



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 02:11 PM EDT

PDB ID : 8EEE  
Title : Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ104-d in complex with ZIKV E glycoprotein  
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Deposited on : 2022-09-07  
Resolution : 2.82 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

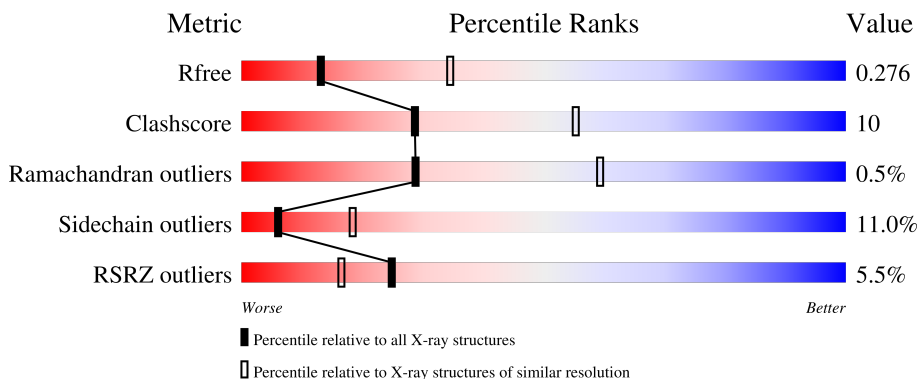
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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.



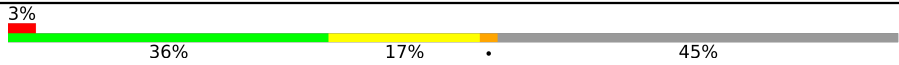
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 of 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	E	405	
1	Z	405	
2	B	220	
2	L	220	
3	A	228	

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Mol	Chain	Length	Quality of chain
3	H	228	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (3%), a green segment (36%), a yellow segment (17%), and a grey segment (45%). The percentages are labeled below each segment.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11031 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Z	393	2919	1826	499	569	25	0	0	0
1	E	392	2929	1832	504	568	25	0	0	0

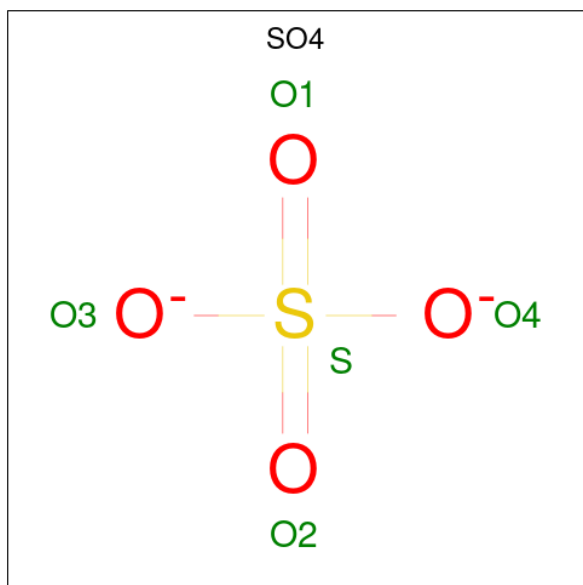
- Molecule 2 is a protein called rhMZ104-D antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	115	874	553	143	175	3	0	0	0
2	B	217	1634	1029	269	331	5	0	0	0

- Molecule 3 is a protein called rhMZ104-D antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	125	963	608	166	183	6	0	0	0
3	A	226	1702	1071	289	334	8	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

