wwPDB X-ray Structure Validation Summary Report (i)

Feb 11, 2024 – 10:40 PM EST

PDB ID	:	3FGN
Title	:	Crystal structure of dethiobiotin synthetase in Mycobacterium tuberculosis
Authors	:	Dey, S.; Sacchettini, J.C.
Deposited on	:	2008-12-08
Resolution	:	1.85 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:

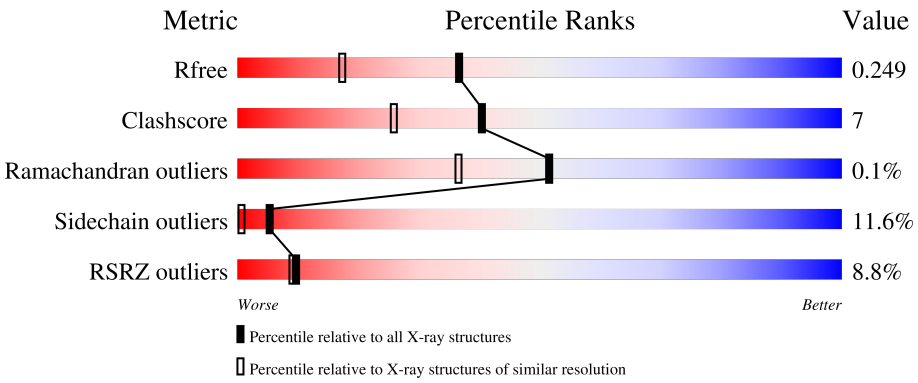
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	251	6% 78% 12% • 8%
1	B	251	6% 75% 12% • 10%
1	C	251	6% 77% 11% • 9%
1	D	251	14% 68% 17% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6648 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 Dethiobiotin synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1613	1007	294	304	8	0	1	0
1	B	225	1568	980	283	297	8	0	0	0
1	C	228	1588	991	288	301	8	0	0	0
1	D	224	1559	974	282	296	7	0	1	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP O06620
A	-23	GLY	-	expression tag	UNP O06620
A	-22	SER	-	expression tag	UNP O06620
A	-21	SER	-	expression tag	UNP O06620
A	-20	HIS	-	expression tag	UNP O06620
A	-19	HIS	-	expression tag	UNP O06620
A	-18	HIS	-	expression tag	UNP O06620
A	-17	HIS	-	expression tag	UNP O06620
A	-16	HIS	-	expression tag	UNP O06620
A	-15	HIS	-	expression tag	UNP O06620
A	-14	SER	-	expression tag	UNP O06620
A	-13	SER	-	expression tag	UNP O06620
A	-12	GLY	-	expression tag	UNP O06620
A	-11	LEU	-	expression tag	UNP O06620
A	-10	GLN	-	expression tag	UNP O06620
A	-9	GLY	-	expression tag	UNP O06620
A	-8	THR	-	expression tag	UNP O06620
A	-7	GLU	-	expression tag	UNP O06620
A	-6	ASN	-	expression tag	UNP O06620
A	-5	LEU	-	expression tag	UNP O06620
A	-4	TYR	-	expression tag	UNP O06620

