



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2020 – 12:09 PM JST

PDB ID : 6M2M  
Title : A role for histone chaperone OsChz1 in histone recognition and deposition  
Authors : Luo, Q.; Wang, B.  
Deposited on : 2020-02-28  
Resolution : 2.85 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

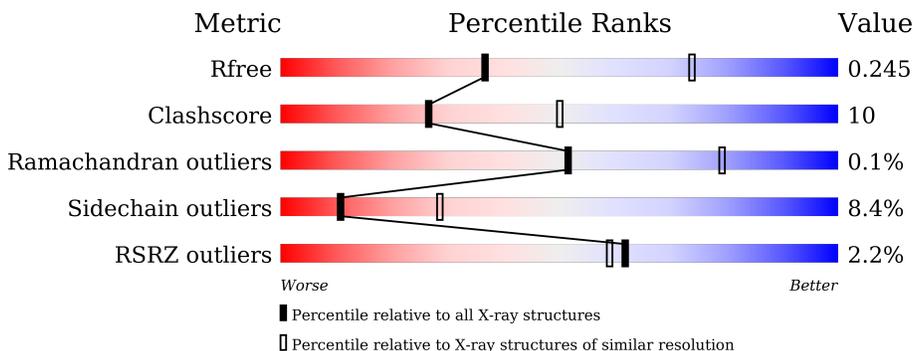
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 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  $\leq 5\%$ . 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	93	
1	C	93	
1	E	93	
1	G	93	
1	I	93	
1	K	93	

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Mol	Chain	Length	Quality of chain
2	B	98	 74% 12% • 12%
2	D	98	 2% 68% 20% • 10%
2	F	98	 66% 19% • 12%
2	H	98	 72% 16% • 10%
2	J	98	 70% 19% • 9%
2	L	98	 3% 78% 12% • 9%
3	M	105	 8% • 90%
3	N	105	 3% 13% • 86%
3	O	105	 9% • 88%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8020 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 Probable histone H2A.3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	E	88	666	421	124	121	0	0	0
1	A	88	666	421	124	121	0	0	0
1	C	88	666	421	124	121	0	0	0
1	G	79	575	369	103	103	0	0	0
1	I	80	582	372	102	108	0	0	0
1	K	81	552	358	97	97	0	0	0

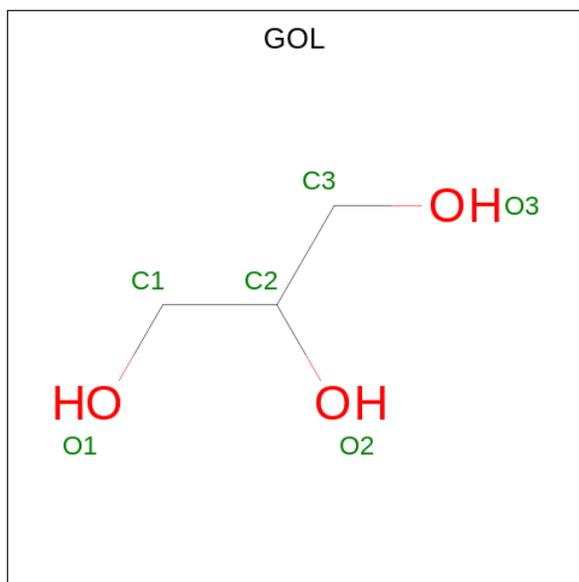
- Molecule 2 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	88	676	435	114	125	2	0	0	0
2	F	86	655	421	110	122	2	0	0	0
2	J	89	649	412	112	123	2	0	0	0
2	H	88	666	427	112	125	2	0	0	0
2	L	89	669	425	115	127	2	0	0	0
2	B	86	664	426	114	122	2	0	0	0

- Molecule 3 is a protein called Expressed protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	10	Total	C	N	O	0	0	0
			81	43	11	27			
3	N	15	Total	C	N	O	0	0	0
			121	67	17	37			
3	O	13	Total	C	N	O	0	0	0
			100	54	15	31			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total	O	0	0
			2	2		
5	A	3	Total	O	0	0
			3	3		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

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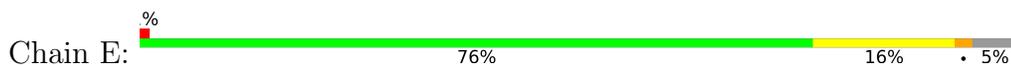
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total O 1 1	0	0
5	I	1	Total O 1 1	0	0
5	F	3	Total O 3 3	0	0
5	H	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0

