



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 27, 2025 – 12:11 PM EST

PDB ID : 8TQ6  
Title : Crystal structure of Fab.B1.23.2 in complex with MHC-I (HLA-B\*44:05)  
Authors : Jiang, J.; Natarajan, K.; Boyd, L.F.; Margulies, D.H.  
Deposited on : 2023-08-06  
Resolution : 3.20 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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

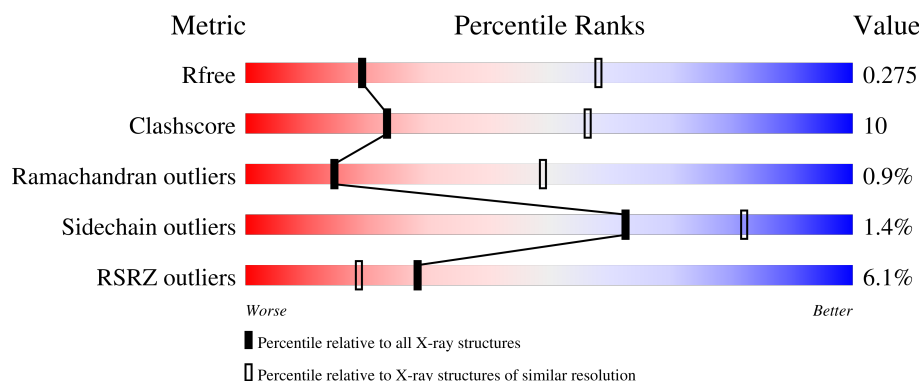
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.






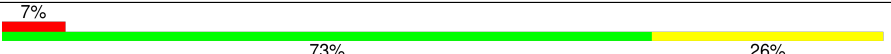
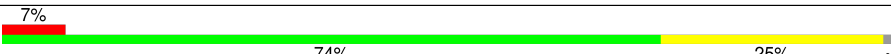
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	274	<div> <div>4%</div> <div>70%</div> <div>29%</div> <div>.</div> </div>
1	C	274	<div> <div>8%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>
2	B	100	<div> <div>4%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
2	D	100	<div> <div>12%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
3	E	9	<div> <div>11%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	9	 89%11%
4	F	213	 5%77%23%
4	H	213	 5%74%25%
5	G	212	 7%73%26%
5	L	212	 7%74%25%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12516 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 HLA class I histocompatibility antigen B alpha chain (HLA-B\*44:05).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2197	1369	394	427	7			
1	C	268	Total	C	N	O	S	11	0	0
			2133	1327	382	417	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q860B7
C	1	GLY	-	expression tag	UNP Q860B7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			820	523	137	157	3			
2	D	100	Total	C	N	O	S	0	0	0
			804	510	136	155	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called MHC class II antigen peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			77	51	12	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	1	0	0
			78	51	12	15			

- Molecule 4 is a protein called Fab B1.23.2 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	213	Total	C	N	O	S	13	0	0
			1573	996	253	316	8			
4	H	213	Total	C	N	O	S	29	0	0
			1584	1001	256	319	8			

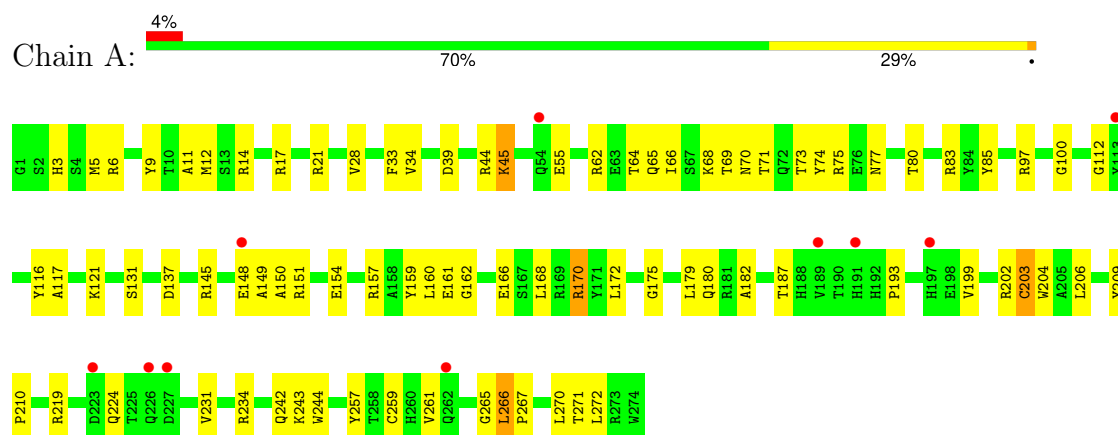
- Molecule 5 is a protein called Fab B1.23.2 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	211	Total	C	N	O	S	0	0	0
			1630	1019	269	334	8			
5	L	210	Total	C	N	O	S	0	0	0
			1620	1012	268	332	8			

