



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:45 AM GMT

PDB ID : 3PSL  
Title : Fine-tuning the stimulation of MLL1 methyltransferase activity by a histone H3 based peptide mimetic  
Authors : Avdic, V.; Zhang, P.; Lanouette, S.; Voronova, A.; Skerjanc, I.; Couture, J.-F.  
Deposited on : 2010-12-01  
Resolution : 1.70 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

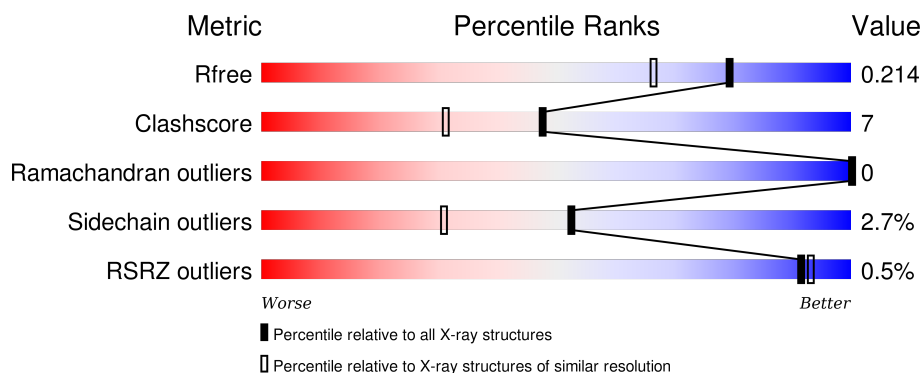
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	318	 79% 13% •• 6%
1	B	318	 80% 13% • 6%
2	C	6	 67% 17% 17%
2	D	6	 67% 17% 17%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5019 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 WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	3	0
			2302	1470	382	439	11			
1	B	298	Total	C	N	O	S	0	0	0
			2299	1470	382	437	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	EXPRESSION TAG	UNP P61964
A	18	ALA	-	EXPRESSION TAG	UNP P61964
A	19	MET	-	EXPRESSION TAG	UNP P61964
A	20	GLY	-	EXPRESSION TAG	UNP P61964
B	17	GLY	-	EXPRESSION TAG	UNP P61964
B	18	ALA	-	EXPRESSION TAG	UNP P61964
B	19	MET	-	EXPRESSION TAG	UNP P61964
B	20	GLY	-	EXPRESSION TAG	UNP P61964

- Molecule 2 is a protein called N-alpha acetylated form of histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			32	19	7	6			
2	D	5	Total	C	N	O	0	0	0
			35	21	8	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total	O	0	0
			197	197		
3	B	146	Total	O	0	0
			146	146		

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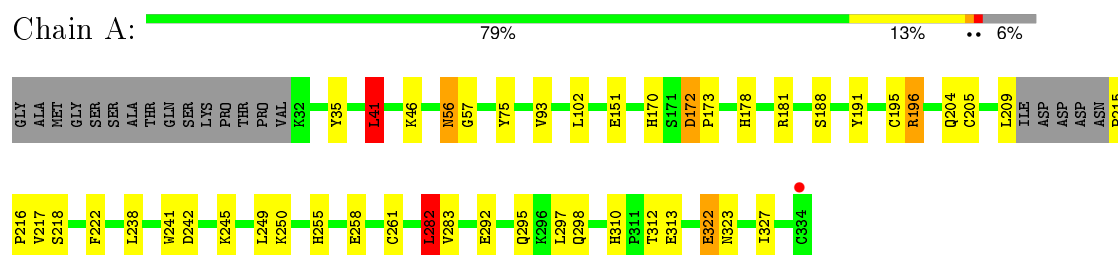
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0

