WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 12:50 am BST

PDB ID	:	5JK2
Title	:	Crystal structure of Treponema pallidum Tp0751 (Pallilysin)
Authors	:	Parker, M.L.; Boulanger, M.J.
Deposited on	:	2016-04-25
Resolution	:	2.15 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

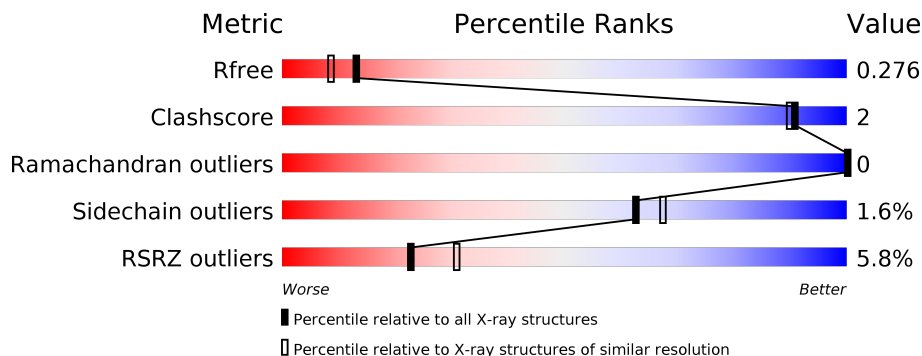|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.15 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.
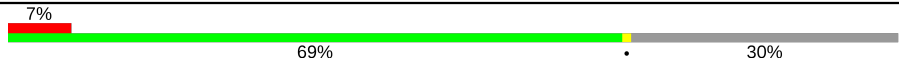
Metric	Percentile Ranks	Value
Rfree		0.276
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		5.8%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	167	2% 72% • 23%
1	B	167	5% 71% • 25%
1	C	167	2% 69% • 27%
1	D	167	5% 70% 7% 23%
1	E	167	2% 74% •• 23%
1	F	167	2% 70% • 26%

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Mol	Chain	Length	Quality of chain
1	G	167	7% · · · · · · · · · 69% · · · · · · · · · · 30%
1	H	167	4% · · · · · · · · · 64% · · · · · · · 7% · 29%
1	I	167	10% · · · · · · · · · 66% · · · · · · · · · 31%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9171 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 Tp0751.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total 1039	C 656	N 196	O 185	S 2	0	0	0
1	B	125	Total 1016	C 642	N 193	O 179	S 2	0	0	0
1	C	122	Total 994	C 627	N 189	O 176	S 2	0	0	0
1	D	128	Total 1034	C 653	N 196	O 183	S 2	0	0	0
1	E	128	Total 1029	C 650	N 195	O 182	S 2	0	0	0
1	F	123	Total 1003	C 636	N 190	O 175	S 2	0	0	0
1	G	117	Total 950	C 602	N 179	O 167	S 2	0	0	0
1	H	119	Total 969	C 612	N 182	O 173	S 2	0	0	0
1	I	116	Total 949	C 602	N 179	O 166	S 2	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	-	expression tag	UNP O83732
A	75	SER	-	expression tag	UNP O83732
A	76	MET	-	expression tag	UNP O83732
A	77	ALA	-	expression tag	UNP O83732
A	199	ALA	GLU	engineered mutation	UNP O83732
A	238	ALA	-	expression tag	UNP O83732
A	239	ALA	-	expression tag	UNP O83732
A	240	ALA	-	expression tag	UNP O83732
B	74	GLY	-	expression tag	UNP O83732
B	75	SER	-	expression tag	UNP O83732
B	76	MET	-	expression tag	UNP O83732