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	expression tag	UNP O06620
A	-2	GLN	-	expression tag	UNP O06620
A	-1	SER	-	expression tag	UNP O06620
A	0	HIS	-	expression tag	UNP O06620
B	-24	MET	-	expression tag	UNP O06620
B	-23	GLY	-	expression tag	UNP O06620
B	-22	SER	-	expression tag	UNP O06620
B	-21	SER	-	expression tag	UNP O06620
B	-20	HIS	-	expression tag	UNP O06620
B	-19	HIS	-	expression tag	UNP O06620
B	-18	HIS	-	expression tag	UNP O06620
B	-17	HIS	-	expression tag	UNP O06620
B	-16	HIS	-	expression tag	UNP O06620
B	-15	HIS	-	expression tag	UNP O06620
B	-14	SER	-	expression tag	UNP O06620
B	-13	SER	-	expression tag	UNP O06620
B	-12	GLY	-	expression tag	UNP O06620
B	-11	LEU	-	expression tag	UNP O06620
B	-10	GLN	-	expression tag	UNP O06620
B	-9	GLY	-	expression tag	UNP O06620
B	-8	THR	-	expression tag	UNP O06620
B	-7	GLU	-	expression tag	UNP O06620
B	-6	ASN	-	expression tag	UNP O06620
B	-5	LEU	-	expression tag	UNP O06620
B	-4	TYR	-	expression tag	UNP O06620
B	-3	PHE	-	expression tag	UNP O06620
B	-2	GLN	-	expression tag	UNP O06620
B	-1	SER	-	expression tag	UNP O06620
B	0	HIS	-	expression tag	UNP O06620
C	-24	MET	-	expression tag	UNP O06620
C	-23	GLY	-	expression tag	UNP O06620
C	-22	SER	-	expression tag	UNP O06620
C	-21	SER	-	expression tag	UNP O06620
C	-20	HIS	-	expression tag	UNP O06620
C	-19	HIS	-	expression tag	UNP O06620
C	-18	HIS	-	expression tag	UNP O06620
C	-17	HIS	-	expression tag	UNP O06620
C	-16	HIS	-	expression tag	UNP O06620
C	-15	HIS	-	expression tag	UNP O06620
C	-14	SER	-	expression tag	UNP O06620
C	-13	SER	-	expression tag	UNP O06620
C	-12	GLY	-	expression tag	UNP O06620

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	LEU	-	expression tag	UNP O06620
C	-10	GLN	-	expression tag	UNP O06620
C	-9	GLY	-	expression tag	UNP O06620
C	-8	THR	-	expression tag	UNP O06620
C	-7	GLU	-	expression tag	UNP O06620
C	-6	ASN	-	expression tag	UNP O06620
C	-5	LEU	-	expression tag	UNP O06620
C	-4	TYR	-	expression tag	UNP O06620
C	-3	PHE	-	expression tag	UNP O06620
C	-2	GLN	-	expression tag	UNP O06620
C	-1	SER	-	expression tag	UNP O06620
C	0	HIS	-	expression tag	UNP O06620
D	-24	MET	-	expression tag	UNP O06620
D	-23	GLY	-	expression tag	UNP O06620
D	-22	SER	-	expression tag	UNP O06620
D	-21	SER	-	expression tag	UNP O06620
D	-20	HIS	-	expression tag	UNP O06620
D	-19	HIS	-	expression tag	UNP O06620
D	-18	HIS	-	expression tag	UNP O06620
D	-17	HIS	-	expression tag	UNP O06620
D	-16	HIS	-	expression tag	UNP O06620
D	-15	HIS	-	expression tag	UNP O06620
D	-14	SER	-	expression tag	UNP O06620
D	-13	SER	-	expression tag	UNP O06620
D	-12	GLY	-	expression tag	UNP O06620
D	-11	LEU	-	expression tag	UNP O06620
D	-10	GLN	-	expression tag	UNP O06620
D	-9	GLY	-	expression tag	UNP O06620
D	-8	THR	-	expression tag	UNP O06620
D	-7	GLU	-	expression tag	UNP O06620
D	-6	ASN	-	expression tag	UNP O06620
D	-5	LEU	-	expression tag	UNP O06620
D	-4	TYR	-	expression tag	UNP O06620
D	-3	PHE	-	expression tag	UNP O06620
D	-2	GLN	-	expression tag	UNP O06620
D	-1	SER	-	expression tag	UNP O06620
D	0	HIS	-	expression tag	UNP O06620