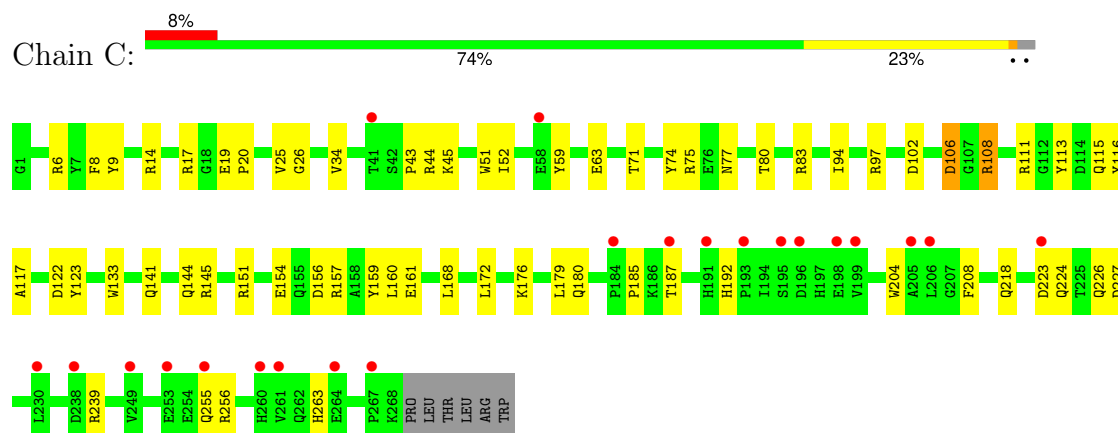
### 3 Residue-property plots

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.

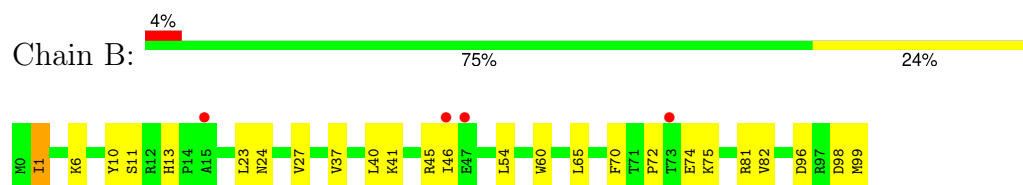
- Molecule 1: HLA class I histocompatibility antigen B alpha chain (HLA-B\*44:05)



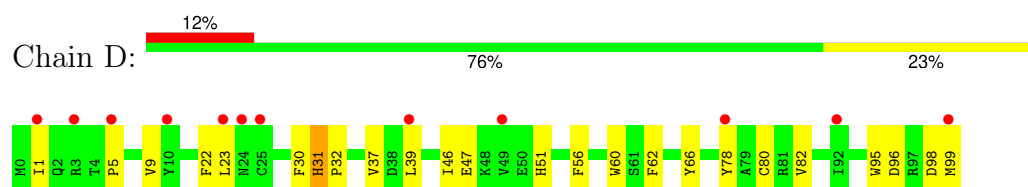
- Molecule 1: HLA class I histocompatibility antigen B alpha chain (HLA-B\*44:05)



