



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2020 – 08:13 PM JST

PDB ID : 7BSD  
Title : Complex structure of 1G5.3 Fab bound to ZIKV NS1c  
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Deposited on : 2020-03-30  
Resolution : 2.53 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

<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
Xtriage (Phenix)	:	1.13
EDS	:	2.15.1
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)	:	2.15.1

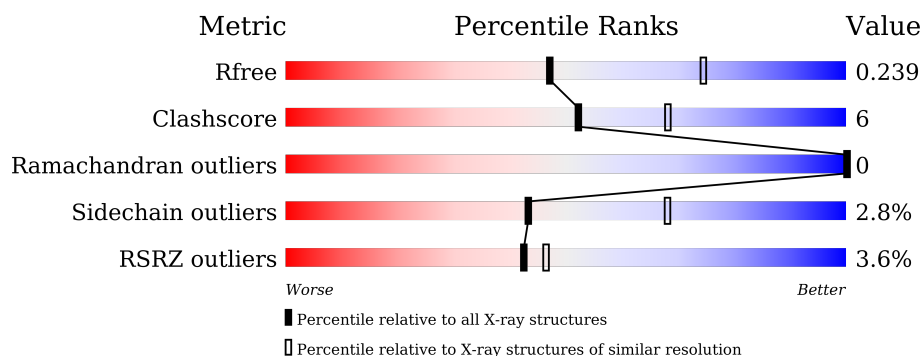
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	223	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	H	223	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>
2	B	218	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> </div>
2	L	218	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>•</div> </div> </div>
3	G	181	<div> <div>•</div> <div> <div>33%</div> <div>• •</div> <div>62%</div> </div> </div>
3	I	181	<div> <div>•</div> <div> <div>31%</div> <div>6%</div> <div>•</div> <div>62%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7896 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 1G5.3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1624	1045	264	310	5			
1	H	215	Total	C	N	O	S	0	0	0
			1669	1070	272	322	5			

- Molecule 2 is a protein called 1G5.3 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1663	1041	281	335	6			
2	L	217	Total	C	N	O	S	0	0	0
			1663	1041	281	335	6			

- Molecule 3 is a protein called NS1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	68	Total	C	N	O	S	0	0	0
			541	333	99	101	8			
3	I	68	Total	C	N	O	S	0	0	0
			541	333	99	101	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	22	Total	O	0	0
			22	22		
4	G	23	Total	O	0	0
			23	23		
4	I	27	Total	O	0	0
			27	27		

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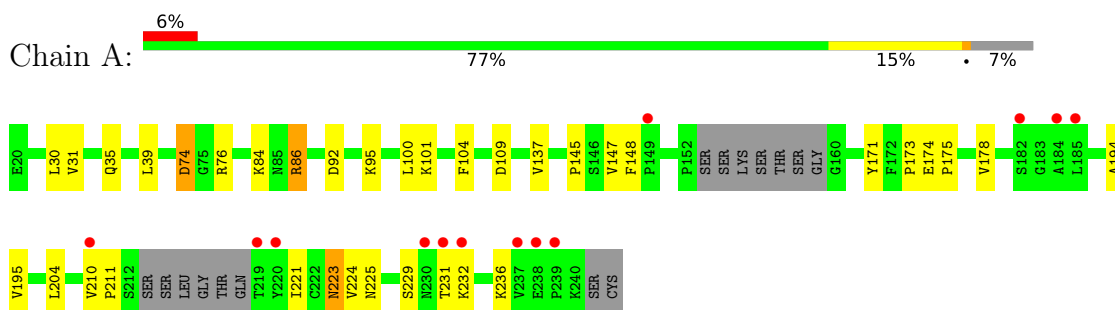
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	55	Total	O	0	0
			55	55		
4	L	34	Total	O	0	0
			34	34		

