wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 04:56 pm BST

PDB ID	:	2WV0
Title	:	Crystal structure of the GntR-HutC family member YvoA from Bacillus subtilis
Authors	:	Resch, M.; Schiltz, E.; Titgemeyer, F.; Muller, Y.A.
Deposited on	:	2009-10-12
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

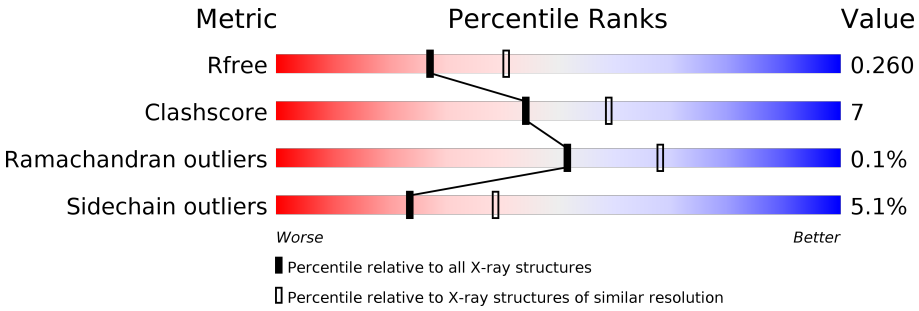
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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%

Mol	Chain	Length	Quality of chain
1	A	243	86% 10% •
1	B	243	88% 10% •
1	C	243	91% 8% •
1	D	243	80% 17% •
1	E	243	79% 15% • •
1	F	243	80% 16% • •
1	G	243	81% 14% • •

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Mol	Chain	Length	Quality of chain
1	H	243	
1	I	243	
1	J	243	

2 Entry composition (i)

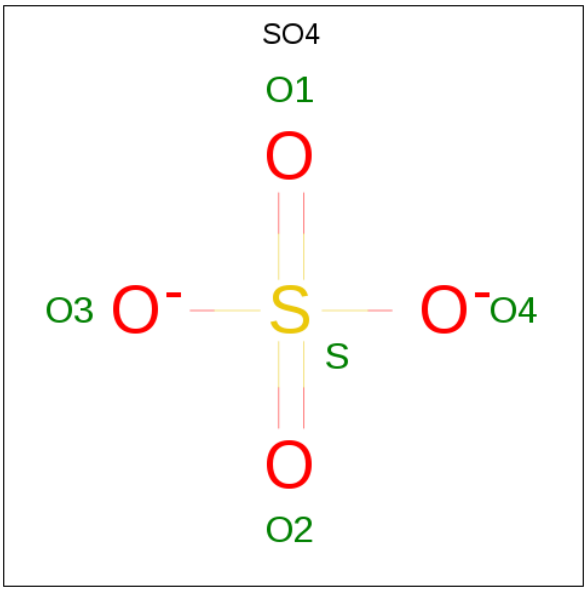
There are 3 unique types of molecules in this entry. The entry contains 18689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	3	0
			1911	1207	330	364	10			
1	B	242	Total	C	N	O	S	0	3	0
			1872	1185	321	355	11			
1	C	242	Total	C	N	O	S	0	0	0
			1871	1180	323	358	10			
1	D	242	Total	C	N	O	S	0	5	0
			1913	1211	330	361	11			
1	E	234	Total	C	N	O	S	0	0	0
			1777	1119	306	343	9			
1	F	237	Total	C	N	O	S	0	2	0
			1853	1171	316	355	11			
1	G	237	Total	C	N	O	S	0	0	0
			1779	1123	302	345	9			
1	H	224	Total	C	N	O	S	0	0	0
			1485	922	267	291	5			
1	I	242	Total	C	N	O	S	0	0	0
			1842	1164	314	354	10			
1	J	235	Total	C	N	O	S	0	0	0
			1542	960	278	296	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

