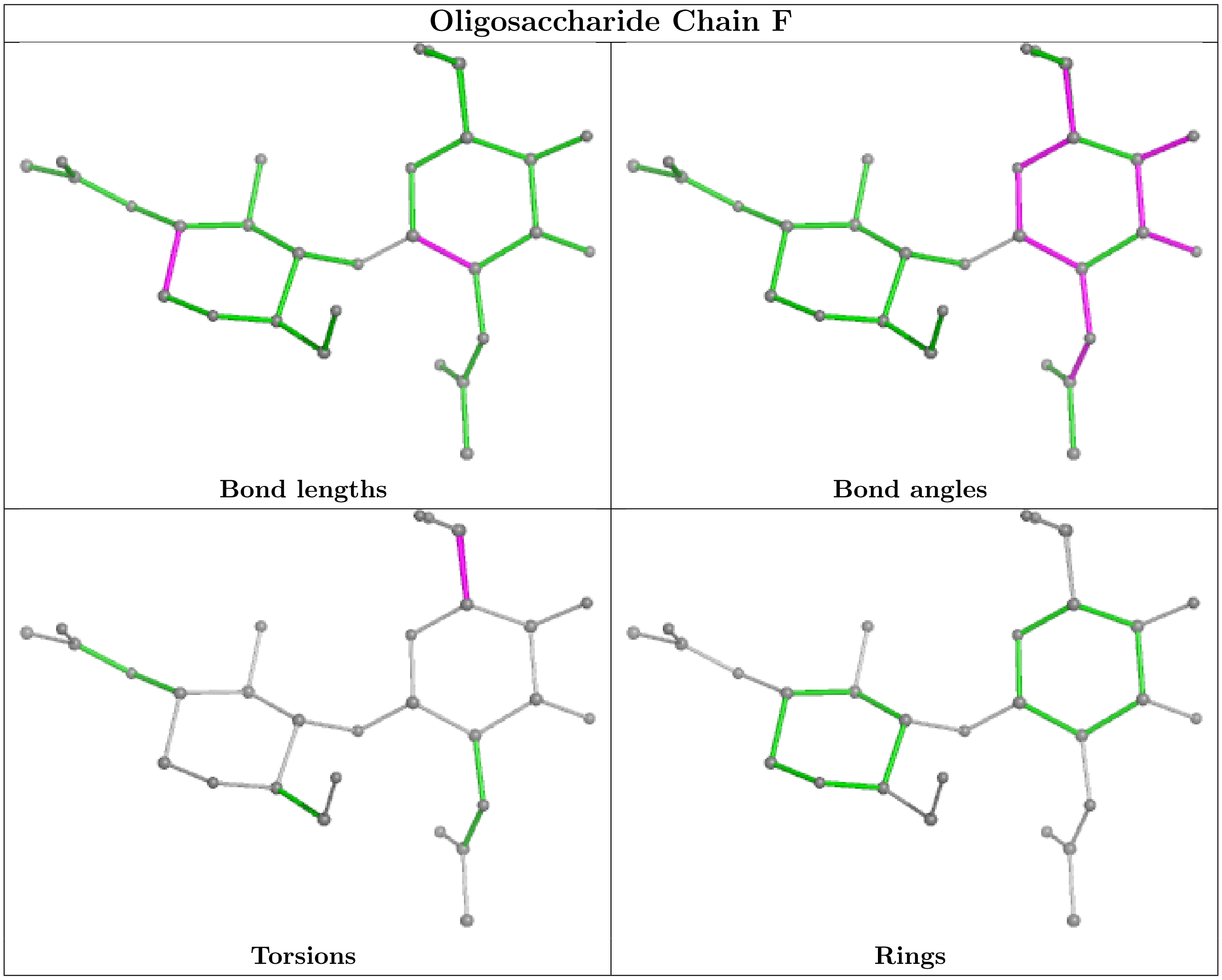
Bond angles



Torsions

Rings

Oligosaccharide Chain F



5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 12 are monoatomic - leaving 25 for Mogul analysis.

