wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 06:35 AM EDT

PDB ID	:	2RJT
Title	:	Crystal Structure Analysis of a Surface Entropy Reduction Mutant of S. pneumoniae FabF
Authors	:	Soisson, S.M.; Parthasarathy, G.; Becker, J.
Deposited on	:	2007-10-15
Resolution	:	1.75 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:

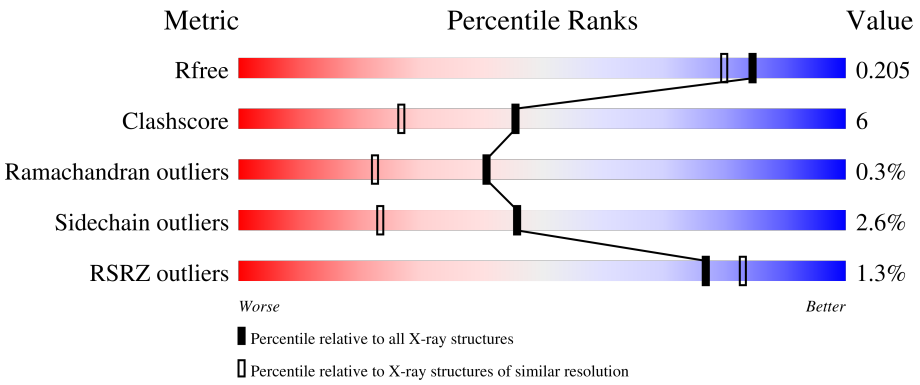
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	428	.% 84% 11% 5%
1	B	428	2% 84% 9% • 5%
1	C	428	.% 83% 12% 5%
1	D	428	.% 86% 9% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14001 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 Beta-ketoacyl-ACP synthase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3047	1927	523	585	12	0	1	0
1	D	408	3053	1930	524	587	12	0	2	0
1	C	408	3057	1933	525	586	13	0	2	0
1	B	408	3053	1930	524	587	12	0	2	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q9FBC2
A	-17	SER	-	expression tag	UNP Q9FBC2
A	-16	SER	-	expression tag	UNP Q9FBC2
A	-15	HIS	-	expression tag	UNP Q9FBC2
A	-14	HIS	-	expression tag	UNP Q9FBC2
A	-13	HIS	-	expression tag	UNP Q9FBC2
A	-12	HIS	-	expression tag	UNP Q9FBC2
A	-11	HIS	-	expression tag	UNP Q9FBC2
A	-10	HIS	-	expression tag	UNP Q9FBC2
A	-9	SER	-	expression tag	UNP Q9FBC2
A	-8	SER	-	expression tag	UNP Q9FBC2
A	-7	GLY	-	expression tag	UNP Q9FBC2
A	-6	LEU	-	expression tag	UNP Q9FBC2
A	-5	VAL	-	expression tag	UNP Q9FBC2
A	-4	PRO	-	expression tag	UNP Q9FBC2
A	-3	ARG	-	expression tag	UNP Q9FBC2
A	-2	GLY	-	expression tag	UNP Q9FBC2
A	-1	SER	-	expression tag	UNP Q9FBC2
A	0	HIS	-	expression tag	UNP Q9FBC2
A	22	ALA	GLU	engineered mutation	UNP Q9FBC2
A	94	ALA	GLU	engineered mutation	UNP Q9FBC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	GLU	engineered mutation	UNP Q9FBC2
A	383	ALA	GLU	engineered mutation	UNP Q9FBC2
A	409	ALA	GLU	engineered mutation	UNP Q9FBC2
D	-18	GLY	-	expression tag	UNP Q9FBC2
D	-17	SER	-	expression tag	UNP Q9FBC2
D	-16	SER	-	expression tag	UNP Q9FBC2
D	-15	HIS	-	expression tag	UNP Q9FBC2
D	-14	HIS	-	expression tag	UNP Q9FBC2
D	-13	HIS	-	expression tag	UNP Q9FBC2
D	-12	HIS	-	expression tag	UNP Q9FBC2
D	-11	HIS	-	expression tag	UNP Q9FBC2
D	-10	HIS	-	expression tag	UNP Q9FBC2
D	-9	SER	-	expression tag	UNP Q9FBC2
D	-8	SER	-	expression tag	UNP Q9FBC2
D	-7	GLY	-	expression tag	UNP Q9FBC2
D	-6	LEU	-	expression tag	UNP Q9FBC2
D	-5	VAL	-	expression tag	UNP Q9FBC2
D	-4	PRO	-	expression tag	UNP Q9FBC2
