



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 3, 2018 – 11:29 PM EST

PDB ID : 5M01  
Title : Crystal structure of murine P14 TCR/ H-2Db complex with PA, modified gp33 peptide from LCMV  
Authors : Achour, A.; Sandalova, T.; Sun, R.; Han, X.  
Deposited on : 2016-10-03  
Resolution : 1.95 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
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) : rb-20030736

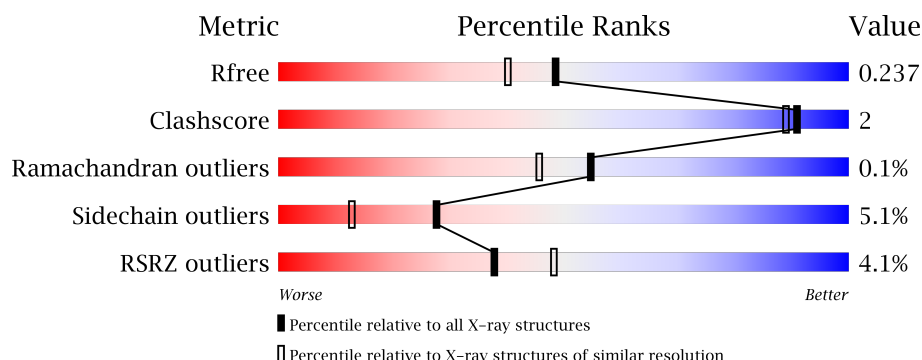
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	276	<div> <div>0.1%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
2	B	119	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>15%</div> </div> </div>
3	G	205	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>8%</div> </div> </div>
4	H	238	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
5	P	9	<div> <div></div> <div> <div></div> <div>100%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	301	-	-	-	X
6	GOL	A	302	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6914 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2273	1435	403	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			833	531	140	154	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P01887
B	-18	ALA	-	expression tag	UNP P01887
B	-17	ARG	-	expression tag	UNP P01887
B	-16	SER	-	expression tag	UNP P01887
B	-15	VAL	-	expression tag	UNP P01887
B	-14	THR	-	expression tag	UNP P01887
B	-13	LEU	-	expression tag	UNP P01887
B	-12	VAL	-	expression tag	UNP P01887
B	-11	PHE	-	expression tag	UNP P01887
B	-10	LEU	-	expression tag	UNP P01887
B	-9	VAL	-	expression tag	UNP P01887
B	-8	LEU	-	expression tag	UNP P01887
B	-7	VAL	-	expression tag	UNP P01887
B	-6	SER	-	expression tag	UNP P01887
B	-5	LEU	-	expression tag	UNP P01887
B	-4	THR	-	expression tag	UNP P01887
B	-3	GLY	-	expression tag	UNP P01887
B	-2	LEU	-	expression tag	UNP P01887
B	-1	MET	-	cloning artifact	UNP P01887
B	0	GLY	-	cloning artifact	UNP P01887

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Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	variant	UNP P01887

- Molecule 3 is a protein called Protein Trav14-1,T-cell receptor alpha chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	188	Total	C	N	O	S	0	0	0
			1476	938	237	293	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	100	LEU	-	linker	UNP A0A0G2JF94
G	101	TYR	-	linker	UNP A0A0G2JF94
G	102	GLY	-	linker	UNP A0A0G2JF94
G	103	ASN	-	linker	UNP A0A0G2JF94
G	104	GLU	-	linker	UNP A0A0G2JF94
G	105	LYS	-	linker	UNP A0A0G2JF94
G	106	ILE	-	linker	UNP A0A0G2JF94
G	107	THR	-	linker	UNP A0A0G2JF94
G	108	PHE	-	linker	UNP A0A0G2JF94
G	109	GLY	-	linker	UNP A0A0G2JF94
G	110	ALA	-	linker	UNP A0A0G2JF94
G	111	GLY	-	linker	UNP A0A0G2JF94
G	112	THR	-	linker	UNP A0A0G2JF94
G	113	LYS	-	linker	UNP A0A0G2JF94
G	114	LEU	-	linker	UNP A0A0G2JF94
G	115	THR	-	linker	UNP A0A0G2JF94
G	116	ILE	-	linker	UNP A0A0G2JF94
G	117	LYS	-	linker	UNP A0A0G2JF94
G	118	PRO	-	linker	UNP A0A0G2JF94
G	119	ASN	-	linker	UNP A0A0G2JF94
G	166	CYS	THR	conflict	UNP P01849