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	$\#\|Z\| > 2$
9	GOL	B	620	-	5,5,5	0.29	0	5,5,5	0.56	0
6	SIN	B	613	-	7,7,7	1.61	1 (14%)	8,8,8	1.29	1 (12%)
9	GOL	A	622[B]	-	5,5,5	0.12	0	5,5,5	0.27	0
9	GOL	A	618	-	5,5,5	0.14	0	5,5,5	0.40	0
5	FC6	B	611	-	12,12,12	0.35	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	FC6	A	611	-	12,12,12	0.67	0	-		
9	GOL	A	619	-	5,5,5	0.18	0	5,5,5	0.40	0
5	FC6	A	612	-	12,12,12	0.66	0	-		
6	SIN	B	614	-	7,7,7	1.48	1 (14%)	8,8,8	0.92	0
9	GOL	A	621	-	5,5,5	0.17	0	5,5,5	0.38	0
10	PEG	B	621	-	6,6,6	0.21	0	5,5,5	0.41	0
9	GOL	A	620[B]	-	5,5,5	0.14	0	5,5,5	0.38	0
9	GOL	A	622[A]	-	5,5,5	0.16	0	5,5,5	0.28	0
9	GOL	A	624[B]	-	5,5,5	0.11	0	5,5,5	0.24	0
9	GOL	B	619	-	5,5,5	0.16	0	5,5,5	0.45	0
6	SIN	A	615	-	7,7,7	1.18	0	8,8,8	1.29	0
5	FC6	B	610	-	12,12,12	0.63	0	-		
6	SIN	A	613	-	7,7,7	1.11	0	8,8,8	1.26	0
6	SIN	B	612	-	7,7,7	1.33	1 (14%)	8,8,8	0.98	0
9	GOL	A	620[A]	-	5,5,5	0.13	0	5,5,5	0.37	0
9	GOL	B	618	-	5,5,5	0.38	0	5,5,5	0.77	0
9	GOL	A	624[A]	-	5,5,5	0.07	0	5,5,5	0.17	0
6	SIN	A	614	-	7,7,7	1.53	1 (14%)	8,8,8	1.21	1 (12%)
10	PEG	A	623	-	6,6,6	0.32	0	5,5,5	0.44	0
6	SIN	B	615	-	7,7,7	1.24	1 (14%)	8,8,8	0.99	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
9	GOL	B	620	-	-	0/4/4/4	-
6	SIN	B	613	-	-	3/5/5/5	-
9	GOL	A	622[B]	-	-	4/4/4/4	-
9	GOL	A	618	-	-	0/4/4/4	-
9	GOL	A	619	-	-	0/4/4/4	-
6	SIN	B	614	-	-	3/5/5/5	-
9	GOL	A	621	-	-	1/4/4/4	-
10	PEG	B	621	-	-	1/4/4/4	-
9	GOL	A	620[B]	-	-	0/4/4/4	-
9	GOL	A	622[A]	-	-	2/4/4/4	-
9	GOL	A	624[B]	-	-	0/4/4/4	-
9	GOL	B	619	-	-	2/4/4/4	-
6	SIN	A	615	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SIN	A	613	-	-	0/5/5/5	-
6	SIN	B	612	-	-	1/5/5/5	-
9	GOL	A	620[A]	-	-	4/4/4/4	-
9	GOL	B	618	-	-	3/4/4/4	-
9	GOL	A	624[A]	-	-	0/4/4/4	-
6	SIN	A	614	-	-	2/5/5/5	-
10	PEG	A	623	-	-	3/4/4/4	-
6	SIN	B	615	-	-	3/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	613	SIN	O3-C4	2.88	1.31	1.22
6	B	614	SIN	O3-C4	2.84	1.31	1.22
6	B	612	SIN	O4-C4	-2.50	1.22	1.30
6	A	614	SIN	O1-C1	2.48	1.30	1.22
6	B	615	SIN	O2-C1	-2.13	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	613	SIN	C2-C3-C4	3.26	120.61	113.60
6	A	614	SIN	C3-C2-C1	2.89	119.82	113.60

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	620[A]	GOL	O1-C1-C2-C3
9	B	618	GOL	O1-C1-C2-C3
9	A	620[A]	GOL	O1-C1-C2-O2
9	A	622[B]	GOL	O1-C1-C2-O2
9	A	622[A]	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	611	FC6	2	0
10	B	621	PEG	2	0

