



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:46 AM UTC

PDB ID : 5DCQ / pdb_00005dcq
Title : Crystal structure of bacterial adhesin, FNE from Streptococcus equi spp. equi.
Authors : Tiouajni, M.; Graille, M.; van Tilbeurgh, H.
Deposited on : 2015-08-24
Resolution : 1.83 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

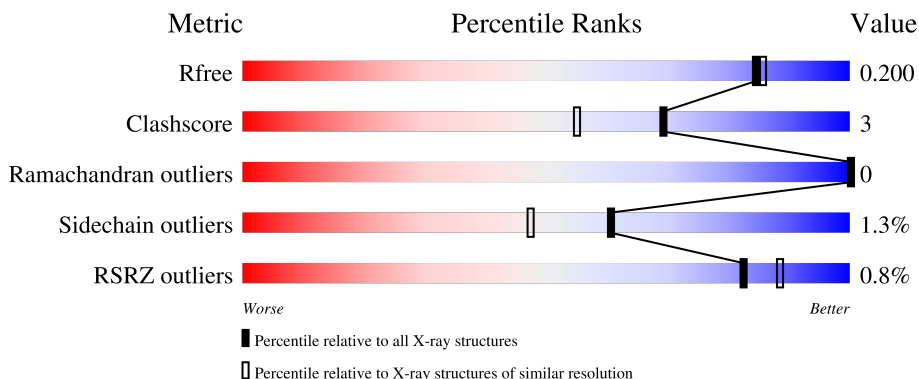
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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.



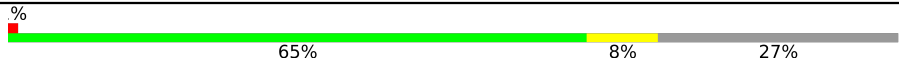
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	170	 89% 8%
1	B	170	 83% 6% 9%
1	C	170	 86% 8% 6%
2	D	271	 70% 27%
2	E	271	 69% 26%

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Mol	Chain	Length	Quality of chain
2	F	271	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '65%', a yellow segment in the middle labeled '8%', and a grey segment on the right labeled '27%'. A small red square is positioned at the beginning of the bar, and a '%' symbol is located above the bar.</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9718 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 artificial repeat proteins (alphaREP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	157	1227	766	218	240	3	0	3	0
1	B	155	1192	742	212	235	3	0	1	0
1	C	159	1235	769	223	240	3	0	1	0

- Molecule 2 is a protein called Fibronectin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	199	1635	1053	259	320	3	0	0	0
2	E	200	1644	1059	261	321	3	0	0	0
2	F	199	1647	1059	261	324	3	0	2	0

There are 21 discrepancies between the modelled and reference sequences:

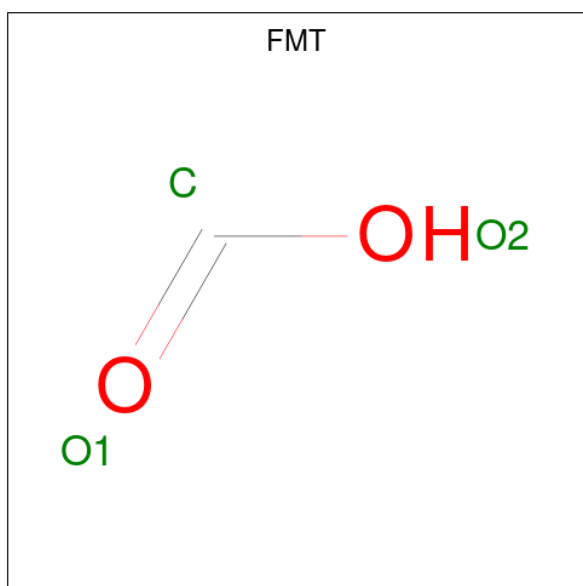
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	expression tag	UNP Q93ED6
D	266	HIS	-	expression tag	UNP Q93ED6
D	267	HIS	-	expression tag	UNP Q93ED6
D	268	HIS	-	expression tag	UNP Q93ED6
D	269	HIS	-	expression tag	UNP Q93ED6
D	270	HIS	-	expression tag	UNP Q93ED6
D	271	HIS	-	expression tag	UNP Q93ED6
E	1	ALA	-	expression tag	UNP Q93ED6
E	266	HIS	-	expression tag	UNP Q93ED6
E	267	HIS	-	expression tag	UNP Q93ED6
E	268	HIS	-	expression tag	UNP Q93ED6
E	269	HIS	-	expression tag	UNP Q93ED6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	270	HIS	-	expression tag	UNP Q93ED6
E	271	HIS	-	expression tag	UNP Q93ED6
F	1	ALA	-	expression tag	UNP Q93ED6
F	266	HIS	-	expression tag	UNP Q93ED6
F	267	HIS	-	expression tag	UNP Q93ED6
F	268	HIS	-	expression tag	UNP Q93ED6
F	269	HIS	-	expression tag	UNP Q93ED6
F	270	HIS	-	expression tag	UNP Q93ED6
F	271	HIS	-	expression tag	UNP Q93ED6

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

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


- Molecule 4 is water.

