



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 PM GMT

PDB ID : 4QTH  
Title : Crystal structure of anti-uPAR Fab 8B12  
Authors : Zhao, B.; Yuan, C.; Luo, Z.; Huang, M.  
Deposited on : 2014-07-08  
Resolution : 2.17 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

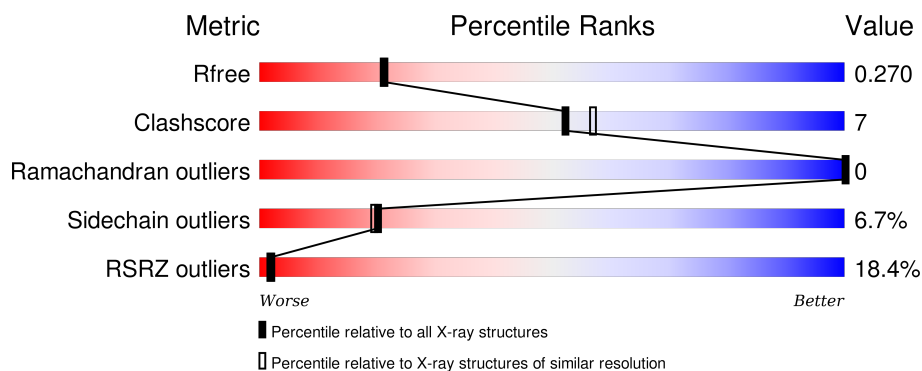
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	A	224	<div> <div>25%</div> <div>83%</div> <div>11%</div> <div>• •</div> </div>
1	H	224	<div> <div>12%</div> <div>72%</div> <div>25%</div> <div>•</div> </div>
2	B	214	<div> <div>28%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
2	L	214	<div> <div>9%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6833 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 anti-uPAR antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	224	Total	C	N	O	S	0	0	0
			1686	1062	276	338	10			
1	A	215	Total	C	N	O	S	0	0	0
			1621	1027	262	323	9			

- Molecule 2 is a protein called anti-uPAR antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1658	1024	280	347	7			
2	B	211	Total	C	N	O	S	0	0	0
			1635	1012	276	341	6			

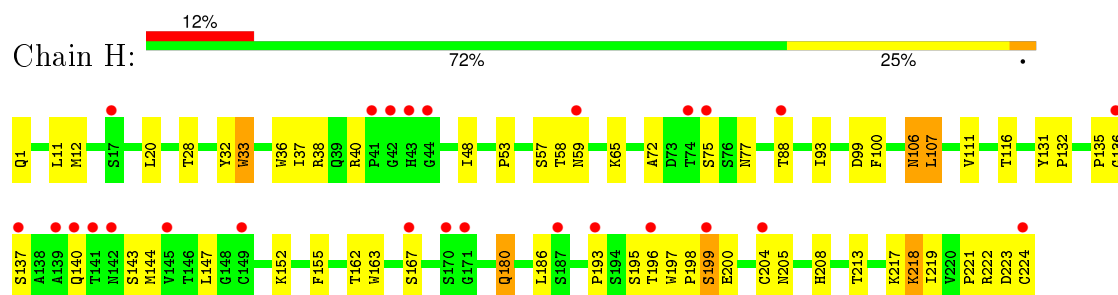
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	64	Total	O	0	0
			64	64		
3	L	63	Total	O	0	0
			63	63		
3	A	38	Total	O	0	0
			38	38		
3	B	68	Total	O	0	0
			68	68		

