



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 PM GMT

PDB ID : 4GQB  
Title : Crystal Structure of the human PRMT5:MEP50 Complex  
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Deposited on : 2012-08-22  
Resolution : 2.06 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

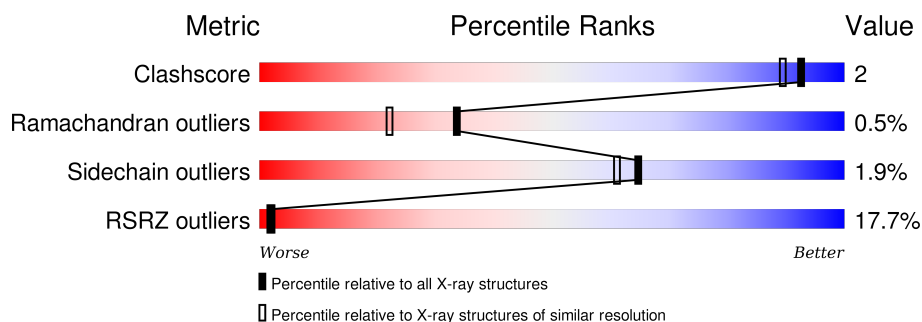
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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))
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	637	<div> <div>17%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
2	B	344	<div> <div>16%</div> <div>82%</div> <div>6%</div> <div>12%</div> </div>
3	C	22	<div> <div>18%</div> <div>23%</div> <div>14%</div> <div>5%</div> <div>59%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7656 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	1	0
			5006	3202	854	926	24			

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2269	1427	387	443	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP Q9BQA1
B	0	SER	-	EXPRESSION TAG	UNP Q9BQA1
B	1	LEU	-	EXPRESSION TAG	UNP Q9BQA1

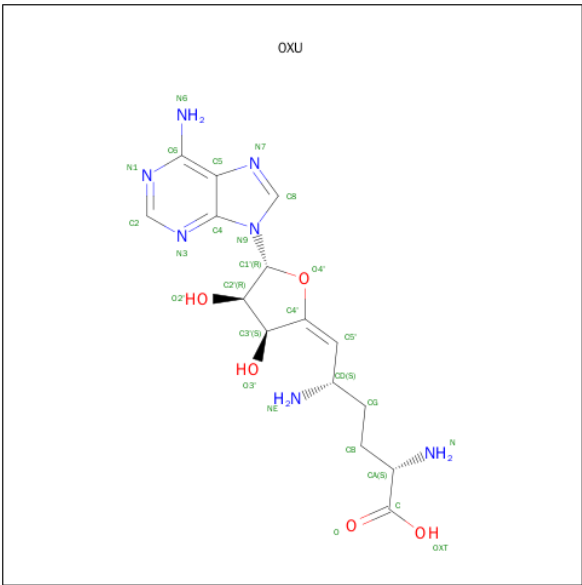
- Molecule 3 is a protein called Histone H4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			54	31	13	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ACE	-	ACETYLATION	UNP P62805

- Molecule 4 is (2S,5S,6E)-2,5-DIAMINO-6-[(3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYDIHYDROFURAN-2(3H)-YLIDENE]HEXANOIC ACID (three-letter code: 0XU) (formula: C<sub>15</sub>H<sub>21</sub>N<sub>7</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	15	7	5		

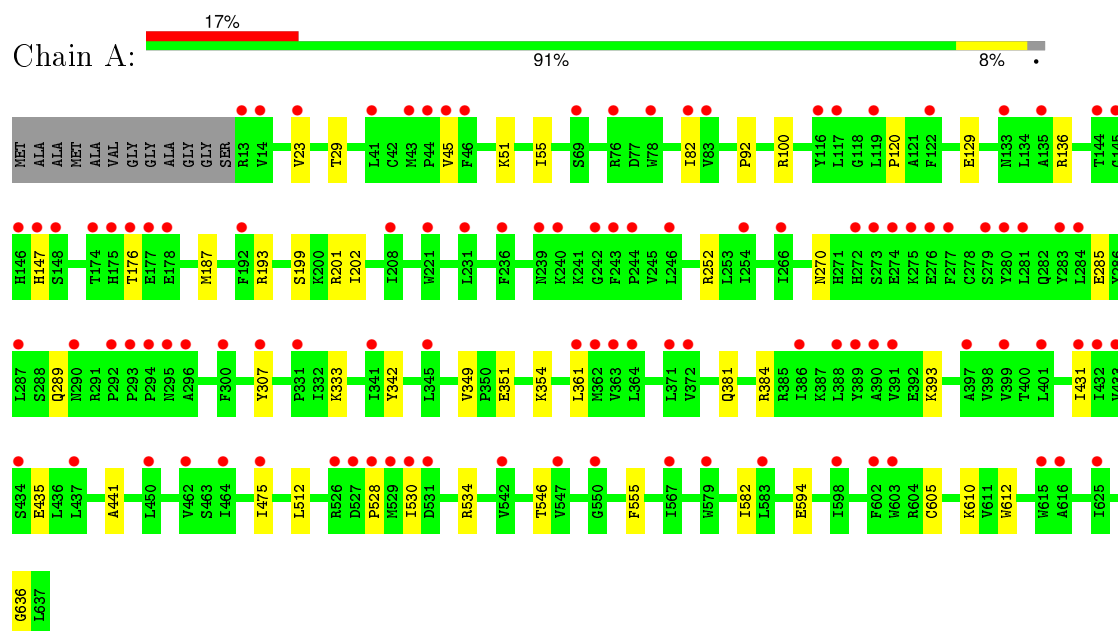
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		
5	B	59	Total	O	0	0
			59	59		
5	C	2	Total	O	0	0
			2	2		