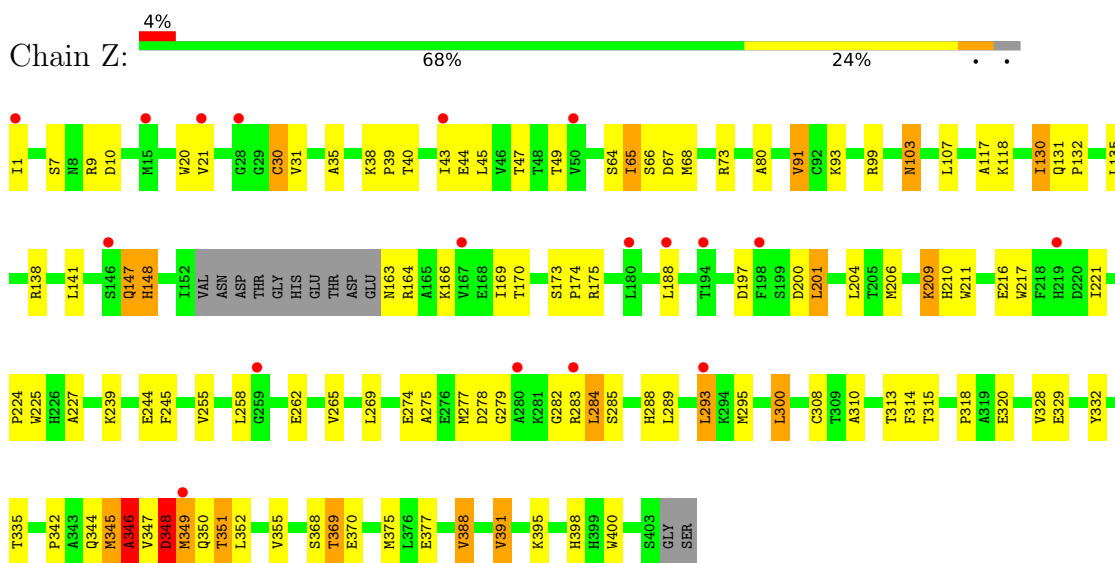


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

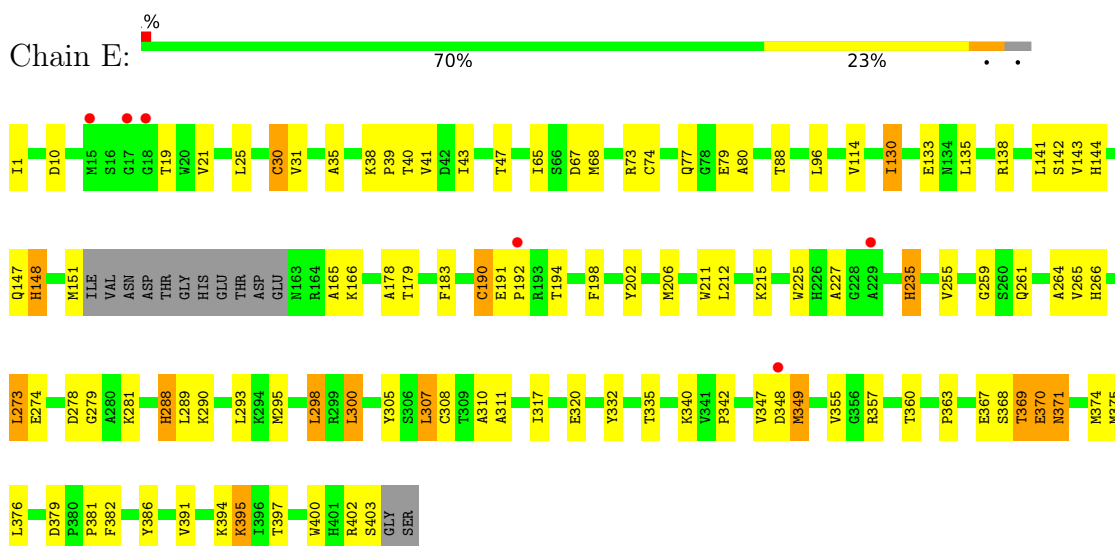
### 3 Residue-property plots [i](#)

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.

