



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:13 am BST

PDB ID : 1Z6B
Title : Crystal structure of Plasmodium falciparum FabZ at 2.1 Å
Authors : Kostrewa, D.; Winkler, F.K.; Folkers, G.; Scapozza, L.; Perozzo, R.
Deposited on : 2005-03-22
Resolution : 2.09 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 following versions of software and data (see [references ⓘ](#)) 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

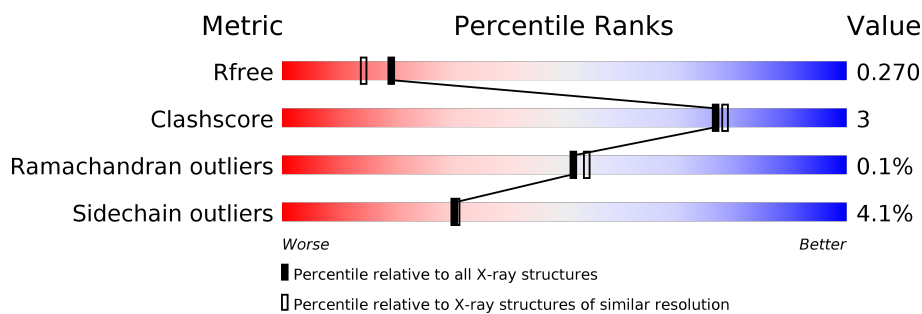
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	154	81% 10% • 8%
1	B	154	76% 8% • 14%
1	C	154	81% 8% • 10%
1	D	154	71% 14% • 14%
1	E	154	81% 7% • 11%
1	F	154	83% 8% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6728 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 fatty acid synthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1101	719	180	197	5			
1	B	132	Total	C	N	O	S	0	0	0
			1024	671	168	180	5			
1	C	138	Total	C	N	O	S	0	0	0
			1072	704	175	188	5			
1	D	132	Total	C	N	O	S	0	0	0
			1030	676	168	181	5			
1	E	137	Total	C	N	O	S	0	0	0
			1067	700	175	187	5			
1	F	142	Total	C	N	O	S	0	0	0
			1107	725	180	197	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	CLONING ARTIFACT	UNP Q965D7
A	78	SER	-	CLONING ARTIFACT	UNP Q965D7
A	79	HIS	-	CLONING ARTIFACT	UNP Q965D7
A	80	MET	-	CLONING ARTIFACT	UNP Q965D7
B	77	GLY	-	CLONING ARTIFACT	UNP Q965D7
B	78	SER	-	CLONING ARTIFACT	UNP Q965D7
B	79	HIS	-	CLONING ARTIFACT	UNP Q965D7
B	80	MET	-	CLONING ARTIFACT	UNP Q965D7
C	77	GLY	-	CLONING ARTIFACT	UNP Q965D7
C	78	SER	-	CLONING ARTIFACT	UNP Q965D7
C	79	HIS	-	CLONING ARTIFACT	UNP Q965D7
C	80	MET	-	CLONING ARTIFACT	UNP Q965D7
D	77	GLY	-	CLONING ARTIFACT	UNP Q965D7
D	78	SER	-	CLONING ARTIFACT	UNP Q965D7
D	79	HIS	-	CLONING ARTIFACT	UNP Q965D7
D	80	MET	-	CLONING ARTIFACT	UNP Q965D7
E	77	GLY	-	CLONING ARTIFACT	UNP Q965D7

Continued on next page...

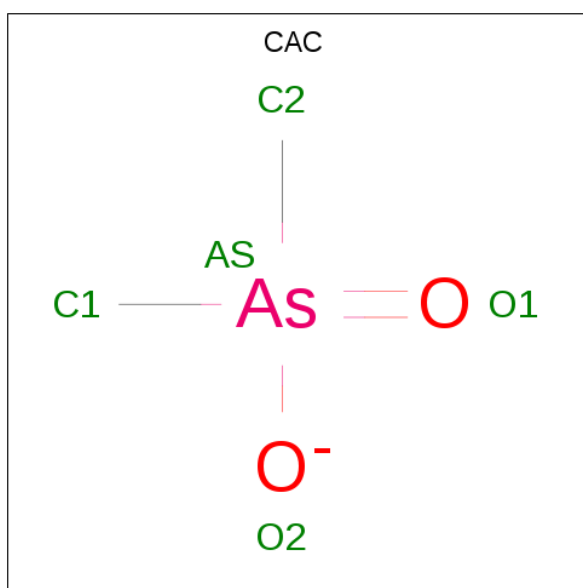
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	78	SER	-	CLONING ARTIFACT	UNP Q965D7
E	79	HIS	-	CLONING ARTIFACT	UNP Q965D7
E	80	MET	-	CLONING ARTIFACT	UNP Q965D7
F	77	GLY	-	CLONING ARTIFACT	UNP Q965D7
F	78	SER	-	CLONING ARTIFACT	UNP Q965D7
F	79	HIS	-	CLONING ARTIFACT	UNP Q965D7
F	80	MET	-	CLONING ARTIFACT	UNP Q965D7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	C	1	Total	As	C	O	0	0
			5	1	2	2		
3	D	1	Total	As	C	O	0	0
			5	1	2	2		
3	E	1	Total	As	C	O	0	0
			5	1	2	2		
3	F	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	44	Total	O	0	0
			44	44		
5	C	36	Total	O	0	0
			36	36		
5	D	51	Total	O	0	0
			51	51		
5	E	40	Total	O	0	0
			40	40		
5	F	46	Total	O	0	0
			46	46		