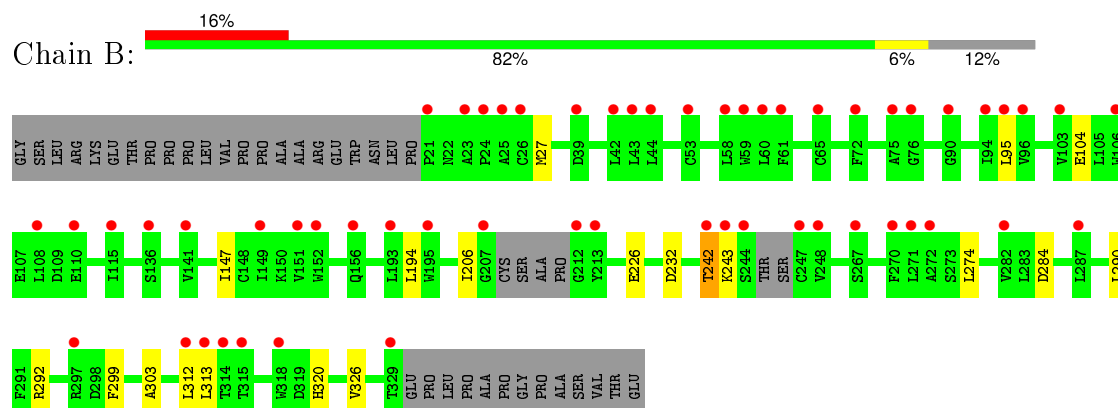
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

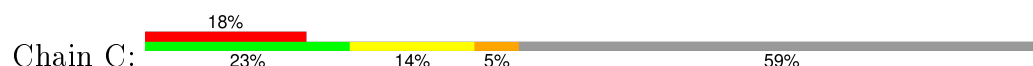
- Molecule 1: Protein arginine N-methyltransferase 5

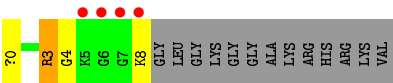


- Molecule 2: Methylosome protein 50



- Molecule 3: Histone H4 peptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.98 Å   138.76 Å   178.47 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.71 – 2.06 19.71 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.71-2.06) 99.6 (19.71-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.06 Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.188   ,   0.222 (Not available)   ,   (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.983	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 77935 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 0XU, 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	0.51	0/5146	0.68	0/7012
2	B	0.46	0/2322	0.73	0/3173
3	C	0.64	0/51	0.80	0/63
All	All	0.50	0/7519	0.70	0/10248

There are no bond length outliers.

There are no bond angle outliers.

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	5006	0	4833	19	0
2	B	2269	0	2157	9	0
3	C	54	0	59	3	0
4	A	27	0	20	1	0
5	A	239	0	0	1	0
5	B	59	0	0	0	0
5	C	2	0	0	0	0
All	All	7656	0	7069	29	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 2.



