



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2021 – 04:23 PM EST

PDB ID : 7KFV  
Title : Structural basis for a germline-biased antibody response to SARS-CoV-2 (RBD:C1A-B12 Fab)  
Authors : Pan, J.; Abraham, J.; Clark, L.; Clark, S.  
Deposited on : 2020-10-15  
Resolution : 2.10 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	:	2.16
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)	:	2.16

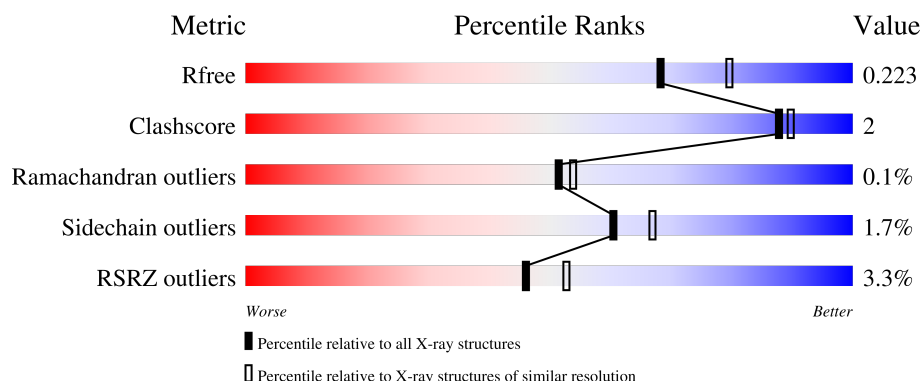
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



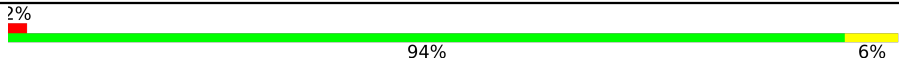
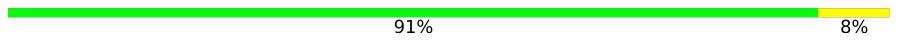
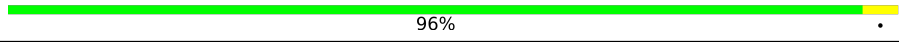
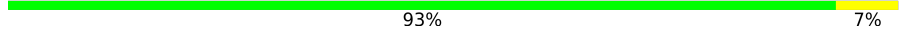
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	A	228	<div> <div>4%</div> <div>81%</div> <div>14%</div> </div>
1	B	228	<div> <div>5%</div> <div>80%</div> <div>5%</div> <div>14%</div> </div>
1	E	228	<div> <div>10%</div> <div>82%</div> <div>14%</div> </div>
2	C	225	<div> <div>4%</div> <div>92%</div> <div>8%</div> </div>
2	F	225	<div> <div>2%</div> <div>90%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	225	 2% 94% 6%
3	D	214	 91% 8%
3	G	214	 96% .
3	L	214	 93% 7%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16494 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	5	0
			1600	1025	270	297	8			
1	B	195	Total	C	N	O	S	0	6	0
			1590	1019	268	295	8			
1	E	195	Total	C	N	O	S	0	3	0
			1570	1004	265	293	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	GLY	-	expression tag	UNP P0DTC2
A	315	SER	-	expression tag	UNP P0DTC2
A	316	GLY	-	expression tag	UNP P0DTC2
A	317	SER	-	expression tag	UNP P0DTC2
A	318	GLY	-	expression tag	UNP P0DTC2
B	314	GLY	-	expression tag	UNP P0DTC2
B	315	SER	-	expression tag	UNP P0DTC2
B	316	GLY	-	expression tag	UNP P0DTC2
B	317	SER	-	expression tag	UNP P0DTC2
B	318	GLY	-	expression tag	UNP P0DTC2
E	314	GLY	-	expression tag	UNP P0DTC2
E	315	SER	-	expression tag	UNP P0DTC2
E	316	GLY	-	expression tag	UNP P0DTC2
E	317	SER	-	expression tag	UNP P0DTC2
E	318	GLY	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of antibody C1A-B12 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	225	Total	C	N	O	S	0	7	0
			1718	1075	294	340	9			

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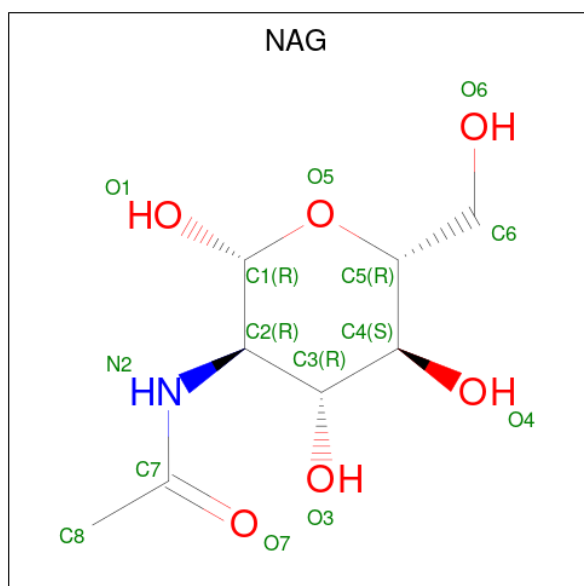
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	219	Total	C	N	O	S	0	3	0
			1652	1039	281	325	7			
2	H	225	Total	C	N	O	S	0	5	0
			1709	1070	293	337	9			

