



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2016 – 06:45 PM EDT

PDB ID : 5FCU  
Title : CRYSTAL STRUCTURE OF THE INNER DOMAIN OF CLADE A/E HIV-1 GP120 IN COMPLEX WITH THE ADCC-POTENT RHESUS MACAQUE ANTIBODY JR4  
Authors : Gohain, N.; Tolbert, W.D.; Pazgier, M.  
Deposited on : 2015-12-15  
Resolution : 1.85 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  
<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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) : rb-20027790

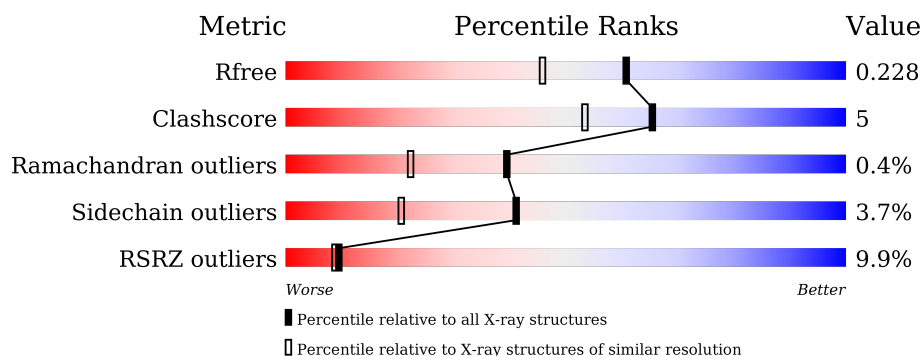
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	G	169	<div> <div>22%</div> <div>46% 13% .. 38%</div> </div>
2	H	233	<div> <div>6%</div> <div>83% 10% 7%</div> </div>
3	L	216	<div> <div>92% 6% .</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
4	NAG	G	501	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4442 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 clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	104	Total	C	N	O	S	0	0	0
			827	519	140	159	9			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	42	VAL	-	expression tag	UNP A0A0M3KKW9
G	43	PRO	-	expression tag	UNP A0A0M3KKW9
G	470	SER	-	expression tag	UNP A0A0M3KKW9
G	471	GLY	-	expression tag	UNP A0A0M3KKW9
G	472	GLY	-	expression tag	UNP A0A0M3KKW9
G	473	GLY	-	expression tag	UNP A0A0M3KKW9
G	474	ASN	-	expression tag	UNP A0A0M3KKW9
G	475	ILE	-	expression tag	UNP A0A0M3KKW9
G	476	LYS	-	expression tag	UNP A0A0M3KKW9
G	477	ASP	-	expression tag	UNP A0A0M3KKW9
G	478	ASN	-	expression tag	UNP A0A0M3KKW9
G	479	TRP	-	expression tag	UNP A0A0M3KKW9
G	480	ARG	-	expression tag	UNP A0A0M3KKW9
G	481	SER	-	expression tag	UNP A0A0M3KKW9
G	482	GLU	-	expression tag	UNP A0A0M3KKW9
G	483	LEU	-	expression tag	UNP A0A0M3KKW9
G	484	TYR	-	expression tag	UNP A0A0M3KKW9
G	485	LYS	-	expression tag	UNP A0A0M3KKW9
G	486	TYR	-	expression tag	UNP A0A0M3KKW9
G	487	LYS	-	expression tag	UNP A0A0M3KKW9
G	488	VAL	-	expression tag	UNP A0A0M3KKW9
G	489	VAL	-	expression tag	UNP A0A0M3KKW9
G	490	GLN	-	expression tag	UNP A0A0M3KKW9
G	491	ILE	-	expression tag	UNP A0A0M3KKW9
G	492	GLU	-	expression tag	UNP A0A0M3KKW9
G	493	PRO	-	expression tag	UNP A0A0M3KKW9
G	494	LEU	-	expression tag	UNP A0A0M3KKW9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	495	GLY	-	expression tag	UNP A0A0M3KKW9
G	496	ILE	-	expression tag	UNP A0A0M3KKW9