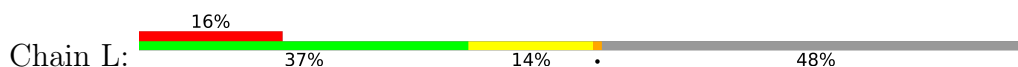
- Molecule 1: Envelope protein E

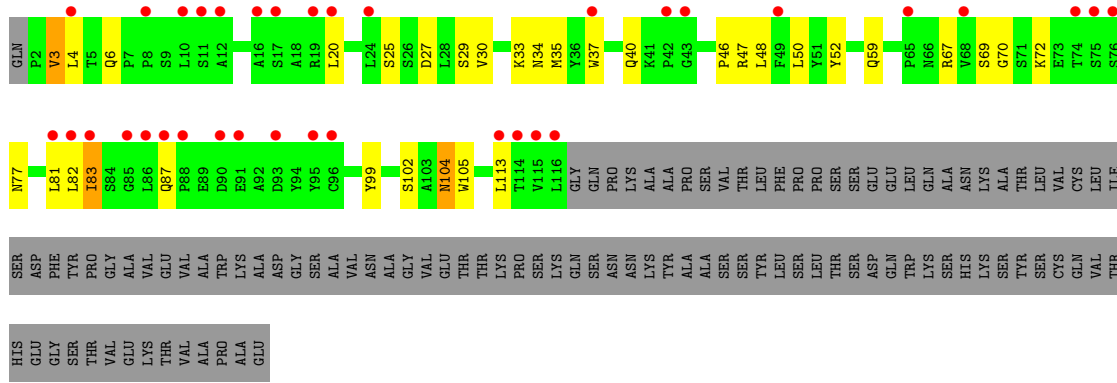


- Molecule 1: Envelope protein E

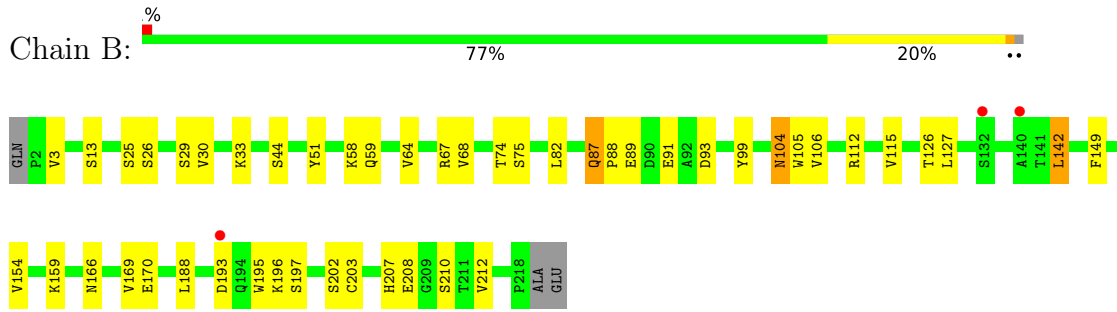


- Molecule 2: rhMZ104-D antibody light chain

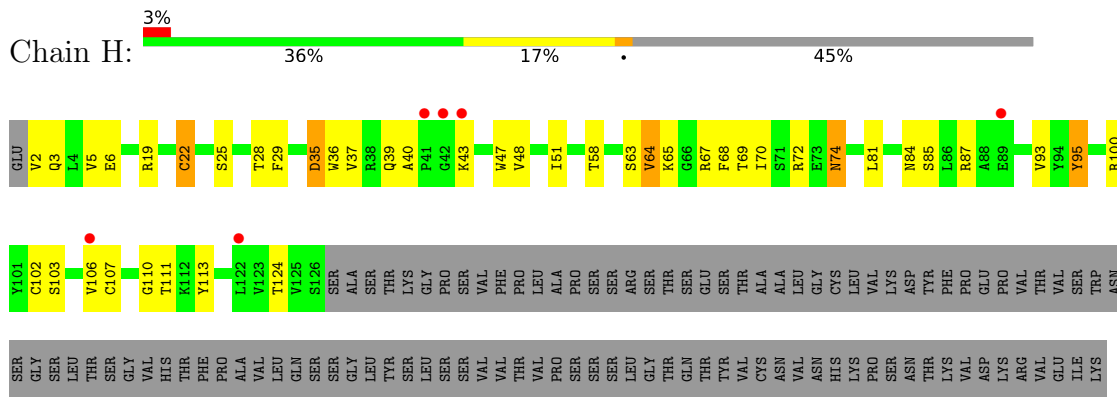




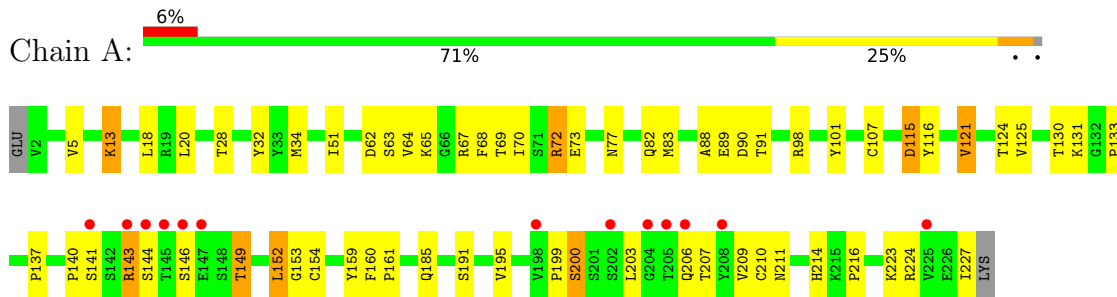
• Molecule 2: rhMZ104-D antibody light chain