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 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: fatty acid synthesis protein

Chain A: 




- Molecule 1: fatty acid synthesis protein

Chain B: 



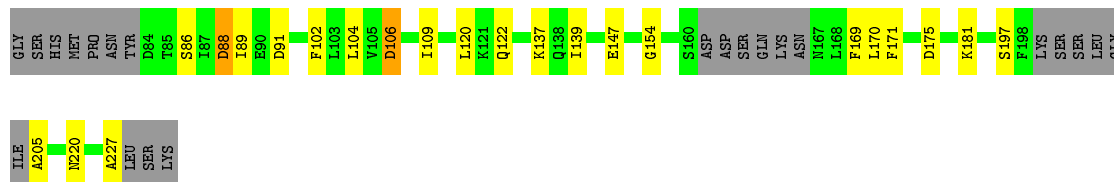
- Molecule 1: fatty acid synthesis protein

Chain C: 




- Molecule 1: fatty acid synthesis protein

Chain D: 



- Molecule 1: fatty acid synthesis protein

Chain E: 



- Molecule 1: fatty acid synthesis protein

Chain F:

83%

8%

•

8%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 127.49Å 173.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.09 86.84 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (87.71-2.09) 99.6 (86.84-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.174 , 0.222 0.237 , 0.270	Depositor DCC
R_{free} test set	2984 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6728	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: CAC, SO4, CL

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	0.66	1/1122 (0.1%)	0.78	3/1517 (0.2%)
1	B	0.62	0/1043	0.76	2/1408 (0.1%)
1	C	0.60	0/1093	0.76	1/1477 (0.1%)
1	D	0.59	0/1050	0.80	3/1419 (0.2%)
1	E	0.59	0/1087	0.78	1/1468 (0.1%)
1	F	0.59	0/1129	0.74	0/1527
All	All	0.61	1/6524 (0.0%)	0.77	10/8816 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	SER	CB-OG	5.95	1.50	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	ASP	CB-CG-OD2	7.88	125.39	118.30
1	E	106	ASP	CB-CG-OD2	6.70	124.33	118.30
1	D	106	ASP	CB-CG-OD2	6.64	124.28	118.30
1	D	175	ASP	CB-CG-OD2	6.55	124.19	118.30
1	D	91	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	106	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	84	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	88	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	106	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	161	ASP	CB-CG-OD2	5.08	122.87	118.30

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	1101	0	1151	9	0
1	B	1024	0	1077	7	0
1	C	1072	0	1129	5	0
1	D	1030	0	1076	11	0
1	E	1067	0	1120	8	0
1	F	1107	0	1155	9	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	39	0	0	0	0
5	B	44	0	0	0	0
5	C	36	0	0	0	0
5	D	51	0	0	0	0
5	E	40	0	0	0	0
5	F	46	0	0	1	0
All	All	6728	0	6708	40	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.