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Chain	Residue	Modelled	Actual	Comment	Reference
B	77	ALA	-	expression tag	UNP O83732
B	199	ALA	GLU	engineered mutation	UNP O83732
B	238	ALA	-	expression tag	UNP O83732
B	239	ALA	-	expression tag	UNP O83732
B	240	ALA	-	expression tag	UNP O83732
C	74	GLY	-	expression tag	UNP O83732
C	75	SER	-	expression tag	UNP O83732
C	76	MET	-	expression tag	UNP O83732
C	77	ALA	-	expression tag	UNP O83732
C	199	ALA	GLU	engineered mutation	UNP O83732
C	238	ALA	-	expression tag	UNP O83732
C	239	ALA	-	expression tag	UNP O83732
C	240	ALA	-	expression tag	UNP O83732
D	74	GLY	-	expression tag	UNP O83732
D	75	SER	-	expression tag	UNP O83732
D	76	MET	-	expression tag	UNP O83732
D	77	ALA	-	expression tag	UNP O83732
D	199	ALA	GLU	engineered mutation	UNP O83732
D	238	ALA	-	expression tag	UNP O83732
D	239	ALA	-	expression tag	UNP O83732
D	240	ALA	-	expression tag	UNP O83732
E	74	GLY	-	expression tag	UNP O83732
E	75	SER	-	expression tag	UNP O83732
E	76	MET	-	expression tag	UNP O83732
E	77	ALA	-	expression tag	UNP O83732
E	199	ALA	GLU	engineered mutation	UNP O83732
E	238	ALA	-	expression tag	UNP O83732
E	239	ALA	-	expression tag	UNP O83732
E	240	ALA	-	expression tag	UNP O83732
F	74	GLY	-	expression tag	UNP O83732
F	75	SER	-	expression tag	UNP O83732
F	76	MET	-	expression tag	UNP O83732
F	77	ALA	-	expression tag	UNP O83732
F	199	ALA	GLU	engineered mutation	UNP O83732
F	238	ALA	-	expression tag	UNP O83732
F	239	ALA	-	expression tag	UNP O83732
F	240	ALA	-	expression tag	UNP O83732
G	74	GLY	-	expression tag	UNP O83732
G	75	SER	-	expression tag	UNP O83732
G	76	MET	-	expression tag	UNP O83732
G	77	ALA	-	expression tag	UNP O83732
G	199	ALA	GLU	engineered mutation	UNP O83732

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Chain	Residue	Modelled	Actual	Comment	Reference
G	238	ALA	-	expression tag	UNP O83732
G	239	ALA	-	expression tag	UNP O83732
G	240	ALA	-	expression tag	UNP O83732
H	74	GLY	-	expression tag	UNP O83732
H	75	SER	-	expression tag	UNP O83732
H	76	MET	-	expression tag	UNP O83732
H	77	ALA	-	expression tag	UNP O83732
H	199	ALA	GLU	engineered mutation	UNP O83732
H	238	ALA	-	expression tag	UNP O83732
H	239	ALA	-	expression tag	UNP O83732
H	240	ALA	-	expression tag	UNP O83732
I	74	GLY	-	expression tag	UNP O83732
I	75	SER	-	expression tag	UNP O83732
I	76	MET	-	expression tag	UNP O83732
I	77	ALA	-	expression tag	UNP O83732
I	199	ALA	GLU	engineered mutation	UNP O83732
I	238	ALA	-	expression tag	UNP O83732
I	239	ALA	-	expression tag	UNP O83732
I	240	ALA	-	expression tag	UNP O83732