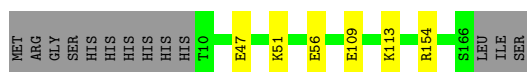
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	156	Total O 156 156	0	0
4	B	164	Total O 164 164	0	0
4	C	161	Total O 161 161	0	0
4	D	185	Total O 185 185	0	0
4	E	198	Total O 198 198	0	0
4	F	238	Total O 238 238	0	0

3 Residue-property plots [i](#)


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 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: artificial repeat proteins (alphaREP3)

Chain A: 




- Molecule 1: artificial repeat proteins (alphaREP3)

Chain B: 



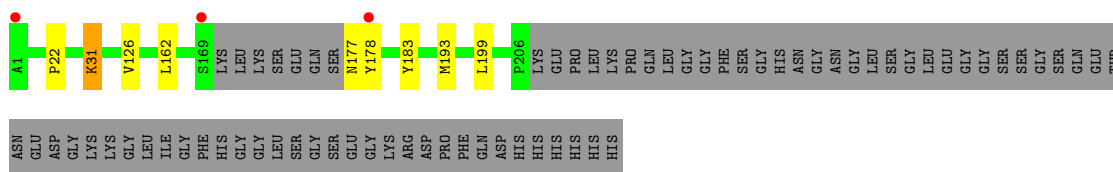
- Molecule 1: artificial repeat proteins (alphaREP3)

Chain C: 



- Molecule 2: Fibronectin-binding protein

Chain D: 



- Molecule 2: Fibronectin-binding protein

Chain E: 



GLU
GLY
GLY
SER
SER
GLY
GLY
SER
GLN
GLU
THR
GLU
ASN
GLU
ASP
GLY
LYS
LYS
GLY
LEU
LEU
ILE
GLY
PHE
HIS
GLY
GLY
LEU
SER
GLY
SER
GLU
GLU
GLY
LYS
LYS
ARG
ASP
GLU
PRO
PHE
PHE
GLN
ASP
ASP
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 2: Fibronectin-binding protein



A1
N7
R11
K31
C38
Q48
S54
Y75
I78
K125
K157
F161
K165
D168
S169
LYS
LEU
LEU
LYS
SER
GLU
GLN
SER
N177
Y178
Y183
H190
K194
Q197
N198
L199
P206
LYS
GLU
PRO
LEU
LYS
PRO
GLN
LEU
GLY
PHE

SER
GLY
HIS
ASN
GLY
ASN
GLY
LEU
SER
GLY
LEU
GLY
GLY
SER
SER
GLY
SER
GLN
THR
ASN
GLU
ASP
GLY
LYS
LYS
GLY
LEU
ILE
GLY
PHE
HIS
GLY
GLY
LEU
SER
GLY
SER
GLU
GLY
LYS
LYS
ARG
ASP
PRO
PHE
GLN
ASP
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	113.69Å 113.69Å 152.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.83 50.00 – 1.83	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-1.83) 97.9 (50.00-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.83Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.167 , 0.203 0.163 , 0.200	Depositor DCC
R_{free} test set	4769 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9718	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.50% 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: FMT

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	0.46	0/1240	0.68	0/1667
1	B	0.48	0/1204	0.66	0/1621
1	C	0.45	0/1247	0.69	0/1677
2	D	0.38	0/1681	0.67	0/2279
2	E	0.42	0/1690	0.70	0/2290
2	F	0.41	0/1693	0.66	0/2295
All	All	0.43	0/8755	0.68	0/11829

There are no bond length outliers.

There are no bond angle outliers.

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	1227	0	1256	5	0
1	B	1192	0	1218	13	0
1	C	1235	0	1271	9	0
2	D	1635	0	1556	6	0
2	E	1644	0	1569	8	0
2	F	1647	0	1564	18	0
3	A	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	1	0	0
3	C	12	0	4	0	0
3	D	3	0	1	0	0
3	E	9	0	3	1	0
3	F	6	0	2	1	0
4	A	156	0	0	4	3
4	B	164	0	0	7	0
4	C	161	0	0	6	1
4	D	185	0	0	2	1
4	E	198	0	0	5	0
4	F	238	0	0	11	1
All	All	9718	0	8446	59	3

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.