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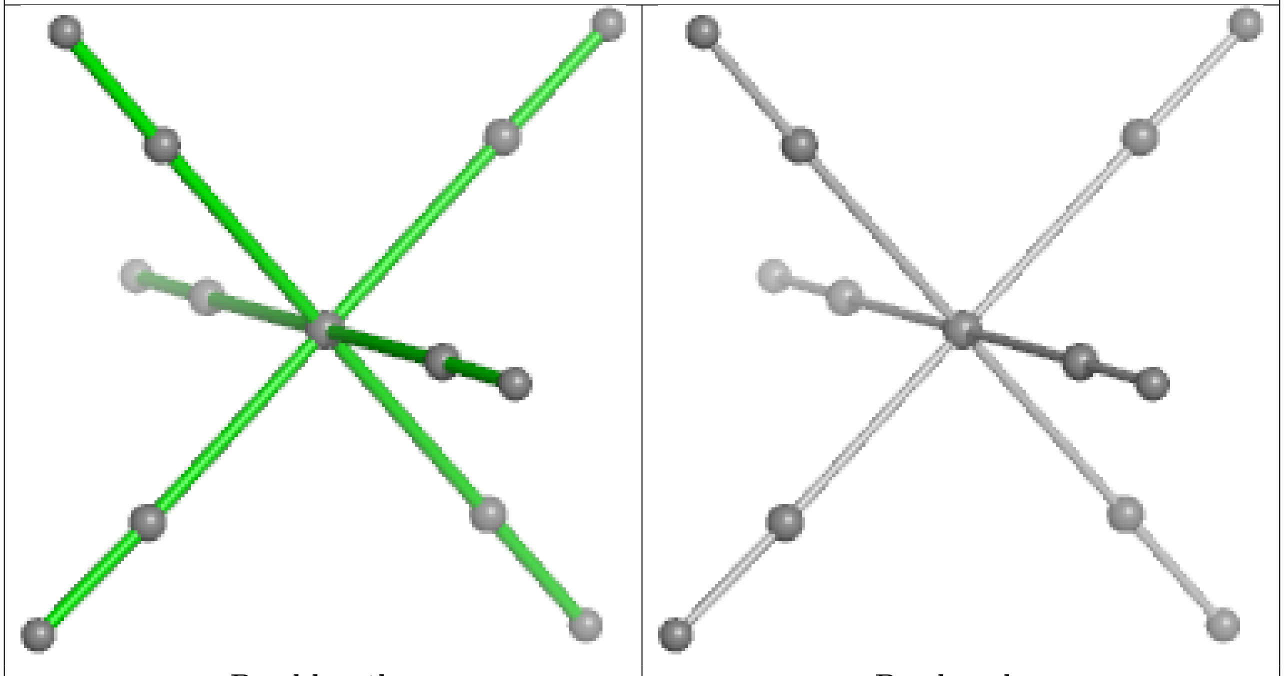
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	610	FC6	1	0
9	A	620[A]	GOL	1	0
6	A	614	SIN	1	0
10	A	623	PEG	1	0
6	B	615	SIN	4	0