All (40) 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:85:THR:HG23	1:A:110:TYR:HA	1.64	0.80
1:E:169:PHE:HB3	1:E:228:LEU:HD23	1.66	0.77
1:F:169:PHE:CB	1:F:228:LEU:HD23	2.20	0.72
1:F:169:PHE:HB3	1:F:228:LEU:HD23	1.73	0.70
1:E:169:PHE:CB	1:E:228:LEU:HD23	2.23	0.68
1:F:87:ILE:HB	1:F:108:VAL:HB	1.82	0.62
1:A:85:THR:CG2	1:A:110:TYR:HA	2.34	0.57
1:A:84:ASP:O	1:A:85:THR:HG22	2.05	0.57
1:B:98:HIS:HE2	3:B:401:CAC:AS	2.52	0.53
1:C:106:ASP:OD1	1:F:125:THR:HG22	2.12	0.50
1:B:125:THR:HG22	1:E:106:ASP:OD1	2.11	0.50
1:F:169:PHE:HB2	1:F:228:LEU:HD23	1.94	0.49
1:F:85:THR:HG22	1:F:87:ILE:HG13	1.93	0.49
1:D:109:ILE:HD11	1:D:120:LEU:HD23	1.94	0.49
1:B:106:ASP:OD1	1:E:125:THR:HG22	2.15	0.47
1:C:169:PHE:HB3	1:C:228:LEU:HD23	1.97	0.47
1:C:87:ILE:HB	1:C:108:VAL:HB	1.95	0.47
1:C:122:GLN:HB3	1:F:122:GLN:HB3	1.97	0.47
1:E:154:GLY:HA3	1:E:169:PHE:CZ	2.51	0.46
1:A:185:PRO:HG2	1:D:89:ILE:HG21	1.99	0.45
1:B:185:PRO:HG2	1:E:89:ILE:HG21	1.99	0.44
1:A:130:PHE:CD1	1:A:138:GLN:HB3	2.53	0.44
1:D:170:LEU:N	1:D:227:ALA:O	2.33	0.44
1:A:122:GLN:HB3	1:D:122:GLN:HB3	1.99	0.43
1:C:114:ASN:ND2	1:C:160:SER:HB3	2.32	0.43
1:D:137:LYS:HD3	1:D:139:ILE:HD11	2.01	0.43
1:D:104:LEU:HD12	1:D:147:GLU:HG3	2.00	0.43
1:F:220:ASN:ND2	5:F:548:HOH:O	2.51	0.43
1:D:104:LEU:HD12	1:D:147:GLU:CG	2.49	0.42
1:B:111:MET:HE1	1:B:113:PRO:HG3	2.02	0.42
1:A:125:THR:HG22	1:D:106:ASP:OD1	2.19	0.42
1:A:154:GLY:HA3	1:A:169:PHE:CZ	2.55	0.41
1:D:154:GLY:HA3	1:D:169:PHE:CZ	2.56	0.41
1:E:130:PHE:CD1	1:E:138:GLN:HB3	2.55	0.41
1:B:182:PRO:HB2	1:B:184:LEU:HD21	2.03	0.41
1:D:88:ASP:C	1:D:88:ASP:OD1	2.58	0.41
1:D:197:SER:O	1:D:205:ALA:HB1	2.20	0.41
1:F:110:TYR:HB3	1:F:118:ILE:HB	2.02	0.41
1:A:174:VAL:HG12	1:B:177:VAL:HB	2.02	0.40
1:E:199:LYS:O	1:E:203:GLY:N	2.54	0.40

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	138/154 (90%)	131 (95%)	6 (4%)	1 (1%)	22	18
1	B	126/154 (82%)	123 (98%)	3 (2%)	0	100	100
1	C	134/154 (87%)	129 (96%)	5 (4%)	0	100	100
1	D	126/154 (82%)	120 (95%)	6 (5%)	0	100	100
1	E	131/154 (85%)	128 (98%)	3 (2%)	0	100	100
1	F	138/154 (90%)	133 (96%)	5 (4%)	0	100	100
All	All	793/924 (86%)	764 (96%)	28 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	THR

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	124/135 (92%)	120 (97%)	4 (3%)	39	41
1	B	114/135 (84%)	108 (95%)	6 (5%)	22	20
1	C	120/135 (89%)	114 (95%)	6 (5%)	24	23
1	D	115/135 (85%)	109 (95%)	6 (5%)	23	21
1	E	119/135 (88%)	117 (98%)	2 (2%)	60	67
1	F	124/135 (92%)	119 (96%)	5 (4%)	31	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	716/810 (88%)	687 (96%)	29 (4%)	30	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	112	GLN
1	A	171	PHE
1	A	220	ASN
1	B	88	ASP
1	B	102	PHE
1	B	136	GLN
1	B	171	PHE
1	B	198	PHE
1	B	204	ILE
1	C	102	PHE
1	C	109	ILE
1	C	168	LEU
1	C	171	PHE
1	C	175	ASP
1	C	200	SER
1	D	86	SER
1	D	88	ASP
1	D	102	PHE
1	D	171	PHE
1	D	181	LYS
1	D	220	ASN
1	E	102	PHE
1	E	171	PHE
1	F	102	PHE
1	F	168	LEU
1	F	171	PHE
1	F	214	ASN
1	F	220	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	B	114	ASN
1	C	114	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	220	ASN
1	D	114	ASN
1	D	214	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\# Z > 2$
4	SO4	B	507	-	4,4,4	0.15	0	6,6,6	0.34	0
3	CAC	F	405	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	D	403	-	0,4,4	0.00	-	0,6,6	0.00	-
4	SO4	F	506	-	4,4,4	0.16	0	6,6,6	0.20	0
4	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.30	0
3	CAC	C	404	-	0,4,4	0.00	-	0,6,6	0.00	-
4	SO4	E	505	-	4,4,4	0.12	0	6,6,6	0.26	0
3	CAC	B	401	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	E	406	-	0,4,4	0.00	-	0,6,6	0.00	-
4	SO4	D	504	-	4,4,4	0.19	0	6,6,6	0.30	0
3	CAC	A	402	-	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.47	0
4	SO4	C	503	-	4,4,4	0.20	0	6,6,6	0.31	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	CAC	1	0

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 ⓘ

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.