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)
2:F:169:SER:OG	4:F:401:HOH:O	1.88	0.91
2:F:1:ALA:N	4:F:402:HOH:O	2.06	0.89
1:B:118:GLU:OE2	4:B:301:HOH:O	1.92	0.86
2:E:54:SER:O	4:E:401:HOH:O	1.93	0.86
1:B:116:LYS:NZ	4:B:304:HOH:O	2.15	0.75

All (3) 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)
4:A:425:HOH:O	4:D:571:HOH:O[5_554]	1.95	0.25
4:A:430:HOH:O	4:C:318:HOH:O[4_664]	2.10	0.10
4:A:318:HOH:O	4:F:504:HOH:O[4_664]	2.16	0.04

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	158/170 (93%)	157 (99%)	1 (1%)	0	100	100
1	B	154/170 (91%)	154 (100%)	0	0	100	100
1	C	159/170 (94%)	159 (100%)	0	0	100	100
2	D	195/271 (72%)	193 (99%)	2 (1%)	0	100	100
2	E	196/271 (72%)	193 (98%)	3 (2%)	0	100	100
2	F	197/271 (73%)	193 (98%)	4 (2%)	0	100	100
All	All	1059/1323 (80%)	1049 (99%)	10 (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	125/134 (93%)	122 (98%)	3 (2%)	43	25
1	B	121/134 (90%)	117 (97%)	4 (3%)	33	15
1	C	126/134 (94%)	124 (98%)	2 (2%)	55	39
2	D	180/236 (76%)	179 (99%)	1 (1%)	78	72
2	E	181/236 (77%)	178 (98%)	3 (2%)	53	37
2	F	182/236 (77%)	181 (100%)	1 (0%)	81	75
All	All	915/1110 (82%)	901 (98%)	14 (2%)	61	42

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	70	LYS
1	C	147	GLU
2	F	31	LYS

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Mol	Chain	Res	Type
2	E	31	LYS
2	E	52	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	GLN
2	E	150	ASN
2	E	186	GLN
2	F	111	GLN
2	F	186	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](#)

12 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	$\# Z > 2$
3	FMT	F	302	-	2,2,2	0.73	0	1,1,1	0.24	0
3	FMT	F	301	-	2,2,2	0.72	0	1,1,1	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	C	201	-	2,2,2	0.72	0	1,1,1	0.25	0
3	FMT	E	301	-	2,2,2	0.69	0	1,1,1	0.35	0
3	FMT	E	302	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	E	303	-	2,2,2	0.72	0	1,1,1	0.24	0
3	FMT	C	203	-	2,2,2	0.70	0	1,1,1	0.08	0
3	FMT	B	201	-	2,2,2	0.72	0	1,1,1	0.17	0
3	FMT	C	202	-	2,2,2	0.55	0	1,1,1	0.63	0
3	FMT	D	301	-	2,2,2	0.73	0	1,1,1	0.23	0
3	FMT	A	201	-	2,2,2	0.71	0	1,1,1	0.23	0
3	FMT	C	204	-	2,2,2	0.71	0	1,1,1	0.21	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	FMT	1	0
3	E	301	FMT	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 [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	157/170 (92%)	-0.46	0 100 100	11, 23, 47, 67	3 (1%)
1	B	155/170 (91%)	-0.35	1 (0%) 85 90	14, 25, 51, 71	1 (0%)
1	C	159/170 (93%)	-0.39	2 (1%) 75 82	8, 25, 51, 66	1 (0%)
2	D	199/271 (73%)	-0.14	3 (1%) 72 79	17, 30, 52, 73	0
2	E	200/271 (73%)	-0.42	1 (0%) 87 92	13, 26, 52, 68	0
2	F	199/271 (73%)	-0.50	2 (1%) 79 86	13, 24, 44, 63	2 (1%)
All	All	1069/1323 (80%)	-0.37	9 (0%) 82 88	8, 26, 50, 73	7 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	ALA	2.9
1	C	165	LYS	2.9
1	C	168	ILE	2.6
2	F	178	TYR	2.6
2	D	178	TYR	2.3

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(Å ²)	Q<0.9
3	FMT	C	202	3/3	0.72	0.19	51,51,56,58	0
3	FMT	B	201	3/3	0.80	0.15	53,53,62,67	0
3	FMT	C	204	3/3	0.84	0.17	54,54,58,59	0
3	FMT	F	302	3/3	0.86	0.11	61,61,63,64	0
3	FMT	E	303	3/3	0.87	0.09	44,44,48,50	0
3	FMT	D	301	3/3	0.87	0.07	71,71,73,73	0
3	FMT	F	301	3/3	0.88	0.19	53,53,59,60	0
3	FMT	C	203	3/3	0.89	0.13	30,30,44,44	0
3	FMT	E	302	3/3	0.90	0.12	62,62,64,66	0
3	FMT	E	301	3/3	0.90	0.11	27,27,40,47	0
3	FMT	A	201	3/3	0.91	0.10	51,51,52,56	0
3	FMT	C	201	3/3	0.96	0.07	28,28,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.