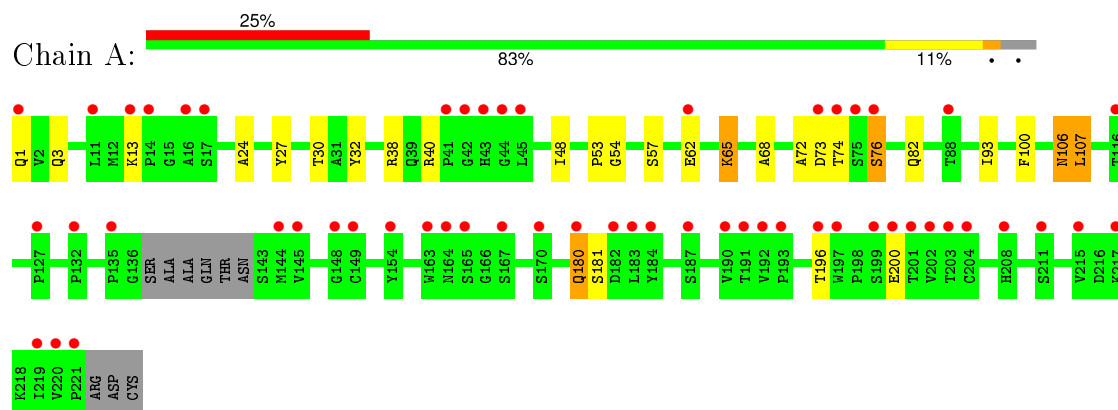
### 3 Residue-property plots [i](#)

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.

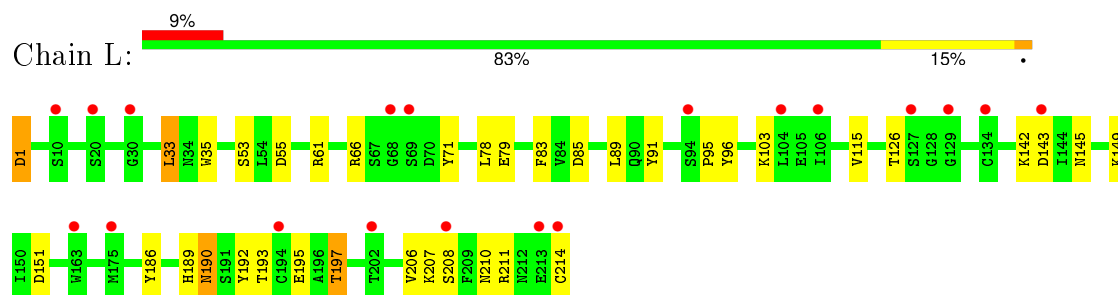
- Molecule 1: anti-uPAR antibody, heavy chain



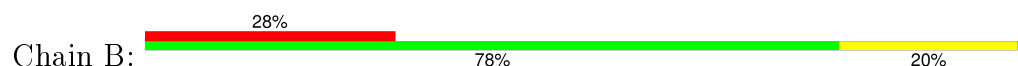
- Molecule 1: anti-uPAR antibody, heavy chain

