



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:16 am GMT

PDB ID : 2IFT  
Title : Crystal structure of putative methylase HI0767 from Haemophilus influenzae. NESG target IR102.  
Authors : Vorobiev, S.M.; Su, M.; Seetharaman, J.; Shastry, R.; Janjua, H.; Cunningham, K.; Ma, L.C.; Xiao, R.; Liu, J.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-09-21  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

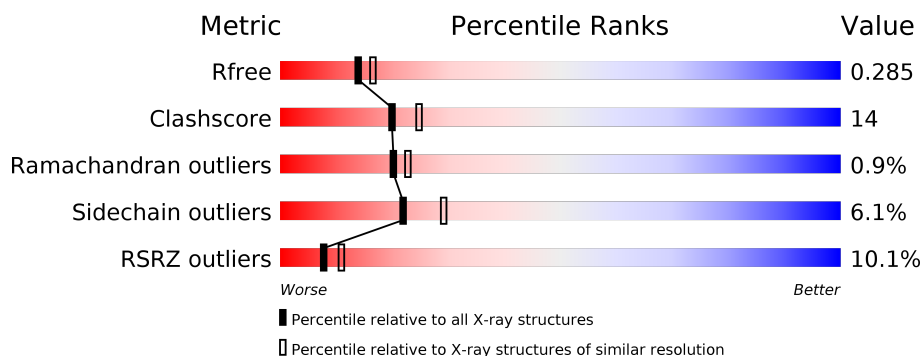
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	201	<div> <div>9%</div> <div>60%</div> <div>24%</div> <div>•</div> <div>12%</div> </div>
1	B	201	<div> <div>7%</div> <div>55%</div> <div>22%</div> <div>•</div> <div>20%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2676 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 Putative methylase HI0767.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	Se	0	0	0
			1332	863	224	241	3	1			
1	B	161	Total	C	N	O	S	Se	0	0	0
			1237	799	206	228	3	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P44869
A	49	MSE	MET	MODIFIED RESIDUE	UNP P44869
A	194	LEU	-	CLONING ARTIFACT	UNP P44869
A	195	GLU	-	CLONING ARTIFACT	UNP P44869
A	196	HIS	-	CLONING ARTIFACT	UNP P44869
A	197	HIS	-	CLONING ARTIFACT	UNP P44869
A	198	HIS	-	CLONING ARTIFACT	UNP P44869
A	199	HIS	-	CLONING ARTIFACT	UNP P44869
A	200	HIS	-	CLONING ARTIFACT	UNP P44869
A	201	HIS	-	CLONING ARTIFACT	UNP P44869
B	1	MSE	MET	MODIFIED RESIDUE	UNP P44869
B	49	MSE	MET	MODIFIED RESIDUE	UNP P44869
B	194	LEU	-	CLONING ARTIFACT	UNP P44869
B	195	GLU	-	CLONING ARTIFACT	UNP P44869
B	196	HIS	-	CLONING ARTIFACT	UNP P44869
B	197	HIS	-	CLONING ARTIFACT	UNP P44869
B	198	HIS	-	CLONING ARTIFACT	UNP P44869
B	199	HIS	-	CLONING ARTIFACT	UNP P44869
B	200	HIS	-	CLONING ARTIFACT	UNP P44869
B	201	HIS	-	CLONING ARTIFACT	UNP P44869

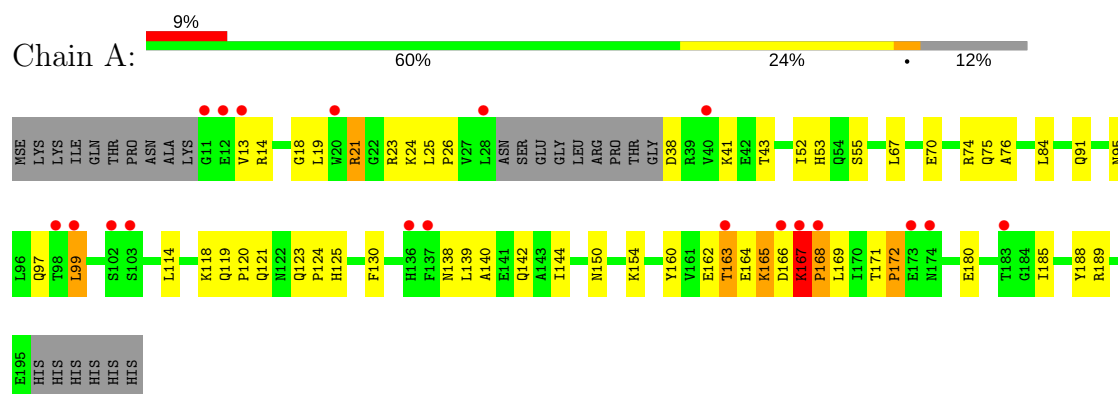
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total 55	O 55	0	0
2	B	52	Total 52	O 52	0	0

