wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 01:55 am BST

PDB ID	:	3FG9
Title	:	The crystal structure of an universal stress protein UspA family protein from Lactobacillus plantarum WCFS1
Authors	:	Tan, K.; Li, H.; Cobb, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-12-05
Resolution	:	1.47 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:

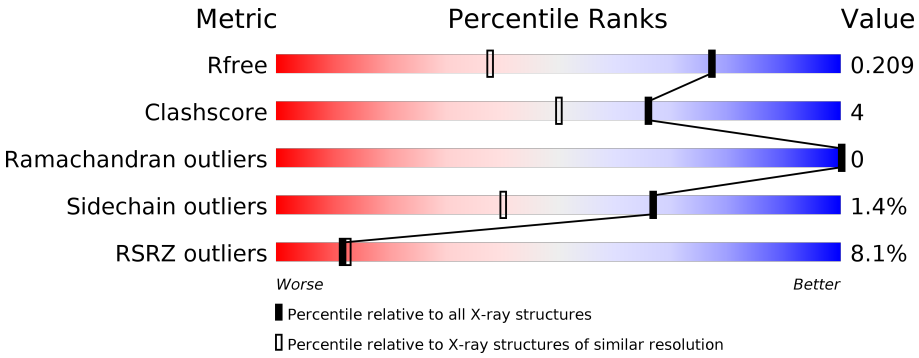
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.47 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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% 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	156	4% 90% 9%
1	B	156	7% 84% 10% 6%
1	C	156	3% 93%
1	D	156	14% 88% 8%
1	E	156	5% 90% 6%
1	F	156	12% 82% 8% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	A	155	-	-	X	-
3	FMT	C	156	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8212 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 protein of universal stress protein UspA family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	11	0
			1282	813	217	248	2	2			
1	B	146	Total	C	N	O	S	Se	0	7	0
			1177	742	198	233	2	2			
1	C	150	Total	C	N	O	S	Se	0	7	0
			1210	768	201	238	2	1			
1	D	150	Total	C	N	O	S	Se	0	4	0
			1197	759	201	234	2	1			
1	E	150	Total	C	N	O	S	Se	0	9	0
			1230	781	211	235	2	1			
1	F	141	Total	C	N	O	S	Se	0	8	0
			1141	721	193	224	2	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q88RY8
A	-1	ASN	-	expression tag	UNP Q88RY8
A	0	ALA	-	expression tag	UNP Q88RY8
B	-2	SER	-	expression tag	UNP Q88RY8
B	-1	ASN	-	expression tag	UNP Q88RY8
B	0	ALA	-	expression tag	UNP Q88RY8
C	-2	SER	-	expression tag	UNP Q88RY8
C	-1	ASN	-	expression tag	UNP Q88RY8
C	0	ALA	-	expression tag	UNP Q88RY8
D	-2	SER	-	expression tag	UNP Q88RY8
D	-1	ASN	-	expression tag	UNP Q88RY8
D	0	ALA	-	expression tag	UNP Q88RY8
E	-2	SER	-	expression tag	UNP Q88RY8
E	-1	ASN	-	expression tag	UNP Q88RY8
E	0	ALA	-	expression tag	UNP Q88RY8
F	-2	SER	-	expression tag	UNP Q88RY8
F	-1	ASN	-	expression tag	UNP Q88RY8

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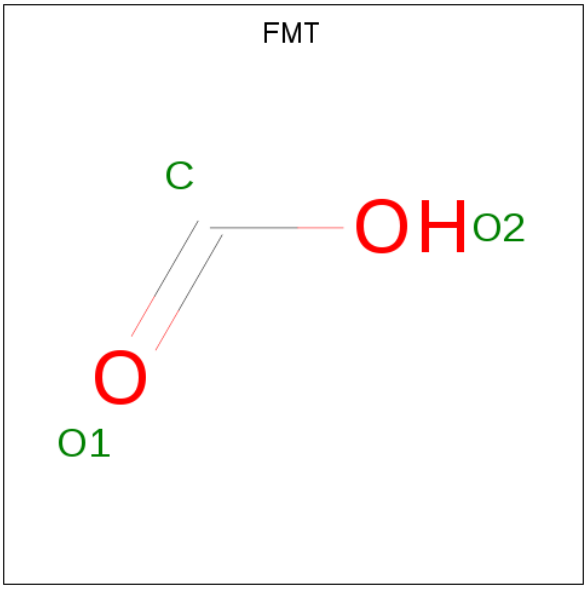
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q88RY8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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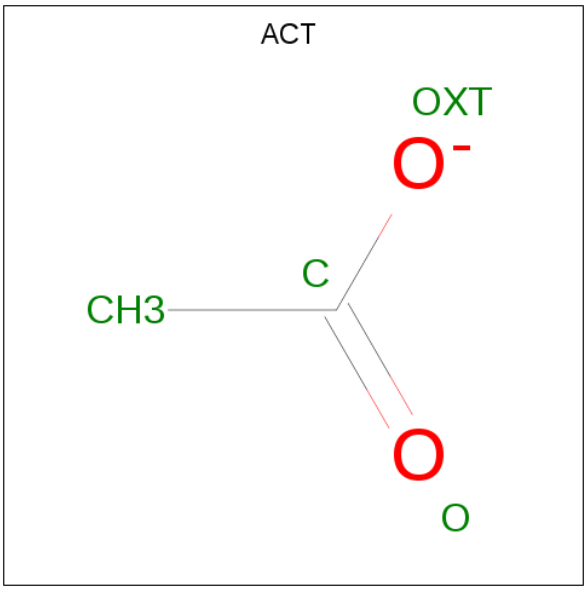
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	209	Total O 209 209	0	0
5	B	148	Total O 148 148	0	0
5	C	176	Total O 176 176	0	0
5	D	132	Total O 132 132	0	0

