wwPDB X-ray Structure Validation Summary Report (i)

Apr 27, 2024 – 01:34 pm BST

PDB ID	:	2VOE
Title	:	Crystal structure of Rv2780 from M. tuberculosis H37Rv
Authors	:	Tripathi, S.M.; Ramachandran, R.
Deposited on	:	2008-02-17
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

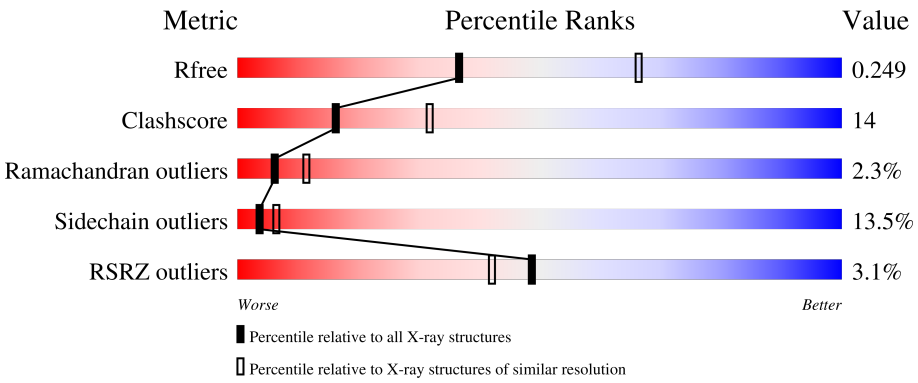
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	371	2%, 70%, 22%, 7%
1	B	371	%, 75%, 16%, 8%
1	C	371	8%, 70%, 22%, 7%
1	D	371	2%, 71%, 21%, 8%
1	E	371	3%, 72%, 21%, 6%

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Mol	Chain	Length	Quality of chain
1	F	371	3% 71% 22% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16386 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 ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	371	2691	1691	473	514	13	0	0	0
1	B	371	2699	1693	476	517	13	0	0	0
1	C	371	2687	1688	470	516	13	0	0	0
1	D	371	2699	1695	476	515	13	0	0	0
1	E	371	2695	1693	473	516	13	0	0	0
1	F	371	2691	1689	473	516	13	0	0	0

- Molecule 2 is water.

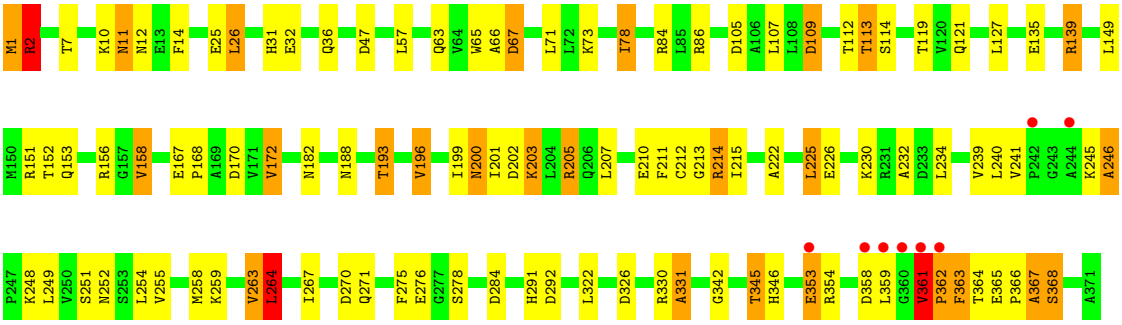
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	31	31	31	0	0
2	B	49	49	49	0	0
2	C	39	39	39	0	0
2	D	30	30	30	0	0
2	E	36	36	36	0	0
2	F	39	39	39	0	0

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.

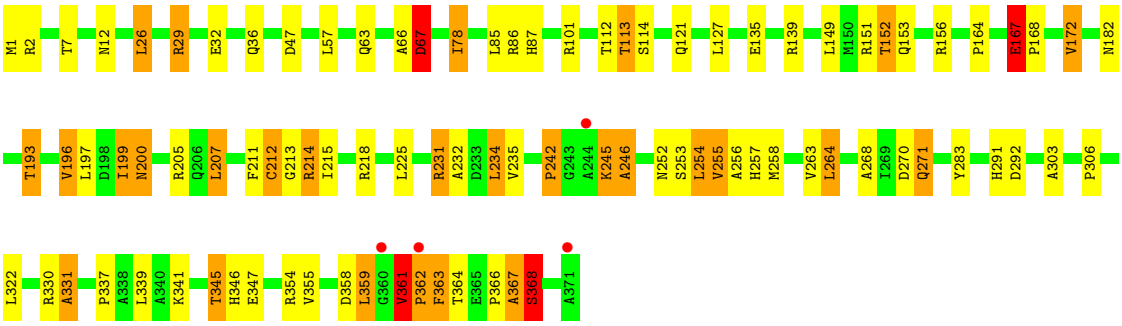
• Molecule 1: ALANINE DEHYDROGENASE

Chain A:



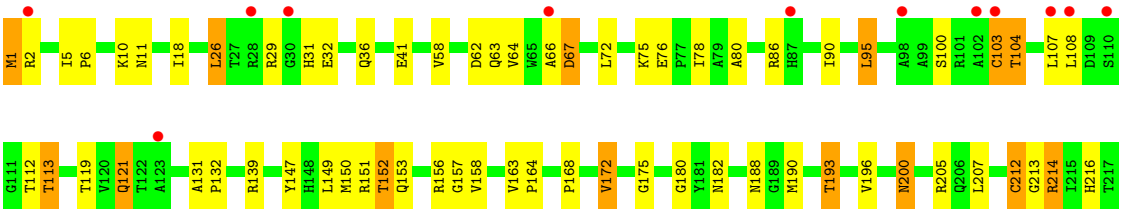
• Molecule 1: ALANINE DEHYDROGENASE

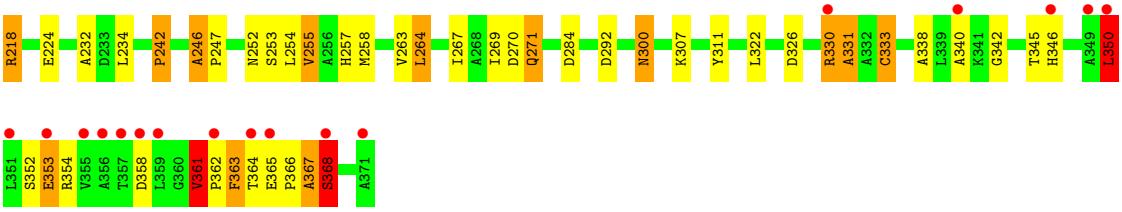
Chain B:



• Molecule 1: ALANINE DEHYDROGENASE

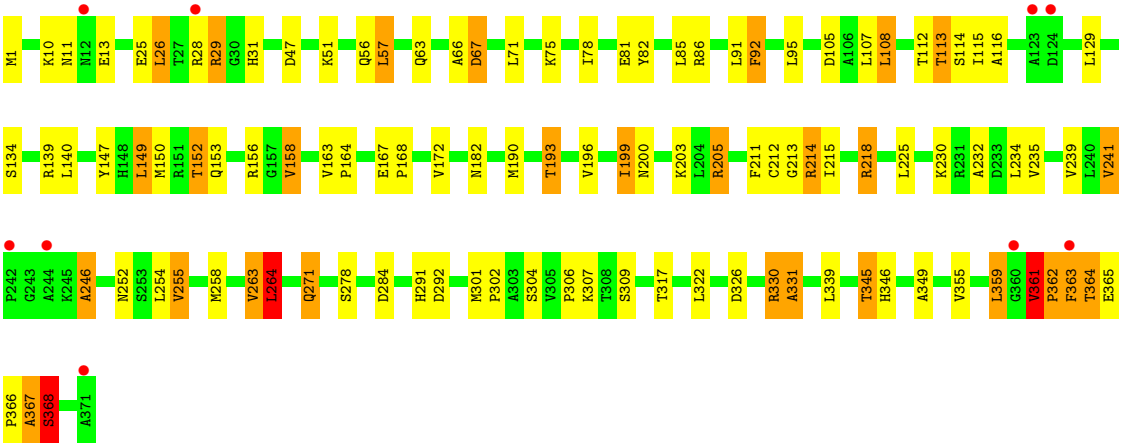
Chain C:





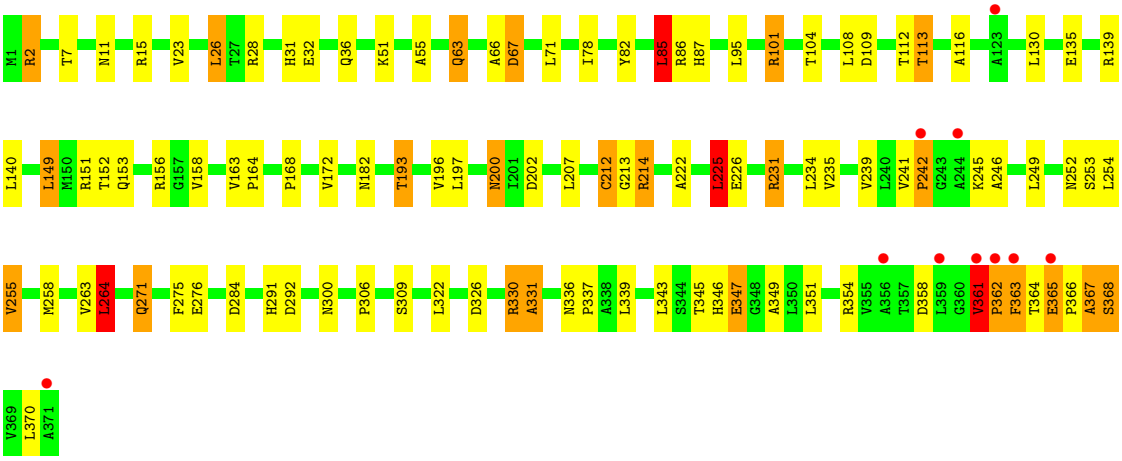
• Molecule 1: ALANINE DEHYDROGENASE

Chain D: 2% 71% 21% 8%



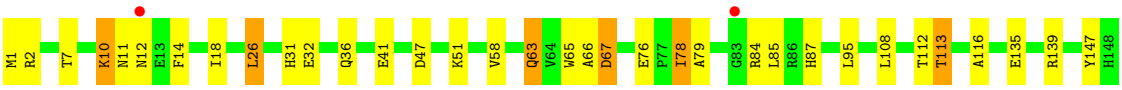
• Molecule 1: ALANINE DEHYDROGENASE

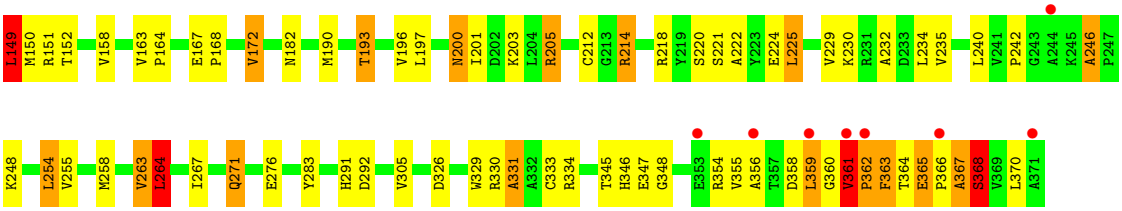
Chain E: 3% 72% 21% 6%



• Molecule 1: ALANINE DEHYDROGENASE

Chain F: 3% 71% 22% 6%




L149
M150
R151
T152
V158
V163
P164
E167
P168
V172
N182
M190
T193
V196
L197
N200
I201
D202
K203
L204
R205
C212
G213
R214
R218
Y219
S220
S221
A222
Y223
E224
L225
V229
K230
R231
A232
D233
L234
V235
L240
V241
P242
G243
A244
K245
A246
P247
K248
L254
V255
M258
V263
L264
I267
Q271
E276
Y283
H291
D292
V305
D326
W329
R330
A331
A332
C333
R334
T345
H346
E347
G348
E353
R354
V355
A356
T357
D358
L359
G360
V361
P362
F363
T364
E365
P366
A367
S368
V369
L370
A371

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.89Å 127.08Å 135.95Å 90.00° 115.04° 90.00°	Depositor
Resolution (Å)	123.09 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (123.09-2.60) 97.3 (40.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.251 0.195 , 0.249	Depositor DCC
R_{free} test set	4005 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16386	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.77	0/2740	0.88	5/3736 (0.1%)
1	B	0.79	3/2747 (0.1%)	0.89	5/3743 (0.1%)
1	C	0.88	1/2735 (0.0%)	0.91	6/3729 (0.2%)
1	D	0.79	0/2748	0.90	5/3746 (0.1%)
1	E	0.82	1/2744 (0.0%)	0.92	5/3741 (0.1%)
1	F	0.81	3/2739 (0.1%)	0.90	7/3733 (0.2%)
All	All	0.81	8/16453 (0.0%)	0.90	33/22428 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	4
1	E	0	1
1	F	0	1
All	All	0	10

