wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2022 – 12:07 PM JST

PDB ID	:	6JC4
Title	:	Crystal structure of the urease accessory protein UreF from Klebsiella pneumoniae
Authors	:	Wu, W.; Zhang, Q.; Bartlam, M.
Deposited on	:	2019-01-28
Resolution	:	2.30 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:

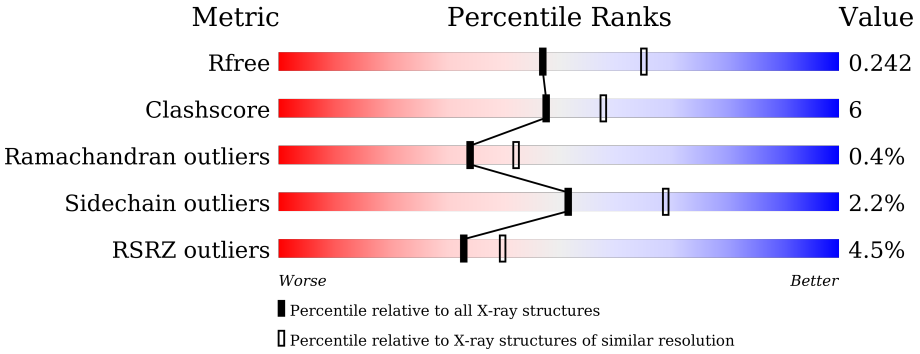
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	257	3% 67% 11% 22%
1	B	257	3% 72% 6% 22%
1	C	257	5% 69% 7% • 22%
1	D	257	4% 69% 9% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6715 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 Urease accessory protein UreF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1591	1010	287	282	12	0	0	0
1	B	200	1591	1010	287	282	12	0	0	0
1	C	200	1591	1010	287	282	12	0	0	0
1	D	200	1591	1010	287	282	12	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP A0A2X3G2L5
A	-31	ALA	-	expression tag	UNP A0A2X3G2L5
A	-30	SER	-	expression tag	UNP A0A2X3G2L5
A	-29	CYS	-	expression tag	UNP A0A2X3G2L5
A	-28	ARG	-	expression tag	UNP A0A2X3G2L5
A	-27	SER	-	expression tag	UNP A0A2X3G2L5
A	-26	SER	-	expression tag	UNP A0A2X3G2L5
A	-25	ARG	-	expression tag	UNP A0A2X3G2L5
A	-24	LYS	-	expression tag	UNP A0A2X3G2L5
A	-23	PRO	-	expression tag	UNP A0A2X3G2L5
A	-22	ALA	-	expression tag	UNP A0A2X3G2L5
A	-21	LEU	-	expression tag	UNP A0A2X3G2L5
A	-20	THR	-	expression tag	UNP A0A2X3G2L5
A	-19	PRO	-	expression tag	UNP A0A2X3G2L5
A	-18	ALA	-	expression tag	UNP A0A2X3G2L5
A	-17	ARG	-	expression tag	UNP A0A2X3G2L5
A	-16	ALA	-	expression tag	UNP A0A2X3G2L5
A	-15	THR	-	expression tag	UNP A0A2X3G2L5
A	-14	VAL	-	expression tag	UNP A0A2X3G2L5
A	-13	ILE	-	expression tag	UNP A0A2X3G2L5
A	-12	ILE	-	expression tag	UNP A0A2X3G2L5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	MET	-	initiating methionine	UNP A0A2X3G2L5
B	-31	ALA	-	expression tag	UNP A0A2X3G2L5
B	-30	SER	-	expression tag	UNP A0A2X3G2L5
B	-29	CYS	-	expression tag	UNP A0A2X3G2L5
B	-28	ARG	-	expression tag	UNP A0A2X3G2L5
B	-27	SER	-	expression tag	UNP A0A2X3G2L5
B	-26	SER	-	expression tag	UNP A0A2X3G2L5
B	-25	ARG	-	expression tag	UNP A0A2X3G2L5
B	-24	LYS	-	expression tag	UNP A0A2X3G2L5
B	-23	PRO	-	expression tag	UNP A0A2X3G2L5
B	-22	ALA	-	expression tag	UNP A0A2X3G2L5