- Molecule 4 is a protein called T-cell receptor beta chain V region C5,T-cell receptor beta-2 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	237	Total	C	N	O	S	0	5	0
			1901	1192	340	363	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	93	ASP	-	linker	UNP P04213
H	94	ALA	-	linker	UNP P04213
H	95	GLY	-	linker	UNP P04213
H	96	GLY	-	linker	UNP P04213
H	97	ARG	-	linker	UNP P04213
H	98	ASN	-	linker	UNP P04213
H	99	THR	-	linker	UNP P04213
H	100	LEU	-	linker	UNP P04213
H	101	TYR	-	linker	UNP P04213
H	102	PHE	-	linker	UNP P04213
H	103	GLY	-	linker	UNP P04213
H	104	ALA	-	linker	UNP P04213
H	105	GLY	-	linker	UNP P04213
H	106	THR	-	linker	UNP P04213
H	107	ARG	-	linker	UNP P04213
H	108	LEU	-	linker	UNP P04213
H	109	SER	-	linker	UNP P04213
H	110	VAL	-	linker	UNP P04213
H	111	LEU	-	linker	UNP P04213
H	168	CYS	SER	conflict	UNP P01851
H	182	SER	CYS	conflict	UNP P01851

- Molecule 5 is a protein called LCMV-DERIVED GP33 ALTERED PEPTIDE LIGAND PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total	C	N	O	S	0	0	0
			66	42	11	12	1			

- Molecule 6 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
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	126	Total	O	0	0
			126	126		
7	B	45	Total	O	0	0
			45	45		
7	G	53	Total	O	0	0
			53	53		
7	H	125	Total	O	0	0
			125	125		
7	P	4	Total	O	0	0
			4	4		

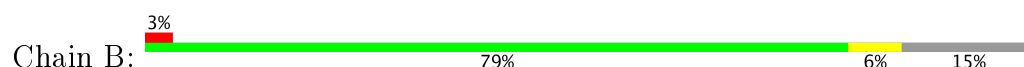
### 3 Residue-property plots [i](#)

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.

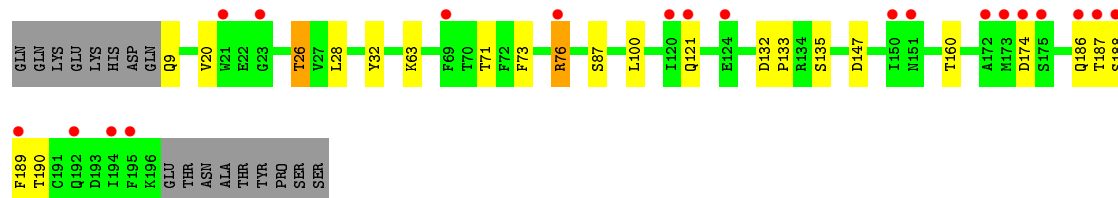
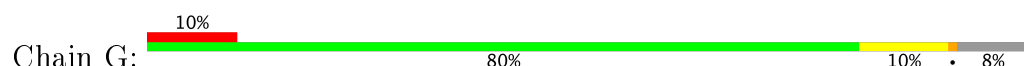
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



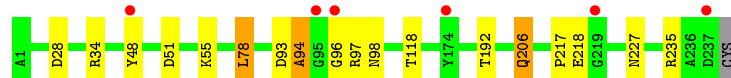
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Protein Trav14-1, T-cell receptor alpha chain C region



- Molecule 4: T-cell receptor beta chain V region C5, T-cell receptor beta-2 chain C region



- Molecule 5: LCMV-DERIVED GP33 ALTERED PEPTIDE LIGAND PA



There are no outlier residues recorded for this chain.