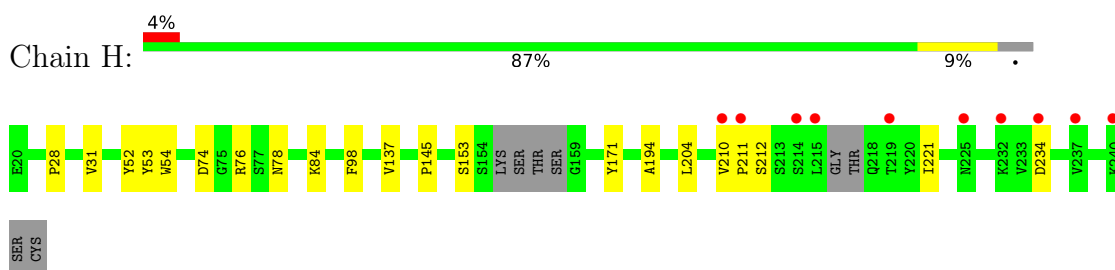
### 3 Residue-property plots [i](#)

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.

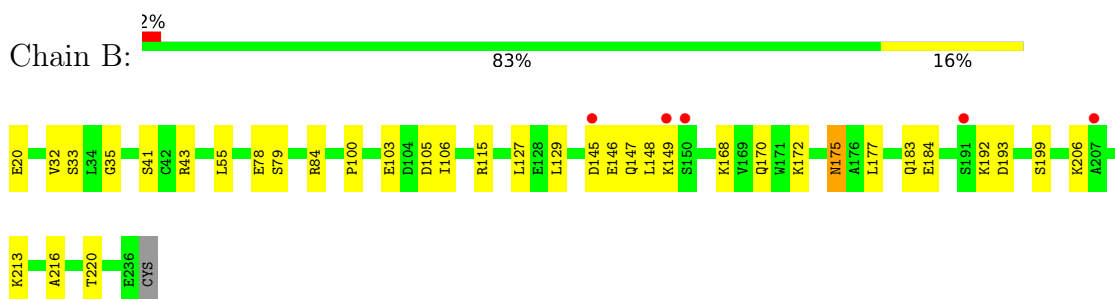
- Molecule 1: 1G5.3 Fab Heavy Chain



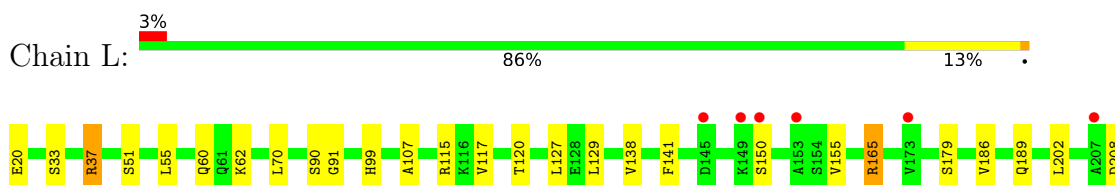
- Molecule 1: 1G5.3 Fab Heavy Chain

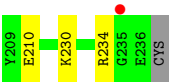


- Molecule 2: 1G5.3 Fab Light Chain

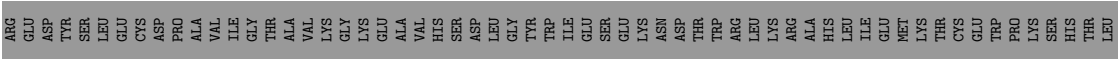


- Molecule 2: 1G5.3 Fab Light Chain

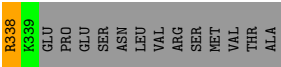
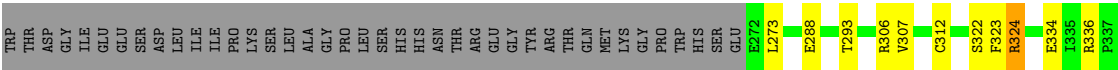