B	-21	LEU	-	expression tag	UNP A0A2X3G2L5
B	-20	THR	-	expression tag	UNP A0A2X3G2L5
B	-19	PRO	-	expression tag	UNP A0A2X3G2L5
B	-18	ALA	-	expression tag	UNP A0A2X3G2L5
B	-17	ARG	-	expression tag	UNP A0A2X3G2L5
B	-16	ALA	-	expression tag	UNP A0A2X3G2L5
B	-15	THR	-	expression tag	UNP A0A2X3G2L5
B	-14	VAL	-	expression tag	UNP A0A2X3G2L5
B	-13	ILE	-	expression tag	UNP A0A2X3G2L5
B	-12	ILE	-	expression tag	UNP A0A2X3G2L5
C	-32	MET	-	initiating methionine	UNP A0A2X3G2L5
C	-31	ALA	-	expression tag	UNP A0A2X3G2L5
C	-30	SER	-	expression tag	UNP A0A2X3G2L5
C	-29	CYS	-	expression tag	UNP A0A2X3G2L5
C	-28	ARG	-	expression tag	UNP A0A2X3G2L5
C	-27	SER	-	expression tag	UNP A0A2X3G2L5
C	-26	SER	-	expression tag	UNP A0A2X3G2L5
C	-25	ARG	-	expression tag	UNP A0A2X3G2L5
C	-24	LYS	-	expression tag	UNP A0A2X3G2L5
C	-23	PRO	-	expression tag	UNP A0A2X3G2L5
C	-22	ALA	-	expression tag	UNP A0A2X3G2L5
C	-21	LEU	-	expression tag	UNP A0A2X3G2L5
C	-20	THR	-	expression tag	UNP A0A2X3G2L5
C	-19	PRO	-	expression tag	UNP A0A2X3G2L5
C	-18	ALA	-	expression tag	UNP A0A2X3G2L5
C	-17	ARG	-	expression tag	UNP A0A2X3G2L5
C	-16	ALA	-	expression tag	UNP A0A2X3G2L5
C	-15	THR	-	expression tag	UNP A0A2X3G2L5
C	-14	VAL	-	expression tag	UNP A0A2X3G2L5
C	-13	ILE	-	expression tag	UNP A0A2X3G2L5
C	-12	ILE	-	expression tag	UNP A0A2X3G2L5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-32	MET	-	initiating methionine	UNP A0A2X3G2L5
D	-31	ALA	-	expression tag	UNP A0A2X3G2L5
D	-30	SER	-	expression tag	UNP A0A2X3G2L5
D	-29	CYS	-	expression tag	UNP A0A2X3G2L5
D	-28	ARG	-	expression tag	UNP A0A2X3G2L5
D	-27	SER	-	expression tag	UNP A0A2X3G2L5
D	-26	SER	-	expression tag	UNP A0A2X3G2L5
D	-25	ARG	-	expression tag	UNP A0A2X3G2L5
D	-24	LYS	-	expression tag	UNP A0A2X3G2L5
D	-23	PRO	-	expression tag	UNP A0A2X3G2L5
D	-22	ALA	-	expression tag	UNP A0A2X3G2L5
D	-21	LEU	-	expression tag	UNP A0A2X3G2L5
D	-20	THR	-	expression tag	UNP A0A2X3G2L5
D	-19	PRO	-	expression tag	UNP A0A2X3G2L5
D	-18	ALA	-	expression tag	UNP A0A2X3G2L5
D	-17	ARG	-	expression tag	UNP A0A2X3G2L5
D	-16	ALA	-	expression tag	UNP A0A2X3G2L5
D	-15	THR	-	expression tag	UNP A0A2X3G2L5
D	-14	VAL	-	expression tag	UNP A0A2X3G2L5
D	-13	ILE	-	expression tag	UNP A0A2X3G2L5
D	-12	ILE	-	expression tag	UNP A0A2X3G2L5

- Molecule 2 is water.

