



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 04:16 AM GMT

PDB ID : 2C4B
Title : INHIBITOR CYSTINE KNOT PROTEIN MCOEETI FUSED TO THE
CATALYTICALLY INACTIVE BARNASE MUTANT H102A
Authors : Niemann, H.H.; Schmoldt, H.U.; Wentzel, A.; Kolmar, H.; Heinz, D.W.
Deposited on : 2005-10-18
Resolution : 1.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

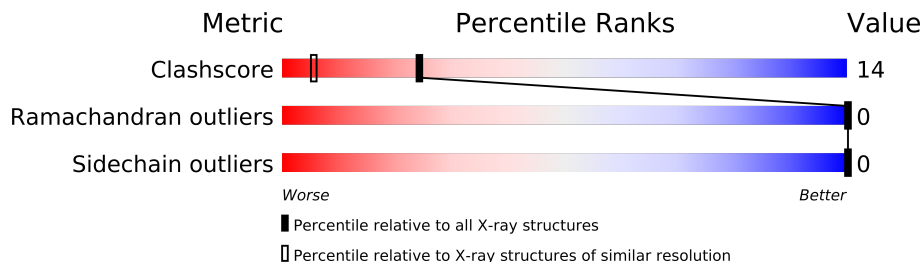
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.30 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	79885	1140 (1.34-1.26)
Ramachandran outliers	78287	1093 (1.34-1.26)
Sidechain outliers	78261	1092 (1.34-1.26)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	143	
1	B	143	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 3057 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

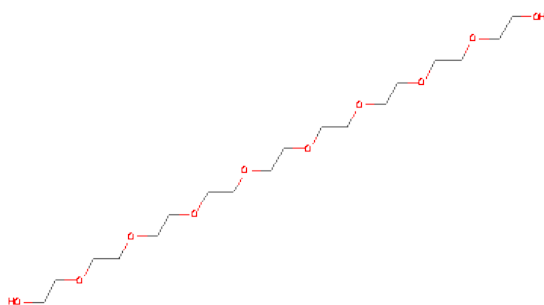
- Molecule 1 is a protein called BARNASE MCOEETI FUSION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	6	0
			1133	713	194	219	7			
1	B	142	Total	C	N	O	S	0	14	0
			1178	739	208	224	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	HIS	ENGINEERED MUTATION	UNP P00648
B	102	ALA	HIS	ENGINEERED MUTATION	UNP P00648

- Molecule 2 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	14	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	1
			20	12	8		
2	B	1	Total	C	O	0	1
			12	7	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



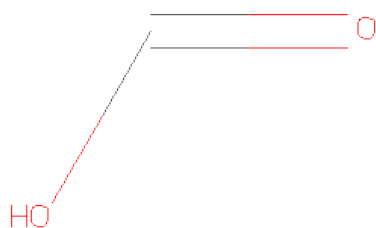
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



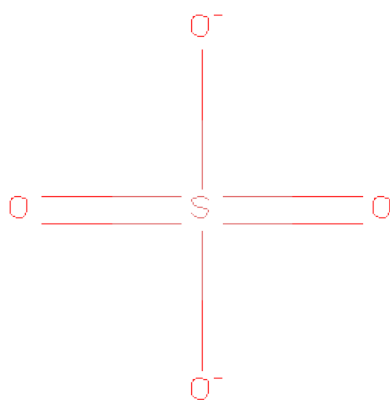
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	1
			5	2	3		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	1
			8	4	4		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	1
			4	1	3		

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



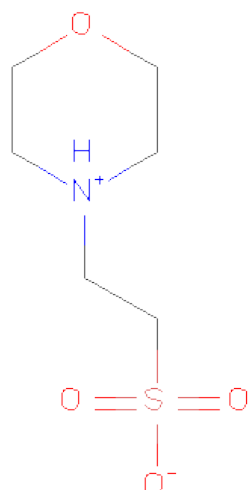
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	15	Total	X	0	0
			15	15		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	257	Total	O	0	0
			257	257		
9	B	249	Total	O	0	0
			249	249		
9	D	3	Total	O	0	0
			3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: BARNASE MCOEETI FUSION