● Molecule 3: NS1C



● Molecule 3: NS1C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.89Å 111.14Å 158.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.53 49.50 – 2.53	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.50-2.53) 96.8 (49.50-2.53)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.221 , 0.239 0.221 , 0.239	Depositor DCC
$R_{free}$ test set	3219 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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](#)

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	0.28	0/1670	0.52	0/2279
1	H	0.27	0/1715	0.51	0/2339
2	B	0.26	0/1699	0.48	0/2305
2	L	0.26	0/1699	0.48	0/2305
3	G	0.41	0/553	0.49	0/744
3	I	0.29	0/553	0.48	0/744
All	All	0.28	0/7889	0.50	0/10716

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	1624	0	1586	21	0
1	H	1669	0	1628	12	0
2	B	1663	0	1616	23	0
2	L	1663	0	1616	19	0
3	G	541	0	520	5	0
3	I	541	0	520	9	0
4	A	34	0	0	1	0
4	B	22	0	0	5	0
4	G	23	0	0	1	0
4	H	55	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	27	0	0	3	0
4	L	34	0	0	0	0
All	All	7896	0	7486	84	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 6.

All (84) 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:170:GLN:HG2	2:B:177:LEU:HD11	1.66	0.77
2:B:184:GLU:HG3	4:B:306:HOH:O	1.84	0.77
2:B:168:LYS:HB2	2:B:220:THR:HB	1.71	0.72
2:B:84:ARG:HG2	4:B:302:HOH:O	1.91	0.71
1:A:145:PRO:HB3	1:A:171:TYR:HB3	1.76	0.68
1:A:147:VAL:HG21	1:A:224:VAL:HG11	1.77	0.66
2:B:78:GLU:OE1	3:G:306:ARG:NH2	2.31	0.64
2:B:84:ARG:N	4:B:302:HOH:O	2.25	0.63
1:A:194:ALA:HA	1:A:204:LEU:HB3	1.82	0.62
3:I:324:ARG:NH2	4:I:402:HOH:O	2.33	0.62
3:G:272:GLU:N	4:G:403:HOH:O	2.35	0.59
1:H:221:ILE:HD11	1:H:234:ASP:HB3	1.84	0.59
1:A:174:GLU:HG2	1:A:175:PRO:HA	1.85	0.59
3:I:288:GLU:OE2	3:I:338:ARG:NH2	2.29	0.57
1:H:145:PRO:HB3	1:H:171:TYR:HB3	1.86	0.56
2:B:20:GLU:N	4:B:304:HOH:O	2.38	0.56
2:B:55:LEU:HD12	2:B:115:ARG:HA	1.87	0.56
2:B:35:GLY:HA2	2:B:100:PRO:HB2	1.90	0.53
2:L:55:LEU:HD12	2:L:115:ARG:HA	1.90	0.53
3:I:322:SER:OG	3:I:324:ARG:NH1	2.43	0.52
2:B:145:ASP:O	2:B:149:LYS:HG3	2.09	0.52
3:G:297:SER:OG	3:G:331:TYR:O	2.26	0.52
1:A:74:ASP:HB2	1:A:76:ARG:HH11	1.75	0.51
2:B:148:LEU:O	2:B:206:LYS:HE3	2.10	0.51
2:L:165:ARG:HH21	2:L:186:VAL:HG21	1.74	0.50
3:I:334:GLU:HG3	4:I:407:HOH:O	2.10	0.50
1:A:221:ILE:HG12	1:A:236:LYS:HB3	1.94	0.49
3:I:306:ARG:NH2	4:I:401:HOH:O	2.25	0.49
1:A:86:ARG:NH2	1:A:109:ASP:OD2	2.45	0.49
1:H:194:ALA:HA	1:H:204:LEU:HB3	1.95	0.49
1:A:30:LEU:HB2	1:A:173:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:O	2:B:175:ASN:ND2	2.46	0.49
2:B:146:GLU:HA	2:B:149:LYS:HE2	1.94	0.48
1:A:195:VAL:HG21	2:B:183:GLN:HB3	1.95	0.48
2:B:106:ILE:HD11	2:B:129:LEU:HD22	1.96	0.48
2:L:37:ARG:HB2	2:L:99:HIS:HB2	1.96	0.48