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total 26　O 26	0	0
2	B	22	Total 22　O 22	0	0
2	C	34	Total 34　O 34	0	0
2	D	15	Total 15　O 15	0	0
2	E	19	Total 19　O 19	0	0
2	F	20	Total 20　O 20	0	0
2	G	22	Total 22　O 22	0	0
2	H	12	Total 12　O 12	0	0
2	I	18	Total 18　O 18	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.
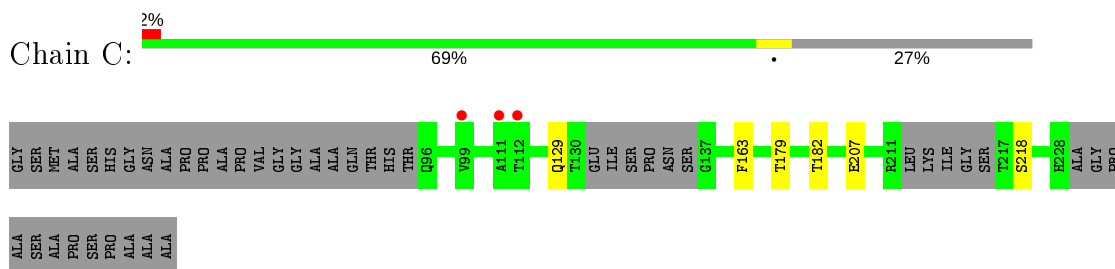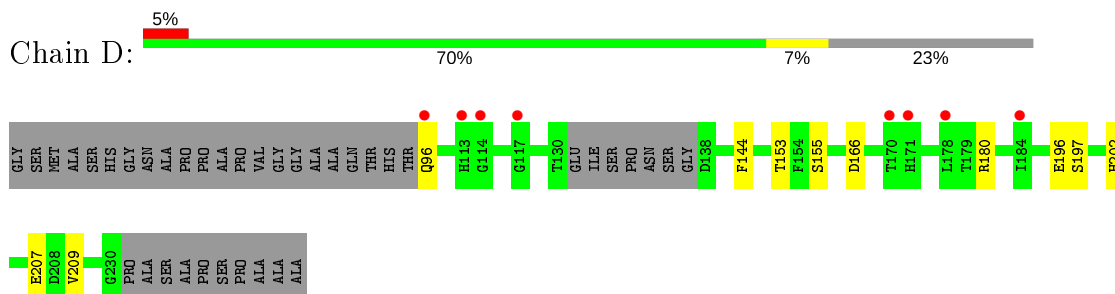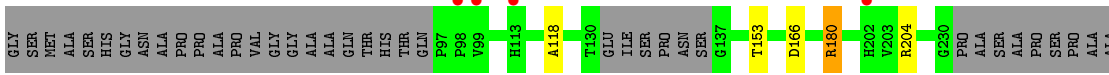
- Molecule 1: Tp0751
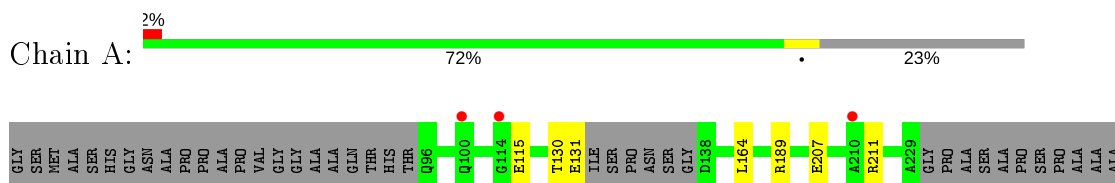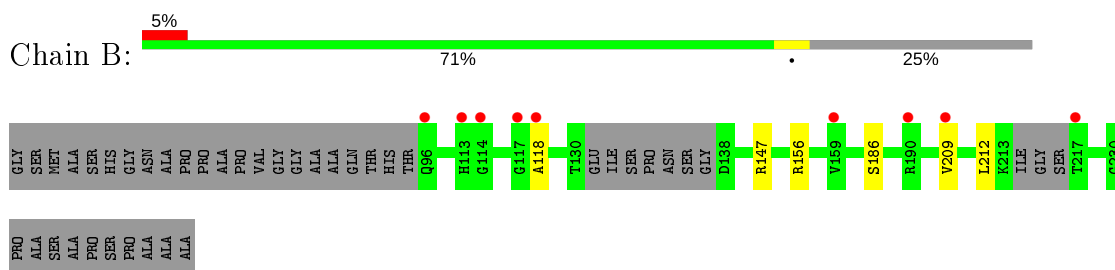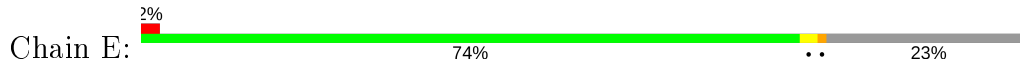

- Molecule 1: Tp0751
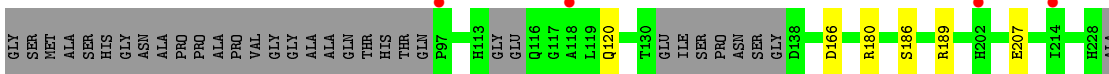

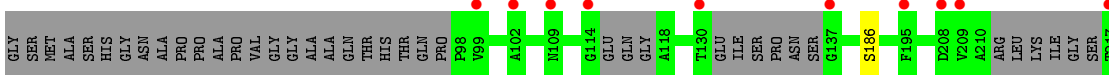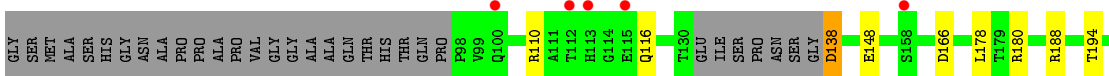- Molecule 1: Tp0751

- Molecule 1: Tp0751

- Molecule 1: Tp0751

Chain E:

- Molecule 1: Tp0751

Chain F:

- Molecule 1: Tp0751

Chain G:

- Molecule 1: Tp0751

Chain H:

- Molecule 1: Tp0751

Chain I:
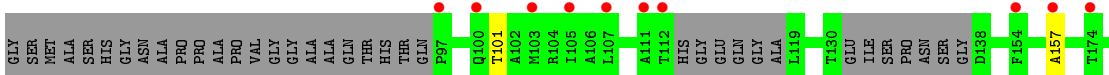
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.72Å 144.72Å 152.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.38 – 2.15 65.38 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.38-2.15) 99.2 (65.38-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.239 , 0.276 0.242 , 0.276	Depositor DCC
R_{free} test set	4990 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.8	EDS
L-test for twinning[2]	$< |L| > = 0.33, < L^2 > = 0.16$	Xtriage
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
Reported twinning fraction	0.440 for -h,-k,l	Depositor
Outliers	0 of 100350 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9171	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 28.55 % 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 1.8080e-03.*

