Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 03:28 AM EDT

PDB ID	:	5XUY
Title	:	Crystal structure of ATG101-ATG13HORMA
Authors	:	Kim, B.-W.; Song, H.K.
Deposited on	:	2017-06-26
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

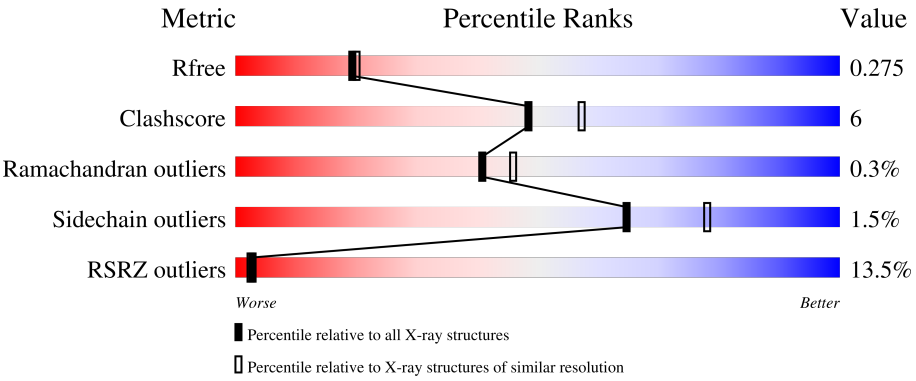
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	190	12% 85% 10% 5%
1	C	190	17% 86% 11% ·
2	B	218	9% 85% 9% 6%
2	D	218	14% 79% 17% ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6039 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 Autophagy-related protein 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1319	842	221	248	8			
1	C	184	Total	C	N	O	S	0	0	0
			1390	888	240	254	8			

- Molecule 2 is a protein called Autophagy-related protein 101.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	205	Total	C	N	O	S	0	0	0
			1576	999	268	300	9			
2	D	215	Total	C	N	O	S	0	0	0
			1653	1042	284	318	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	40	ALA	LYS	engineered mutation	UNP Q9BSB4
B	41	ALA	LYS	engineered mutation	UNP Q9BSB4
B	42	ALA	GLU	engineered mutation	UNP Q9BSB4
D	40	ALA	LYS	engineered mutation	UNP Q9BSB4
D	41	ALA	LYS	engineered mutation	UNP Q9BSB4
D	42	ALA	GLU	engineered mutation	UNP Q9BSB4

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	27	Total	O	0	0
			27	27		
3	C	23	Total	O	0	0
			23	23		

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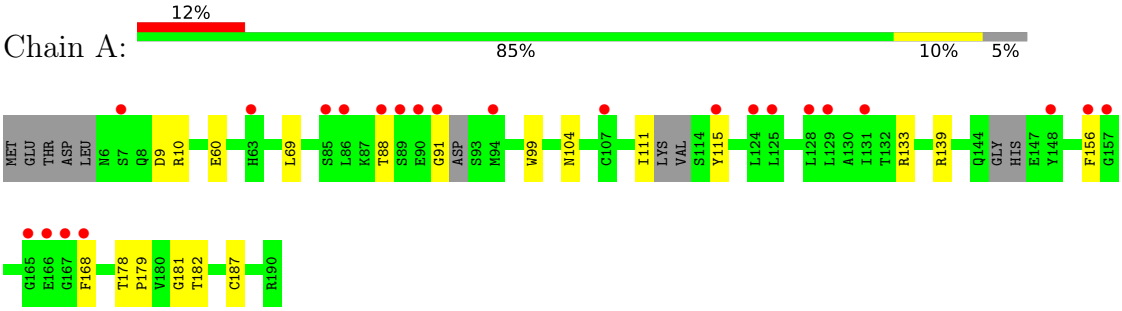
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	31	Total O 31 31	0	0