3:G:333:MET:HE2	3:G:333:MET:HB2	1.68	0.48
2:L:210:GLU:OE2	2:L:234:ARG:NH1	2.46	0.47
3:G:273:LEU:HD11	3:G:323:PHE:HB3	1.96	0.47
2:B:145:ASP:HA	2:B:148:LEU:HD12	1.94	0.47
1:H:210:VAL:HG22	1:H:211:PRO:HD2	1.96	0.47
1:H:53:TYR:OH	1:H:76:ARG:NH2	2.40	0.47
1:A:148:PHE:CE2	2:B:147:GLN:HG3	2.50	0.47
2:L:62:LYS:HD3	2:L:107:ALA:HB2	1.97	0.47
1:A:31:VAL:O	1:A:137:VAL:HA	2.15	0.47
2:B:105:ASP:O	2:B:127:LEU:HD23	2.15	0.46
2:L:37:ARG:NH1	2:L:99:HIS:ND1	2.63	0.46
2:L:129:LEU:O	2:L:189:GLN:NE2	2.48	0.46
2:L:155:VAL:CG1	2:L:202:LEU:HB3	2.46	0.46
1:A:39:LEU:HD12	1:A:100:LEU:HD23	1.97	0.46
1:A:178:VAL:HA	1:A:223:ASN:O	2.17	0.45
1:H:78:ASN:OD1	2:L:117:VAL:HG11	2.16	0.45
3:I:273:LEU:HD11	3:I:323:PHE:HB3	1.98	0.45
2:L:141:PHE:O	2:L:155:VAL:HG23	2.17	0.45
2:L:51:SER:OG	2:L:51:SER:O	2.33	0.45
2:B:103:GLU:O	2:B:106:ILE:HG13	2.16	0.45
1:H:28:PRO:O	4:H:302:HOH:O	2.21	0.45
2:L:155:VAL:HG13	2:L:202:LEU:HB3	2.00	0.44
2:L:60:GLN:HB2	2:L:70:LEU:HD11	2.00	0.44
1:A:101:LYS:NZ	4:A:301:HOH:O	2.32	0.44
1:A:86:ARG:HH22	1:A:109:ASP:CG	2.20	0.44
1:H:84:LYS:HB3	1:H:84:LYS:HE2	1.70	0.43
2:L:127:LEU:HD12	2:L:127:LEU:HA	1.86	0.43
2:B:192:LYS:HG2	2:B:193:ASP:H	1.84	0.43
2:B:183:GLN:OE1	4:B:301:HOH:O	2.21	0.43
2:L:138:VAL:O	2:L:230:LYS:HD2	2.19	0.42
1:A:210:VAL:HG22	1:A:211:PRO:HD2	2.02	0.42
1:A:194:ALA:HB2	1:A:204:LEU:HD23	2.02	0.42
2:L:90:SER:OG	2:L:91:GLY:N	2.52	0.42
1:H:54:TRP:HB3	1:H:98:PHE:CZ	2.55	0.42
1:A:229:SER:OG	1:A:231:THR:OG1	2.31	0.41
2:B:32:VAL:O	2:B:129:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:O	1:A:104:PHE:HA	2.20	0.41
1:H:74:ASP:OD1	1:H:76:ARG:NH1	2.53	0.41
3:I:307:VAL:HG23	1:H:52:TYR:OH	2.21	0.41
3:I:312:CYS:HB3	3:I:338:ARG:HG3	2.01	0.41
1:A:225:ASN:ND2	1:A:232:LYS:HD3	2.36	0.40
2:B:172:LYS:HB2	2:B:216:ALA:HB3	2.03	0.40
2:L:20:GLU:HG3	2:L:120:THR:HG21	2.02	0.40
2:L:234:ARG:HG2	2:L:234:ARG:NH1	2.37	0.40
2:L:165:ARG:NH2	2:L:186:VAL:HG21	2.36	0.40
1:A:92:ASP:OD2	1:A:95:LYS:HD2	2.22	0.40
1:H:31:VAL:O	1:H:137:VAL:HA	2.21	0.40
3:I:293:THR:O	3:I:336:ARG:HD2	2.22	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	202/223 (91%)	191 (95%)	11 (5%)	0	100	100
1	H	209/223 (94%)	203 (97%)	6 (3%)	0	100	100
2	B	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
2	L	215/218 (99%)	208 (97%)	7 (3%)	0	100	100
3	G	66/181 (36%)	66 (100%)	0	0	100	100
3	I	66/181 (36%)	65 (98%)	1 (2%)	0	100	100
All	All	973/1244 (78%)	942 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	185/198 (93%)	181 (98%)	4 (2%)	52	75
1	H	191/198 (96%)	189 (99%)	2 (1%)	76	89
2	B	188/189 (100%)	181 (96%)	7 (4%)	34	57
2	L	188/189 (100%)	182 (97%)	6 (3%)	39	63
3	G	60/160 (38%)	57 (95%)	3 (5%)	24	44
3	I	60/160 (38%)	58 (97%)	2 (3%)	38	62
All	All	872/1094 (80%)	848 (97%)	24 (3%)	43	68