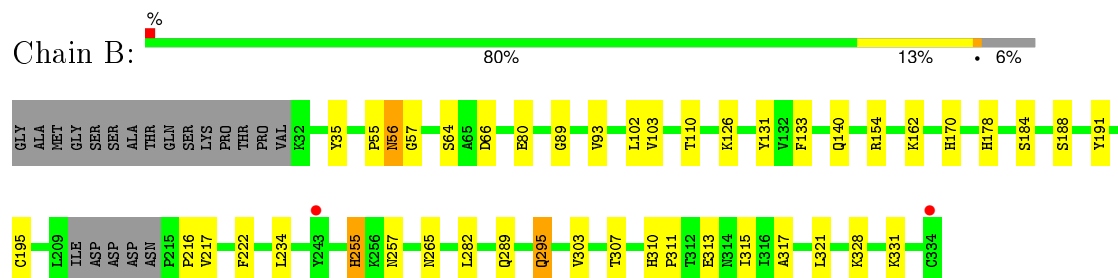
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

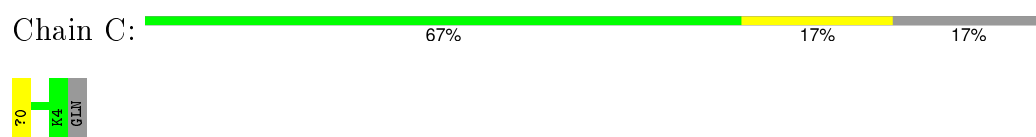
- Molecule 1: WD repeat-containing protein 5



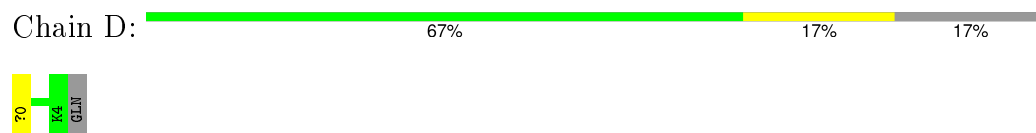
- Molecule 1: WD repeat-containing protein 5



- Molecule 2: N-alpha acetylated form of histone H3



- Molecule 2: N-alpha acetylated form of histone H3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.95Å 48.61Å 63.31Å 98.79° 90.95° 117.48°	Depositor
Resolution (Å)	35.64 – 1.70 35.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (35.64-1.70) 90.4 (35.64-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.51 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.155 , 0.205 0.162 , 0.214	Depositor DCC
$R_{free}$ test set	2575 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.6	EDS
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50439 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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	1.16	2/2372 (0.1%)	1.02	5/3216 (0.2%)
1	B	1.04	2/2354 (0.1%)	0.94	2/3192 (0.1%)
2	C	1.82	1/29 (3.4%)	1.00	0/38
2	D	1.86	1/32 (3.1%)	1.44	1/41 (2.4%)
All	All	1.11	6/4787 (0.1%)	0.99	8/6487 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	0	ACE	C-N	8.53	1.53	1.34
1	A	322	GLU	CD-OE1	6.59	1.32	1.25
2	C	0	ACE	C-N	6.41	1.48	1.34
1	B	184	SER	CA-CB	5.46	1.61	1.52
1	A	241	TRP	CB-CG	-5.19	1.41	1.50
1	B	133	PHE	CE2-CZ	5.17	1.47	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	282	LEU	CB-CG-CD1	6.95	122.81	111.00
1	A	41	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	46	LYS	CD-CE-NZ	-5.88	98.18	111.70
1	B	154	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	D	0	ACE	O-C-N	-5.71	113.57	122.70
1	A	238	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	B	131	TYR	CB-CG-CD1	-5.13	117.92	121.00

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	2302	0	2269	34	0
1	B	2299	0	2266	35	0
2	C	32	0	32	0	0
2	D	35	0	41	0	0
3	A	197	0	0	5	0
3	B	146	0	0	8	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
All	All	5019	0	4608	69	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.

