



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:01 PM UTC

PDB ID : 1SXN / pdb_00001sxn
Title : REDUCED BOVINE SUPEROXIDE DISMUTASE AT PH 5.0
Authors : Ferraroni, M.; Rypniewski, W.R.; Bruni, B.; Orioli, P.; Wilson, K.S.; Mangani, S.
Deposited on : 1997-09-17
Resolution : 1.90 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

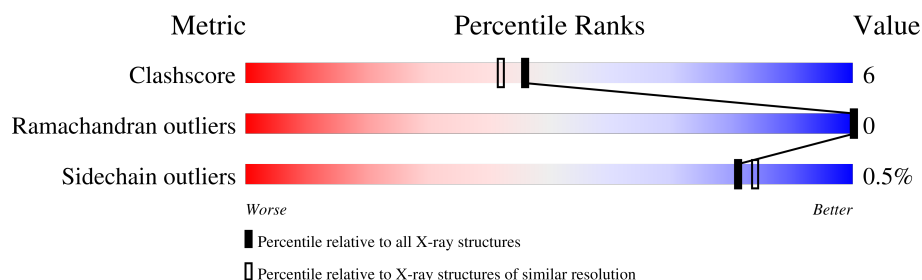
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	151	 66% 31% .
1	B	151	 70% 26% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2508 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 CU, ZN SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	1	0
			1076	661	191	220	4			
1	B	151	Total	C	N	O	S	0	0	0
			1058	651	188	215	4			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

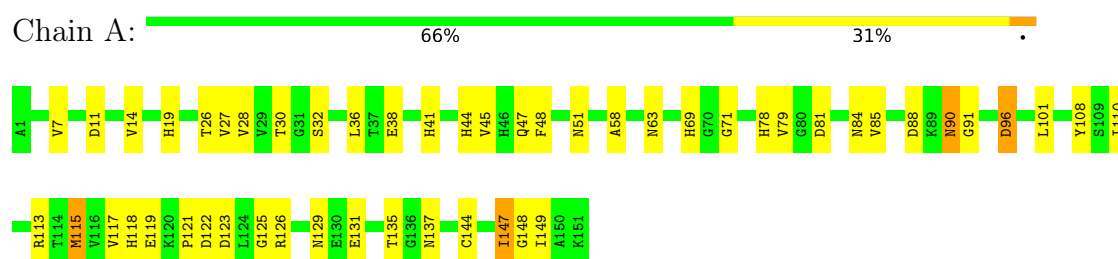
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	248	Total 248	O 248	0	0
5	B	120	Total 120	O 120	0	0

3 Residue-property plots

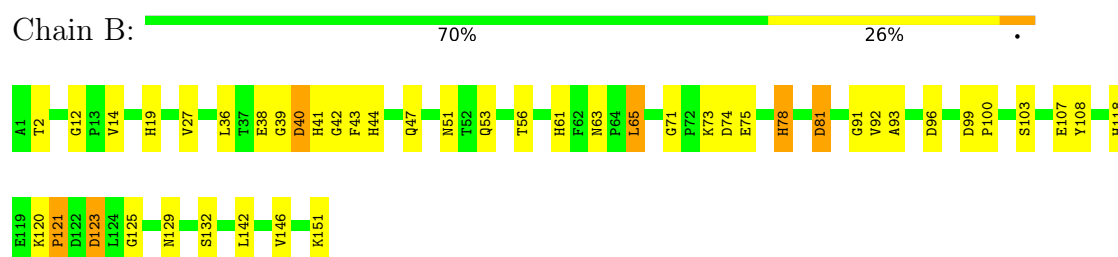
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: CU, ZN SUPEROXIDE DISMUTASE



• Molecule 1: CU, ZN SUPEROXIDE DISMUTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.69Å 197.80Å 50.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	98.0 (10.00-1.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.95	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2508	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: CA, CU, ZN