D	-3	ARG	-	expression tag	UNP Q9FBC2
D	-2	GLY	-	expression tag	UNP Q9FBC2
D	-1	SER	-	expression tag	UNP Q9FBC2
D	0	HIS	-	expression tag	UNP Q9FBC2
D	22	ALA	GLU	engineered mutation	UNP Q9FBC2
D	94	ALA	GLU	engineered mutation	UNP Q9FBC2
D	325	ALA	GLU	engineered mutation	UNP Q9FBC2
D	383	ALA	GLU	engineered mutation	UNP Q9FBC2
D	409	ALA	GLU	engineered mutation	UNP Q9FBC2
C	-18	GLY	-	expression tag	UNP Q9FBC2
C	-17	SER	-	expression tag	UNP Q9FBC2
C	-16	SER	-	expression tag	UNP Q9FBC2
C	-15	HIS	-	expression tag	UNP Q9FBC2
C	-14	HIS	-	expression tag	UNP Q9FBC2
C	-13	HIS	-	expression tag	UNP Q9FBC2
C	-12	HIS	-	expression tag	UNP Q9FBC2
C	-11	HIS	-	expression tag	UNP Q9FBC2
C	-10	HIS	-	expression tag	UNP Q9FBC2
C	-9	SER	-	expression tag	UNP Q9FBC2
C	-8	SER	-	expression tag	UNP Q9FBC2
C	-7	GLY	-	expression tag	UNP Q9FBC2
C	-6	LEU	-	expression tag	UNP Q9FBC2
C	-5	VAL	-	expression tag	UNP Q9FBC2
C	-4	PRO	-	expression tag	UNP Q9FBC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP Q9FBC2
C	-2	GLY	-	expression tag	UNP Q9FBC2
C	-1	SER	-	expression tag	UNP Q9FBC2
C	0	HIS	-	expression tag	UNP Q9FBC2
C	22	ALA	GLU	engineered mutation	UNP Q9FBC2
C	94	ALA	GLU	engineered mutation	UNP Q9FBC2
C	325	ALA	GLU	engineered mutation	UNP Q9FBC2
C	383	ALA	GLU	engineered mutation	UNP Q9FBC2
C	409	ALA	GLU	engineered mutation	UNP Q9FBC2
B	-18	GLY	-	expression tag	UNP Q9FBC2
B	-17	SER	-	expression tag	UNP Q9FBC2
B	-16	SER	-	expression tag	UNP Q9FBC2
B	-15	HIS	-	expression tag	UNP Q9FBC2
B	-14	HIS	-	expression tag	UNP Q9FBC2
B	-13	HIS	-	expression tag	UNP Q9FBC2
B	-12	HIS	-	expression tag	UNP Q9FBC2
B	-11	HIS	-	expression tag	UNP Q9FBC2
B	-10	HIS	-	expression tag	UNP Q9FBC2
B	-9	SER	-	expression tag	UNP Q9FBC2
B	-8	SER	-	expression tag	UNP Q9FBC2
B	-7	GLY	-	expression tag	UNP Q9FBC2
B	-6	LEU	-	expression tag	UNP Q9FBC2
B	-5	VAL	-	expression tag	UNP Q9FBC2
B	-4	PRO	-	expression tag	UNP Q9FBC2
B	-3	ARG	-	expression tag	UNP Q9FBC2
B	-2	GLY	-	expression tag	UNP Q9FBC2
B	-1	SER	-	expression tag	UNP Q9FBC2
B	0	HIS	-	expression tag	UNP Q9FBC2
B	22	ALA	GLU	engineered mutation	UNP Q9FBC2
B	94	ALA	GLU	engineered mutation	UNP Q9FBC2
B	325	ALA	GLU	engineered mutation	UNP Q9FBC2
B	383	ALA	GLU	engineered mutation	UNP Q9FBC2
B	409	ALA	GLU	engineered mutation	UNP Q9FBC2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	507	507	507	0	0
2	D	472	472	472	0	0
2	C	408	408	408	0	0