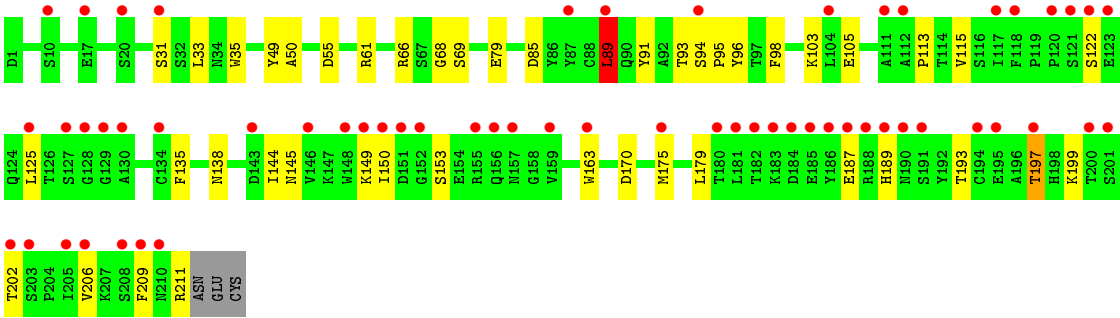


- Molecule 2: anti-uPAR antibody, light chain



- Molecule 2: anti-uPAR antibody, light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.08Å 72.92Å 85.55Å 90.00° 105.37° 90.00°	Depositor
Resolution (Å)	41.31 – 2.17 41.20 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.31-2.17) 99.6 (41.20-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.229 , 0.273 0.227 , 0.270	Depositor DCC
$R_{free}$ test set	2547 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50229 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.59	0/1664	0.68	0/2275
1	H	0.66	2/1730 (0.1%)	0.76	0/2366
2	B	0.63	1/1668 (0.1%)	0.73	1/2261 (0.0%)
2	L	0.59	1/1691 (0.1%)	0.71	0/2292
All	All	0.62	4/6753 (0.1%)	0.72	1/9194 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	TRP	CD2-CE2	5.73	1.48	1.41
1	H	197	TRP	CD2-CE2	5.53	1.48	1.41
1	H	33	TRP	CD2-CE2	5.28	1.47	1.41
2	L	35	TRP	CD2-CE2	5.20	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	LEU	CB-CG-CD2	6.48	122.02	111.00

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	1621	0	1572	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1686	0	1630	35	0
2	B	1635	0	1569	22	0
2	L	1658	0	1585	21	0
3	A	38	0	0	0	0
3	B	68	0	0	2	0
3	H	64	0	0	0	0
3	L	63	0	0	1	0
All	All	6833	0	6356	87	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 7.