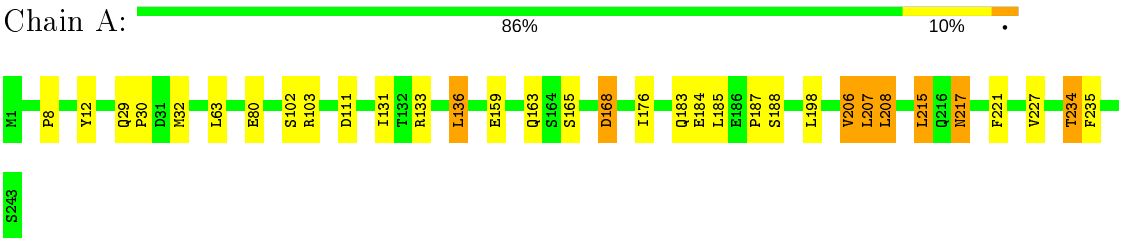
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	132	Total O 132 132	0	0
3	B	109	Total O 109 109	0	0
3	C	103	Total O 103 103	0	0
3	D	113	Total O 113 113	0	0
3	E	50	Total O 50 50	0	0
3	F	93	Total O 93 93	0	0
3	G	38	Total O 38 38	0	0
3	H	24	Total O 24 24	0	0
3	I	80	Total O 80 80	0	0
3	J	27	Total O 27 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

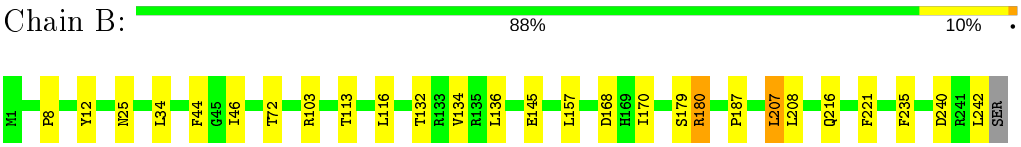
- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain A:



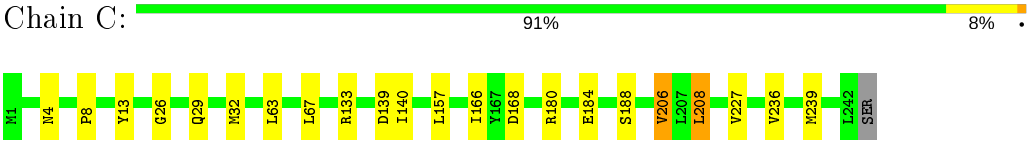
- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain B:



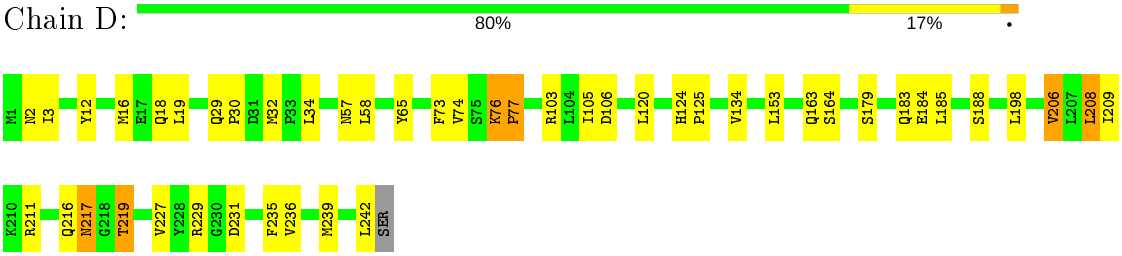
- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain C:



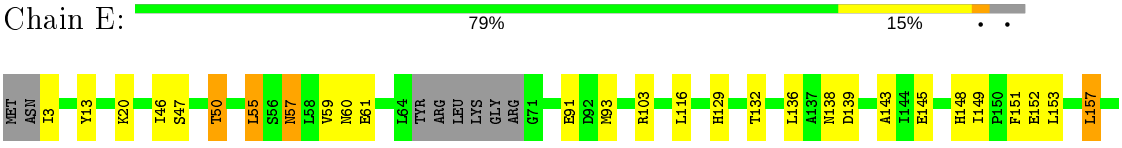
- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