Chain A: 



- Molecule 1: BARNASE MCOEETI FUSION

Chain B: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	74.02Å 217.71Å 58.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 1.30	Depositor
% Data completeness (in resolution range)	100.0 (39.84-1.30)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.132 , 0.164	Depositor
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.318	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 114402 reflections	Xtriage
Total number of atoms	3057	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, UNX, FMT, EDO, 2PE, SO4, MES

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	0.92	1/1174 (0.1%)	0.97	1/1582 (0.1%)
1	B	0.84	2/1239 (0.2%)	0.90	1/1663 (0.1%)
All	All	0.88	3/2413 (0.1%)	0.94	2/3245 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	SER	CB-OG	-5.63	1.34	1.42
1	A	3	VAL	CB-CG1	-5.21	1.42	1.52
1	B	3	VAL	CB-CG1	-5.05	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	12	ASP	CB-CG-OD2	-5.70	113.17	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1133	0	0	6	0
1	B	1178	0	0	5	0
2	A	28	0	0	0	0
2	B	32	0	0	3	0
3	A	6	0	0	1	0
4	A	21	0	0	2	0
4	B	28	0	0	0	0
5	A	6	0	0	0	0
5	B	4	0	0	0	0
6	A	35	0	0	1	0
6	B	50	0	0	7	0
7	B	12	0	0	1	0
8	D	15	0	0	12	0
9	A	257	0	0	2	0
9	B	249	0	0	9	0
9	D	3	0	0	0	0
All	All	3057	0	0	32	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 32 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:104[B]:GLN:NE2	9:B:2164:HOH:O	1.92	1.01
6:B:1155:SO4:O1	9:B:2215:HOH:O	1.86	0.92
6:B:1165:SO4:O1	9:B:2230:HOH:O	1.88	0.91
6:B:1171:SO4:S	6:B:1172:SO4:O4	2.35	0.83
6:A:1163:SO4:O3	1:B:125[C]:ARG:NH2	2.13	0.82