All (87) 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:H:218:LYS:HD3	1:H:218:LYS:H	1.29	0.96
2:B:85:ASP:OD1	2:B:103:LYS:HD3	1.69	0.93
2:L:145:ASN:HB2	2:L:197:THR:HG22	1.55	0.89
2:L:190:ASN:ND2	2:L:210:ASN:OD1	2.10	0.85
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.61	0.83
2:L:85:ASP:OD1	2:L:103:LYS:HD3	1.79	0.82
2:B:66:ARG:HD2	2:B:68:GLY:O	1.82	0.80
1:H:198:PRO:HB3	1:H:221:PRO:HG3	1.73	0.70
1:H:224:CYS:HA	2:L:214:CYS:HB3	1.74	0.67
2:B:145:ASN:HB2	2:B:197:THR:HG22	1.78	0.66
1:H:152:LYS:HE2	1:H:180:GLN:NE2	2.13	0.64
2:B:69:SER:HB2	3:B:337:HOH:O	1.97	0.63
1:H:224:CYS:HA	2:L:214:CYS:CB	2.29	0.63
2:L:145:ASN:CB	2:L:197:THR:HG22	2.28	0.63
1:H:224:CYS:CA	2:L:214:CYS:HB3	2.27	0.63
2:L:143:ASP:HB2	3:L:355:HOH:O	1.98	0.63
1:H:32:TYR:OH	1:H:107:LEU:HG	2.00	0.61
1:H:163:TRP:CZ3	1:H:204:CYS:HB3	2.34	0.61
2:L:149:LYS:HB2	2:L:193:THR:HB	1.83	0.60
1:H:147:LEU:HD22	1:H:219:ILE:HG21	1.84	0.59
1:H:218:LYS:CD	1:H:218:LYS:H	2.10	0.59
1:H:106:ASN:H	1:H:106:ASN:HD22	1.50	0.59
2:L:78:LEU:HD13	2:L:83:PHE:CZ	2.39	0.58
1:H:198:PRO:HB3	1:H:221:PRO:CG	2.33	0.58
1:H:152:LYS:HE2	1:H:180:GLN:HE22	1.70	0.57
1:A:106:ASN:HD22	1:A:106:ASN:H	1.52	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:GLU:O	2:B:211:ARG:NH1	2.37	0.56
1:A:62:GLU:HA	1:A:65:LYS:HD3	1.89	0.55
1:A:38:ARG:HB2	1:A:48:ILE:HD11	1.88	0.54
2:B:163:TRP:CD1	2:B:175:MET:HG3	2.43	0.54
1:H:162:THR:OG1	1:H:205:ASN:HB2	2.09	0.53
2:L:151:ASP:OD2	2:L:189:HIS:HD2	1.91	0.53
1:H:135:PRO:HD3	1:H:147:LEU:HD23	1.89	0.53
2:B:149:LYS:HB2	2:B:193:THR:HB	1.90	0.53
1:H:36:TRP:C	1:H:37:ILE:HD12	2.31	0.50
2:B:105:GLU:HB3	3:B:317:HOH:O	2.11	0.50
1:A:196:THR:O	1:A:200:GLU:HG2	2.12	0.49
2:B:193:THR:HG23	2:B:206:VAL:HG13	1.93	0.49
2:L:61:ARG:CZ	2:L:79:GLU:HG3	2.42	0.49
2:B:61:ARG:CZ	2:B:79:GLU:HG3	2.43	0.49
1:H:100:PHE:HB2	1:H:107:LEU:HB3	1.94	0.49
1:H:186:LEU:C	1:H:186:LEU:HD12	2.34	0.48
2:L:151:ASP:OD2	2:L:189:HIS:CD2	2.66	0.48
1:A:53:PRO:HB3	1:A:72:ALA:CB	2.42	0.48
2:L:186:TYR:CZ	2:L:211:ARG:HD2	2.48	0.48
1:H:199:SER:HB3	1:H:200:GLU:HG2	1.96	0.48
2:B:49:TYR:O	2:B:50:ALA:C	2.52	0.47
2:B:89:LEU:HG	2:B:98:PHE:CE2	2.50	0.47
1:H:33:TRP:HB2	1:H:99:ASP:HB3	1.97	0.47
1:A:24:ALA:HB1	1:A:27:TYR:CE1	2.50	0.47
1:H:75:SER:OG	2:B:199:LYS:HD2	2.15	0.47
1:H:208:HIS:HB3	1:H:213:THR:HB	1.97	0.47
1:A:73:ASP:OD1	1:A:76:SER:OG	2.33	0.46
2:B:94:SER:HA	2:B:95:PRO:C	2.36	0.46
1:A:100:PHE:HB2	1:A:107:LEU:HB3	1.97	0.46
1:H:11:LEU:HD21	1:H:155:PHE:HZ	1.81	0.46
2:B:150:ILE:HD11	2:B:179:LEU:HD21	1.97	0.46
1:A:30:THR:HA	1:A:53:PRO:O	2.16	0.46
2:B:115:VAL:HA	2:B:135:PHE:O	2.15	0.45
2:L:91:TYR:HA	2:L:96:TYR:CD1	2.51	0.45
2:B:150:ILE:CG2	2:B:189:HIS:HB3	2.47	0.44
1:H:58:THR:O	1:H:59:ASN:OD1	2.34	0.44
1:H:223:ASP:O	1:H:224:CYS:HB2	2.17	0.44
1:A:53:PRO:HA	1:A:54:GLY:HA2	1.79	0.44
1:H:38:ARG:HB2	1:H:48:ILE:HD11	2.00	0.44
2:L:115:VAL:HG12	2:L:207:LYS:HG3	1.99	0.44
2:L:33:LEU:HD22	2:L:71:TYR:HB3	2.00	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:SER:HA	2:B:125:LEU:HD12	2.00	0.43
2:B:91:TYR:HA	2:B:96:TYR:CD1	2.53	0.43
1:H:131:TYR:HA	1:H:132:PRO:HD3	1.79	0.43
2:B:138:ASN:ND2	2:B:170:ASP:OD2	2.51	0.43
2:B:113:PRO:HG3	2:B:144:ILE:HD11	2.01	0.42
1:A:68:ALA:HA	1:A:82:GLN:O	2.20	0.42
1:H:223:ASP:O	1:H:224:CYS:CB	2.67	0.42
1:A:32:TYR:OH	1:A:107:LEU:HG	2.20	0.41
1:H:193:PRO:O	1:H:196:THR:HB	2.21	0.41
1:H:218:LYS:HD3	1:H:218:LYS:N	2.12	0.41
2:B:31:SER:O	2:B:50:ALA:HA	2.21	0.41
2:L:192:TYR:O	2:L:208:SER:HA	2.20	0.41
1:H:11:LEU:HD21	1:H:155:PHE:CZ	2.55	0.41
1:H:53:PRO:HB3	1:H:72:ALA:HB1	2.02	0.41
1:H:20:LEU:HD22	1:H:116:THR:HG21	2.02	0.40
1:A:180:GLN:HB3	1:A:181:SER:H	1.66	0.40
1:H:136:GLY:HA2	1:H:222:ARG:HD3	2.04	0.40
2:L:1:ASP:HB3	2:L:95:PRO:HG2	2.04	0.40
2:L:193:THR:HA	2:L:207:LYS:O	2.22	0.40
1:H:144:MET:HE1	1:H:193:PRO:HD3	2.03	0.40

