



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 05:39 AM UTC

PDB ID : 1BXZ / pdb_00001bxz
Title : CRYSTAL STRUCTURE OF A THERMOPHILIC ALCOHOL DEHYDROGENASE SUBSTRATE COMPLEX FROM THERMOANAEROBACTER BROCKII
Authors : Li, C.; Heatwole, J.; Soelaiman, S.; Shoham, M.
Deposited on : 1998-10-09
Resolution : 2.99 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

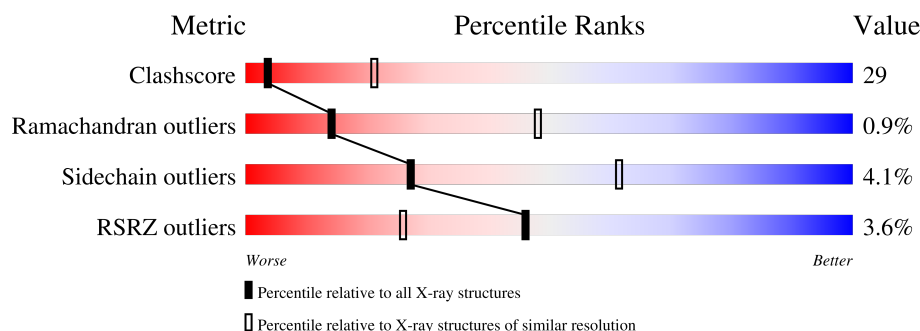
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	2% 53% 41% 6%
1	B	352	6% 54% 41% 5%
1	C	352	4% 51% 43% 6%
1	D	352	3% 51% 42% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10852 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 NADP-DEPENDENT ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2643	1693	455	476	19			
1	B	352	Total	C	N	O	S	0	0	0
			2643	1693	455	476	19			
1	C	352	Total	C	N	O	S	0	0	0
			2643	1693	455	476	19			
1	D	352	Total	C	N	O	S	0	0	0
			2643	1693	455	476	19			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

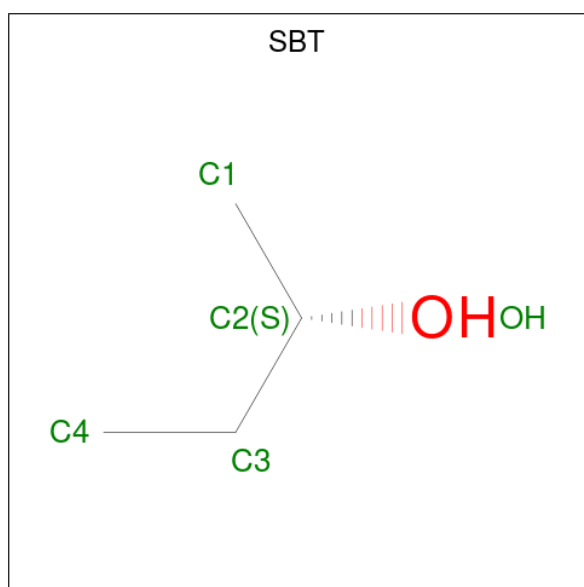
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-BUTANOL (CCD ID: SBT) (formula: C₄H₁₀O).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		