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	1.41	8/1099 (0.7%)	2.46	68/1489 (4.6%)
1	B	1.06	2/1076 (0.2%)	2.25	48/1459 (3.3%)
All	All	1.25	10/2175 (0.5%)	2.36	116/2948 (3.9%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	HIS	ND1-CE1	7.34	1.39	1.32
1	A	78	HIS	CG-ND1	7.14	1.46	1.38
1	A	78	HIS	CE1-NE2	-5.75	1.26	1.32
1	B	44	HIS	CG-CD2	5.54	1.42	1.35
1	A	81	ASP	CA-C	-5.46	1.45	1.52
1	A	79	VAL	C-N	5.29	1.41	1.33
1	A	118	HIS	ND1-CE1	5.29	1.37	1.32
1	A	135	THR	CA-C	-5.17	1.45	1.52
1	A	125	GLY	C-N	-5.08	1.27	1.33
1	A	41	HIS	C-N	-5.04	1.29	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	HIS	CB-CG-CD2	-9.39	118.99	131.20
1	A	79	VAL	O-C-N	-9.26	112.89	121.87
1	A	147	ILE	CA-C-N	-8.95	114.50	122.47
1	A	147	ILE	C-N-CA	-8.95	114.50	122.47
1	A	47	GLN	N-CA-C	8.91	120.60	111.07
1	A	79	VAL	CA-C-O	8.76	130.06	120.95
1	A	84	ASN	OD1-CG-ND2	-8.55	114.05	122.60
1	B	27	VAL	N-CA-C	-8.46	95.93	108.12
1	B	96	ASP	N-CA-CB	8.42	125.97	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ASN	N-CA-CB	-8.33	101.30	110.71
1	A	118	HIS	CB-CG-CD2	-8.29	120.42	131.20
1	A	96	ASP	CA-CB-CG	-8.09	104.51	112.60
1	B	121	PRO	N-CA-CB	8.02	110.79	103.33
1	B	19	HIS	CA-CB-CG	-7.54	106.26	113.80
1	B	63	ASN	OD1-CG-ND2	7.50	130.10	122.60
1	A	38	GLU	CA-C-O	-7.48	113.36	121.44
1	B	92	VAL	CA-C-O	7.40	128.66	120.59
1	A	81	ASP	CB-CG-OD1	7.22	135.01	118.40
1	B	103	SER	N-CA-CB	-7.22	99.13	111.69
1	B	47	GLN	CA-C-O	-7.20	113.28	120.70
1	B	108	TYR	CA-C-O	-7.17	110.77	119.59
1	B	129	ASN	N-CA-CB	7.17	123.94	111.39
1	A	137	ASN	OD1-CG-ND2	-7.17	115.43	122.60
1	A	27	VAL	O-C-N	-7.13	115.56	123.26
1	A	58	ALA	O-C-N	-7.05	112.73	122.46
1	B	44	HIS	CB-CG-ND1	6.97	133.16	122.70
1	A	85	VAL	N-CA-C	-6.87	98.44	108.89
1	A	123	ASP	CA-C-O	6.85	127.72	119.43
1	B	75	GLU	CA-C-O	6.73	128.21	120.00
1	A	148	GLY	O-C-N	-6.72	117.45	123.29
1	A	11	ASP	CA-CB-CG	-6.66	105.94	112.60
1	A	26	THR	CA-CB-OG1	-6.64	99.64	109.60
1	A	90	ASN	CA-CB-CG	-6.57	106.03	112.60
1	A	126	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	A	115	MET	CA-CB-CG	6.48	127.06	114.10
1	B	78	HIS	O-C-N	-6.45	115.50	122.85
1	A	101	LEU	O-C-N	6.44	130.99	122.36
1	B	41	HIS	O-C-N	6.41	130.81	123.31
1	A	137	ASN	CB-CG-ND2	6.39	125.99	116.40
1	A	149	ILE	O-C-N	-6.36	115.67	122.61
1	A	117	VAL	N-CA-CB	6.34	119.88	111.25
1	B	120	LYS	CA-C-N	6.33	126.24	119.85
1	B	120	LYS	C-N-CA	6.33	126.24	119.85
1	A	149	ILE	CA-CB-CG1	-6.29	99.70	110.40
1	A	101	LEU	CA-C-O	-6.29	112.13	119.24
1	B	56	THR	CA-CB-OG1	6.26	119.00	109.60
1	A	14	VAL	CA-C-N	-6.25	110.94	121.75
1	A	14	VAL	C-N-CA	-6.25	110.94	121.75
1	A	28	VAL	O-C-N	6.24	129.96	123.03
1	A	81	ASP	OD1-CG-OD2	-6.23	107.94	122.90