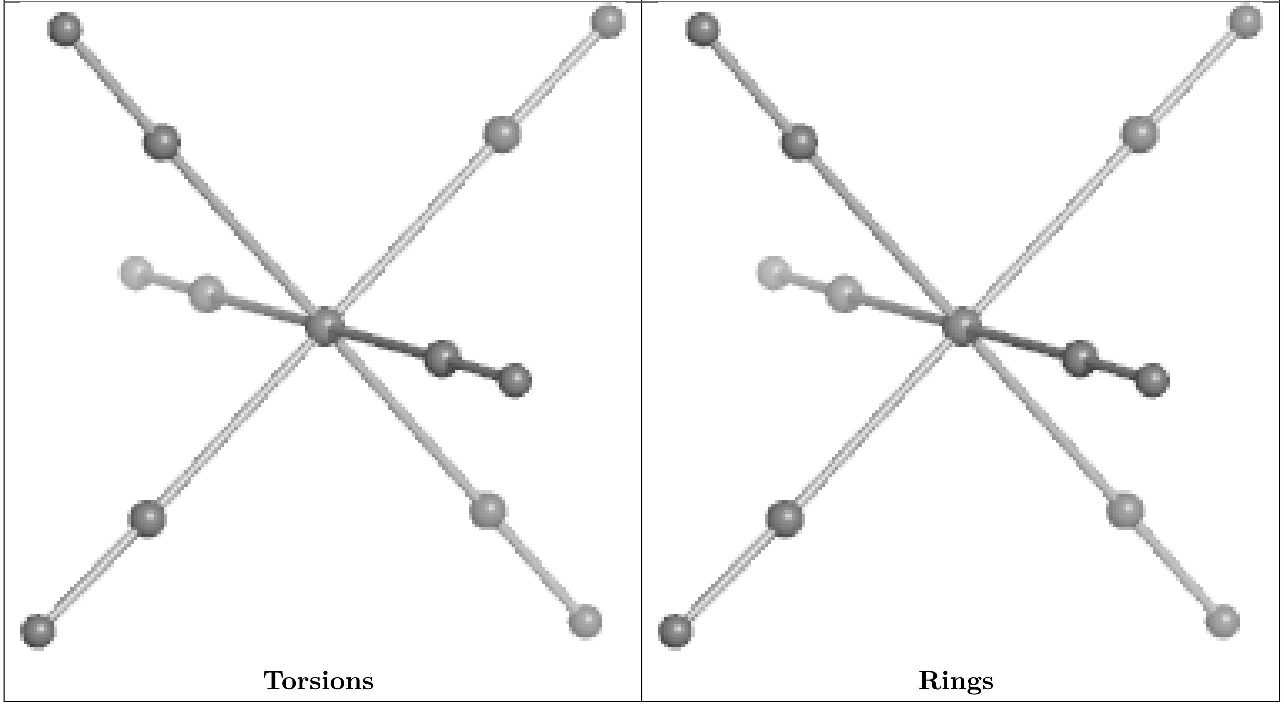
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FC6 B 611