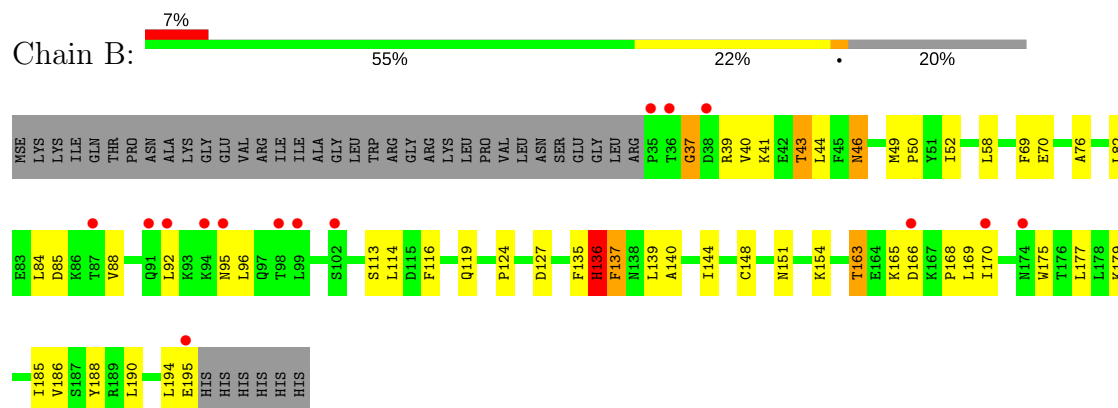
### 3 Residue-property plots [i](#)

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: Putative methylase HI0767



#### • Molecule 1: Putative methylase HI0767



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.34Å 57.87Å 47.52Å 90.00° 107.36° 90.00°	Depositor
Resolution (Å)	29.34 – 2.30 29.34 – 2.28	Depositor EDS
% Data completeness (in resolution range)	90.3 (29.34-2.30) 96.8 (29.34-2.28)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.73 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.266 0.236 , 0.285	Depositor DCC
$R_{free}$ test set	646 reflections (3.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.38	0/1361	0.75	5/1859 (0.3%)
1	B	0.40	0/1266	0.78	4/1725 (0.2%)
All	All	0.39	0/2627	0.77	9/3584 (0.3%)

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	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	135	PHE	C-N-CA	-9.59	97.72	121.70
1	A	166	ASP	N-CA-C	7.35	130.84	111.00
1	A	169	LEU	N-CA-C	6.86	129.53	111.00
1	B	37	GLY	N-CA-C	-6.83	96.02	113.10
1	B	136	HIS	N-CA-C	6.46	128.45	111.00
1	A	167	LYS	N-CA-C	6.31	128.05	111.00
1	B	137	PHE	N-CA-CB	-6.15	99.53	110.60
1	A	168	PRO	N-CA-C	5.61	126.70	112.10
1	A	172	PRO	N-CA-C	-5.23	98.51	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	136	HIS	Mainchain

## 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	1332	0	1267	38	0
1	B	1237	0	1181	34	0
2	A	55	0	0	3	0
2	B	52	0	0	4	0
All	All	2676	0	2448	71	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.