1	A	30	THR	CA-C-N	-6.15	113.84	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	THR	C-N-CA	-6.15	113.84	121.83
1	A	44	HIS	O-C-N	6.14	130.59	123.17
1	A	81	ASP	O-C-N	6.13	130.47	122.68
1	A	110	ILE	CA-CB-CG2	-6.09	100.15	110.50
1	A	78	HIS	ND1-CE1-NE2	6.07	114.47	108.40
1	B	107	GLU	N-CA-C	6.02	117.84	111.28
1	B	47	GLN	N-CA-C	6.00	117.61	111.14
1	B	121	PRO	CA-C-O	5.87	128.83	121.67
1	A	135	THR	CA-C-O	5.86	125.65	119.03
1	B	53	GLN	O-C-N	5.84	129.59	121.83
1	B	146	VAL	O-C-N	-5.83	115.84	122.72
1	A	69	HIS	CB-CG-ND1	5.82	131.43	122.70
1	B	108	TYR	O-C-N	5.80	129.80	122.37
1	B	43	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	108	TYR	N-CA-C	-5.78	106.45	112.93
1	B	61	HIS	CA-CB-CG	-5.75	108.05	113.80
1	A	129	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	126	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	B	129	ASN	N-CA-C	-5.67	99.81	108.76
1	A	81	ASP	CA-C-O	-5.65	115.05	120.92
1	B	74	ASP	CA-C-O	-5.64	115.16	121.81
1	A	44	HIS	CA-C-O	-5.62	115.05	121.40
1	B	42	GLY	O-C-N	5.60	129.97	122.70
1	A	28	VAL	CA-C-O	-5.59	114.58	120.57
1	A	19	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	131	GLU	CB-CG-CD	-5.59	103.09	112.60
1	B	71	GLY	CA-C-N	5.56	125.22	119.05
1	B	71	GLY	C-N-CA	5.56	125.22	119.05
1	A	71	GLY	CA-C-N	5.54	125.37	119.28
1	A	71	GLY	C-N-CA	5.54	125.37	119.28
1	A	108	TYR	CA-CB-CG	-5.52	103.96	113.90
1	B	118	HIS	N-CA-C	5.50	118.60	110.46
1	A	118	HIS	CB-CG-ND1	5.49	130.94	122.70
1	B	123	ASP	CA-C-O	5.48	126.30	119.12
1	B	2	THR	CA-C-O	-5.47	112.88	118.90
1	B	71	GLY	N-CA-C	-5.45	101.23	112.34
1	A	123	ASP	O-C-N	-5.44	115.37	122.39
1	A	119	GLU	N-CA-CB	-5.41	102.15	110.16
1	A	121	PRO	O-C-N	-5.39	116.32	123.01
1	A	47	GLN	O-C-N	5.39	127.62	122.07
1	A	27	VAL	CA-C-N	5.38	129.71	122.93
1	A	27	VAL	C-N-CA	5.38	129.71	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	VAL	CA-C-N	-5.38	114.61	122.19
1	A	7	VAL	C-N-CA	-5.38	114.61	122.19
1	A	113	ARG	O-C-N	-5.38	115.01	122.76
1	B	12	GLY	CA-C-O	5.35	129.17	121.52
1	B	123	ASP	O-C-N	-5.29	114.56	122.39
1	A	32	SER	CA-C-O	5.26	126.68	120.89
1	A	48	PHE	CA-C-O	5.24	126.62	120.80
1	A	144	CYS	CA-C-O	-5.24	115.62	121.23
1	A	69	HIS	ND1-CG-CD2	-5.24	100.86	106.10
1	B	78	HIS	N-CA-CB	-5.22	102.52	110.45
1	B	93	ALA	O-C-N	-5.21	117.14	123.29
1	B	123	ASP	CA-C-N	5.20	131.21	123.05
1	B	123	ASP	C-N-CA	5.20	131.21	123.05
1	B	81	ASP	CB-CG-OD1	5.18	130.32	118.40
1	A	144	CYS	O-C-N	5.14	128.92	123.42
1	B	56	THR	N-CA-CB	5.11	117.72	110.16
1	B	63	ASN	N-CA-CB	-5.08	104.19	110.79
1	A	122	ASP	N-CA-C	-5.05	101.08	109.46
1	A	88	ASP	CA-C-N	5.04	127.53	120.28
1	A	88	ASP	C-N-CA	5.04	127.53	120.28
1	B	65	LEU	CA-C-N	5.04	129.97	122.82
1	B	65	LEU	C-N-CA	5.04	129.97	122.82
1	B	40	ASP	CA-CB-CG	-5.03	107.57	112.60