Bond lengths

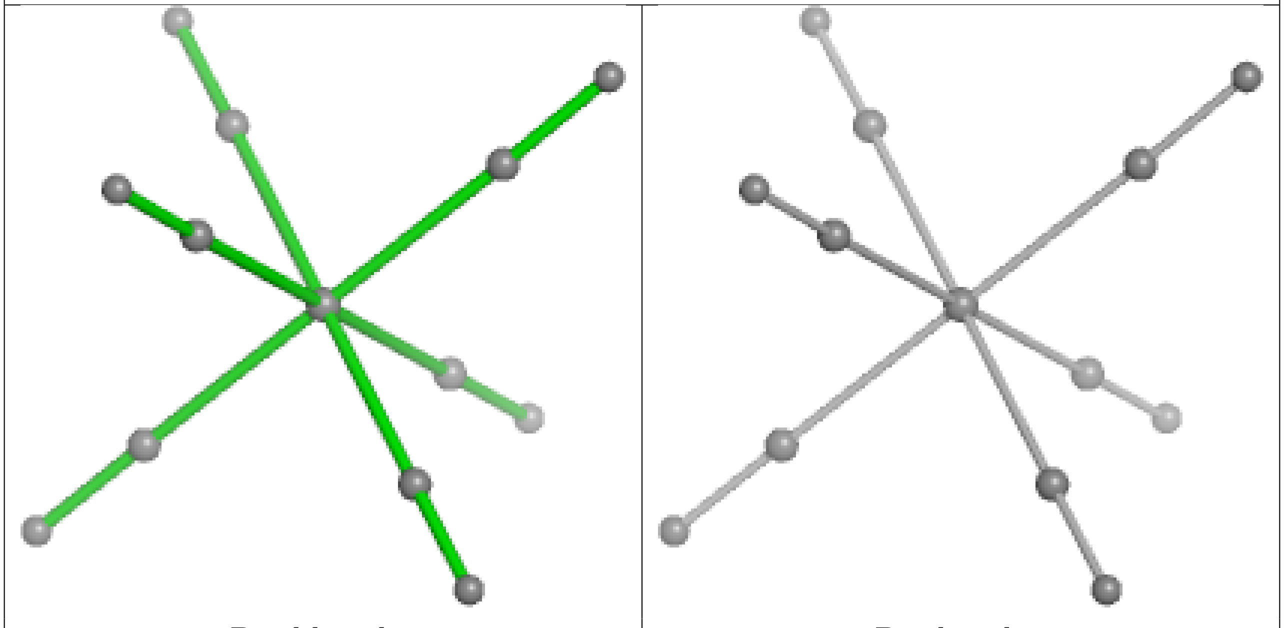
Bond angles



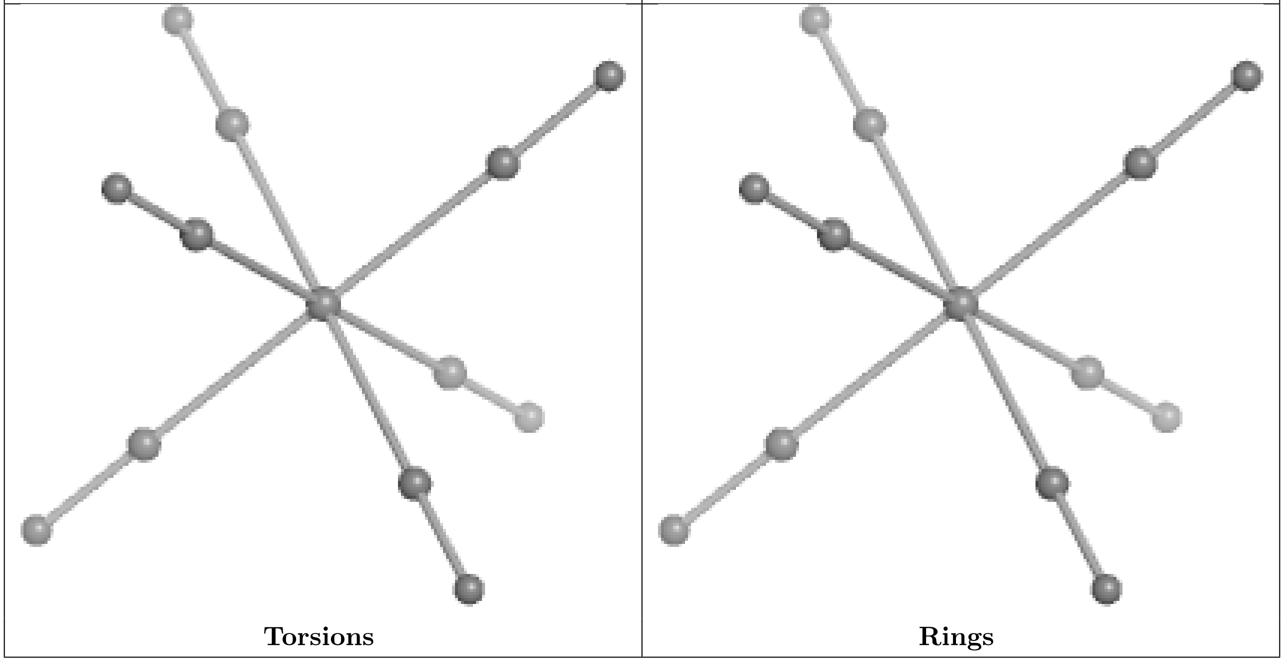
Torsions

Rings

Ligand FC6 A 611