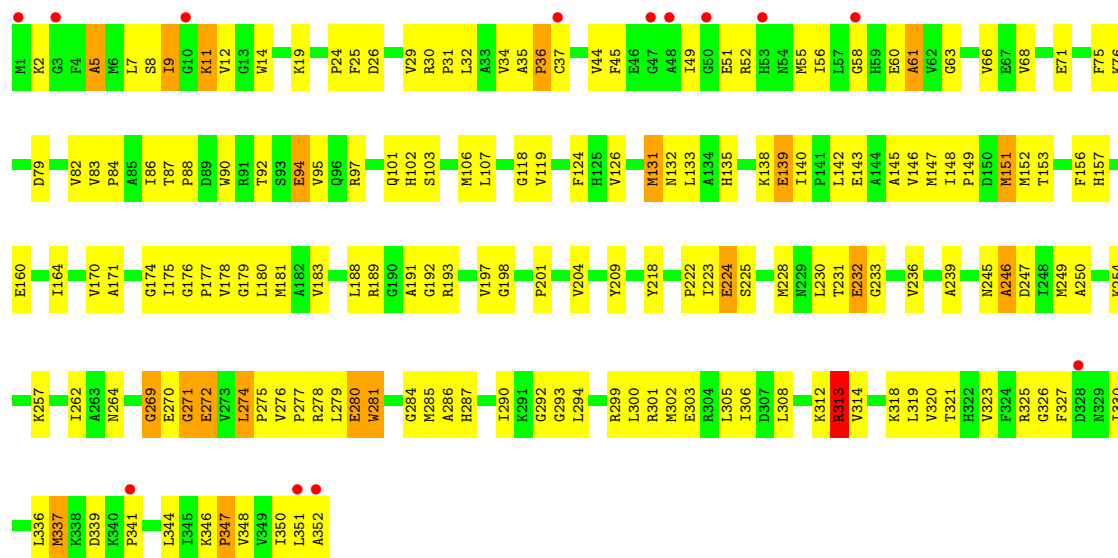
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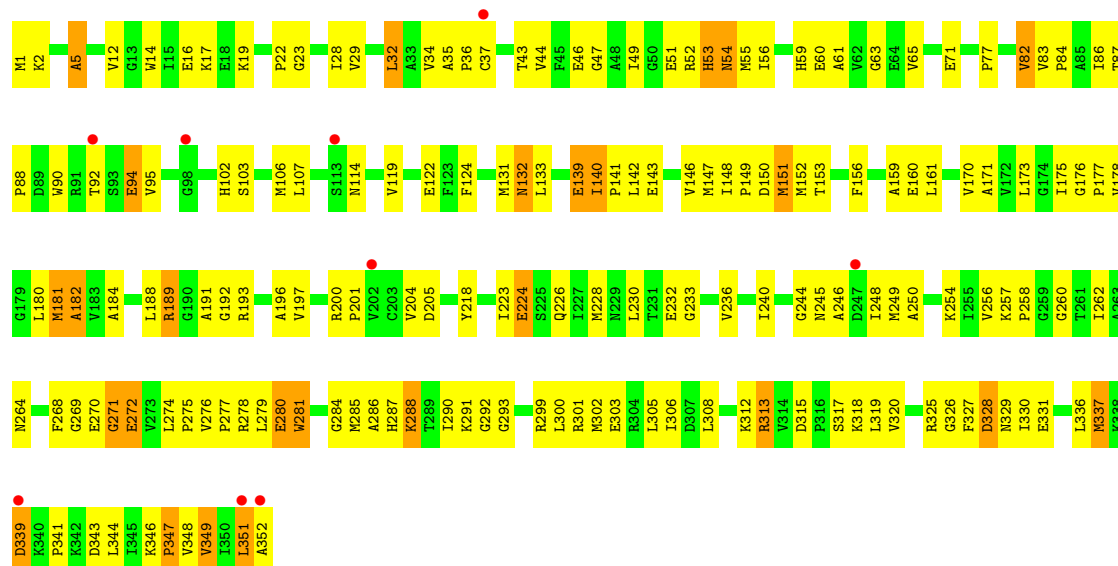
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	63	Total 63	O 63	0	0
6	C	44	Total 44	O 44	0	0
6	D	66	Total 66	O 66	0	0



● Molecule 1: NADP-DEPENDENT ALCOHOL DEHYDROGENASE



● Molecule 1: NADP-DEPENDENT ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.45Å 123.08Å 168.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.99 50.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	86.3 (50.00-2.99) 83.4 (50.00-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.96Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.214 , 0.264 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10852	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, CL, SBT, 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	0.83	7/2701 (0.3%)	1.16	25/3654 (0.7%)
1	B	0.72	3/2701 (0.1%)	1.11	8/3654 (0.2%)
1	C	0.84	6/2701 (0.2%)	1.14	18/3654 (0.5%)
1	D	0.75	7/2701 (0.3%)	1.10	15/3654 (0.4%)
All	All	0.79	23/10804 (0.2%)	1.13	66/14616 (0.5%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	ILE	CA-CB	14.13	1.68	1.54
1	D	328	ASP	C-O	10.28	1.36	1.24
1	A	157	HIS	ND1-CE1	9.88	1.42	1.32
1	A	157	HIS	CG-ND1	-8.97	1.28	1.38
1	D	54	ASN	C-O	7.92	1.33	1.23

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	LEU	O-C-N	-8.93	111.21	122.82
1	D	328	ASP	O-C-N	8.07	131.39	122.11
1	B	315	ASP	CA-C-N	8.02	127.66	119.56
1	B	315	ASP	C-N-CA	8.02	127.66	119.56
1	B	281	TRP	N-CA-C	-7.56	103.36	112.59

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	2643	0	2690	175	0
1	B	2643	0	2690	159	0
1	C	2643	0	2689	176	0
1	D	2643	0	2689	167	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	10	0	0
5	B	5	0	10	0	0
5	C	5	0	10	0	0
5	D	5	0	10	0	0
6	A	75	0	0	2	0
6	B	63	0	0	2	0
6	C	44	0	0	1	0
6	D	66	0	0	2	0
All	All	10852	0	10798	625	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 29.