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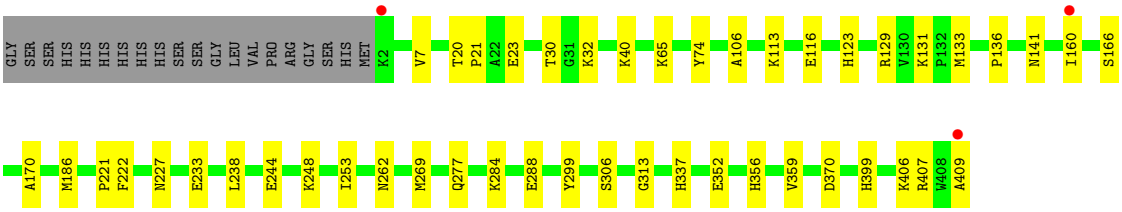
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	404	404	404	0	0

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.

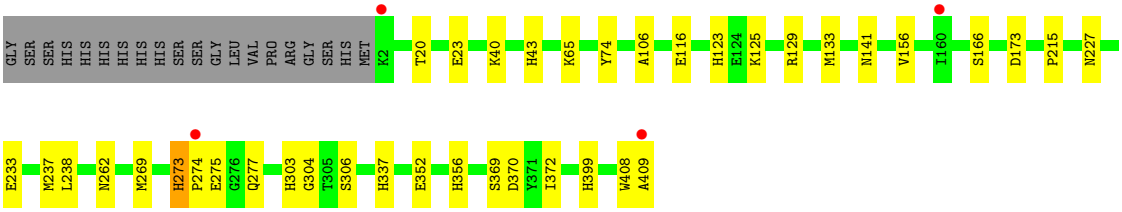
• Molecule 1: Beta-ketoacyl-ACP synthase II

Chain A:



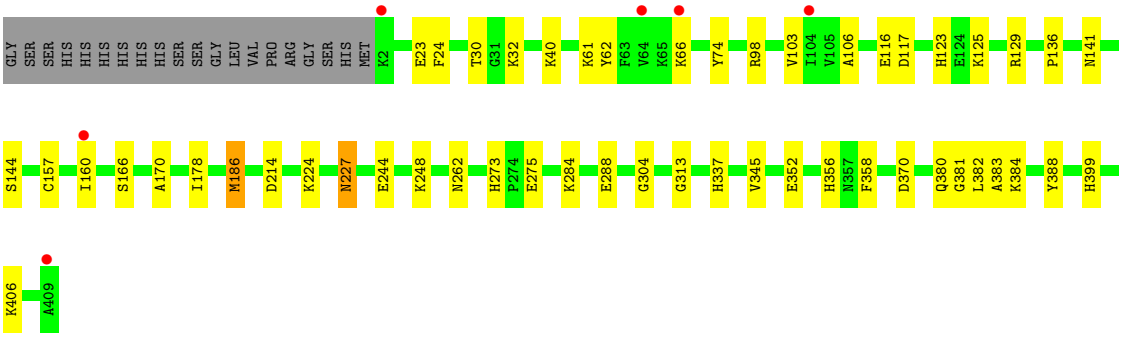
• Molecule 1: Beta-ketoacyl-ACP synthase II

Chain D:



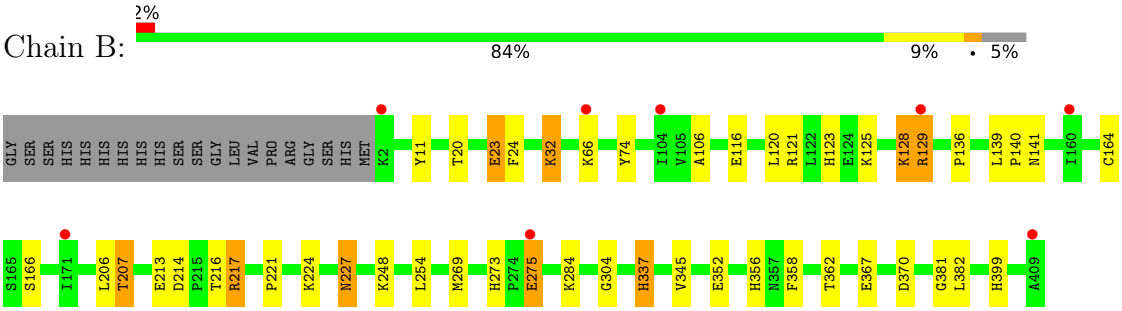
• Molecule 1: Beta-ketoacyl-ACP synthase II

