



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:23 pm BST

PDB ID : 6ERB
Title : Enterococcus faecalis FIC protein (H111A) in complex with sulfate.
Authors : Veyron, S.; Cherfils, J.
Deposited on : 2017-10-17
Resolution : 2.20 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

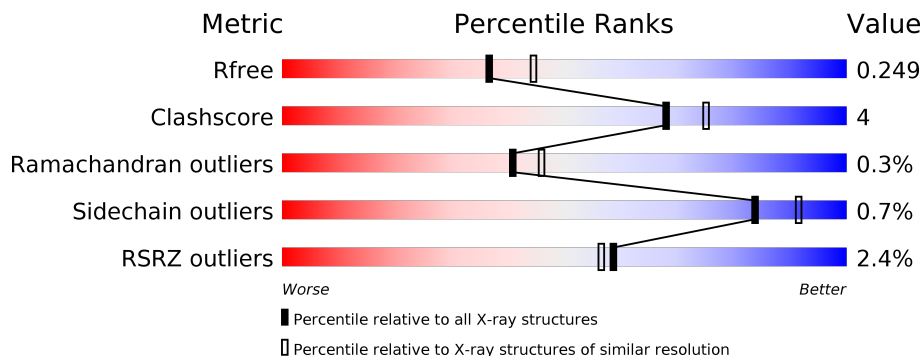
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	207	
1	B	207	
1	C	207	
1	D	207	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6918 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 Fic family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1645	1051	277	312	5	0	0	0
1	D	198	1645	1051	277	312	5	0	0	0
1	B	200	1661	1062	279	314	6	0	0	0
1	C	198	1653	1056	280	312	5	0	1	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP U6S0Y1
A	2	HIS	-	expression tag	UNP U6S0Y1
A	3	HIS	-	expression tag	UNP U6S0Y1
A	4	HIS	-	expression tag	UNP U6S0Y1
A	5	HIS	-	expression tag	UNP U6S0Y1
A	6	HIS	-	expression tag	UNP U6S0Y1
A	7	HIS	-	expression tag	UNP U6S0Y1
A	32	ASN	LYS	conflict	UNP U6S0Y1
A	35	ARG	GLN	conflict	UNP U6S0Y1
A	45	ILE	VAL	conflict	UNP U6S0Y1
A	47	VAL	ILE	conflict	UNP U6S0Y1
A	118	ALA	HIS	conflict	UNP U6S0Y1
A	142	ARG	GLN	conflict	UNP U6S0Y1
A	150	ASN	ASP	conflict	UNP U6S0Y1
A	205	ASP	GLU	conflict	UNP U6S0Y1
A	206	GLU	ASP	conflict	UNP U6S0Y1
D	1	MET	-	initiating methionine	UNP U6S0Y1
D	2	HIS	-	expression tag	UNP U6S0Y1
D	3	HIS	-	expression tag	UNP U6S0Y1
D	4	HIS	-	expression tag	UNP U6S0Y1
D	5	HIS	-	expression tag	UNP U6S0Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	HIS	-	expression tag	UNP U6S0Y1
D	7	HIS	-	expression tag	UNP U6S0Y1
D	32	ASN	LYS	conflict	UNP U6S0Y1
D	35	ARG	GLN	conflict	UNP U6S0Y1
D	45	ILE	VAL	conflict	UNP U6S0Y1
D	47	VAL	ILE	conflict	UNP U6S0Y1
D	118	ALA	HIS	conflict	UNP U6S0Y1
D	142	ARG	GLN	conflict	UNP U6S0Y1
D	150	ASN	ASP	conflict	UNP U6S0Y1
D	205	ASP	GLU	conflict	UNP U6S0Y1
D	206	GLU	ASP	conflict	UNP U6S0Y1
B	1	MET	-	initiating methionine	UNP U6S0Y1
B	2	HIS	-	expression tag	UNP U6S0Y1
B	3	HIS	-	expression tag	UNP U6S0Y1
B	4	HIS	-	expression tag	UNP U6S0Y1
B	5	HIS	-	expression tag	UNP U6S0Y1
B	6	HIS	-	expression tag	UNP U6S0Y1
B	7	HIS	-	expression tag	UNP U6S0Y1
B	32	ASN	LYS	conflict	UNP U6S0Y1
B	35	ARG	GLN	conflict	UNP U6S0Y1
B	45	ILE	VAL	conflict	UNP U6S0Y1
B	47	VAL	ILE	conflict	UNP U6S0Y1
B	118	ALA	HIS	conflict	UNP U6S0Y1
B	142	ARG	GLN	conflict	UNP U6S0Y1
B	150	ASN	ASP	conflict	UNP U6S0Y1
B	205	ASP	GLU	conflict	UNP U6S0Y1
B	206	GLU	ASP	conflict	UNP U6S0Y1
C	1	MET	-	initiating methionine	UNP U6S0Y1
C	2	HIS	-	expression tag	UNP U6S0Y1
C	3	HIS	-	expression tag	UNP U6S0Y1
C	4	HIS	-	expression tag	UNP U6S0Y1
C	5	HIS	-	expression tag	UNP U6S0Y1
C	6	HIS	-	expression tag	UNP U6S0Y1
C	7	HIS	-	expression tag	UNP U6S0Y1
C	32	ASN	LYS	conflict	UNP U6S0Y1
C	35	ARG	GLN	conflict	UNP U6S0Y1
C	45	ILE	VAL	conflict	UNP U6S0Y1
C	47	VAL	ILE	conflict	UNP U6S0Y1
C	118	ALA	HIS	conflict	UNP U6S0Y1
C	142	ARG	GLN	conflict	UNP U6S0Y1
C	150	ASN	ASP	conflict	UNP U6S0Y1
C	205	ASP	GLU	conflict	UNP U6S0Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	GLU	ASP	conflict	UNP U6S0Y1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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


- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	85	Total O 85 85	0	0
3	D	70	Total O 70 70	0	0
3	B	79	Total O 79 79	0	0
3	C	60	Total O 60 60	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 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.

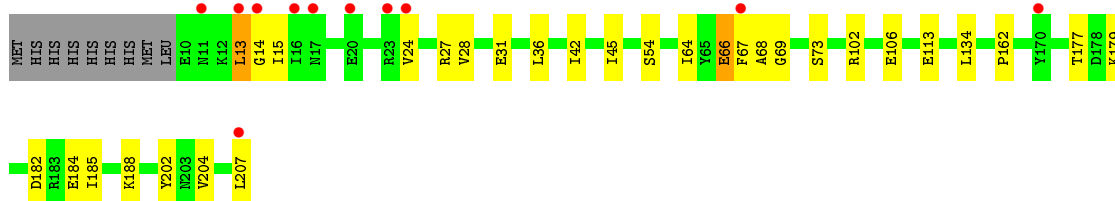
- Molecule 1: Fic family protein

Chain A: 

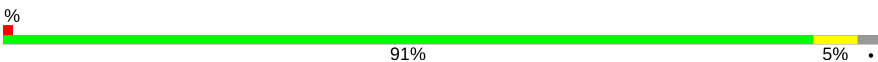


- Molecule 1: Fic family protein

Chain D: 




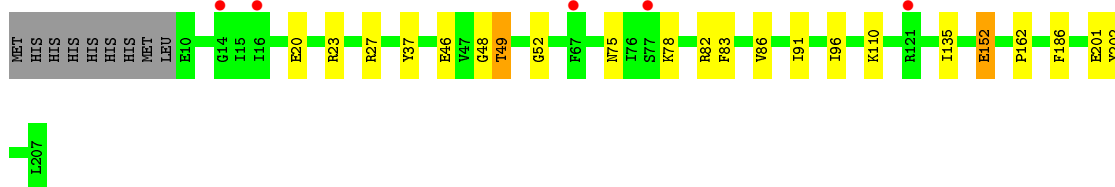
- Molecule 1: Fic family protein

Chain B: 