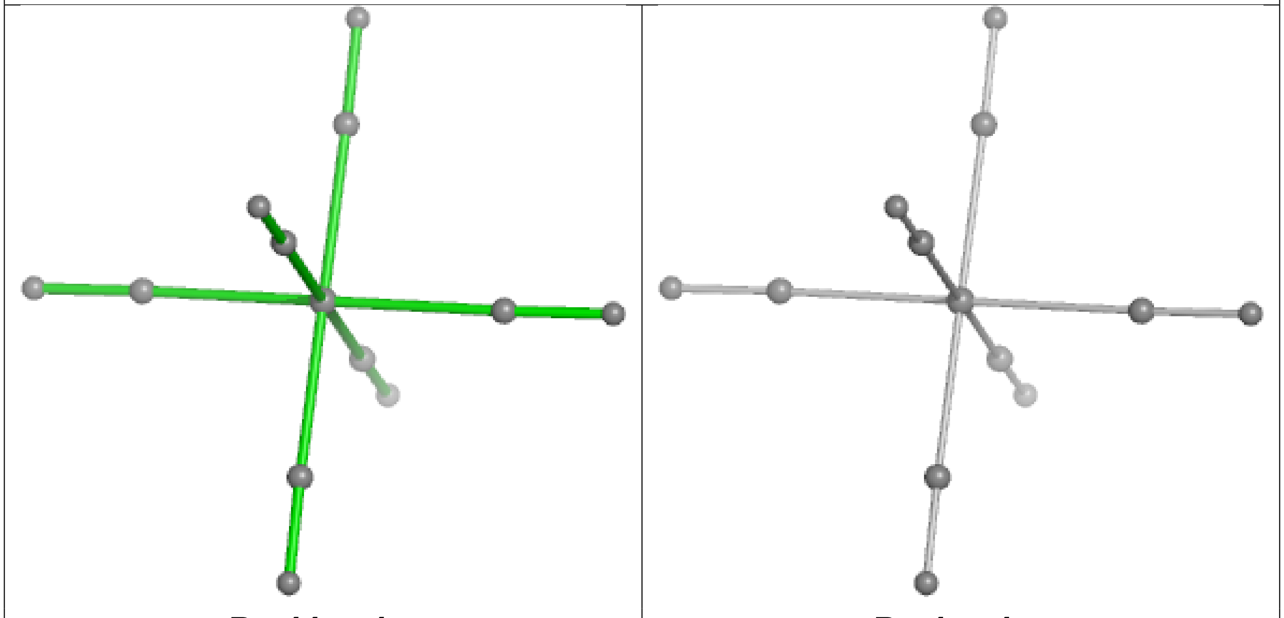


Bond lengths **Bond angles**



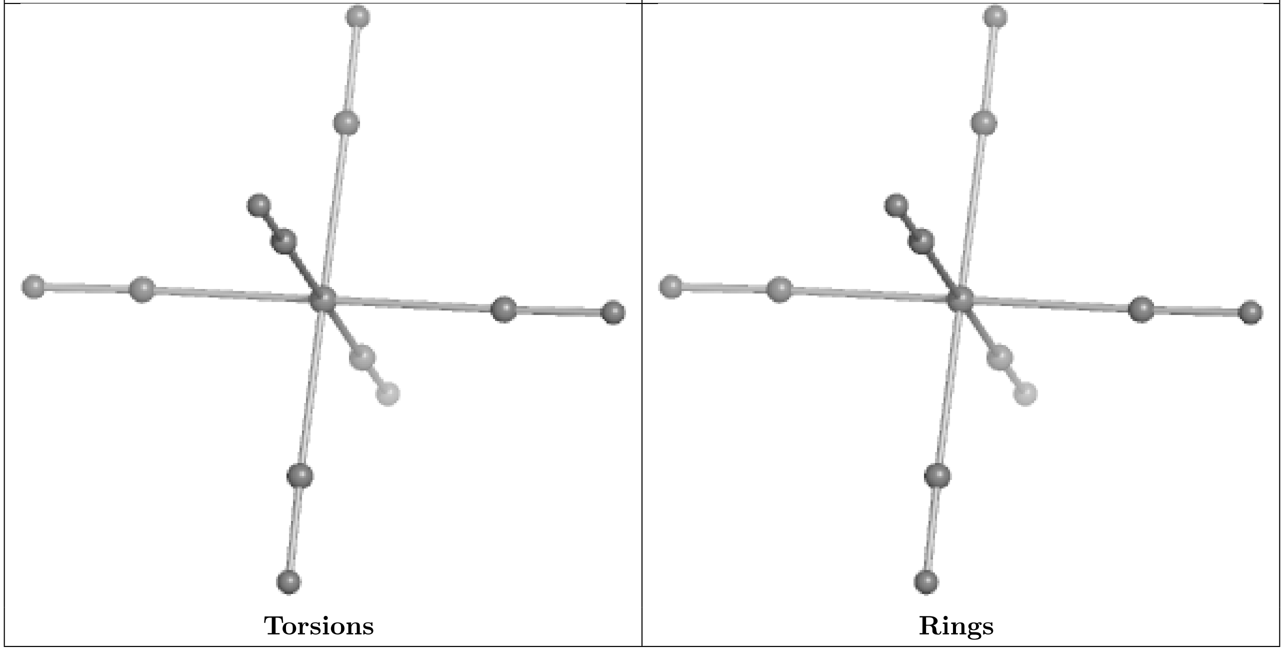
Torsions **Rings**

Ligand FC6 A 612