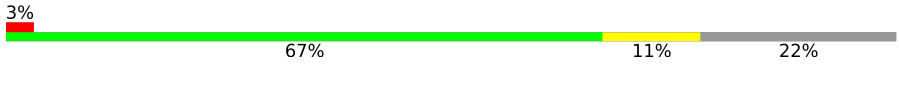
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	98	98	98	0	0
			Total	O		
2	B	90	90	90	0	0
			Total	O		
2	C	74	74	74	0	0
			Total	O		
2	D	89	89	89	0	0

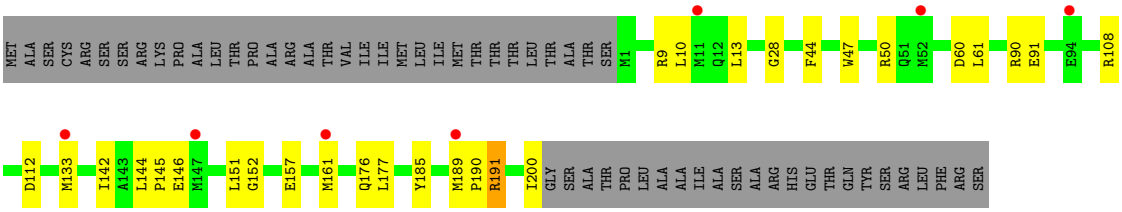
3 Residue-property plots (i)

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: Urease accessory protein UreF

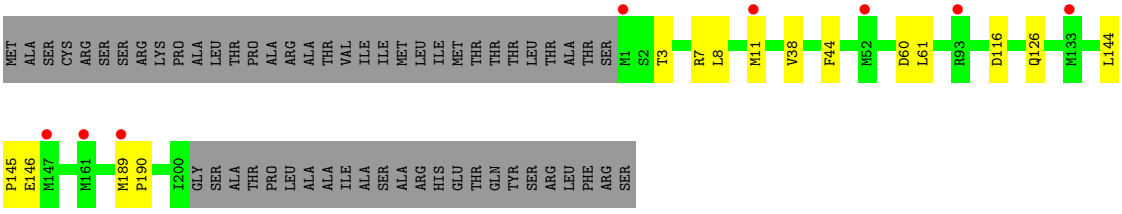
Chain A:





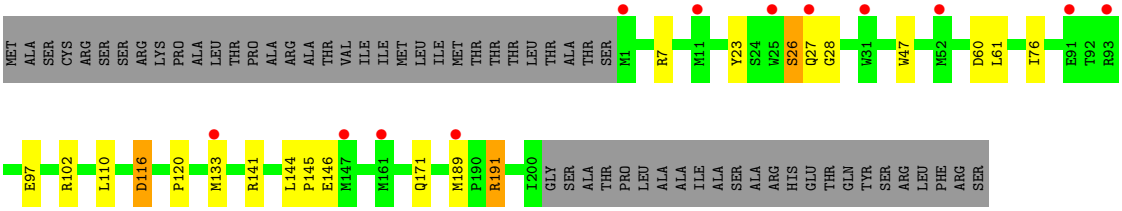
• Molecule 1: Urease accessory protein UreF

Chain B:



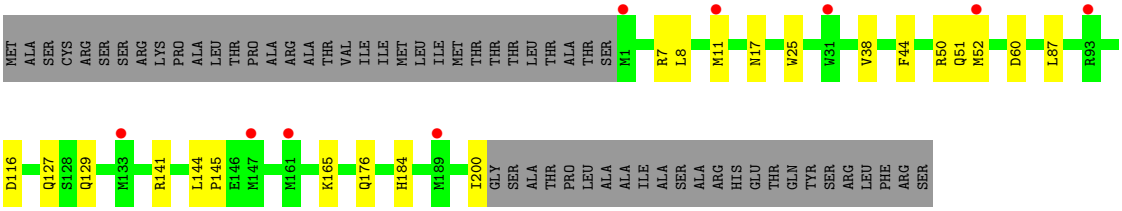
• Molecule 1: Urease accessory protein UreF

Chain C:



• Molecule 1: Urease accessory protein UreF

Chain D:


MET
ALA
SER
CYS
ARG
SER
SER
ARG
LYS
PRO
ALA
LEU
THR
PRO
ALA
ARG
ALA
THR
VAL
ILE
ILE
MET
LEU
ILE
MET
THR
THR
THR
LEU
THR
ALA
THR
SER
M1
R7
L8
M11
N17
W25
W31
V38
F44
R50
Q51
M52
D60
L87
R93

D116
Q127
S128
Q129
M133
R141
L144
P145
E146
M147
M161
K165
Q176
H184
M189
I200
GLY
SER
ALA
THR
PRO
LEU
ALA
ALA
ILE
ALA
SER
ALA
ARG
HIS
GLU
THR
GLN
TYR
SER
ARG
LEU
PHE
ARG
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	121.89Å 121.89Å 63.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.03 – 2.30 44.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.03-2.30) 99.9 (44.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.08 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0241	Depositor
R, R_{free}	0.200 , 0.242 0.205 , 0.242	Depositor DCC
R_{free} test set	1984 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.19% 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	0.70	0/1633	0.84	1/2220 (0.0%)
1	B	0.70	0/1633	0.84	0/2220
1	C	0.69	0/1633	0.84	1/2220 (0.0%)
1	D	0.70	0/1633	0.85	0/2220
All	All	0.70	0/6532	0.84	2/8880 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	C	116	ASP	N-CA-CB	-5.15	101.33	110.60

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	1591	0	1555	39	0
1	B	1591	0	1555	11	0
1	C	1591	0	1555	17	0
1	D	1591	0	1555	21	0
2	A	98	0	0	5	0
2	B	90	0	0	1	0
2	C	74	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	89	0	0	3	0
All	All	6715	0	6220	76	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 76 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:52:MET:HE1	1:D:184:HIS:CD2	1.68	1.26
1:D:52:MET:SD	2:D:373:HOH:O	2.08	1.10
1:A:161:MET:HE1	1:D:17:ASN:HB2	1.36	1.07
1:C:23:TYR:O	1:C:26:SER:OG	1.72	1.06
1:D:52:MET:HE1	1:D:184:HIS:HD2	0.99	1.03

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	198/257 (77%)	194 (98%)	4 (2%)	0	100	100
1	B	198/257 (77%)	194 (98%)	3 (2%)	1 (0%)	29	35
1	C	198/257 (77%)	193 (98%)	4 (2%)	1 (0%)	29	35
1	D	198/257 (77%)	195 (98%)	2 (1%)	1 (0%)	29	35
All	All	792/1028 (77%)	776 (98%)	13 (2%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ASP

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Mol	Chain	Res	Type
1	C	116	ASP
1	D	116	ASP

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	158/204 (78%)	156 (99%)	2 (1%)	69	82
1	B	158/204 (78%)	156 (99%)	2 (1%)	69	82
1	C	158/204 (78%)	152 (96%)	6 (4%)	33	47
1	D	158/204 (78%)	154 (98%)	4 (2%)	47	65
All	All	632/816 (78%)	618 (98%)	14 (2%)	52	69

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	133	MET
1	C	141	ARG
1	D	165	LYS
1	D	60	ASP
1	D	141	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	101	ASN
1	D	127	GLN
1	D	184	HIS
1	D	17	ASN
1	D	27	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	200/257 (77%)	-0.03	7 (3%)	44	51	18, 28, 52, 71	6 (3%)
1	B	200/257 (77%)	0.07	8 (4%)	38	45	18, 32, 61, 76	7 (3%)
1	C	200/257 (77%)	0.12	12 (6%)	21	28	19, 33, 63, 87	7 (3%)
1	D	200/257 (77%)	0.08	9 (4%)	33	40	16, 31, 56, 77	7 (3%)
All	All	800/1028 (77%)	0.06	36 (4%)	33	40	16, 31, 59, 87	27 (3%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	MET	8.7
1	D	161	MET	8.3
1	C	1	MET	8.0
1	A	133	MET	8.0
1	D	52	MET	7.6

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.