• Molecule 3: rhMZ104-D antibody heavy chain



• Molecule 3: rhMZ104-D antibody heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.32Å 130.42Å 109.71Å 90.00° 104.17° 90.00°	Depositor
Resolution (Å)	14.99 – 2.82 49.25 – 2.82	Depositor EDS
% Data completeness (in resolution range)	73.1 (14.99-2.82) 73.3 (49.25-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.76 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.217 , 0.275 0.221 , 0.276	Depositor DCC
$R_{free}$ test set	2000 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	11031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: SO4

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	E	0.28	0/2992	0.56	0/4065
1	Z	0.29	0/2981	0.59	0/4053
2	B	0.27	0/1677	0.48	0/2289
2	L	0.27	0/898	0.50	0/1225
3	A	0.28	0/1743	0.50	0/2371
3	H	0.26	0/986	0.50	0/1333
All	All	0.28	0/11277	0.54	0/15336

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	E	0	2
1	Z	0	5
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Z	197	ASP	Peptide
1	Z	345	MET	Peptide
1	Z	346	ALA	Peptide
1	Z	348	ASP	Peptide
1	Z	351	THR	Peptide

## 5.2 Too-close contacts [i](#)

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	E	2929	0	2795	61	0
1	Z	2919	0	2777	65	0
2	B	1634	0	1576	18	0
2	L	874	0	838	18	0
3	A	1702	0	1647	32	0
3	H	963	0	916	27	0
4	A	5	0	0	0	0
4	H	5	0	0	0	0
All	All	11031	0	10549	210	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 210 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:88:THR:HG23	3:H:106:VAL:HG12	1.39	1.04
1:Z:30:CYS:SG	1:Z:31:VAL:N	2.53	0.80
1:Z:262:GLU:HG2	1:E:259:GLY:HA3	1.65	0.78
3:H:106:VAL:HG12	3:H:106:VAL:O	1.85	0.75
3:H:3:GLN:HE21	3:H:25:SER:HB2	1.53	0.73

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	E	388/405 (96%)	344 (89%)	43 (11%)	1 (0%)	41	70
1	Z	389/405 (96%)	344 (88%)	39 (10%)	6 (2%)	10	31
2	B	215/220 (98%)	205 (95%)	10 (5%)	0	100	100
2	L	113/220 (51%)	103 (91%)	10 (9%)	0	100	100
3	A	224/228 (98%)	206 (92%)	18 (8%)	0	100	100
3	H	123/228 (54%)	112 (91%)	11 (9%)	0	100	100
All	All	1452/1706 (85%)	1314 (90%)	131 (9%)	7 (0%)	29	59

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	347	VAL
1	Z	348	ASP
1	Z	300	LEU
1	Z	346	ALA
1	Z	349	MET

### 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	E	312/338 (92%)	280 (90%)	32 (10%)	7	21
1	Z	310/338 (92%)	278 (90%)	32 (10%)	7	21
2	B	183/185 (99%)	164 (90%)	19 (10%)	7	20
2	L	98/185 (53%)	88 (90%)	10 (10%)	7	21
3	A	188/190 (99%)	166 (88%)	22 (12%)	5	16
3	H	98/190 (52%)	82 (84%)	16 (16%)	2	7
All	All	1189/1426 (83%)	1058 (89%)	131 (11%)	6	18

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	44	SER

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Mol	Chain	Res	Type
2	B	75	SER
2	B	212	VAL
1	E	265	VAL
1	E	255	VAL

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

Mol	Chain	Res	Type
1	Z	331	GLN
3	H	3	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 monosaccharides 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	$\# Z  > 2$
4	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.06	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	E	392/405 (96%)	-0.14	6 (1%) 73 67	15, 41, 84, 116	0
1	Z	393/405 (97%)	0.20	18 (4%) 32 22	15, 62, 102, 128	0
2	B	217/220 (98%)	-0.20	3 (1%) 75 69	12, 36, 68, 98	0
2	L	115/220 (52%)	1.41	35 (30%) 0 0	44, 98, 179, 199	0
3	A	226/228 (99%)	0.10	13 (5%) 23 15	13, 39, 93, 127	0
3	H	125/228 (54%)	0.27	6 (4%) 30 21	51, 79, 93, 113	0
All	All	1468/1706 (86%)	0.14	81 (5%) 25 16	12, 49, 105, 199	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	116	LEU	8.1
2	L	12	ALA	7.9
2	L	86	LEU	7.7
2	L	65	PRO	6.2
2	L	17	SER	5.1

### 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	SO4	H	301	5/5	0.96	0.13	90,91,93,94	0
4	SO4	A	301	5/5	0.96	0.11	68,68,72,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.