All (69) 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:204:GLN:HB2	3:A:452:HOH:O	1.62	0.98
1:A:178:HIS:HD2	1:A:222:PHE:H	1.16	0.89
1:A:323:ASN:HB3	3:A:442:HOH:O	1.73	0.87
1:B:140:GLN:OE1	3:B:357:HOH:O	1.94	0.84
1:B:178:HIS:HD2	1:B:222:PHE:H	1.27	0.80
1:A:178:HIS:CD2	1:A:222:PHE:H	2.01	0.79
1:B:310:HIS:HD2	1:B:313:GLU:H	1.28	0.77
1:B:110:THR:HG22	1:B:126:LYS:HD3	1.67	0.77
1:B:170:HIS:HE1	1:B:188:SER:OG	1.67	0.77
1:B:178:HIS:CD2	1:B:222:PHE:H	2.09	0.71
1:A:292:GLU:OE1	3:A:497:HOH:O	2.09	0.70
1:A:310:HIS:HD2	1:A:313:GLU:H	1.39	0.68
1:A:35:TYR:H	1:A:295:GLN:HE22	1.40	0.68
1:B:140:GLN:HG3	3:B:357:HOH:O	1.95	0.66
1:A:196:ARG:NH2	3:A:520:HOH:O	2.32	0.63
1:A:255:HIS:CD2	1:A:255:HIS:H	2.16	0.63
1:B:110:THR:CG2	1:B:126:LYS:HD3	2.29	0.63
1:B:310:HIS:CD2	1:B:313:GLU:H	2.15	0.61
1:A:255:HIS:HE1	3:A:363:HOH:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:CD2	1:A:313:GLU:H	2.18	0.61
1:A:195[B]:CYS:SG	1:A:217:VAL:HG11	2.41	0.61
1:B:93:VAL:HG22	1:B:102:LEU:HD22	1.83	0.60
1:B:89:GLY:HA3	3:B:3:HOH:O	2.01	0.60
1:B:255:HIS:H	1:B:255:HIS:CD2	2.20	0.59
1:B:35:TYR:H	1:B:295:GLN:HE22	1.49	0.58
1:A:204:GLN:HG3	1:A:205:CYS:N	2.18	0.58
1:B:170:HIS:CE1	1:B:188:SER:OG	2.54	0.58
1:A:242:ASP:CG	1:A:245:LYS:HG3	2.25	0.58
1:B:140:GLN:CG	3:B:357:HOH:O	2.50	0.57
1:A:310:HIS:CD2	1:A:312:THR:H	2.23	0.57
1:A:57:GLY:O	1:A:310:HIS:HE1	1.90	0.55
1:A:283:VAL:HB	1:A:297:LEU:HB2	1.89	0.54
1:A:310:HIS:HD2	1:A:312:THR:H	1.55	0.54
1:A:322:GLU:H	1:A:322:GLU:CD	2.11	0.54
1:A:170:HIS:HE1	1:A:188:SER:OG	1.91	0.53
1:B:64:SER:HB3	1:B:66:ASP:OD1	2.08	0.53
1:B:80:GLU:OE1	3:B:421:HOH:O	2.19	0.52
1:A:255:HIS:HD2	1:A:255:HIS:H	1.55	0.52
1:B:55:PRO:O	1:B:311:PRO:HG3	2.10	0.52
1:A:249:LEU:O	1:A:250:LYS:HG3	2.10	0.52
1:B:55:PRO:HG3	3:B:387:HOH:O	2.11	0.51
1:A:93:VAL:HG22	1:A:102:LEU:HD22	1.93	0.49
1:B:265:ASN:ND2	1:B:307:THR:OG1	2.45	0.49
1:A:35:TYR:N	1:A:295:GLN:HE22	2.10	0.49
1:B:191:TYR:HA	1:B:216:PRO:HB3	1.95	0.49
1:A:75:TYR:HE2	1:A:313:GLU:HG3	1.77	0.48
1:B:195:CYS:SG	1:B:217:VAL:HG11	2.54	0.47
1:B:56:ASN:HD22	1:B:56:ASN:C	2.18	0.47
1:B:255:HIS:H	1:B:255:HIS:HD2	1.60	0.46
1:A:56:ASN:HD22	1:A:56:ASN:C	2.19	0.45
1:B:303:VAL:HB	1:B:321:LEU:HD12	1.98	0.45
1:A:151:GLU:HG2	1:A:172:ASP:C	2.37	0.45
1:B:315:ILE:HG12	1:B:331:LYS:HD2	1.99	0.45
1:A:191:TYR:HA	1:A:216:PRO:HB3	1.98	0.44
1:B:317:ALA:HA	1:B:328:LYS:O	2.18	0.44
1:B:93:VAL:CG2	1:B:102:LEU:HD22	2.48	0.44
1:A:178:HIS:CD2	1:A:222:PHE:N	2.79	0.43
1:A:242:ASP:OD2	1:A:245:LYS:HG3	2.18	0.43
1:A:218:SER:HB2	1:A:261:CYS:HA	2.00	0.43
1:A:41:LEU:HB2	1:A:327:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PRO:C	1:B:57:GLY:H	2.21	0.43
1:B:289:GLN:HG2	3:B:395:HOH:O	2.18	0.42
1:B:93:VAL:HA	1:B:103:VAL:O	2.20	0.41
1:A:282:LEU:HD12	1:A:298:GLN:HA	2.02	0.41
1:B:55:PRO:C	1:B:57:GLY:N	2.73	0.41
1:A:209:LEU:HD22	1:A:209:LEU:N	2.36	0.41
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.89	0.41
1:B:57:GLY:O	1:B:310:HIS:HE1	2.04	0.40
1:B:140:GLN:CD	3:B:357:HOH:O	2.50	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	297/318 (93%)	284 (96%)	13 (4%)	0	100	100
1	B	294/318 (92%)	281 (96%)	13 (4%)	0	100	100
2	C	3/6 (50%)	3 (100%)	0	0	100	100
2	D	3/6 (50%)	3 (100%)	0	0	100	100
All	All	597/648 (92%)	571 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	258/276 (94%)	250 (97%)	8 (3%)	47	25
1	B	255/276 (92%)	249 (98%)	6 (2%)	57	36
2	C	2/4 (50%)	2 (100%)	0	100	100
2	D	3/4 (75%)	3 (100%)	0	100	100
All	All	518/560 (92%)	504 (97%)	14 (3%)	52	31