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	84	LYS
1	A	86	ARG
1	A	223	ASN
2	B	33	SER
2	B	41	SER
2	B	43	ARG
2	B	79	SER
2	B	175	ASN
2	B	199	SER
2	B	213	LYS
3	G	284	LYS
3	G	297	SER
3	G	339	LYS
3	I	324	ARG
3	I	338	ARG
1	H	153	SER
1	H	212	SER
2	L	33	SER
2	L	37	ARG
2	L	150	SER
2	L	165	ARG

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Mol	Chain	Res	Type
2	L	179	SER
2	L	208	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

There are no ligands in this entry.

### 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	208/223 (93%)	0.39	13 (6%) 20 21	24, 47, 90, 110	0
1	H	215/223 (96%)	0.33	10 (4%) 31 34	23, 42, 94, 103	0
2	B	217/218 (99%)	0.28	5 (2%) 60 64	30, 53, 83, 99	0
2	L	217/218 (99%)	0.21	7 (3%) 47 52	28, 49, 81, 94	0
3	G	68/181 (37%)	-0.06	1 (1%) 73 76	21, 33, 48, 70	0
3	I	68/181 (37%)	-0.06	0 100 100	22, 33, 47, 75	0
All	All	993/1244 (79%)	0.25	36 (3%) 42 46	21, 46, 87, 110	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	ALA	4.6
1	H	215	LEU	4.3
2	B	150	SER	4.1
1	H	232	LYS	3.9
1	A	220	TYR	3.8
2	L	207	ALA	3.8
1	H	240	LYS	3.6
1	A	182	SER	3.4
1	A	237	VAL	3.1
2	L	149	LYS	2.8
1	A	219	THR	2.8
2	L	173	VAL	2.8
1	H	219	THR	2.7
1	A	149	PRO	2.6
2	L	150	SER	2.6
1	A	210	VAL	2.5
1	A	239	PRO	2.5
1	A	232	LYS	2.4
2	B	145	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	191	SER	2.4
1	H	211	PRO	2.4
2	B	149	LYS	2.3
1	H	214	SER	2.3
1	H	237	VAL	2.3
2	B	207	ALA	2.3
1	H	234	ASP	2.2
2	L	153	ALA	2.2
1	H	210	VAL	2.2
1	A	185	LEU	2.2
1	A	238	GLU	2.2
1	H	225	ASN	2.1
2	L	145	ASP	2.1
2	L	235	GLY	2.1
1	A	230	ASN	2.1
1	A	231	THR	2.0
3	G	272	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.