The worst 5 of 625 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:C:254:LYS:HG2	1:C:280:GLU:HG3	1.33	1.11
1:C:151:MET:HE2	1:C:177:PRO:HB2	1.42	1.02
1:B:153:THR:HG22	1:B:301:ARG:HE	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:MET:HE1	1:B:346:LYS:HG2	1.43	0.97
1:A:36:PRO:HB2	1:A:337:MET:HG3	1.46	0.96

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	350/352 (99%)	318 (91%)	31 (9%)	1 (0%)	36	70
1	B	350/352 (99%)	316 (90%)	31 (9%)	3 (1%)	14	48
1	C	350/352 (99%)	308 (88%)	37 (11%)	5 (1%)	9	36
1	D	350/352 (99%)	311 (89%)	35 (10%)	4 (1%)	11	43
All	All	1400/1408 (99%)	1253 (90%)	134 (10%)	13 (1%)	14	48

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	ALA
1	B	246	ALA
1	C	246	ALA
1	D	351	LEU
1	C	271	GLY

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	274/274 (100%)	266 (97%)	8 (3%)	37	70
1	B	274/274 (100%)	263 (96%)	11 (4%)	28	62
1	C	274/274 (100%)	262 (96%)	12 (4%)	25	60
1	D	274/274 (100%)	260 (95%)	14 (5%)	21	55
All	All	1096/1096 (100%)	1051 (96%)	45 (4%)	27	61

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	ARG
1	D	224	GLU
1	C	337	MET
1	D	94	GLU
1	D	272	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	102	HIS
1	D	96	GLN
1	C	53	HIS
1	D	59	HIS
1	B	329	ASN

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

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\# Z > 2$
5	SBT	D	353	-	4,4,4	1.09	0	4,4,4	0.21	0
5	SBT	C	353	-	4,4,4	1.34	0	4,4,4	1.18	1 (25%)
5	SBT	A	353	-	4,4,4	0.77	0	4,4,4	0.27	0
5	SBT	B	353	-	4,4,4	0.85	0	4,4,4	0.88	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
5	SBT	D	353	-	-	0/2/2/2	-
5	SBT	C	353	-	-	0/2/2/2	-
5	SBT	A	353	-	-	0/2/2/2	-
5	SBT	B	353	-	-	0/2/2/2	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	353	SBT	OH-C2-C1	2.07	118.38	109.45

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/352 (100%)	0.30	8 (2%) 61 38	15, 39, 61, 70	0
1	B	352/352 (100%)	0.42	21 (5%) 27 14	17, 40, 63, 78	0
1	C	352/352 (100%)	0.37	13 (3%) 45 25	19, 42, 65, 78	0
1	D	352/352 (100%)	0.31	9 (2%) 57 34	20, 40, 63, 72	0
All	All	1408/1408 (100%)	0.35	51 (3%) 46 26	15, 40, 63, 78	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	ALA	6.7
1	B	48	ALA	4.4
1	B	352	ALA	3.9
1	C	1	MET	3.9
1	A	49	ILE	3.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	356	1/1	0.80	0.23	34,34,34,34	0
2	ZN	B	354	1/1	0.82	0.35	27,27,27,27	0
4	MG	D	356	1/1	0.87	0.22	33,33,33,33	0
2	ZN	A	354	1/1	0.88	0.29	26,26,26,26	0
4	MG	B	356	1/1	0.88	0.24	35,35,35,35	0
4	MG	A	356	1/1	0.89	0.14	19,19,19,19	0
5	SBT	C	353	5/5	0.89	0.14	44,44,48,49	0
5	SBT	B	353	5/5	0.90	0.12	25,29,33,35	0
5	SBT	D	353	5/5	0.90	0.13	41,42,44,46	0
2	ZN	C	354	1/1	0.91	0.30	26,26,26,26	0
3	CL	D	355	1/1	0.92	0.22	45,45,45,45	0
5	SBT	A	353	5/5	0.93	0.13	36,37,38,39	0
2	ZN	D	354	1/1	0.93	0.33	28,28,28,28	0
3	CL	C	355	1/1	0.96	0.14	29,29,29,29	0
3	CL	A	355	1/1	0.97	0.19	27,27,27,27	0
3	CL	B	355	1/1	0.97	0.17	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.