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	56	ASN
1	A	172	ASP
1	A	173	PRO
1	A	181	ARG
1	A	215	PRO
1	A	258	GLU
1	A	282	LEU
1	B	56	ASN
1	B	162	LYS
1	B	255	HIS
1	B	257	ASN
1	B	282	LEU
1	B	295	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	170	HIS
1	A	178	HIS
1	A	255	HIS
1	A	265	ASN
1	A	289	GLN
1	A	295	GLN
1	A	310	HIS
1	A	323	ASN
1	B	56	ASN
1	B	140	GLN
1	B	170	HIS
1	B	178	HIS

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Mol	Chain	Res	Type
1	B	255	HIS
1	B	265	ASN
1	B	289	GLN
1	B	295	GLN
1	B	310	HIS
1	B	323	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 [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, 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	298/318 (93%)	-0.37	1 (0%) 94 95	7, 14, 29, 39	2 (0%)
1	B	298/318 (93%)	-0.08	2 (0%) 89 91	9, 22, 38, 47	3 (1%)
2	C	4/6 (66%)	-0.56	0 100 100	9, 10, 11, 18	0
2	D	4/6 (66%)	-0.39	0 100 100	10, 13, 14, 21	0
All	All	604/648 (93%)	-0.23	3 (0%) 91 93	7, 18, 35, 47	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	CYS	4.8
1	B	243	TYR	3.8
1	A	334	CYS	3.3

### 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.