- Molecule 1: Fic family protein

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.93Å 131.16Å 136.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.05 – 2.20 43.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.05-2.20) 99.9 (43.05-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.213 , 0.249 0.213 , 0.249	Depositor DCC
R_{free} test set	2733 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtrriage
Anisotropy	0.547	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.002 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6918	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	0.45	0/1674	0.63	2/2253 (0.1%)
1	B	0.45	0/1690	0.66	1/2274 (0.0%)
1	C	0.43	0/1685	0.60	0/2267
1	D	0.48	0/1674	0.62	0/2253
All	All	0.45	0/6723	0.63	3/9047 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	82	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	B	82	ARG	NE-CZ-NH1	5.20	122.90	120.30

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	1645	0	1640	11	0
1	B	1661	0	1660	8	0
1	C	1653	0	1653	15	0
1	D	1645	0	1640	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	85	0	0	3	0
3	B	79	0	0	0	0
3	C	60	0	0	1	0
3	D	70	0	0	0	0
All	All	6918	0	6593	50	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.

All (50) 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:20:GLU:OE1	1:C:23:ARG:NH1	2.13	0.80
1:B:41:ASP:OD1	1:B:44:ARG:NH1	2.23	0.71
1:A:23:ARG:NH1	3:A:401:HOH:O	2.18	0.66
1:C:46:GLU:OE1	1:C:49:THR:HG21	1.97	0.64
1:D:13:LEU:HD13	1:D:14:GLY:H	1.65	0.62
1:A:162:PRO:O	1:C:82[B]:ARG:NH2	2.34	0.60
1:C:78:LYS:HB3	1:C:83:PHE:HE2	1.67	0.60
1:C:49:THR:HG22	1:C:52:GLY:H	1.69	0.58
1:D:27:ARG:NH1	1:D:31:GLU:OE1	2.37	0.58
1:B:20:GLU:O	1:B:24:VAL:HG23	2.04	0.58
1:D:66:GLU:O	1:D:68:ALA:N	2.40	0.55
1:D:179:LYS:HB3	1:D:182:ASP:HB2	1.89	0.53
1:B:179:LYS:HB3	1:B:182:ASP:HB2	1.90	0.53
1:A:20:GLU:HG3	3:A:401:HOH:O	2.09	0.51
1:A:179:LYS:HB3	1:A:182:ASP:HB2	1.92	0.51
1:D:15:ILE:CD1	1:D:24:VAL:HG21	2.41	0.51
1:A:101:GLN:OE1	1:A:110:LYS:NZ	2.38	0.50
1:A:177:THR:HG21	1:A:185:ILE:HD13	1.94	0.50
1:B:87:MET:HG3	1:B:88:TYR:CD2	2.47	0.49
1:D:184:GLU:OE2	1:D:188:LYS:HB2	2.13	0.49
1:A:31:GLU:OE1	3:A:402:HOH:O	2.20	0.48
1:D:45:ILE:HD11	1:D:134:LEU:CD1	2.44	0.48
1:D:113:GLU:CD	1:B:82:ARG:HH22	2.16	0.48
1:D:54:SER:OG	1:D:69:GLY:O	2.25	0.48
1:A:205:ASP:OD1	1:A:205:ASP:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:MET:HG3	1:A:88:TYR:CD2	2.48	0.47
1:D:162:PRO:O	1:B:82:ARG:HD2	2.13	0.47
1:D:27:ARG:HB2	1:D:202:TYR:CE2	2.50	0.46
1:A:82:ARG:HD2	1:C:162:PRO:O	2.16	0.46
1:C:96:ILE:O	1:C:110:LYS:HE3	2.16	0.46
1:C:75:ASN:OD1	1:C:86:VAL:HG23	2.16	0.46
1:C:27:ARG:HB2	1:C:202:TYR:CE1	2.51	0.45
1:D:27:ARG:HB2	1:D:202:TYR:CZ	2.52	0.44
1:C:91:ILE:H	1:C:91:ILE:HD12	1.82	0.44
1:C:82[B]:ARG:NH2	3:C:404:HOH:O	2.34	0.43
1:D:204:VAL:HA	1:D:207:LEU:HD12	2.00	0.43
1:A:159:GLU:OE1	1:B:80:ASN:ND2	2.52	0.43
1:C:37:TYR:HB2	1:C:186:PHE:CE2	2.54	0.43
1:D:36:LEU:HG	1:D:42:ILE:HB	2.00	0.43
1:C:23:ARG:HG3	1:C:201:GLU:CD	2.39	0.42
1:D:66:GLU:C	1:D:68:ALA:H	2.23	0.42
1:D:177:THR:HG21	1:D:185:ILE:HD13	2.01	0.42
1:C:152:GLU:H	1:C:152:GLU:CD	2.23	0.41
1:D:13:LEU:HD12	1:D:15:ILE:CG1	2.51	0.41
1:D:102:ARG:NH2	1:D:106:GLU:OE2	2.36	0.41
1:C:48:GLY:HA2	1:C:135:ILE:HD11	2.02	0.41
1:D:13:LEU:HD13	1:D:14:GLY:N	2.32	0.41
1:D:45:ILE:HD13	1:D:45:ILE:HG21	1.87	0.41
1:B:45:ILE:HG12	1:B:55:TYR:CD1	2.56	0.40
1:D:28:VAL:HB	1:D:64:ILE:HD11	2.03	0.40