- Molecule 3 is a protein called light chain of antibody C1A-B3 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	3	0
			1653	1035	276	337	5			
3	G	214	Total	C	N	O	S	0	4	0
			1663	1041	279	338	5			
3	L	214	Total	C	N	O	S	0	3	0
			1655	1038	276	336	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



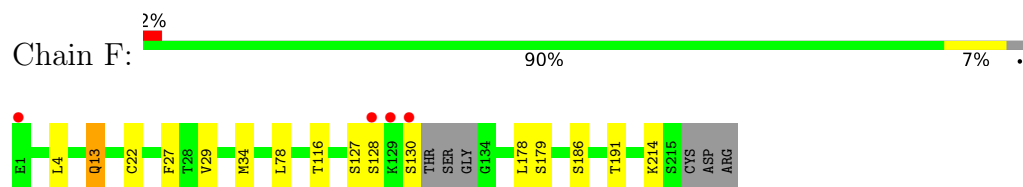
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

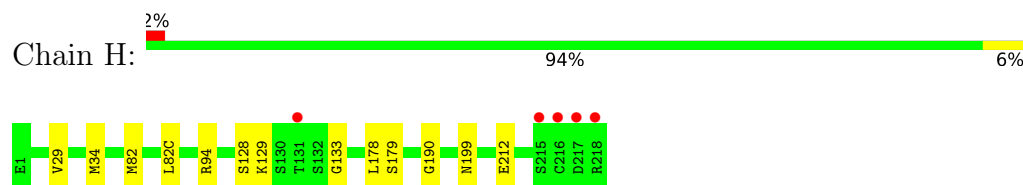
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total 165	O 165	0	0
5	B	154	Total 154	O 154	0	0
5	C	202	Total 202	O 202	0	0
5	D	237	Total 237	O 237	0	0
5	E	88	Total 88	O 88	0	0
5	F	128	Total 128	O 128	0	0
5	G	187	Total 187	O 187	0	0
5	H	250	Total 250	O 250	0	0
5	L	231	Total 231	O 231	0	0



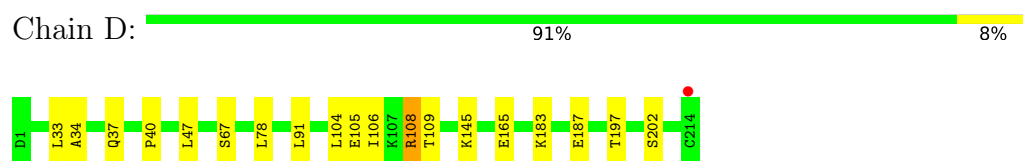
- Molecule 2: Heavy chain of antibody C1A-B12 Fab



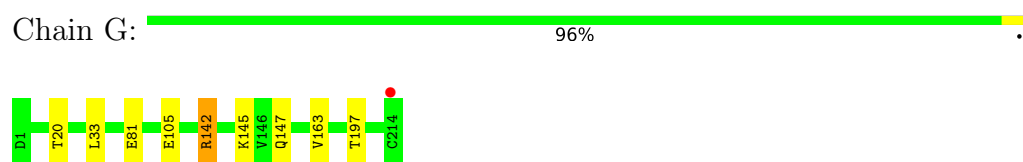
- Molecule 2: Heavy chain of antibody C1A-B12 Fab



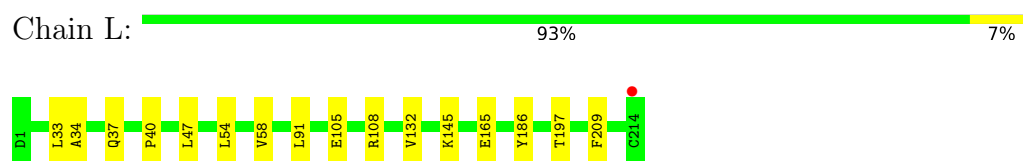
- Molecule 3: light chain of antibody C1A-B3 Fab



- Molecule 3: light chain of antibody C1A-B3 Fab



- Molecule 3: light chain of antibody C1A-B3 Fab





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.83Å 113.25Å 268.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.44 – 2.10 134.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (134.44-2.10) 98.7 (134.44-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.183 , 0.215 0.188 , 0.223	Depositor DCC
$R_{free}$ test set	7437 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: 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	A	0.38	0/1645	0.52	0/2235
1	B	0.39	0/1637	0.53	0/2224
1	E	0.34	0/1614	0.52	0/2195
2	C	0.43	0/1762	0.61	0/2395
2	F	0.37	0/1692	0.63	0/2301
2	H	0.45	0/1750	0.62	0/2379
3	D	0.44	0/1687	0.63	0/2289
3	G	0.42	0/1697	0.63	0/2303
3	L	0.46	0/1689	0.63	0/2292
All	All	0.41	0/15173	0.60	0/20613