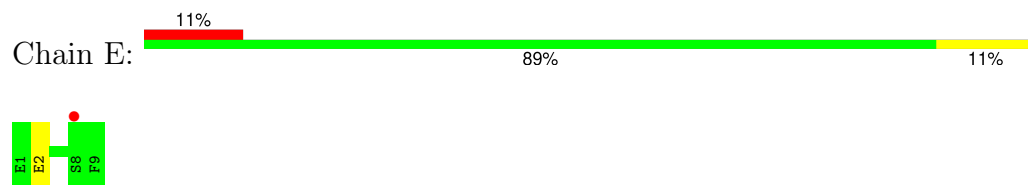
- Molecule 2: Beta-2-microglobulin



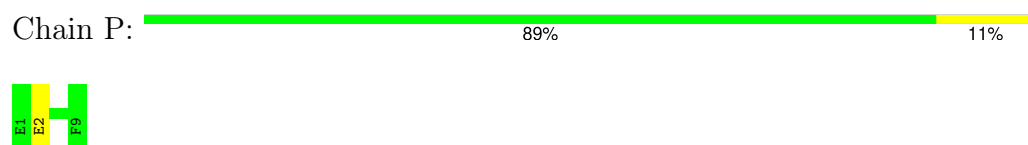
- Molecule 2: Beta-2-microglobulin



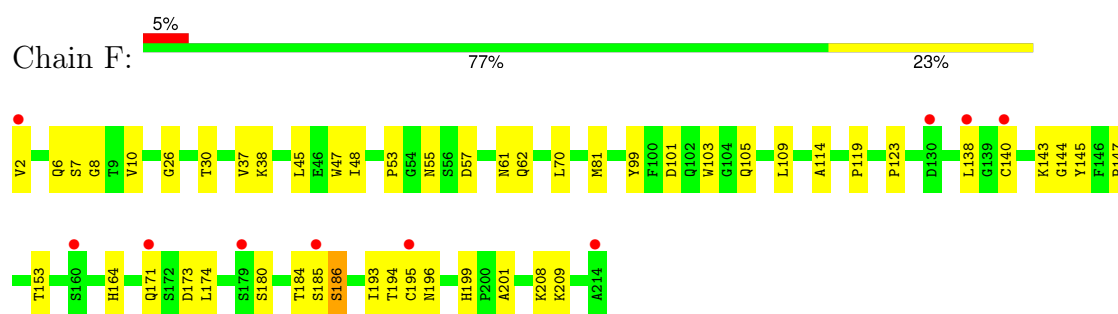
- Molecule 3: MHC class II antigen peptide



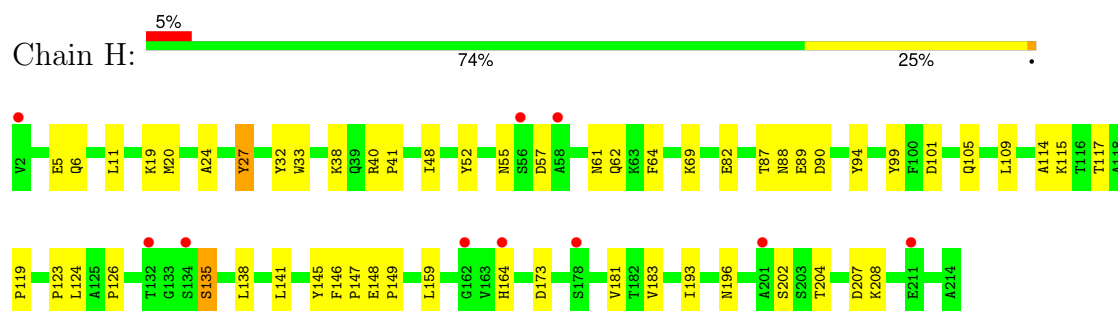
- Molecule 3: MHC class II antigen peptide



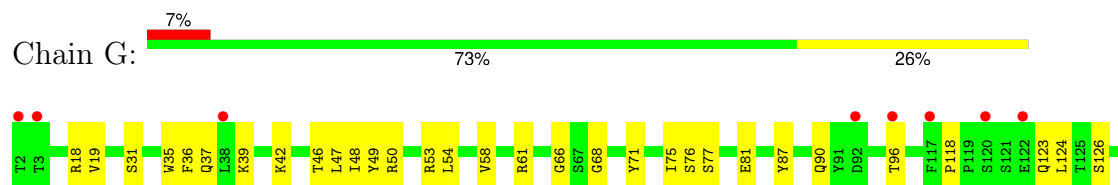
- Molecule 4: Fab B1.23.2 Heavy Chain

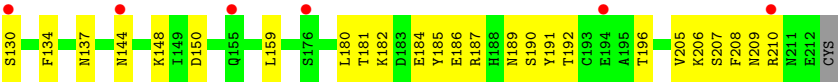


- Molecule 4: Fab B1.23.2 Heavy Chain

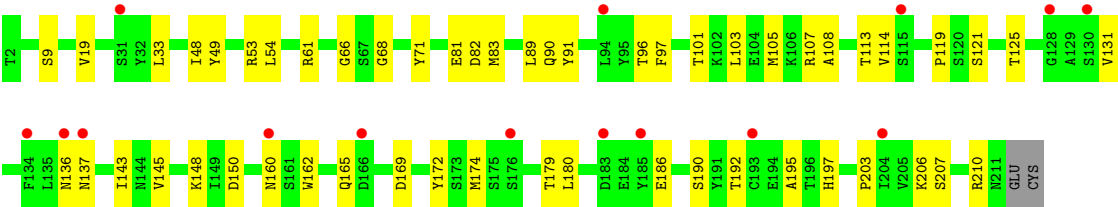


- Molecule 5: Fab B1.23.2 Light Chain





● Molecule 5: Fab B1.23.2 Light Chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.50Å 92.84Å 229.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.21 – 3.20 72.21 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (72.21-3.20) 95.8 (72.21-3.20)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.240 , 0.268 0.242 , 0.275	Depositor DCC
$R_{free}$ test set	1616 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.766	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	12516	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 3.19% 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	0.30	0/2254	0.59	0/3069
1	C	0.26	0/2189	0.54	0/2982
2	B	0.25	0/843	0.49	0/1143
2	D	0.26	0/826	0.51	0/1120
3	E	0.32	0/79	0.56	0/102
3	P	0.37	0/80	0.59	0/103
4	F	0.26	0/1615	0.51	0/2214
4	H	0.26	0/1626	0.50	0/2228
5	G	0.29	0/1666	0.55	0/2262
5	L	0.27	0/1656	0.52	0/2248
All	All	0.27	0/12834	0.53	0/17471