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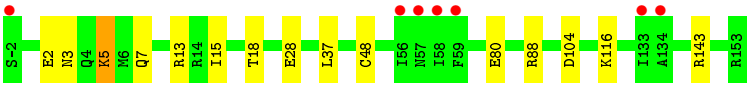
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	183	Total O 183 183	0	0
5	F	95	Total O 95 95	0	0

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 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 (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.

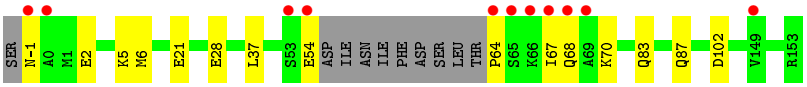
- Molecule 1: protein of universal stress protein UspA family

Chain A:



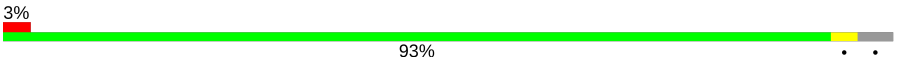
- Molecule 1: protein of universal stress protein UspA family

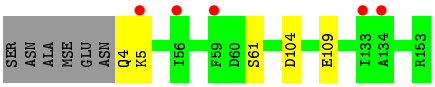
Chain B:



- Molecule 1: protein of universal stress protein UspA family

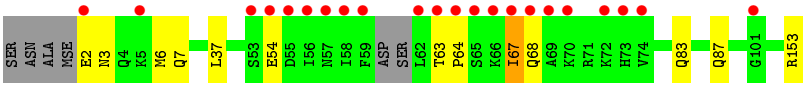
Chain C:





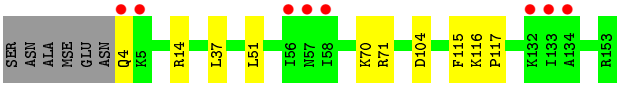
- Molecule 1: protein of universal stress protein UspA family

Chain D:



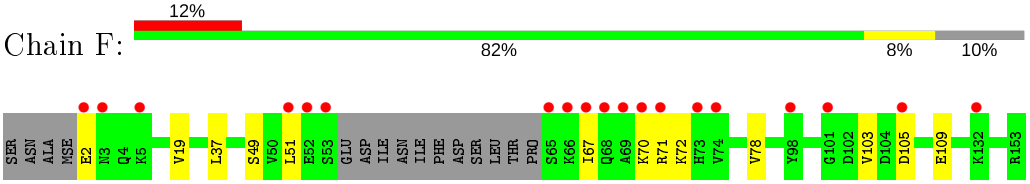
- Molecule 1: protein of universal stress protein UspA family

Chain E:



- Molecule 1: protein of universal stress protein UspA family

Chain F:


12%
82%
8%
10%
SER ASN ALA MSE E2 N3 Q4 K5 V19 L37 S49 V50 L51 E52 S53 GLU ASP ILE ASN ILE PHE ASP SER LEU THR PRO S65 K66 I67 Q68 A69 K70 R71 K72 H73 V74 V78 Y98 G101 D102 V103 D104 D105 E109 K132 R153

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	38.35Å 118.95Å 191.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.60 – 1.47 37.61 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.60-1.47) 99.5 (37.61-1.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.177 , 0.212 0.175 , 0.209	Depositor DCC
R_{free} test set	7512 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8212	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8343e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FMT, MG, ACT

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	0.64	0/1332	0.75	1/1801 (0.1%)
1	B	0.65	0/1214	0.74	1/1642 (0.1%)
1	C	0.58	0/1250	0.72	0/1697
1	D	0.59	0/1227	0.73	0/1665
1	E	0.60	0/1276	0.69	0/1727
1	F	0.57	0/1181	0.68	0/1600
All	All	0.60	0/7480	0.72	2/10132 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	102	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	88	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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	1282	0	1327	14	0
1	B	1177	0	1192	13	0
1	C	1210	0	1233	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1197	0	1211	9	0
1	E	1230	0	1272	9	0
1	F	1141	0	1163	10	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	2	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	2	2	0
3	B	3	0	1	0	0
3	C	6	0	2	3	0
3	D	6	0	2	1	0
4	C	4	0	3	0	0
5	A	209	0	0	5	0
5	B	148	0	0	1	0
5	C	176	0	0	0	0
5	D	132	0	0	1	0
5	E	183	0	0	4	0
5	F	95	0	0	2	0
All	All	8212	0	7408	59	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 4.