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 [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	A	1600	0	1519	5	0
1	B	1590	0	1520	8	0
1	E	1570	0	1486	5	0
2	C	1718	0	1680	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1652	0	1618	6	0
2	H	1709	0	1671	6	0
3	D	1653	0	1617	10	0
3	G	1663	0	1627	5	0
3	L	1655	0	1623	9	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	E	14	0	13	0	0
5	A	165	0	0	0	0
5	B	154	0	0	1	0
5	C	202	0	0	0	0
5	D	237	0	0	0	0
5	E	88	0	0	1	0
5	F	128	0	0	0	0
5	G	187	0	0	0	0
5	H	250	0	0	0	0
5	L	231	0	0	4	0
All	All	16494	0	14400	59	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 59 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:C:133:GLY:HA2	3:G:81:GLU:HB3	1.72	0.72
3:L:209:PHE:HZ	5:L:482:HOH:O	1.75	0.67
3:L:186:TYR:HE1	5:L:482:HOH:O	1.78	0.67
3:D:108:ARG:HG2	3:D:109:THR:N	2.12	0.63
3:G:20:THR:HB	2:H:190:GLY:HA3	1.80	0.63

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	199/228 (87%)	194 (98%)	5 (2%)	0	100	100
1	B	199/228 (87%)	193 (97%)	6 (3%)	0	100	100
1	E	196/228 (86%)	188 (96%)	8 (4%)	0	100	100
2	C	230/225 (102%)	228 (99%)	2 (1%)	0	100	100
2	F	218/225 (97%)	215 (99%)	2 (1%)	1 (0%)	29	26
2	H	228/225 (101%)	226 (99%)	1 (0%)	1 (0%)	34	32
3	D	215/214 (100%)	209 (97%)	6 (3%)	0	100	100
3	G	216/214 (101%)	208 (96%)	8 (4%)	0	100	100
3	L	215/214 (100%)	209 (97%)	6 (3%)	0	100	100
All	All	1916/2001 (96%)	1870 (98%)	44 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	116	THR
2	H	133	GLY

### 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	174/198 (88%)	171 (98%)	3 (2%)	60	67
1	B	174/198 (88%)	173 (99%)	1 (1%)	86	90
1	E	171/198 (86%)	170 (99%)	1 (1%)	86	90
2	C	193/186 (104%)	188 (97%)	5 (3%)	46	50
2	F	184/186 (99%)	178 (97%)	6 (3%)	38	40
2	H	191/186 (103%)	185 (97%)	6 (3%)	40	43
3	D	189/186 (102%)	186 (98%)	3 (2%)	62	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	190/186 (102%)	186 (98%)	4 (2%)	53	59
3	L	189/186 (102%)	186 (98%)	3 (2%)	62	69
All	All	1655/1710 (97%)	1623 (98%)	32 (2%)	60	63

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	178	LEU
2	F	186	SER
3	L	33	LEU
2	F	179[B]	SER
2	F	191	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	370	ASN
3	L	189	HIS
2	F	13	GLN
1	B	354	ASN
1	E	388	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	NAG	B	601	1	14,14,15	0.32	0	17,19,21	0.78	1 (5%)
4	NAG	E	601	1	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
4	NAG	A	601	1	14,14,15	0.30	0	17,19,21	0.85	1 (5%)

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	B	601	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	3.15	116.47	112.19
4	B	601	NAG	C1-O5-C5	2.86	116.07	112.19
4	E	601	NAG	C1-O5-C5	2.83	116.03	112.19

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	195/228 (85%)	0.12	9 (4%) 32 38	23, 44, 100, 130	0
1	B	195/228 (85%)	0.20	11 (5%) 24 29	22, 45, 96, 111	0
1	E	195/228 (85%)	0.53	23 (11%) 4 5	32, 68, 116, 128	0
2	C	225/225 (100%)	-0.08	8 (3%) 42 49	23, 34, 81, 137	0
2	F	219/225 (97%)	-0.07	4 (1%) 68 72	32, 51, 79, 120	0
2	H	225/225 (100%)	-0.15	5 (2%) 62 66	23, 35, 64, 119	0
3	D	214/214 (100%)	-0.22	1 (0%) 91 92	23, 38, 57, 82	0
3	G	214/214 (100%)	-0.27	1 (0%) 91 92	24, 39, 65, 96	0
3	L	214/214 (100%)	-0.21	1 (0%) 91 92	20, 37, 56, 81	0
All	All	1896/2001 (94%)	-0.03	63 (3%) 46 53	20, 41, 94, 137	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	449	TYR	7.2
2	H	218	ARG	7.2
2	H	217	ASP	7.1
2	H	216	CYS	6.9
1	E	369	TYR	6.2

### 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	NAG	E	601	14/15	0.78	0.17	141,141,141,141	0
4	NAG	B	601	14/15	0.86	0.16	72,74,74,74	0
4	NAG	A	601	14/15	0.88	0.20	81,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.