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	A	1076	0	1017	11	0
1	B	1058	0	994	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	248	0	0	4	0
5	B	120	0	0	3	1
All	All	2508	0	2011	24	1

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 6.

All (24) 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:45:VAL:HG22	1:A:115:MET:HE1	1.32	1.09
1:A:51:ASN:HB2	5:A:471:HOH:O	1.82	0.79
1:B:14:VAL:HG21	1:B:142:LEU:HB3	1.74	0.70
1:B:151:LYS:NZ	5:B:184:HOH:O	2.20	0.69
1:A:96:ASP:OD1	5:A:515:HOH:O	2.11	0.69
1:A:115:MET:CE	1:A:147:ILE:HD11	2.23	0.68
1:B:51:ASN:HB2	5:B:163:HOH:O	1.93	0.67
1:A:115:MET:HE3	1:A:147:ILE:HD11	1.78	0.66
1:A:115:MET:HE2	1:A:115:MET:HA	1.81	0.63
1:A:115:MET:HE2	1:A:115:MET:CA	2.29	0.62
1:B:65:LEU:HD12	5:B:219:HOH:O	2.00	0.62
1:B:36:LEU:O	1:B:91:GLY:HA2	2.00	0.61
1:A:45:VAL:HG22	1:A:115:MET:CE	2.20	0.58
1:A:96:ASP:CG	5:A:515:HOH:O	2.50	0.55
1:B:78:HIS:HB2	1:B:81:ASP:CG	2.33	0.53
1:A:90:ASN:HB3	5:A:502:HOH:O	2.12	0.49
1:B:36:LEU:O	1:B:91:GLY:CA	2.61	0.49
1:B:99:ASP:HA	1:B:100:PRO:HD3	1.69	0.47
1:B:123:ASP:OD1	1:B:132:SER:OG	2.33	0.44
1:B:14:VAL:HG21	1:B:142:LEU:HD13	1.99	0.44
1:B:40:ASP:CB	1:B:121:PRO:HB3	2.49	0.43
1:A:36:LEU:O	1:A:91:GLY:HA2	2.19	0.42
1:B:38:GLU:HG2	1:B:39:GLY:N	2.35	0.41
1:B:125:GLY:HA2	1:B:132:SER:O	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:203:HOH:O	5:B:203:HOH:O[4_556]	2.07	0.13

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	150/151 (99%)	148 (99%)	2 (1%)	0	100	100
1	B	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
All	All	299/302 (99%)	290 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	111/117 (95%)	111 (100%)	0	100	100
1	B	107/117 (92%)	106 (99%)	1 (1%)	70	73
All	All	218/234 (93%)	217 (100%)	1 (0%)	81	84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	B	53	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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.