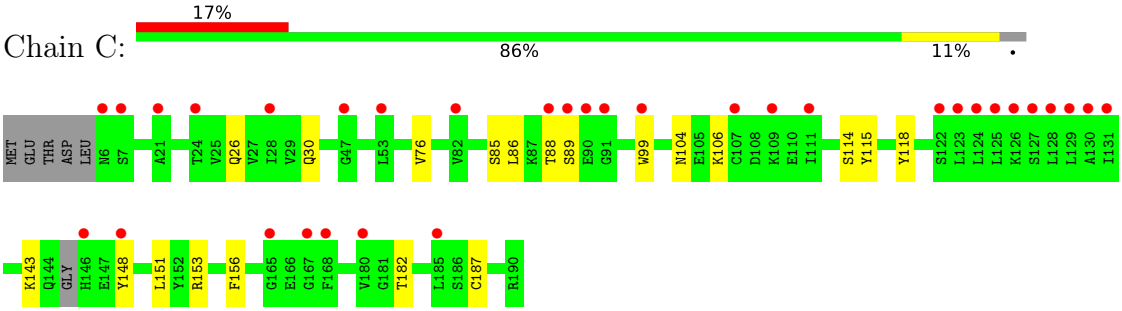
3 Residue-property plots (i)

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.

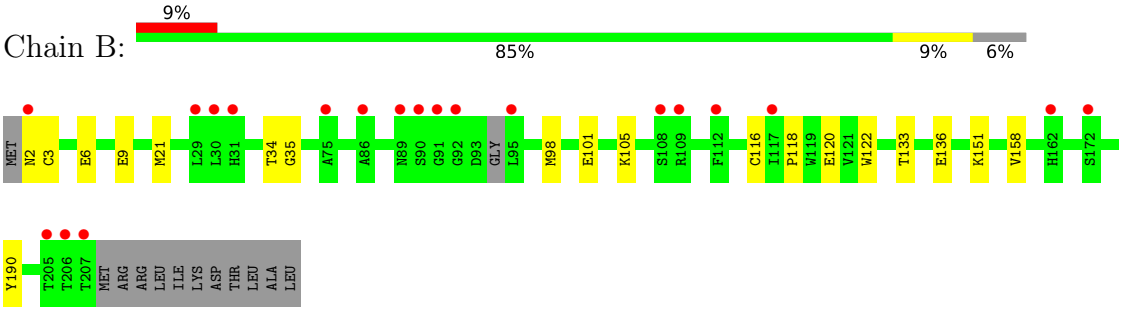
• Molecule 1: Autophagy-related protein 13



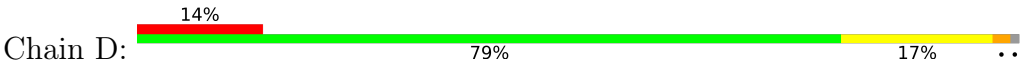
• Molecule 1: Autophagy-related protein 13

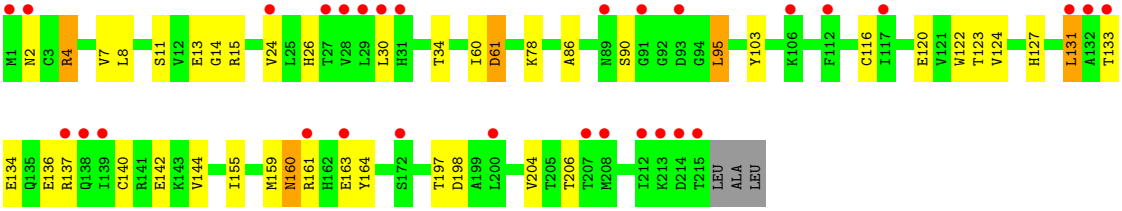


• Molecule 2: Autophagy-related protein 101



• Molecule 2: Autophagy-related protein 101




M1
N2
C3
R4
V7
L8
S11
V12
E13
G14
R15
V24
L25
H26
T27
V28
L29
L30
H31
T34
I60
D61
K78
A86
N89
S90
G91
G92
D93
G94
L95
Y103
K106
F112
C116
I117
E120
V121
W122
T123
V124
H127
L131
A132
T133