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	147/143 (103%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	154/143 (108%)	149 (97%)	5 (3%)	0	100	100
All	All	301/286 (105%)	289 (96%)	12 (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	125/119 (105%)	125 (100%)	0	100	100
1	B	133/119 (112%)	133 (100%)	0	100	100
All	All	258/238 (108%)	258 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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 chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 15 are unknown and 4 are modelled with single atom - leaving 38 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
2	2PE	A	1145	-	20,20,27	0.62	0	18,19,26	0.95	0
2	2PE	A	1146	-	6,6,27	0.85	0	5,5,26	0.72	0
3	GOL	A	1148	4	5,5,5	0.41	0	5,5,5	0.97	0
4	EDO	A	1153	-	3,3,3	0.61	0	2,2,2	0.50	0
4	EDO	A	1154[A]	3	3,3,3	0.68	0	2,2,2	0.24	0
4	EDO	A	1154[B]	-	3,3,3	0.43	0	2,2,2	0.84	0
4	EDO	A	1156	-	3,3,3	0.79	0	2,2,2	0.47	0
5	FMT	A	1157	-	2,2,2	0.47	0	1,1,1	0.34	0
5	FMT	A	1158	-	2,2,2	0.57	0	1,1,1	0.16	0
6	SO4	A	1159	-	4,4,4	0.73	0	6,6,6	0.43	0
6	SO4	A	1160	-	4,4,4	0.49	0	6,6,6	0.71	0
6	SO4	A	1161	-	4,4,4	0.53	0	6,6,6	0.28	0
6	SO4	A	1162	-	4,4,4	0.25	0	6,6,6	0.19	0
6	SO4	A	1163	-	4,4,4	0.19	0	6,6,6	0.39	0
6	SO4	A	1164	-	4,4,4	0.54	0	6,6,6	0.67	0
6	SO4	A	1165	-	4,4,4	0.46	0	6,6,6	0.83	0
6	SO4	B	1155	-	4,4,4	0.70	0	6,6,6	0.40	0
2	2PE	B	1156[A]	-	3,3,27	1.60	0	2,2,26	1.31	0
2	2PE	B	1156[B]	-	3,3,27	1.01	0	2,2,26	0.60	0
2	2PE	B	1157[A]	-	3,4,27	1.14	0	2,3,26	1.16	0
2	2PE	B	1157[B]	-	3,4,27	0.73	0	2,3,26	1.22	0
7	MES	B	1158	6	12,12,12	1.97	1 (8%)	16,16,16	1.90	7 (43%)
4	EDO	B	1159	-	3,3,3	0.56	0	2,2,2	0.24	0
4	EDO	B	1160	-	3,3,3	1.59	0	2,2,2	2.61	2 (100%)
4	EDO	B	1161	-	3,3,3	0.62	0	2,2,2	0.61	0
4	EDO	B	1162	-	3,3,3	0.52	0	2,2,2	0.41	0
4	EDO	B	1163[A]	-	3,3,3	0.65	0	2,2,2	0.24	0
4	EDO	B	1163[B]	-	3,3,3	0.55	0	2,2,2	0.18	0
4	EDO	B	1164	-	3,3,3	0.60	0	2,2,2	0.37	0
6	SO4	B	1165	-	4,4,4	0.85	0	6,6,6	0.70	0
6	SO4	B	1166	-	4,4,4	0.69	0	6,6,6	0.46	0
6	SO4	B	1167	-	4,4,4	0.37	0	6,6,6	0.41	0
6	SO4	B	1168	-	4,4,4	0.20	0	6,6,6	0.17	0
6	SO4	B	1169	1,7	4,4,4	1.17	0	6,6,6	0.74	0
6	SO4	B	1170	-	4,4,4	0.30	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	B	1171	6	4,4,4	0.43	0	6,6,6	0.77	0
6	SO4	B	1172	6	4,4,4	0.30	0	6,6,6	0.69	0
6	SO4	B	1173	-	4,4,4	0.28	0	6,6,6	0.51	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
2	2PE	A	1145	-	-	0/18/18/25	0/0/0/0
2	2PE	A	1146	-	-	0/4/4/25	0/0/0/0
3	GOL	A	1148	4	-	0/4/4/4	0/0/0/0
4	EDO	A	1153	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1154[A]	3	-	0/1/1/1	0/0/0/0
4	EDO	A	1154[B]	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1156	-	-	0/1/1/1	0/0/0/0
5	FMT	A	1157	-	-	0/0/0/0	0/0/0/0
5	FMT	A	1158	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1159	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1160	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1161	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1162	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1163	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1164	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1165	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1155	-	-	0/0/0/0	0/0/0/0
2	2PE	B	1156[A]	-	-	0/1/1/25	0/0/0/0
2	2PE	B	1156[B]	-	-	0/1/1/25	0/0/0/0
2	2PE	B	1157[A]	-	-	0/2/2/25	0/0/0/0
2	2PE	B	1157[B]	-	-	0/2/2/25	0/0/0/0
7	MES	B	1158	6	-	0/6/14/14	1/1/1/1
4	EDO	B	1159	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1160	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1161	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1162	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1163[A]	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1163[B]	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1164	-	-	0/1/1/1	0/0/0/0
6	SO4	B	1165	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1166	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1167	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1168	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	1169	1,7	-	0/0/0/0	0/0/0/0
6	SO4	B	1170	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1171	6	-	0/0/0/0	0/0/0/0
6	SO4	B	1172	6	-	0/0/0/0	0/0/0/0
6	SO4	B	1173	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1158	MES	C8-S	-5.94	1.67	1.78

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1158	MES	O1-C2-C3	3.08	115.02	111.34
4	B	1160	EDO	O1-C1-C2	-2.92	91.73	112.13
7	B	1158	MES	C7-N4-C5	2.82	119.04	111.66
7	B	1158	MES	C8-C7-N4	2.70	117.05	112.44
7	B	1158	MES	O2S-S-O1S	-2.67	107.28	112.44

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1158	MES	C2-C3-C5-C6-N4-O1

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 will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.