All (71) 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:A:25:LEU:HD21	1:A:99:LEU:HD21	1.33	1.11
1:A:119:GLN:HE21	1:A:121:GLN:HE22	1.21	0.86
1:B:165:LYS:HD2	1:B:185:ILE:HA	1.60	0.81
1:B:127:ASP:OD1	1:B:154:LYS:HD2	1.84	0.77
1:A:124:PRO:HB2	1:A:154:LYS:HG2	1.66	0.76
1:B:82:LEU:HD11	1:B:116:PHE:CD1	2.22	0.75
1:A:114:LEU:HD11	1:A:139:LEU:HD22	1.70	0.72
1:B:165:LYS:CD	1:B:185:ILE:HA	2.18	0.72
1:B:92:LEU:O	1:B:96:LEU:HD13	1.93	0.69
1:A:140:ALA:O	1:A:144:ILE:HG12	1.92	0.68
1:B:43:THR:HG21	1:B:179:LYS:NZ	2.13	0.64
1:B:49:MSE:HB2	1:B:50:PRO:HD3	1.79	0.64
1:A:119:GLN:HB2	1:B:119:GLN:HB2	1.81	0.63
1:B:114:LEU:HD11	1:B:139:LEU:HD22	1.80	0.62
1:A:25:LEU:HD21	1:A:99:LEU:CD2	2.21	0.62
1:A:163:THR:HG23	1:A:164:GLU:N	2.15	0.62
1:B:44:LEU:HD13	1:B:190:LEU:HD11	1.82	0.61
1:B:85:ASP:HB3	1:B:88:VAL:HG12	1.84	0.59
1:B:166:ASP:O	1:B:168:PRO:HD3	2.02	0.59
1:B:46:ASN:HA	1:B:49:MSE:HG3	1.85	0.58
1:B:85:ASP:HB3	1:B:88:VAL:CG1	2.37	0.55
1:B:40:VAL:HG22	1:B:179:LYS:HD2	1.90	0.54
1:A:160:TYR:CE1	1:A:162:GLU:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:CG2	1:A:164:GLU:N	2.71	0.54
1:B:140:ALA:O	1:B:144:ILE:HG13	2.09	0.53
1:A:52:ILE:HD12	1:A:55:SER:OG	2.09	0.52
1:B:82:LEU:HD13	1:B:113:SER:OG	2.09	0.52
1:A:171:THR:O	1:A:172:PRO:C	2.48	0.51
1:A:52:ILE:HD11	1:A:76:ALA:HB2	1.93	0.50
1:A:23:ARG:HG2	1:A:24:LYS:N	2.27	0.50
1:A:165:LYS:N	1:A:185:ILE:O	2.39	0.49
1:A:70:GLU:O	1:A:74:ARG:HG3	2.12	0.49
1:B:169:LEU:HD22	2:B:397:HOH:O	2.13	0.49
1:A:123:GLN:HG2	2:A:433:HOH:O	2.13	0.48
1:A:53:HIS:HB2	2:A:406:HOH:O	2.14	0.48
1:A:123:GLN:O	1:A:125:HIS:CD2	2.67	0.48
1:B:39:ARG:O	1:B:43:THR:HG23	2.14	0.48
1:B:170:ILE:N	1:B:170:ILE:HD12	2.28	0.48
1:B:163:THR:HG22	2:B:355:HOH:O	2.14	0.47
1:B:186:VAL:HG13	1:B:188:TYR:CE1	2.49	0.47
1:A:123:GLN:O	1:A:125:HIS:HD2	1.95	0.47
1:A:14:ARG:HA	1:A:23:ARG:O	2.14	0.47
1:A:18:GLY:O	1:A:21:ARG:HG2	2.15	0.47
1:A:95:ASN:O	1:A:99:LEU:HG	2.15	0.47
1:A:13:VAL:O	1:A:24:LYS:HA	2.15	0.46
1:A:38:ASP:N	1:A:41:LYS:HZ1	2.14	0.46
1:B:194:LEU:O	1:B:195:GLU:CB	2.64	0.45
1:A:118:LYS:O	1:A:120:PRO:HD3	2.15	0.45
1:A:26:PRO:O	1:A:91:GLN:NE2	2.48	0.45
1:B:41:LYS:O	1:B:44:LEU:HB3	2.17	0.45
1:B:169:LEU:HA	1:B:169:LEU:HD23	1.73	0.45
1:A:19:LEU:HG	1:A:75:GLN:OE1	2.17	0.44
1:B:186:VAL:HG11	1:B:188:TYR:OH	2.17	0.44
1:A:52:ILE:HG23	1:A:53:HIS:N	2.33	0.44
1:B:144:ILE:HG23	1:B:175:TRP:CH2	2.53	0.43
1:B:124:PRO:HB2	1:B:154:LYS:HG2	2.00	0.43
1:A:120:PRO:HA	1:A:150:ASN:HB3	2.01	0.43
1:A:23:ARG:HH11	1:A:23:ARG:HG3	1.84	0.43
1:B:52:ILE:O	1:B:76:ALA:HA	2.19	0.43
1:A:180:GLU:HA	1:A:188:TYR:O	2.19	0.43
1:A:167:LYS:N	1:A:168:PRO:CD	2.83	0.42
1:A:138:ASN:O	1:A:142:GLN:HG3	2.18	0.42
1:B:43:THR:HG21	1:B:179:LYS:HZ3	1.81	0.42
1:B:137:PHE:N	2:B:307:HOH:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASP:C	1:B:168:PRO:HD3	2.40	0.42
1:A:167:LYS:CB	2:A:460:HOH:O	2.68	0.41
1:A:67:LEU:HD13	1:A:130:PHE:HB3	2.02	0.41
1:A:180:GLU:HG3	1:A:189:ARG:HG2	2.03	0.41
1:B:40:VAL:HG23	2:B:440:HOH:O	2.21	0.41
1:A:41:LYS:HB2	1:A:41:LYS:HE3	1.81	0.40
1:B:69:PHE:CZ	1:B:95:ASN:ND2	2.89	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	172/201 (86%)	161 (94%)	9 (5%)	2 (1%)	15	16
1	B	159/201 (79%)	145 (91%)	13 (8%)	1 (1%)	28	34
All	All	331/402 (82%)	306 (92%)	22 (7%)	3 (1%)	20	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	LYS
1	A	167	LYS
1	B	37	GLY