The worst 5 of 59 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:15[B]:ILE:HD11	1:A:37:LEU:HD22	1.23	1.11
1:A:80:GLU:OE1	1:B:-1:ASN:HB3	1.49	1.08
1:C:61:SER:H	3:C:156:FMT:H	0.97	1.07
1:A:18[B]:THR:HG22	1:A:48[B]:CYS:SG	1.97	1.03
1:C:61:SER:N	3:C:156:FMT:H	1.80	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	165/156 (106%)	163 (99%)	2 (1%)	0	100	100
1	B	149/156 (96%)	148 (99%)	1 (1%)	0	100	100
1	C	155/156 (99%)	153 (99%)	2 (1%)	0	100	100
1	D	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	E	157/156 (101%)	155 (99%)	2 (1%)	0	100	100
1	F	145/156 (93%)	144 (99%)	1 (1%)	0	100	100
All	All	921/936 (98%)	910 (99%)	11 (1%)	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	148/135 (110%)	144 (97%)	4 (3%)	44	14
1	B	134/135 (99%)	134 (100%)	0	100	100
1	C	139/135 (103%)	137 (99%)	2 (1%)	67	40
1	D	136/135 (101%)	134 (98%)	2 (2%)	65	37
1	E	141/135 (104%)	139 (99%)	2 (1%)	67	40
1	F	131/135 (97%)	129 (98%)	2 (2%)	65	37
All	All	829/810 (102%)	817 (99%)	12 (1%)	67	40

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	109	GLU
1	D	63	THR
1	E	104	ASP
1	C	104	ASP
1	E	4	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	HIS
1	E	91	ASN
1	D	91	ASN
1	B	68	GLN
1	D	87	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)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\#\|Z\|>2$
3	FMT	C	156	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	155	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	156	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	155	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	155	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	155	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACT	C	157	-	1,3,3	1.21	0	0,3,3	0.00	-
3	FMT	A	156	-	0,2,2	0.00	-	0,1,1	0.00	-

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	156	FMT	3	0
3	D	156	FMT	1	0
3	A	155	FMT	2	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

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, 95^{th} 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	154/156 (98%)	0.24	7 (4%) 33 36	8, 15, 26, 32	0
1	B	144/156 (92%)	0.72	11 (7%) 13 15	8, 14, 30, 36	0
1	C	149/156 (95%)	0.25	5 (3%) 45 49	10, 16, 29, 37	0
1	D	149/156 (95%)	1.09	22 (14%) 2 2	11, 20, 36, 38	0
1	E	149/156 (95%)	0.31	8 (5%) 25 28	11, 18, 29, 38	0
1	F	140/156 (89%)	0.84	19 (13%) 3 3	12, 22, 35, 38	0
All	All	885/936 (94%)	0.57	72 (8%) 12 13	8, 17, 33, 38	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	LEU	14.4
1	D	63	THR	12.7
1	F	67	ILE	12.6
1	D	64	PRO	12.2
1	D	67	ILE	11.4

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

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

6.3 Carbohydrates

There are no carbohydrates 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, 95^{th} 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(Å^2)	Q<0.9
3	FMT	D	155	3/3	0.65	0.20	25,25,27,29	0
3	FMT	A	155	3/3	0.82	0.18	25,25,25,27	3
2	MG	F	154	1/1	0.84	0.10	22,22,22,22	1
4	ACT	C	157	4/4	0.88	0.13	21,22,22,23	4
3	FMT	B	155	3/3	0.88	0.12	23,23,23,24	3
3	FMT	C	155	3/3	0.90	0.16	16,16,21,24	0
3	FMT	C	156	3/3	0.90	0.17	24,24,25,25	3
3	FMT	A	156	3/3	0.90	0.14	23,23,24,24	3
3	FMT	D	156	3/3	0.91	0.11	24,24,24,25	3
2	MG	E	155	1/1	0.94	0.24	26,26,26,26	1
2	MG	A	154	1/1	0.94	0.13	19,19,19,19	1
2	MG	D	154	1/1	0.97	0.13	24,24,24,24	1
2	MG	E	154	1/1	0.98	0.18	21,21,21,21	1
2	MG	C	154	1/1	0.98	0.12	19,19,19,19	1
2	MG	B	154	1/1	0.99	0.05	14,14,14,14	1

6.5 Other polymers (i)

There are no such residues in this entry.