All (29) 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:B:194:LEU:HB2	2:B:206:ILE:HD11	1.84	0.59
1:A:55:ILE:HD13	5:A:1025:HOH:O	2.03	0.58
2:B:284:ASP:HB3	2:B:290:LEU:HD11	1.88	0.55
1:A:610:LYS:HD3	1:A:636:GLY:HA2	1.89	0.54
1:A:307:TYR:HE1	3:C:8:LYS:HG3	1.73	0.54
2:B:226:GLU:HB3	2:B:242:THR:HB	1.90	0.54
1:A:92:PRO:O	1:A:100:ARG:HG3	2.09	0.52
3:C:0:ACE:H1	3:C:4:GLY:O	2.10	0.52
1:A:82:ILE:O	1:A:120:PRO:HD2	2.10	0.51
1:A:351:GLU:O	1:A:354:LYS:HB2	2.11	0.51
1:A:129:GLU:HG3	1:A:187[B]:MET:CE	2.40	0.51
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.95	0.48
1:A:361:LEU:HD11	1:A:431:ILE:HD12	1.96	0.47
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.80	0.46
2:B:232:ASP:C	2:B:232:ASP:OD1	2.54	0.46
1:A:23:VAL:HG22	1:A:29:THR:HG21	1.98	0.45
1:A:51:LYS:HB3	2:B:299:PHE:HE2	1.81	0.45
4:A:701:OXU:H11	3:C:3:ARG:NH2	2.14	0.44
2:B:312:LEU:HD22	2:B:326:VAL:HG12	2.00	0.44
1:A:349:VAL:O	1:A:384:ARG:NH1	2.50	0.44
2:B:303:ALA:HB1	2:B:313:LEU:HD11	2.00	0.44
1:A:147:HIS:HA	1:A:201:ARG:NH2	2.33	0.43
1:A:285:GLU:O	1:A:289:GLN:HG2	2.18	0.43
1:A:512:LEU:HD22	1:A:546:THR:HG21	2.01	0.43
2:B:27:MET:HG3	2:B:320:HIS:HE1	1.86	0.41
2:B:95:LEU:HD12	2:B:104:GLU:O	2.21	0.41
1:A:342:TYR:CD1	1:A:381:GLN:HG3	2.56	0.41
1:A:199:SER:HB3	1:A:202:ILE:HD12	2.03	0.40
1:A:605:CYS:HB2	1:A:612:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	624/637 (98%)	599 (96%)	23 (4%)	2 (0%)	46	36
2	B	297/344 (86%)	284 (96%)	10 (3%)	3 (1%)	19	8
3	C	7/22 (32%)	5 (71%)	2 (29%)	0	100	100
All	All	928/1003 (92%)	888 (96%)	35 (4%)	5 (0%)	34	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	A	530	ILE
2	B	243	LYS
2	B	242	THR
1	A	528	PRO

### 5.3.2 Protein sidechains ⓘ

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	543/562 (97%)	531 (98%)	12 (2%)	60	55
2	B	248/291 (85%)	246 (99%)	2 (1%)	86	86
3	C	4/12 (33%)	3 (75%)	1 (25%)	1	0
All	All	795/865 (92%)	780 (98%)	15 (2%)	65	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	136	ARG
1	A	176	THR
1	A	193	ARG
1	A	252	ARG

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Mol	Chain	Res	Type
1	A	270	ASN
1	A	333	LYS
1	A	393	LYS
1	A	435	GLU
1	A	475	ILE
1	A	582	ILE
1	A	594	GLU
2	B	274	LEU
2	B	292	ARG
3	C	3	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
2	B	224	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	0XU	A	701	-	19,29,29	0.84	1 (5%)	14,42,42	1.55	3 (21%)

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	0XU	A	701	-	-	0/8/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	0XU	C6-N6	2.70	1.43	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	0XU	C1'-N9-C4	-2.97	122.46	126.94
4	A	701	0XU	N3-C2-N1	-2.17	127.23	128.89
4	A	701	0XU	O3'-C3'-C2'	-2.05	109.33	113.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	0XU	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 ⓘ