### 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	134/179 (75%)	128 (96%)	6 (4%)	32	44
1	B	129/179 (72%)	119 (92%)	10 (8%)	15	18
All	All	263/358 (74%)	247 (94%)	16 (6%)	22	29

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	43	THR
1	A	84	LEU
1	A	97	GLN
1	A	99	LEU
1	A	163	THR
1	B	43	THR
1	B	46	ASN
1	B	58	LEU
1	B	70	GLU
1	B	84	LEU
1	B	136	HIS
1	B	148	CYS
1	B	151	ASN
1	B	163	THR
1	B	177	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	119	GLN
1	A	125	HIS
1	A	142	GLN
1	A	192	GLN
1	B	46	ASN
1	B	110	ASN
1	B	111	GLN
1	B	151	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 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	175/201 (87%)	0.75	19 (10%) 6 9	13, 30, 55, 63	1 (0%)
1	B	160/201 (79%)	0.65	15 (9%) 9 12	14, 29, 54, 60	0
All	All	335/402 (83%)	0.70	34 (10%) 8 11	13, 30, 55, 63	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	LEU	7.3
1	A	168	PRO	4.6
1	B	99	LEU	4.5
1	A	11	GLY	4.1
1	B	36	THR	3.9
1	B	35	PRO	3.8
1	B	195	GLU	3.7
1	B	98	THR	3.7
1	A	40	VAL	3.6
1	B	94	LYS	3.3
1	A	28	LEU	3.0
1	A	166	ASP	3.0
1	B	174	ASN	3.0
1	A	13	VAL	2.9
1	A	98	THR	2.9
1	A	136	HIS	2.9
1	A	103	SER	2.8
1	A	12	GLU	2.7
1	B	91	GLN	2.6
1	A	174	ASN	2.6
1	A	137	PHE	2.5
1	A	20	TRP	2.5
1	A	163	THR	2.5
1	B	38	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	166	ASP	2.3
1	A	102	SER	2.3
1	B	87	THR	2.2
1	B	95	ASN	2.1
1	A	173	GLU	2.1
1	B	92	LEU	2.1
1	B	102	SER	2.1
1	B	170	ILE	2.0
1	A	167	LYS	2.0
1	A	183	THR	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 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.