E134
Q135
E136
R137
Q138
I139
C140
R141
E142
K143
V144
I155
M159
N160
R161
H162
E163
Y164
S172
T197
D198
A199
L200
V204
T205
T206
T207
M208
I212
K213
D214
T215
LEU
ALA
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	87.99Å 125.18Å 100.76Å 90.00° 102.08° 90.00°	Depositor
Resolution (Å)	31.46 – 2.20 31.46 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (31.46-2.20) 98.7 (31.46-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.237 , 0.275 0.237 , 0.275	Depositor DCC
R_{free} test set	1998 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.4	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	0.95	EDS
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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

5.1 Standard geometry

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	0.26	0/1337	0.47	0/1815
1	C	0.26	0/1412	0.48	0/1914
2	B	0.26	0/1605	0.45	0/2179
2	D	0.32	0/1683	0.60	2/2284 (0.1%)
All	All	0.28	0/6037	0.51	2/8192 (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})
2	D	131	LEU	CB-CG-CD1	-13.29	88.42	111.00
2	D	95	LEU	CA-CB-CG	5.61	128.19	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1319	0	1279	9	0
1	C	1390	0	1383	14	0
2	B	1576	0	1507	12	0
2	D	1653	0	1579	35	0
3	A	20	0	0	1	0
3	B	27	0	0	2	0
3	C	23	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	0	3	0
All	All	6039	0	5748	70	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.