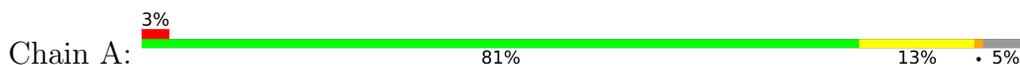
### 3 Residue-property plots [i](#)

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: Probable histone H2A.3



- Molecule 1: Probable histone H2A.3



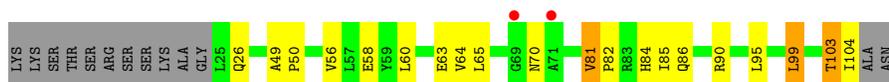
- Molecule 1: Probable histone H2A.3



- Molecule 1: Probable histone H2A.3



- Molecule 1: Probable histone H2A.3



- Molecule 1: Probable histone H2A.3



- Molecule 2: Histone H2B.1



- Molecule 2: Histone H2B.1



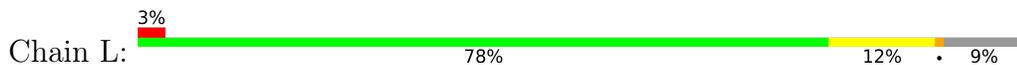
- Molecule 2: Histone H2B.1



- Molecule 2: Histone H2B.1



- Molecule 2: Histone H2B.1



- Molecule 2: Histone H2B.1



- Molecule 3: Expressed protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.36Å 116.34Å 101.90Å 90.00° 114.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 29.36 – 2.84	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.85) 93.5 (29.36-2.84)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.194 , 0.253 0.206 , 0.245	Depositor DCC
$R_{free}$ test set	1890 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.447 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.450 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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](#)

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

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	0.88	0/674	0.83	0/910
1	C	0.80	0/674	0.93	1/910 (0.1%)
1	E	0.83	0/674	0.91	0/910
1	G	0.67	0/583	0.88	1/793 (0.1%)
1	I	0.69	0/590	0.88	0/805
1	K	0.66	0/560	0.85	0/766
2	B	0.76	0/674	0.78	0/908
2	D	0.76	0/687	0.79	0/927
2	F	0.87	0/665	0.75	0/898
2	H	0.83	0/676	0.82	0/914
2	J	0.86	0/659	0.86	0/893
2	L	0.70	0/679	0.82	0/917
3	M	0.57	0/80	0.69	0/107
3	N	0.77	0/120	0.74	0/162
3	O	0.81	0/99	0.86	0/133
All	All	0.78	0/8094	0.84	2/10953 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	101	ASP	N-CA-C	-5.20	96.97	111.00
1	C	73	ARG	CB-CA-C	-5.00	100.40	110.40

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	666	0	694	10	0
1	C	666	0	694	10	0
1	E	666	0	694	19	0
1	G	575	0	575	31	0
1	I	582	0	570	31	0
1	K	552	0	528	18	0
2	B	664	0	691	8	0
2	D	676	0	695	19	0
2	F	655	0	671	23	0
2	H	666	0	678	14	0
2	J	649	0	626	21	0
2	L	669	0	673	8	0
3	M	81	0	50	2	0
3	N	121	0	86	0	0
3	O	100	0	66	6	0
4	A	6	0	8	1	0
4	C	6	0	8	0	0
4	F	6	0	8	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	3	0	0	2	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
All	All	8020	0	8015	165	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 10.

The worst 5 of 165 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:E:99:LEU:HD21	2:F:89:PHE:CE1	1.62	1.34
1:I:81:VAL:HG22	1:I:82:PRO:CD	1.69	1.22
1:E:99:LEU:HD21	2:F:89:PHE:CD1	1.74	1.21
1:I:64:VAL:HG12	2:J:86:MET:HE3	1.13	1.11
1:I:64:VAL:CG1	2:J:86:MET:CE	2.28	1.11

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	86/93 (92%)	84 (98%)	2 (2%)	0	100	100
1	C	86/93 (92%)	84 (98%)	2 (2%)	0	100	100
1	E	86/93 (92%)	85 (99%)	1 (1%)	0	100	100
1	G	77/93 (83%)	70 (91%)	7 (9%)	0	100	100
1	I	78/93 (84%)	70 (90%)	8 (10%)	0	100	100
1	K	79/93 (85%)	70 (89%)	9 (11%)	0	100	100
2	B	84/98 (86%)	81 (96%)	3 (4%)	0	100	100
2	D	86/98 (88%)	83 (96%)	3 (4%)	0	100	100
2	F	84/98 (86%)	80 (95%)	4 (5%)	0	100	100
2	H	86/98 (88%)	84 (98%)	2 (2%)	0	100	100
2	J	87/98 (89%)	83 (95%)	4 (5%)	0	100	100
2	L	87/98 (89%)	81 (93%)	6 (7%)	0	100	100
3	M	8/105 (8%)	6 (75%)	2 (25%)	0	100	100
3	N	13/105 (12%)	11 (85%)	2 (15%)	0	100	100
3	O	11/105 (10%)	9 (82%)	1 (9%)	1 (9%)	1	1
All	All	1038/1461 (71%)	981 (94%)	56 (5%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	O	433	GLU