Bond lengths

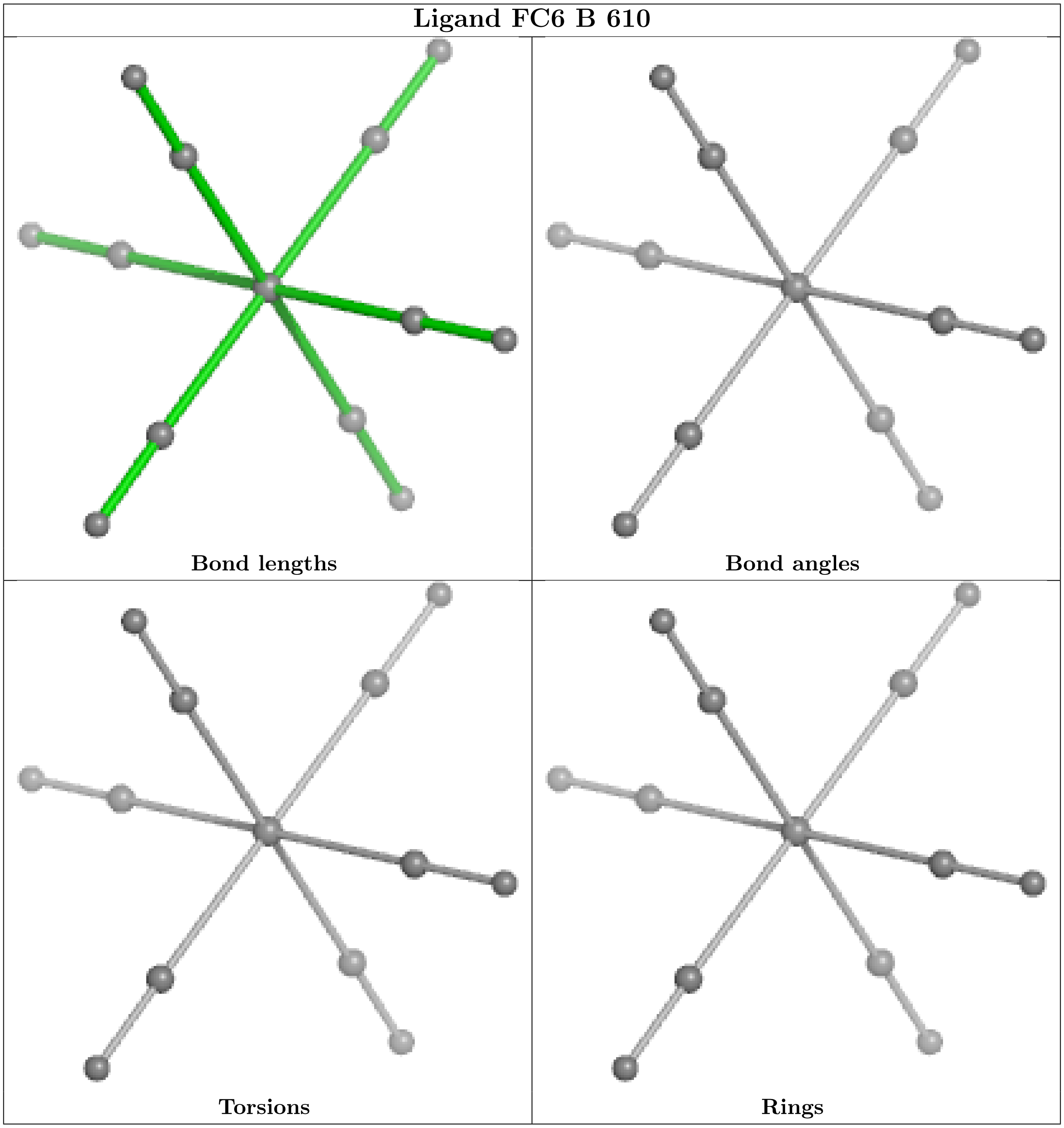
Bond angles



Torsions

Rings

Ligand FC6 B 610



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.