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	114	114	114	0	0

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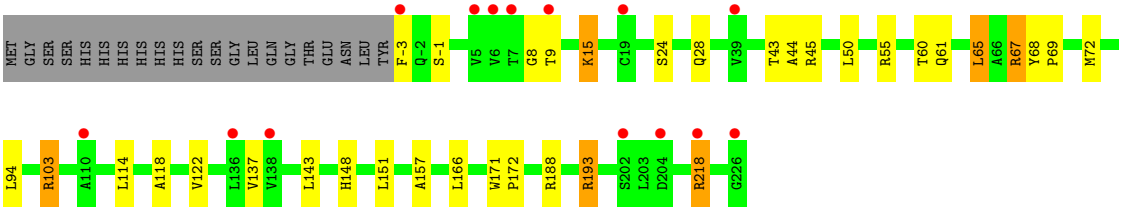
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	96	96	96	0	0
			Total	O		
2	C	73	73	73	0	0
			Total	O		
2	D	37	37	37	0	0

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.

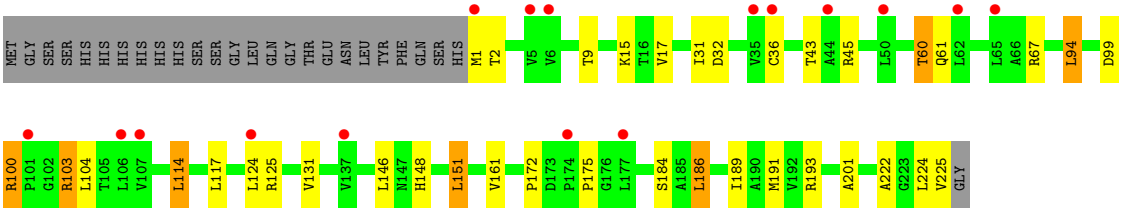
• Molecule 1: Dethiobiotin synthetase

Chain A:



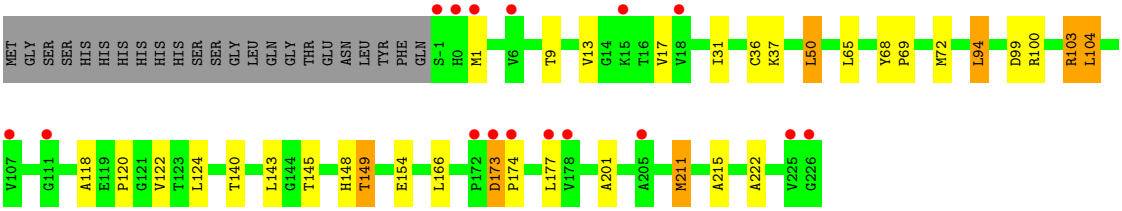
• Molecule 1: Dethiobiotin synthetase

Chain B:



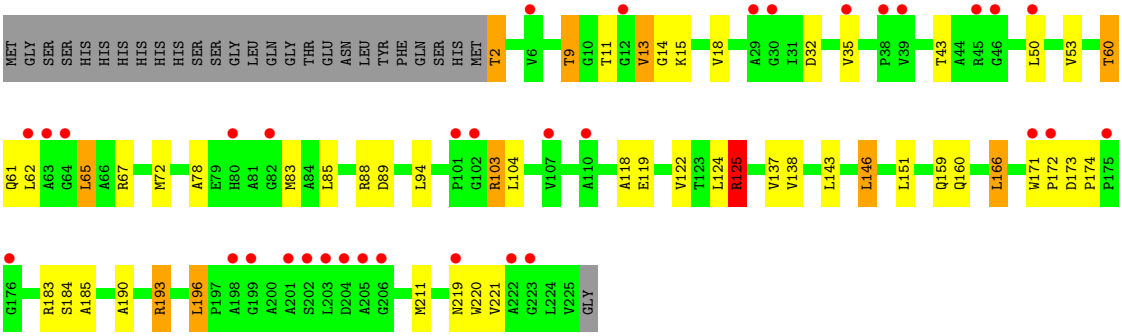
• Molecule 1: Dethiobiotin synthetase

Chain C:



• Molecule 1: Dethiobiotin synthetase

Chain D:


MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
LEU
GLN
GLY
THR
GLU
ASN
LEU
TYR
PHE
GLN
SER
HIS
MET
T2
V6
T9
G10
T11
G12
V13
G14
K15
V18
A29
G30
I31
D32
V35
P38
V39
T43
A44
R45
G46
L50
V53
T60
Q61
L62
A63
G64
L65
A66
R67
M72
A78
E79
H80
A81
G82
M83
A84
L85
R88
D89
L94
P101
G102
R103
L104
V107
A110
A118
E119
V122
T123
L124
R125
V137
V138
L143
L146
L151
Q159
Q160
L166
W171
P172
D173
P174
P175
G176
R183
S184
A185
A190
R193
L196
P197
A198
G199
A200
A201
S202
L203
D204
A205
G206
M211
N219
W220
V221
A222
G223
L224
V225
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.38Å 104.68Å 151.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.70 – 1.85 31.25 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.1 (31.70-1.85) 97.1 (31.25-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.253 0.211 , 0.249	Depositor DCC
R_{free} test set	3701 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6648	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.50	0/1640	0.69	4/2241 (0.2%)
1	B	0.46	0/1587	0.64	0/2171
1	C	0.44	0/1608	0.61	0/2199
1	D	0.42	0/1584	0.64	1/2168 (0.0%)
All	All	0.46	0/6419	0.65	5/8779 (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	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	103	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	D	125	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	103	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	193	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	173	ASP	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	1613	0	1660	19	0
1	B	1568	0	1623	22	0
1	C	1588	0	1638	26	0
1	D	1559	0	1605	30	0
2	A	114	0	0	2	0
2	B	96	0	0	1	0
2	C	73	0	0	0	0
2	D	37	0	0	3	0
All	All	6648	0	6526	93	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 7.

The worst 5 of 93 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:9:THR:HG21	2:D:229:HOH:O	1.53	1.08
1:D:88[B]:ARG:HG2	1:D:88[B]:ARG:HH11	1.06	1.08
1:A:218:ARG:HA	1:A:218:ARG:HE	1.23	1.02
1:C:145:THR:O	1:C:149:THR:HG23	1.71	0.89
1:B:100:ARG:CG	1:B:100:ARG:HH11	1.86	0.89

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	229/251 (91%)	224 (98%)	5 (2%)	0	100	100
1	B	223/251 (89%)	219 (98%)	4 (2%)	0	100	100
1	C	226/251 (90%)	221 (98%)	4 (2%)	1 (0%)	34	19
1	D	223/251 (89%)	220 (99%)	3 (1%)	0	100	100
All	All	901/1004 (90%)	884 (98%)	16 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	PRO

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	157/174 (90%)	142 (90%)	15 (10%)	8	1
1	B	152/174 (87%)	135 (89%)	17 (11%)	6	1
1	C	154/174 (88%)	142 (92%)	12 (8%)	12	2
1	D	151/174 (87%)	124 (82%)	27 (18%)	2	0
All	All	614/696 (88%)	543 (88%)	71 (12%)	5	1

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	124	LEU
1	D	137	VAL
1	D	183	ARG
1	B	124	LEU
1	B	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	80	HIS
1	D	160	GLN
1	D	219	ASN
1	A	80	HIS
1	A	-2	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	230/251 (91%)	0.55	14 (6%)	21	20	22, 30, 44, 56	1 (0%)
1	B	225/251 (89%)	0.49	16 (7%)	16	15	23, 34, 48, 62	0
1	C	228/251 (90%)	0.56	16 (7%)	16	15	28, 37, 50, 78	1 (0%)
1	D	224/251 (89%)	0.86	34 (15%)	2	2	23, 34, 50, 66	4 (1%)
All	All	907/1004 (90%)	0.61	80 (8%)	10	9	22, 34, 49, 78	6 (0%)

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	ASP	5.7
1	C	177	LEU	5.6
1	C	174	PRO	5.5
1	D	171	TRP	5.1
1	A	6	VAL	5.0

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.