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	2197	0	2046	60	0
1	C	2133	0	1957	42	0
2	B	820	0	770	17	0
2	D	804	0	741	17	0
3	E	77	0	64	1	0
3	P	78	0	67	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1573	0	1500	28	0
4	H	1584	0	1518	35	0
5	G	1630	0	1536	37	0
5	L	1620	0	1532	31	0
All	All	12516	0	11731	243	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 243 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:D:5:PRO:HB3	2:D:30:PHE:HB3	1.70	0.73
4:H:164:HIS:NE2	5:L:136:ASN:OD1	2.21	0.72
1:C:6:ARG:NH1	1:C:102:ASP:OD1	2.23	0.72
4:F:144:GLY:HA2	4:F:174:LEU:HD13	1.70	0.72
4:F:10:VAL:HG13	4:F:109:LEU:HD13	1.72	0.72

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	272/274 (99%)	255 (94%)	17 (6%)	0	100	100
1	C	266/274 (97%)	251 (94%)	14 (5%)	1 (0%)	30	64
2	B	98/100 (98%)	92 (94%)	5 (5%)	1 (1%)	13	47
2	D	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	13	47
3	E	7/9 (78%)	7 (100%)	0	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	9	40
4	H	211/213 (99%)	192 (91%)	17 (8%)	2 (1%)	14	49
5	G	209/212 (99%)	194 (93%)	12 (6%)	3 (1%)	9	40
5	L	208/212 (98%)	194 (93%)	11 (5%)	3 (1%)	9	40
All	All	1587/1616 (98%)	1475 (93%)	98 (6%)	14 (1%)	14	49

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	185	SER
4	H	147	PRO
5	L	137	ASN
5	G	137	ASN
5	L	190	SER

### 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	226/235 (96%)	220 (97%)	6 (3%)	40	69
1	C	216/235 (92%)	211 (98%)	5 (2%)	45	72
2	B	91/95 (96%)	91 (100%)	0	100	100
2	D	87/95 (92%)	85 (98%)	2 (2%)	45	72
3	E	6/7 (86%)	6 (100%)	0	100	100
3	P	7/7 (100%)	7 (100%)	0	100	100
4	F	174/180 (97%)	171 (98%)	3 (2%)	56	78
4	H	177/180 (98%)	176 (99%)	1 (1%)	84	92
5	G	182/190 (96%)	181 (100%)	1 (0%)	86	93
5	L	182/190 (96%)	181 (100%)	1 (0%)	86	93
All	All	1348/1414 (95%)	1329 (99%)	19 (1%)	62	82

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	164	HIS
4	H	27	TYR
5	L	150	ASP
5	G	54	LEU
1	C	226	GLN

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

Mol	Chain	Res	Type
1	A	3	HIS
1	A	65	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 oligosaccharides 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	274/274 (100%)	0.52	10 (3%) 46 32	22, 39, 68, 86	0
1	C	267/274 (97%)	0.81	22 (8%) 19 13	8, 45, 95, 111	2 (0%)
2	B	100/100 (100%)	0.49	4 (4%) 43 29	20, 42, 71, 82	0
2	D	100/100 (100%)	1.04	12 (12%) 10 7	32, 62, 89, 98	0
3	E	9/9 (100%)	0.46	1 (11%) 12 8	30, 35, 48, 48	0
3	P	9/9 (100%)	0.49	0 100 100	23, 31, 35, 43	1 (11%)
4	F	211/213 (99%)	0.63	10 (4%) 37 25	12, 39, 67, 77	1 (0%)
4	H	210/213 (98%)	0.76	10 (4%) 36 25	10, 47, 73, 83	3 (1%)
5	G	211/212 (99%)	0.75	14 (6%) 26 17	24, 43, 67, 84	0
5	L	210/212 (99%)	0.77	15 (7%) 23 16	22, 49, 78, 87	0
All	All	1601/1616 (99%)	0.71	98 (6%) 28 19	8, 44, 79, 111	7 (0%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	GLU	17.8
1	C	199	VAL	10.9
4	H	132	THR	6.0
5	L	137	ASN	4.1
4	F	160	SER	4.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.