### 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	66/71 (93%)	62 (94%)	4 (6%)	18	43
1	C	66/71 (93%)	63 (96%)	3 (4%)	27	57
1	E	66/71 (93%)	61 (92%)	5 (8%)	13	33
1	G	52/71 (73%)	47 (90%)	5 (10%)	8	22
1	I	53/71 (75%)	49 (92%)	4 (8%)	13	34
1	K	44/71 (62%)	36 (82%)	8 (18%)	1	4
2	B	72/87 (83%)	64 (89%)	8 (11%)	6	16
2	D	73/87 (84%)	69 (94%)	4 (6%)	21	49
2	F	70/87 (80%)	60 (86%)	10 (14%)	3	8
2	H	71/87 (82%)	67 (94%)	4 (6%)	21	47
2	J	64/87 (74%)	58 (91%)	6 (9%)	8	23
2	L	71/87 (82%)	68 (96%)	3 (4%)	30	60
3	M	9/90 (10%)	8 (89%)	1 (11%)	6	16
3	N	14/90 (16%)	13 (93%)	1 (7%)	14	36
3	O	11/90 (12%)	10 (91%)	1 (9%)	9	25
All	All	802/1218 (66%)	735 (92%)	67 (8%)	11	28

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	99	LEU
2	F	107	TYR
2	B	117	GLU
1	K	103	THR

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Mol	Chain	Res	Type
2	F	72	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	119	GLN
1	G	91	ASN
2	L	119	GLN
1	G	70	ASN
1	I	70	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GOL	F	201	-	5,5,5	0.65	0	5,5,5	0.79	0
4	GOL	A	201	-	5,5,5	0.50	0	5,5,5	0.48	0
4	GOL	C	201	-	5,5,5	0.68	0	5,5,5	1.21	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	201	-	-	4/4/4/4	-
4	GOL	A	201	-	-	0/4/4/4	-
4	GOL	C	201	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	GOL	O3-C3-C2	2.05	120.02	110.20

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	GOL	C1-C2-C3-O3
4	C	201	GOL	O1-C1-C2-O2
4	C	201	GOL	O1-C1-C2-C3
4	C	201	GOL	C1-C2-C3-O3
4	C	201	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	GOL	1	0

## 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	88/93 (94%)	0.19	3 (3%) 45 39	27, 44, 75, 95	0
1	C	88/93 (94%)	0.15	0 100 100	26, 44, 77, 87	0
1	E	88/93 (94%)	0.17	1 (1%) 80 80	26, 43, 74, 89	0
1	G	79/93 (84%)	0.43	4 (5%) 28 23	38, 79, 123, 134	0
1	I	80/93 (86%)	0.33	2 (2%) 57 54	37, 81, 123, 140	0
1	K	81/93 (87%)	0.39	3 (3%) 41 36	37, 78, 121, 133	0
2	B	86/98 (87%)	0.08	0 100 100	30, 48, 73, 92	0
2	D	88/98 (89%)	0.26	2 (2%) 60 57	29, 49, 106, 111	0
2	F	86/98 (87%)	0.14	0 100 100	30, 50, 75, 97	0
2	H	88/98 (89%)	0.15	0 100 100	31, 49, 82, 91	0
2	J	89/98 (90%)	0.16	0 100 100	28, 50, 109, 122	0
2	L	89/98 (90%)	0.26	3 (3%) 45 39	28, 48, 106, 119	0
3	M	10/105 (9%)	0.74	1 (10%) 7 5	89, 95, 115, 117	0
3	N	15/105 (14%)	0.96	3 (20%) 1 0	85, 104, 145, 147	0
3	O	13/105 (12%)	0.46	1 (7%) 13 10	88, 95, 116, 128	0
All	All	1068/1461 (73%)	0.24	23 (2%) 62 59	26, 54, 109, 147	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	71	ALA	4.9
1	A	23	ALA	4.0
1	K	64	VAL	3.3
2	L	83	MET	3.2
1	I	71	ALA	3.1

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	F	201	6/6	0.85	0.17	61,70,76,76	0
4	GOL	A	201	6/6	0.85	0.19	58,60,62,65	0
4	GOL	C	201	6/6	0.87	0.17	63,65,71,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.