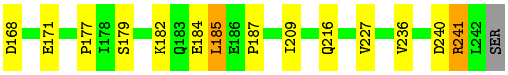
Chain D:



- Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

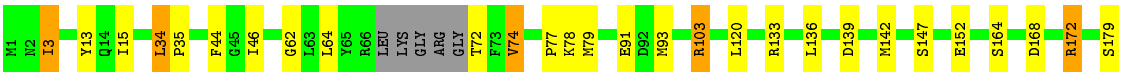
Chain E:





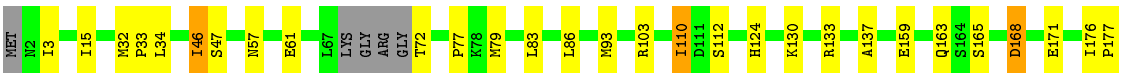
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain F:



• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain G:

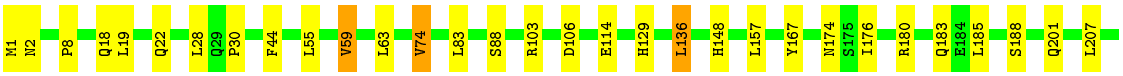


• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain H:

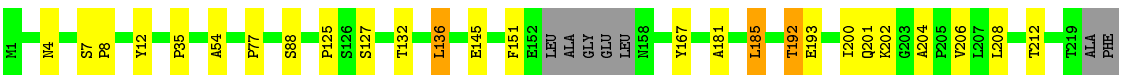
• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

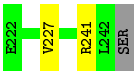
Chain I:



• Molecule 1: HTH-TYPE TRANSCRIPTIONAL REPRESSOR YVOA

Chain J:




E222
V227
R241
L242
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.41Å 137.08Å 120.19Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	114.00 – 2.40 45.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (114.00-2.40) 99.3 (45.09-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.255 0.260 , 0.260	Depositor DCC
R_{free} test set	6247 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18689	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4

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	0.49	0/1957	0.64	1/2650 (0.0%)
1	B	0.46	0/1918	0.61	1/2601 (0.0%)
1	C	0.48	0/1908	0.63	0/2586
1	D	0.52	0/1966	0.70	0/2661
1	E	0.40	0/1812	0.61	1/2460 (0.0%)
1	F	0.45	0/1895	0.61	1/2566 (0.0%)
1	G	0.38	0/1813	0.54	0/2463
1	H	1.50	25/1504 (1.7%)	0.92	14/2057 (0.7%)
1	I	0.66	3/1879 (0.2%)	0.66	3/2549 (0.1%)
1	J	0.51	1/1567 (0.1%)	0.58	4/2144 (0.2%)
All	All	0.64	29/18219 (0.2%)	0.65	25/24737 (0.1%)

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	133	ARG	CZ-NH1	21.03	1.60	1.33
1	H	215	LEU	C-O	16.61	1.54	1.23
1	H	226	SER	CB-OG	15.30	1.62	1.42
1	H	102	SER	CB-OG	14.95	1.61	1.42
1	I	217	ASN	CG-OD1	13.10	1.52	1.24

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	221	PHE	CB-CG-CD2	-13.12	111.61	120.80
1	I	180	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	H	221	PHE	CG-CD2-CE2	-8.52	111.43	120.80
1	H	167	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	J	136	LEU	CA-CB-CG	7.51	132.58	115.30

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	1911	0	1895	39	0
1	B	1872	0	1829	18	0
1	C	1871	0	1831	15	0
1	D	1913	0	1904	37	0
1	E	1777	0	1699	23	0
1	F	1853	0	1818	31	0
1	G	1779	0	1690	27	0
1	H	1485	0	1220	36	0
1	I	1842	0	1780	22	0
1	J	1542	0	1222	14	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	I	10	0	0	0	0
3	A	132	0	0	3	0
3	B	109	0	0	0	0
3	C	103	0	0	2	0
3	D	113	0	0	1	0
3	E	50	0	0	0	0
3	F	93	0	0	2	0
3	G	38	0	0	3	0
3	H	24	0	0	0	0
3	I	80	0	0	5	0
3	J	27	0	0	0	0
All	All	18689	0	16888	228	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 7.