Chain C:



• Molecule 1: Beta-ketoacyl-ACP synthase II

Chain B:


2%
84%
9%
5%
GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET K2 Y11 T20 E23 F24 K32 K66 Y74 I104 V105 A106 E116 L120 R121 L122 H123 E124 K125 K128 R129 P136 L139 P140 N141 I160 C164
S165 S166 I171 L206 T207 E213 D214 P215 T216 R217 P221 K224 N227 K248 L254 M269 H273 P274 E275 K284 G304 H337 V345 E352 H356 N357 F358 T362 E367 D370 G381 L382 H399 A409

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	112.42Å 115.87Å 278.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 1.75 45.89 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.90-1.75) 99.5 (45.89-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 1.75Å)	Xtriage
Refinement program	TNT, BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.167 , 0.207 0.166 , 0.205	Depositor DCC
R_{free} test set	9058 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14001	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 (i)

5.1 Standard geometry (i)

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	0.72	1/3110 (0.0%)	0.79	0/4218
1	B	0.63	0/3116	0.76	0/4226
1	C	0.62	0/3120	0.75	0/4230
1	D	0.72	0/3116	0.79	1/4226 (0.0%)
All	All	0.67	1/12462 (0.0%)	0.77	1/16900 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	MET	CG-SD	-5.71	1.66	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	273	HIS	C-N-CD	-6.38	106.56	120.60

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	3047	0	2993	40	0
1	B	3053	0	2997	55	0
1	C	3057	0	3008	46	0
1	D	3053	0	2997	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	507	0	0	10	0
2	B	404	0	0	14	0
2	C	408	0	0	14	0
2	D	472	0	0	8	0
All	All	14001	0	11995	154	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 6.

The worst 5 of 154 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:D:141:ASN:HD22	1:C:399:HIS:HE1	1.10	0.93
1:D:273:HIS:CD2	1:D:274:PRO:HD2	2.06	0.91
1:A:399:HIS:HE1	1:B:141:ASN:HD22	1.23	0.87
1:A:407:ARG:O	1:A:409:ALA:HB3	1.78	0.82
1:D:141:ASN:HD22	1:C:399:HIS:CE1	1.96	0.81

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	407/428 (95%)	397 (98%)	9 (2%)	1 (0%)	47	29
1	B	408/428 (95%)	399 (98%)	8 (2%)	1 (0%)	47	29
1	C	408/428 (95%)	399 (98%)	8 (2%)	1 (0%)	47	29
1	D	408/428 (95%)	397 (97%)	9 (2%)	2 (0%)	29	12
All	All	1631/1712 (95%)	1592 (98%)	34 (2%)	5 (0%)	41	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	304	GLY
1	C	304	GLY
1	D	306	SER
1	A	306	SER
1	D	304	GLY

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	314/332 (95%)	308 (98%)	6 (2%)	57	37
1	B	315/332 (95%)	301 (96%)	14 (4%)	28	8
1	C	316/332 (95%)	307 (97%)	9 (3%)	43	20
1	D	315/332 (95%)	311 (99%)	4 (1%)	69	54
All	All	1260/1328 (95%)	1227 (97%)	33 (3%)	46	23

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	227	ASN
1	B	248	LYS
1	B	382	LEU
1	C	144	SER
1	C	74	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	123	HIS
1	B	356	HIS
1	B	399	HIS
1	B	273	HIS
1	D	399	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	408/428 (95%)	-0.32	3 (0%)	87	92	16, 22, 35, 74	0
1	B	408/428 (95%)	-0.06	8 (1%)	65	72	19, 29, 46, 82	0
1	C	408/428 (95%)	-0.08	6 (1%)	73	80	19, 29, 46, 84	0
1	D	408/428 (95%)	-0.25	4 (0%)	82	87	15, 23, 40, 78	0
All	All	1632/1712 (95%)	-0.18	21 (1%)	77	83	15, 26, 42, 84	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	6.0
1	C	2	LYS	4.4
1	B	2	LYS	4.1
1	D	409	ALA	4.0
1	A	409	ALA	3.9

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.