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	GLU	CG-CD	6.96	1.62	1.51
1	F	333	CYS	CB-SG	-6.74	1.70	1.82
1	C	212	CYS	CB-SG	6.20	1.92	1.82
1	E	212	CYS	CB-SG	6.12	1.92	1.82
1	B	167	GLU	CB-CG	5.64	1.62	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	LEU	CA-CB-CG	7.67	132.93	115.30
1	C	264	LEU	CA-CB-CG	7.62	132.81	115.30
1	F	225	LEU	CA-CB-CG	7.42	132.38	115.30
1	F	264	LEU	CA-CB-CG	7.38	132.29	115.30
1	D	205	ARG	NE-CZ-NH1	6.89	123.75	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	VAL	Peptide
1	B	361	VAL	Peptide
1	B	368	SER	Peptide
1	C	361	VAL	Peptide
1	D	241	VAL	Peptide

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	2691	0	2680	95	0
1	B	2699	0	2687	77	0
1	C	2687	0	2667	81	0
1	D	2699	0	2696	84	0
1	E	2695	0	2684	81	0
1	F	2691	0	2671	75	0
2	A	31	0	0	2	0
2	B	49	0	0	0	0
2	C	39	0	0	0	0
2	D	30	0	0	2	0
2	E	36	0	0	1	0
2	F	39	0	0	1	0
All	All	16386	0	16085	464	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 14.

The worst 5 of 464 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:E:231:ARG:HH11	1:E:231:ARG:HG3	1.17	1.08
1:C:213:GLY:HA3	1:F:214:ARG:NH2	1.71	1.06
1:A:214:ARG:HH22	1:E:213:GLY:HA3	1.16	1.03
1:F:113:THR:HB	1:F:346:HIS:HD2	1.23	1.02
1:B:66:ALA:O	1:B:67:ASP:HB2	1.55	1.01

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	369/371 (100%)	343 (93%)	18 (5%)	8 (2%)	6 12
1	B	369/371 (100%)	349 (95%)	11 (3%)	9 (2%)	6 10
1	C	369/371 (100%)	342 (93%)	17 (5%)	10 (3%)	5 8
1	D	369/371 (100%)	348 (94%)	13 (4%)	8 (2%)	6 12
1	E	369/371 (100%)	343 (93%)	17 (5%)	9 (2%)	6 10
1	F	369/371 (100%)	347 (94%)	14 (4%)	8 (2%)	6 12
All	All	2214/2226 (100%)	2072 (94%)	90 (4%)	52 (2%)	6 11

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	331	ALA
1	A	362	PRO
1	A	363	PHE
1	A	367	ALA

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	269/276 (98%)	235 (87%)	34 (13%)	4	8
1	B	270/276 (98%)	237 (88%)	33 (12%)	5	9
1	C	268/276 (97%)	230 (86%)	38 (14%)	3	5
1	D	271/276 (98%)	230 (85%)	41 (15%)	3	4
1	E	270/276 (98%)	231 (86%)	39 (14%)	3	5
1	F	268/276 (97%)	235 (88%)	33 (12%)	4	9
All	All	1616/1656 (98%)	1398 (86%)	218 (14%)	4	6

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	92	PHE
1	D	345	THR
1	F	167	GLU
1	D	149	LEU
1	D	225	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	153	GLN
1	F	89	GLN
1	D	11	ASN
1	F	87	HIS
1	F	271	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 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	371/371 (100%)	-0.30	8 (2%)	62	56	16, 37, 62, 77	0
1	B	371/371 (100%)	-0.23	4 (1%)	80	78	16, 36, 61, 77	0
1	C	371/371 (100%)	0.06	29 (7%)	13	9	15, 37, 62, 77	0
1	D	371/371 (100%)	-0.20	9 (2%)	59	53	16, 37, 62, 77	0
1	E	371/371 (100%)	-0.12	10 (2%)	54	48	15, 36, 62, 77	0
1	F	371/371 (100%)	-0.30	10 (2%)	54	48	15, 37, 62, 77	0
All	All	2226/2226 (100%)	-0.18	70 (3%)	49	42	15, 37, 62, 77	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	371	ALA	6.3
1	A	360	GLY	5.2
1	F	371	ALA	5.0
1	C	359	LEU	4.9
1	A	361	VAL	4.6

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 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.