All (70) 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)
2:D:95:LEU:HD23	2:D:197:THR:HG23	1.39	1.05
1:C:104:ASN:ND2	1:C:182:THR:OG1	2.05	0.90
2:D:95:LEU:HD23	2:D:197:THR:CG2	2.08	0.84
2:D:131:LEU:HD11	2:D:137:ARG:CD	2.11	0.80
2:D:4:ARG:HH21	2:D:161:ARG:HH11	1.30	0.79
1:C:86:LEU:HD11	1:C:148:TYR:HB2	1.65	0.79
1:C:153:ARG:NH1	3:C:201:HOH:O	2.18	0.76
1:C:104:ASN:HD21	1:C:182:THR:HG1	1.36	0.73
2:D:4:ARG:NH2	2:D:120:GLU:OE1	2.21	0.72
2:D:131:LEU:HD11	2:D:137:ARG:HD2	1.73	0.70
2:D:160:ASN:ND2	3:D:302:HOH:O	2.25	0.69
2:B:133:THR:HG23	2:B:136:GLU:H	1.56	0.69
2:D:161:ARG:HG3	2:D:163:GLU:H	1.59	0.68
2:D:164:TYR:O	3:D:301:HOH:O	2.14	0.65
2:B:9:GLU:O	2:B:151:LYS:NZ	2.32	0.62
2:B:116:CYS:SG	3:B:326:HOH:O	2.56	0.61
1:A:60:GLU:OE1	1:A:60:GLU:N	2.29	0.60
2:D:60:ILE:HG23	2:D:144:VAL:HG23	1.83	0.60
2:B:105:LYS:NZ	3:B:302:HOH:O	2.35	0.60
2:D:8:LEU:HB2	2:D:124:VAL:HG12	1.85	0.59
1:A:88:THR:HG23	1:A:91:GLY:H	1.67	0.58
2:D:120:GLU:OE1	2:D:161:ARG:NH1	2.37	0.58
2:D:13:GLU:OE2	2:D:15:ARG:NE	2.37	0.57
2:D:4:ARG:HH21	2:D:161:ARG:NH1	2.02	0.55
2:B:3:CYS:HB2	2:B:118:PRO:O	2.10	0.52
2:B:6:GLU:HG3	2:B:158:VAL:HG11	1.92	0.52
1:C:99:TRP:CE3	1:C:187:CYS:HB2	2.45	0.51
1:A:133:ARG:NH1	3:A:201:HOH:O	2.41	0.51
2:B:2:ASN:O	2:B:2:ASN:ND2	2.44	0.50
1:A:10:ARG:O	1:A:10:ARG:HG3	2.11	0.50
1:C:88:THR:OG1	1:C:89:SER:N	2.45	0.49
2:D:13:GLU:HG3	2:D:131:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:LEU:HD11	2:D:137:ARG:HD3	1.91	0.49
2:D:133:THR:HG22	2:D:136:GLU:OE1	2.12	0.49
2:D:7:VAL:HA	2:D:123:THR:O	2.13	0.49
2:D:24:VAL:HG11	2:D:124:VAL:HG11	1.95	0.49
1:C:26:GLN:NE2	1:C:30:GLN:HE21	2.12	0.48
1:A:111:ILE:HG21	1:A:179:PRO:HG3	1.96	0.48
2:D:197:THR:OG1	2:D:198:ASP:N	2.46	0.48
1:A:99:TRP:CE3	1:A:187:CYS:HB2	2.48	0.48
1:C:115:TYR:HA	1:C:118:TYR:HB3	1.95	0.48
1:C:26:GLN:HE21	1:C:30:GLN:HE21	1.62	0.47
1:A:104:ASN:HB3	1:A:182:THR:OG1	2.14	0.47
2:D:78:LYS:NZ	3:D:303:HOH:O	2.35	0.47
2:D:86:ALA:O	2:D:90:SER:HB3	2.15	0.47
2:D:140:CYS:O	2:D:144:VAL:HG22	2.15	0.46
2:D:2:ASN:O	2:D:2:ASN:ND2	2.47	0.46
1:C:106:LYS:O	1:C:182:THR:HG23	2.16	0.44
2:D:61:ASP:OD2	2:D:142:GLU:HG2	2.17	0.44
2:D:133:THR:OG1	2:D:134:GLU:N	2.51	0.44
2:B:34:THR:OG1	2:B:35:GLY:N	2.51	0.43
2:B:151:LYS:HA	2:B:151:LYS:HD3	1.89	0.43
2:D:134:GLU:O	2:D:137:ARG:HB2	2.17	0.43
2:D:120:GLU:OE2	2:D:122:TRP:NE1	2.46	0.43
2:B:101:GLU:O	2:B:190:TYR:HA	2.19	0.43
2:D:206:THR:H	2:D:206:THR:HG23	1.58	0.43
2:D:13:GLU:HG2	2:D:14:GLY:N	2.34	0.42
2:D:4:ARG:HD3	2:D:4:ARG:H	1.84	0.42
2:D:26:HIS:O	2:D:30:LEU:N	2.51	0.42
2:D:103:TYR:CD2	2:D:116:CYS:HB3	2.55	0.42
1:A:69:LEU:HD23	1:A:156:PHE:CZ	2.55	0.42
1:C:85:SER:OG	1:C:151:LEU:HB2	2.20	0.42
2:B:120:GLU:OE2	2:B:122:TRP:NE1	2.47	0.42
1:C:114:SER:C	1:C:115:TYR:CG	2.94	0.42
1:C:143:LYS:HD2	1:C:143:LYS:HA	1.64	0.42
2:D:11:SER:HA	2:D:127:HIS:O	2.20	0.41
2:B:21:MET:HE1	2:B:98:MET:HB2	2.01	0.41
1:A:178:THR:OG1	1:A:181:GLY:O	2.32	0.41
1:C:104:ASN:ND2	1:C:182:THR:O	2.54	0.41
2:D:155:ILE:O	2:D:159:MET:HB2	2.22	0.40

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	172/190 (90%)	168 (98%)	4 (2%)	0	100	100
1	C	180/190 (95%)	175 (97%)	5 (3%)	0	100	100
2	B	201/218 (92%)	194 (96%)	7 (4%)	0	100	100
2	D	213/218 (98%)	203 (95%)	8 (4%)	2 (1%)	17	16
All	All	766/816 (94%)	740 (97%)	24 (3%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	61	ASP
2	D	204	VAL

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	135/167 (81%)	131 (97%)	4 (3%)	41	53
1	C	145/167 (87%)	143 (99%)	2 (1%)	67	80
2	B	166/194 (86%)	166 (100%)	0	100	100
2	D	174/194 (90%)	171 (98%)	3 (2%)	60	74
All	All	620/722 (86%)	611 (98%)	9 (2%)	65	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	115	TYR
1	A	139	ARG
1	A	168	PHE
1	C	76	VAL
1	C	156	PHE
2	D	4	ARG
2	D	34	THR
2	D	160	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	26	GLN
1	C	104	ASN
1	C	119	ASN