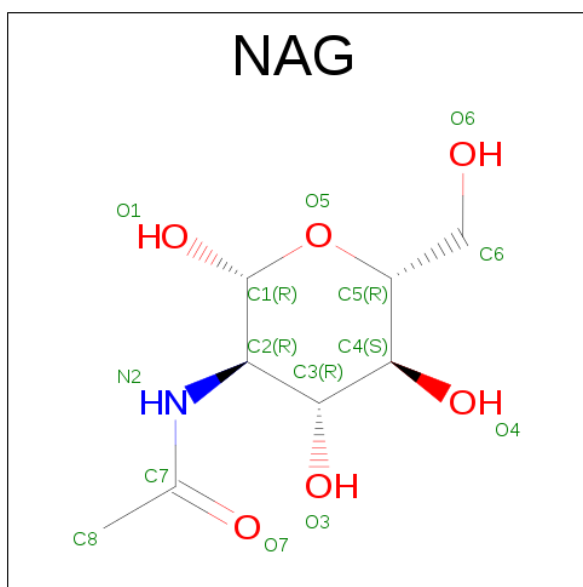
- Molecule 2 is a protein called JR4 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1641	1043	273	321	4			

- Molecule 3 is a protein called JR4 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1566	979	263	320	4			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	3	Total	Cl	0	0
			3	3		

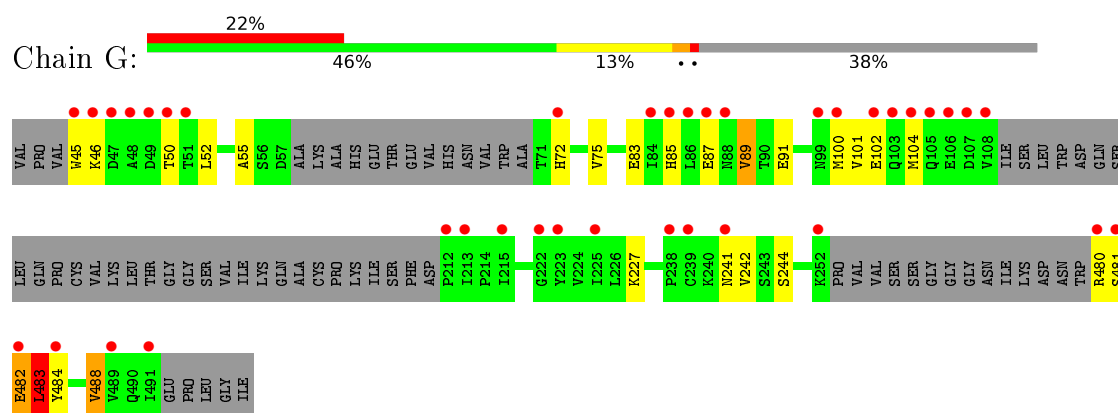
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	19	Total	O	0	0
			19	19		
7	H	123	Total	O	0	0
			123	123		
7	L	234	Total	O	0	0
			234	234		

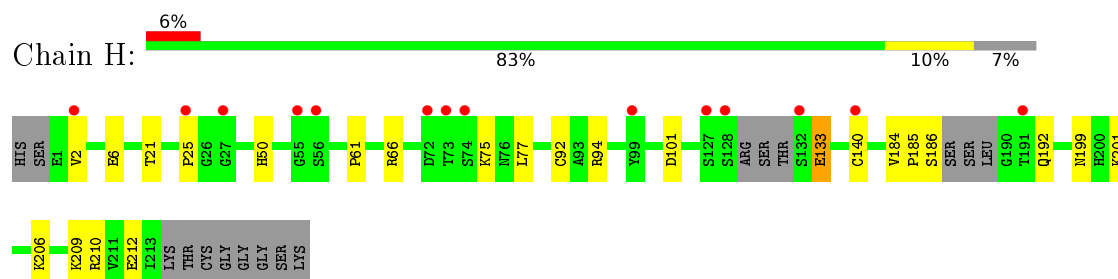
### 3 Residue-property plots [i](#)

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.

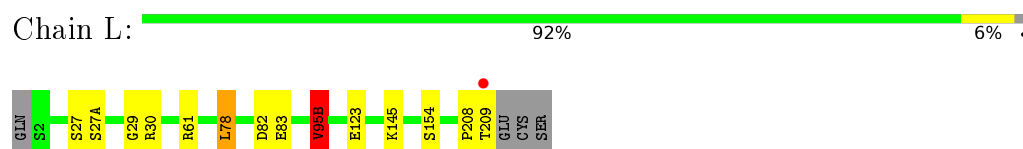
- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



- Molecule 2: JR4 FAB HEAVY CHAIN



- Molecule 3: JR4 FAB LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.45Å 89.85Å 180.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.85 49.46 – 1.85	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.85) 94.3 (49.46-1.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.184 , 0.223 0.192 , 0.228	Depositor DCC
$R_{free}$ test set	2617 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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: CL, SO4, NAG