### 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	625/637 (98%)	0.99	106 (16%) 2 2	31, 52, 86, 116	0
2	B	303/344 (88%)	1.12	56 (18%) 2 1	47, 64, 94, 137	0
3	C	8/22 (36%)	2.61	4 (50%) 0 0	37, 49, 72, 95	0
All	All	936/1003 (93%)	1.04	166 (17%) 2 2	31, 57, 89, 137	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	CYS	10.9
2	B	244	SER	7.6
2	B	271	LEU	7.4
1	A	529	MET	7.2
2	B	58	LEU	6.6
2	B	25	ALA	6.2
2	B	59	TRP	5.7
1	A	530	ILE	5.4
1	A	293	PRO	5.3
1	A	345	LEU	5.1
3	C	6	GLY	5.0
1	A	280	TYR	5.0
1	A	145	GLY	5.0
1	A	296	ALA	4.9
2	B	207	GLY	4.9
3	C	7	GLY	4.9
2	B	44	LEU	4.8
1	A	528	PRO	4.8
1	A	292	PRO	4.8
1	A	273	SER	4.7
2	B	312	LEU	4.6
1	A	284	LEU	4.6
3	C	8	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	361	LEU	4.4
1	A	254	ILE	4.4
1	A	246	LEU	4.4
1	A	175	HIS	4.4
1	A	431	ILE	4.4
1	A	45	VAL	4.3
2	B	329	THR	4.3
2	B	60	LEU	4.3
2	B	313	LEU	4.2
2	B	23	ALA	4.2
2	B	141	VAL	4.1
1	A	147	HIS	4.1
1	A	341	ILE	4.1
2	B	110	GLU	4.1
1	A	433	VAL	4.0
1	A	231	LEU	4.0
2	B	43	LEU	4.0
1	A	527	ASP	4.0
1	A	294	PRO	4.0
1	A	236	PHE	3.9
2	B	75	ALA	3.9
1	A	266	ILE	3.8
1	A	307	TYR	3.8
1	A	274	GLU	3.8
1	A	176	THR	3.8
2	B	212	GLY	3.8
2	B	94	ILE	3.8
1	A	432	ILE	3.7
1	A	281	LEU	3.7
2	B	72	PHE	3.7
1	A	372	VAL	3.7
1	A	437	LEU	3.6
1	A	119	LEU	3.6
1	A	364	LEU	3.6
2	B	248	VAL	3.6
1	A	243	PHE	3.5
2	B	149	ILE	3.5
2	B	103	VAL	3.4
2	B	156	GLN	3.4
1	A	526	ARG	3.4
1	A	283	TYR	3.4
1	A	221	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	146	HIS	3.3
1	A	174	THR	3.3
2	B	272	ALA	3.2
2	B	243	LYS	3.2
2	B	115	ILE	3.2
1	A	363	VAL	3.2
1	A	399	VAL	3.2
1	A	386	ILE	3.2
2	B	318	TRP	3.1
1	A	69	SER	3.1
1	A	23	VAL	3.1
1	A	135	ALA	3.1
1	A	401	LEU	3.0
2	B	108	LEU	3.0
2	B	267	SER	3.0
1	A	331	PRO	3.0
1	A	41	LEU	3.0
1	A	287	LEU	3.0
2	B	270	PHE	3.0
2	B	53	CYS	2.9
1	A	116	TYR	2.9
1	A	242	GLY	2.9
2	B	76	GLY	2.9
1	A	290	ASN	2.9
1	A	13	ARG	2.8
1	A	82	ILE	2.8
1	A	277	PHE	2.7
1	A	177	GLU	2.7
2	B	24	PRO	2.7
1	A	276	GLU	2.7
2	B	242	THR	2.7
1	A	300	PHE	2.7
2	B	314	THR	2.7
1	A	76	ARG	2.6
1	A	602	PHE	2.6
1	A	475	ILE	2.6
2	B	106	TRP	2.6
1	A	550	GLY	2.6
1	A	397	ALA	2.6
1	A	603	TRP	2.5
1	A	464	ILE	2.5
1	A	615	TRP	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	122	PHE	2.5
2	B	61	PHE	2.5
1	A	117	LEU	2.5
1	A	275	LYS	2.5
2	B	26	CYS	2.5
1	A	295	ASN	2.5
1	A	192	PHE	2.5
1	A	244	PRO	2.5
2	B	21	PRO	2.5
1	A	388	LEU	2.4
2	B	193	LEU	2.4
2	B	287	LEU	2.4
1	A	44	PRO	2.4
1	A	43	MET	2.4
2	B	136	SER	2.4
1	A	208	ILE	2.4
1	A	371	LEU	2.4
1	A	462	VAL	2.3
2	B	96	VAL	2.3
2	B	282	VAL	2.3
2	B	90	GLY	2.3
2	B	213	TYR	2.3
1	A	279	SER	2.3
3	C	5	LYS	2.3
1	A	46	PHE	2.3
1	A	616	ALA	2.3
1	A	133	ASN	2.3
1	A	547	VAL	2.3
1	A	362	MET	2.3
2	B	95	LEU	2.3
1	A	14	VAL	2.2
2	B	297	ARG	2.2
2	B	151	VAL	2.2
2	B	42	LEU	2.2
1	A	272	HIS	2.2
2	B	315	THR	2.2
1	A	542	VAL	2.2
1	A	450	LEU	2.2
1	A	598	ILE	2.2
1	A	178	GLU	2.1
2	B	152	TRP	2.1
1	A	148	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	240	LYS	2.1
2	B	65	CYS	2.1
1	A	83	VAL	2.1
2	B	39	ASP	2.1
1	A	239	ASN	2.1
1	A	579	TRP	2.1
1	A	390	ALA	2.1
2	B	195	TRP	2.1
1	A	583	LEU	2.1
1	A	567	ILE	2.0
1	A	625	ILE	2.0
1	A	144	THR	2.0
1	A	391	VAL	2.0
1	A	78	TRP	2.0
1	A	389	TYR	2.0
1	A	434	SER	2.0
1	A	531	ASP	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	0XU	A	701	27/27	0.94	0.13	-0.93	28,39,54,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.