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	180/190 (94%)	0.68	23 (12%) 3 3	46, 84, 141, 173	0
1	C	184/190 (96%)	0.81	33 (17%) 1 1	42, 67, 126, 167	0
2	B	205/218 (94%)	0.46	20 (9%) 7 6	42, 70, 117, 183	0
2	D	215/218 (98%)	0.77	30 (13%) 2 2	42, 79, 139, 153	0
All	All	784/816 (96%)	0.68	106 (13%) 3 2	42, 75, 135, 183	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	6.7
2	B	205	THR	5.8
2	D	215	THR	5.5
2	B	112	PHE	5.4
2	B	207	THR	5.0
1	A	7	SER	4.4
2	D	132	ALA	4.4
2	D	163	GLU	4.2
2	D	2	ASN	4.2
1	C	90	GLU	4.2
1	A	156	PHE	4.1
1	A	91	GLY	4.1
2	D	30	LEU	3.9
1	C	111	ILE	3.9
1	A	107	CYS	3.8
2	B	172	SER	3.8
2	B	92	GLY	3.7
1	A	168	PHE	3.7
1	A	88	THR	3.6
2	B	206	THR	3.6
1	C	91	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	168	PHE	3.5
2	D	31	HIS	3.5
1	C	167	GLY	3.5
1	C	125	LEU	3.5
1	C	129	LEU	3.5
1	A	167	GLY	3.4
1	C	128	LEU	3.4
1	A	148	TYR	3.3
2	D	212	ILE	3.3
2	D	91	GLY	3.3
2	D	27	THR	3.3
2	D	139	ILE	3.3
2	B	86	ALA	3.2
1	C	99	TRP	3.2
1	A	90	GLU	3.2
2	B	91	GLY	3.2
2	D	208	MET	3.2
1	C	146	HIS	3.2
2	B	2	ASN	3.2
2	D	89	ASN	3.1
2	D	131	LEU	3.1
2	D	93	ASP	3.0
1	C	127	SER	3.0
1	A	85	SER	3.0
1	A	157	GLY	3.0
1	C	7	SER	2.9
2	D	28	VAL	2.9
2	B	30	LEU	2.9
1	A	86	LEU	2.9
1	C	130	ALA	2.9
2	D	214	ASP	2.9
2	B	109	ARG	2.9
2	B	31	HIS	2.8
1	A	128	LEU	2.8
1	C	82	VAL	2.8
2	D	29	LEU	2.8
1	A	166	GLU	2.8
1	C	28	ILE	2.8
2	B	95	LEU	2.7
1	A	89	SER	2.7
2	D	172	SER	2.6
2	B	75	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	90	SER	2.6
1	C	131	ILE	2.6
2	D	106	LYS	2.5
1	C	107	CYS	2.5
2	B	29	LEU	2.5
1	A	115	TYR	2.5
1	C	89	SER	2.5
1	C	148	TYR	2.5
2	B	89	ASN	2.5
1	C	24	THR	2.4
2	D	133	THR	2.4
2	D	161	ARG	2.4
1	A	94	MET	2.4
2	D	117	ILE	2.4
1	A	129	LEU	2.4
1	C	109	LYS	2.3
1	C	88	THR	2.3
2	D	24	VAL	2.3
1	A	124	LEU	2.3
1	C	21	ALA	2.3
1	C	124	LEU	2.3
1	A	63	HIS	2.3
1	A	125	LEU	2.3
1	C	126	LYS	2.3
2	D	137	ARG	2.2
1	C	122	SER	2.2
1	A	131	ILE	2.2
2	B	117	ILE	2.2
2	D	213	LYS	2.2
2	D	200	LEU	2.2
2	D	112	PHE	2.2
1	C	180	VAL	2.2
1	C	47	GLY	2.2
1	A	165	GLY	2.2
1	C	6	ASN	2.2
1	C	53	LEU	2.1
2	D	207	THR	2.1
1	C	123	LEU	2.1
1	C	185	LEU	2.1
2	B	162	HIS	2.1
1	C	165	GLY	2.1
2	B	108	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	138	GLN	2.0

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.