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	G	0.66	0/845	0.82	0/1145
2	H	0.89	0/1685	0.87	3/2306 (0.1%)
3	L	1.10	4/1602 (0.2%)	0.94	4/2185 (0.2%)
All	All	0.94	4/4132 (0.1%)	0.89	7/5636 (0.1%)

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	G	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	83	GLU	CD-OE1	7.75	1.34	1.25
3	L	83	GLU	CD-OE2	6.91	1.33	1.25
3	L	154	SER	CB-OG	-5.26	1.35	1.42
3	L	123	GLU	CD-OE2	5.11	1.31	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	ARG	NE-CZ-NH2	-7.02	116.79	120.30
3	L	61	ARG	NE-CZ-NH1	6.75	123.68	120.30
2	H	66	ARG	NE-CZ-NH1	6.47	123.54	120.30
3	L	78	LEU	CB-CG-CD2	6.23	121.59	111.00
3	L	95(B)	VAL	CB-CA-C	-6.12	99.78	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	482	GLU	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	G	827	0	783	21	0
2	H	1641	0	1601	10	0
3	L	1566	0	1529	10	0
4	G	14	0	13	0	0
5	L	15	0	0	0	0
6	L	3	0	0	0	0
7	G	19	0	0	1	0
7	H	123	0	0	0	0
7	L	234	0	0	1	0
All	All	4442	0	3926	40	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 5.

The worst 5 of 40 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:G:481:SER:HB2	1:G:482:GLU:HA	1.56	0.87
1:G:101:VAL:HG13	1:G:483:LEU:CD2	2.11	0.80
3:L:208:PRO:O	3:L:209:THR:OG1	2.00	0.78
1:G:101:VAL:HG13	1:G:483:LEU:HD21	1.65	0.77
1:G:481:SER:HB2	1:G:483:LEU:HB3	1.73	0.71

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	G	96/169 (57%)	90 (94%)	4 (4%)	2 (2%)	9	1
2	H	211/233 (91%)	207 (98%)	4 (2%)	0	100	100
3	L	210/216 (97%)	205 (98%)	5 (2%)	0	100	100
All	All	517/618 (84%)	502 (97%)	13 (2%)	2 (0%)	39	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	483	LEU
1	G	89	VAL

### 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	G	96/151 (64%)	87 (91%)	9 (9%)	11	1
2	H	188/201 (94%)	182 (97%)	6 (3%)	46	27
3	L	178/182 (98%)	176 (99%)	2 (1%)	80	72
All	All	462/534 (86%)	445 (96%)	17 (4%)	41	20

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	483	LEU

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Mol	Chain	Res	Type
1	G	488	VAL
2	H	201	LYS
1	G	480	ARG
2	H	212	GLU

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

Mol	Chain	Res	Type
2	H	3	GLN
2	H	171	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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	NAG	G	501	1	14,14,15	0.72	0	15,19,21	1.21	1 (6%)
5	SO4	L	301	-	4,4,4	0.94	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	L	302	-	4,4,4	0.33	0	6,6,6	0.48	0
5	SO4	L	303	-	4,4,4	0.61	0	6,6,6	0.46	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
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
5	SO4	L	301	-	-	0/0/0/0	0/0/0/0
5	SO4	L	302	-	-	0/0/0/0	0/0/0/0
5	SO4	L	303	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	501	NAG	C1-O5-C5	3.98	118.00	112.14

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	G	104/169 (61%)	1.63	38 (36%) 0 0	40, 70, 92, 100	0
2	H	217/233 (93%)	0.31	14 (6%) 22 21	21, 42, 78, 94	0
3	L	212/216 (98%)	0.03	1 (0%) 91 91	16, 27, 48, 67	0
All	All	533/618 (86%)	0.46	53 (9%) 9 9	16, 39, 86, 100	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	48	ALA	5.8
2	H	55	GLY	5.1
1	G	45	TRP	5.0
1	G	491	ILE	4.7
1	G	46	LYS	4.7

### 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	501	14/15	0.89	0.19	4.22	38,47,52,55	0
5	SO4	L	301	5/5	0.99	0.14	-0.85	21,25,29,30	0
6	CL	L	304	1/1	0.95	0.09	-1.02	66,66,66,66	0
5	SO4	L	302	5/5	0.99	0.06	-1.31	44,46,50,52	0
5	SO4	L	303	5/5	0.97	0.08	-	51,53,57,64	0
6	CL	L	306	1/1	0.92	0.11	-	68,68,68,68	1
6	CL	L	305	1/1	0.96	0.08	-	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.