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.93 Å   46.54 Å   89.40 Å 90.00°   94.34°   90.00°	Depositor
Resolution (Å)	127.60 – 1.95 50.12 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (127.60-1.95) 98.7 (50.12-1.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.196   ,   0.229 0.204   ,   0.237	Depositor DCC
$R_{free}$ test set	3830 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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 ⓘ

### 5.1 Standard geometry ⓘ

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	0.76	0/2343	0.97	7/3180 (0.2%)
2	B	0.70	0/859	0.84	1/1163 (0.1%)
3	G	0.70	1/1511 (0.1%)	0.81	2/2049 (0.1%)
4	H	0.74	0/1956	0.87	4/2657 (0.2%)
5	P	0.59	0/67	0.70	0/88
All	All	0.73	1/6736 (0.0%)	0.89	14/9137 (0.2%)

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
4	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	133	PRO	N-CD	5.22	1.55	1.47

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	A	234	ARG	NE-CZ-NH1	13.71	127.15	120.30
4	H	94[A]	ALA	N-CA-C	-6.70	92.90	111.00
4	H	94[B]	ALA	N-CA-C	-6.70	92.90	111.00
1	A	272	LEU	CA-CB-CG	6.54	130.34	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	217	PRO	Peptide

## 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	2273	0	2149	12	0
2	B	833	0	808	4	0
3	G	1476	0	1420	5	0
4	H	1901	0	1811	11	0
5	P	66	0	68	0	0
6	A	12	0	16	0	0
7	A	126	0	0	0	0
7	B	45	0	0	0	0
7	G	53	0	0	0	0
7	H	125	0	0	2	0
7	P	4	0	0	0	0
All	All	6914	0	6272	26	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.

The worst 5 of 26 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)
4:H:93[A]:ASP:O	7:H:301:HOH:O	2.09	0.71
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.29	0.67
1:A:51:TRP:HD1	1:A:178:THR:HG1	1.44	0.64
4:H:206:GLN:HG2	4:H:227:ASN:OD1	1.99	0.62
3:G:20:VAL:HG21	3:G:26:THR:HB	1.87	0.56

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	275/276 (100%)	270 (98%)	5 (2%)	0	100	100
2	B	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
3	G	186/205 (91%)	174 (94%)	11 (6%)	1 (0%)	32	19
4	H	240/238 (101%)	235 (98%)	5 (2%)	0	100	100
5	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	807/847 (95%)	782 (97%)	24 (3%)	1 (0%)	55	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	186	GLN

### 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	235/234 (100%)	225 (96%)	10 (4%)	33	19
2	B	95/111 (86%)	92 (97%)	3 (3%)	44	31
3	G	167/184 (91%)	152 (91%)	15 (9%)	11	3
4	H	205/204 (100%)	197 (96%)	8 (4%)	37	22
5	P	6/6 (100%)	6 (100%)	0	100	100
All	All	708/739 (96%)	672 (95%)	36 (5%)	28	13

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	63	LYS
3	G	135	SER
4	H	118	THR
3	G	76	ARG
3	G	147	ASP

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

Mol	Chain	Res	Type
4	H	69	GLN
4	H	208	HIS

### 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](#)

2 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	$\# Z  > 2$
6	GOL	A	301	-	5,5,5	0.36	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	302	-	5,5,5	0.40	0	5,5,5	0.25	0

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
6	GOL	A	301	-	-	0/4/4/4	0/0/0/0
6	GOL	A	302	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	276/276 (100%)	0.31	4 (1%) 75 83	19, 32, 53, 77	0
2	B	101/119 (84%)	0.24	3 (2%) 51 61	20, 39, 62, 69	0
3	G	188/205 (91%)	0.77	20 (10%) 7 11	24, 46, 86, 107	0
4	H	237/238 (99%)	0.30	6 (2%) 58 67	24, 34, 52, 67	0
5	P	9/9 (100%)	0.25	0 100 100	21, 22, 28, 29	0
All	All	811/847 (95%)	0.41	33 (4%) 38 48	19, 36, 66, 107	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	172	ALA	8.7
3	G	173	MET	6.6
3	G	187	THR	6.3
2	B	-1	MET	6.1
3	G	189	PHE	6.1

### 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 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
6	GOL	A	302	6/6	0.79	0.39	18.31	39,42,52,55	0
6	GOL	A	301	6/6	0.79	0.26	5.85	59,65,68,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.