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	196/207 (95%)	195 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	198/207 (96%)	197 (100%)	1 (0%)	0	100	100
1	C	197/207 (95%)	196 (100%)	1 (0%)	0	100	100
1	D	196/207 (95%)	193 (98%)	1 (0%)	2 (1%)	15	14
All	All	787/828 (95%)	781 (99%)	4 (0%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	67	PHE
1	D	66	GLU

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	178/187 (95%)	177 (99%)	1 (1%)	86	93
1	B	180/187 (96%)	180 (100%)	0	100	100
1	C	179/187 (96%)	177 (99%)	2 (1%)	73	85
1	D	178/187 (95%)	176 (99%)	2 (1%)	73	85
All	All	715/748 (96%)	710 (99%)	5 (1%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ASP
1	D	13	LEU
1	D	73	SER
1	C	49	THR
1	C	152	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	147	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](#)

4 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	301	-	4,4,4	0.27	0	6,6,6	0.32	0
2	SO4	A	301	-	4,4,4	0.38	0	6,6,6	0.40	0
2	SO4	D	301	-	4,4,4	0.20	0	6,6,6	0.33	0
2	SO4	B	301	-	4,4,4	0.20	0	6,6,6	0.40	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 [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, 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	198/207 (95%)	-0.08	1 (0%) 91 90	37, 51, 69, 77	0
1	B	200/207 (96%)	-0.04	2 (1%) 82 81	35, 52, 68, 77	0
1	C	198/207 (95%)	0.03	5 (2%) 57 55	38, 54, 78, 96	0
1	D	198/207 (95%)	0.26	11 (5%) 24 23	36, 54, 87, 97	0
All	All	794/828 (95%)	0.04	19 (2%) 59 56	35, 53, 76, 97	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	LEU	5.3
1	D	67	PHE	4.0
1	D	24	VAL	3.9
1	C	14	GLY	3.8
1	D	16	ILE	3.7
1	D	14	GLY	3.7
1	C	16	ILE	3.6
1	B	141	LYS	2.9
1	A	102	ARG	2.8
1	D	11	ASN	2.6
1	D	23	ARG	2.5
1	D	207	LEU	2.4
1	C	121	ARG	2.3
1	D	17	ASN	2.3
1	C	77	SER	2.3
1	D	20	GLU	2.2
1	D	170	TYR	2.2
1	B	102	ARG	2.1
1	C	67	PHE	2.1

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 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, 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(\AA^2)	Q<0.9
2	SO4	A	301	5/5	0.94	0.12	52,52,52,52	0
2	SO4	B	301	5/5	0.96	0.16	51,51,51,51	0
2	SO4	D	301	5/5	0.98	0.10	59,59,59,59	0
2	SO4	C	301	5/5	0.98	0.07	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.