The worst 5 of 228 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:G:93:MET:CE	1:G:137:ALA:HB2	1.63	1.27
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.03	1.17
1:H:176:ILE:HG22	1:H:177:PRO:HD2	1.15	1.14
1:G:93:MET:HE3	1:G:137:ALA:HB2	1.10	1.08
1:H:176:ILE:CG2	1:H:177:PRO:HD2	1.86	1.05

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	244/243 (100%)	240 (98%)	4 (2%)	0	100	100
1	B	243/243 (100%)	239 (98%)	4 (2%)	0	100	100
1	C	240/243 (99%)	238 (99%)	2 (1%)	0	100	100
1	D	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	34	48
1	E	230/243 (95%)	223 (97%)	7 (3%)	0	100	100
1	F	235/243 (97%)	230 (98%)	5 (2%)	0	100	100
1	G	233/243 (96%)	230 (99%)	3 (1%)	0	100	100
1	H	216/243 (89%)	202 (94%)	13 (6%)	1 (0%)	29	41
1	I	240/243 (99%)	236 (98%)	4 (2%)	0	100	100
1	J	229/243 (94%)	214 (93%)	15 (7%)	0	100	100
All	All	2355/2430 (97%)	2289 (97%)	64 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	128	ILE
1	D	77	PRO

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	207/213 (97%)	196 (95%)	11 (5%)	22	37
1	B	198/213 (93%)	191 (96%)	7 (4%)	36	55
1	C	200/213 (94%)	192 (96%)	8 (4%)	31	49
1	D	208/213 (98%)	192 (92%)	16 (8%)	13	20
1	E	186/213 (87%)	173 (93%)	13 (7%)	15	24
1	F	200/213 (94%)	190 (95%)	10 (5%)	24	40
1	G	183/213 (86%)	177 (97%)	6 (3%)	38	57
1	H	114/213 (54%)	108 (95%)	6 (5%)	22	37
1	I	193/213 (91%)	184 (95%)	9 (5%)	26	42
1	J	111/213 (52%)	105 (95%)	6 (5%)	22	36
All	All	1800/2130 (84%)	1708 (95%)	92 (5%)	24	39

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	242	LEU
1	E	168	ASP
1	I	188	SER
1	E	3	ILE
1	E	57	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	108	GLN
1	F	53	GLN
1	J	4	ASN
1	E	148	HIS
1	E	163	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
2	SO4	C	1243	-	4,4,4	0.15	0	6,6,6	0.44	0
2	SO4	E	1243	-	4,4,4	0.11	0	6,6,6	0.35	0
2	SO4	G	1243	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	D	1243	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	F	1244	-	4,4,4	0.16	0	6,6,6	0.41	0
2	SO4	D	1244	-	4,4,4	0.20	0	6,6,6	0.40	0
2	SO4	B	1244	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	B	1243	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	I	1244	-	4,4,4	0.10	0	6,6,6	0.51	0
2	SO4	A	1245	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	I	1243	-	4,4,4	0.12	0	6,6,6	0.28	0
2	SO4	A	1244	-	4,4,4	0.21	0	6,6,6	0.50	0
2	SO4	G	1244	-	4,4,4	0.21	0	6,6,6	0.22	0
2	SO4	C	1244	-	4,4,4	0.24	0	6,6,6	0.37	0
2	SO4	F	1243	-	4,4,4	0.19	0	6,6,6	0.36	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	87:THR	C	88:SER	N	1.60

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.