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[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	0.25	0/1063	0.46	0/1441
1	B	0.23	0/1039	0.43	0/1407
1	C	0.24	0/1017	0.44	0/1378
1	D	0.24	0/1058	0.43	0/1434
1	E	0.23	0/1053	0.42	0/1426
1	F	0.23	0/1026	0.43	0/1389
1	G	0.23	0/971	0.42	0/1314
1	H	0.23	0/991	0.42	0/1342
1	I	0.21	0/970	0.40	0/1313
All	All	0.23	0/9188	0.43	0/12444

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	1039	0	1023	2	0
1	B	1016	0	1000	5	0
1	C	994	0	971	4	0
1	D	1034	0	1020	5	1
1	E	1029	0	1016	2	0
1	F	1003	0	995	3	1
1	G	950	0	931	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	969	0	946	6	0
1	I	949	0	936	3	0
2	A	26	0	0	0	0
2	B	22	0	0	3	0
2	C	34	0	0	2	0
2	D	15	0	0	1	0
2	E	19	0	0	1	0
2	F	20	0	0	1	0
2	G	22	0	0	1	0
2	H	12	0	0	0	0
2	I	18	0	0	2	0
All	All	9171	0	8838	30	1

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 2.

The worst 5 of 30 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:H:138:ASP:N	1:H:138:ASP:OD2	2.27	0.68
1:E:166:ASP:OD1	1:E:180:ARG:NH1	2.27	0.66
1:I:211:ARG:NH1	2:I:303:HOH:O	2.32	0.63
1:F:166:ASP:OD1	1:F:180:ARG:NH1	2.32	0.62
1:C:129:GLN:O	2:C:301:HOH:O	2.16	0.60

All (1) 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)
1:D:207:GLU:OE2	1:F:186:SER:OG[4_545]	2.13	0.07

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	124/167 (74%)	114 (92%)	10 (8%)	0	100	100
1	B	119/167 (71%)	111 (93%)	8 (7%)	0	100	100
1	C	116/167 (70%)	108 (93%)	8 (7%)	0	100	100
1	D	124/167 (74%)	114 (92%)	10 (8%)	0	100	100
1	E	124/167 (74%)	115 (93%)	9 (7%)	0	100	100
1	F	117/167 (70%)	113 (97%)	4 (3%)	0	100	100
1	G	109/167 (65%)	99 (91%)	10 (9%)	0	100	100
1	H	113/167 (68%)	107 (95%)	6 (5%)	0	100	100
1	I	108/167 (65%)	103 (95%)	5 (5%)	0	100	100
All	All	1054/1503 (70%)	984 (93%)	70 (7%)	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	110/133 (83%)	107 (97%)	3 (3%)	44	46
1	B	107/133 (80%)	106 (99%)	1 (1%)	78	83
1	C	105/133 (79%)	104 (99%)	1 (1%)	76	81
1	D	109/133 (82%)	107 (98%)	2 (2%)	59	63
1	E	108/133 (81%)	105 (97%)	3 (3%)	43	44
1	F	107/133 (80%)	107 (100%)	0	100	100
1	G	100/133 (75%)	100 (100%)	0	100	100
1	H	103/133 (77%)	99 (96%)	4 (4%)	32	30
1	I	101/133 (76%)	100 (99%)	1 (1%)	76	81
All	All	950/1197 (79%)	935 (98%)	15 (2%)	62	67

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	197	SER
1	E	153	THR
1	H	178	LEU
1	D	155	SER
1	H	148	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	128/167 (76%)	0.45	3 (2%)	60	68	21, 35, 65, 75	0
1	B	125/167 (74%)	0.64	9 (7%)	15	21	22, 40, 64, 77	0
1	C	122/167 (73%)	0.54	3 (2%)	57	65	20, 37, 61, 67	0
1	D	128/167 (76%)	0.64	8 (6%)	20	27	24, 41, 71, 77	0
1	E	128/167 (76%)	0.57	4 (3%)	49	58	21, 40, 65, 76	0
1	F	123/167 (73%)	0.60	4 (3%)	46	55	26, 44, 64, 81	0
1	G	117/167 (70%)	0.97	11 (9%)	8	12	29, 49, 74, 88	0
1	H	119/167 (71%)	0.58	6 (5%)	28	37	23, 47, 76, 87	0
1	I	116/167 (69%)	0.94	16 (13%)	2	3	30, 50, 74, 98	0
All	All	1106/1503 (73%)	0.66	64 (5%)	23	31	20, 42, 71, 98	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	107	LEU	4.6
1	B	114	GLY	4.3
1	H	100	GLN	3.7
1	F	214	ILE	3.6
1	B	118	ALA	3.6

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.