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	211/224 (94%)	198 (94%)	13 (6%)	0	100	100
1	H	222/224 (99%)	210 (95%)	12 (5%)	0	100	100
2	B	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
2	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	854/876 (98%)	816 (96%)	38 (4%)	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	185/192 (96%)	173 (94%)	12 (6%)	21	21
1	H	192/192 (100%)	171 (89%)	21 (11%)	8	6
2	B	189/192 (98%)	181 (96%)	8 (4%)	36	42
2	L	192/192 (100%)	182 (95%)	10 (5%)	29	31
All	All	758/768 (99%)	707 (93%)	51 (7%)	20	19

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	12	MET
1	H	28	THR
1	H	40	ARG
1	H	57	SER
1	H	65	LYS
1	H	77	ASN
1	H	88	THR
1	H	93	ILE
1	H	106	ASN
1	H	107	LEU
1	H	111	VAL
1	H	137	SER
1	H	140	GLN
1	H	143	SER
1	H	167	SER
1	H	180	GLN
1	H	195	SER
1	H	199	SER
1	H	217	LYS
1	H	218	LYS
2	L	1	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	33	LEU
2	L	53	SER
2	L	55	ASP
2	L	66	ARG
2	L	89	LEU
2	L	126	THR
2	L	142	LYS
2	L	190	ASN
2	L	197	THR
1	A	1	GLN
1	A	3	GLN
1	A	13	LYS
1	A	40	ARG
1	A	57	SER
1	A	65	LYS
1	A	74	THR
1	A	76	SER
1	A	93	ILE
1	A	106	ASN
1	A	107	LEU
1	A	180	GLN
2	B	33	LEU
2	B	55	ASP
2	B	89	LEU
2	B	93	THR
2	B	153	SER
2	B	197	THR
2	B	202	THR
2	B	209	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	5	GLN
1	H	106	ASN
1	H	180	GLN
2	L	3	GLN
2	L	156	GLN
2	L	189	HIS
1	A	1	GLN
1	A	5	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	77	ASN
1	A	106	ASN
2	B	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 carbohydrates 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	215/224 (95%)	1.45	55 (25%) 1 1	24, 59, 99, 124	16 (7%)
1	H	224/224 (100%)	0.85	26 (11%) 6 7	24, 42, 74, 119	16 (7%)
2	B	211/214 (98%)	1.54	59 (27%) 1 1	20, 46, 108, 119	14 (6%)
2	L	214/214 (100%)	0.78	19 (8%) 12 13	23, 44, 66, 98	14 (6%)
All	All	864/876 (98%)	1.15	159 (18%) 2 2	20, 47, 97, 124	60 (6%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	129	GLY	7.8
1	H	44	GLY	7.3
2	L	208	SER	7.0
1	H	149	CYS	7.0
2	L	134	CYS	6.7
1	A	149	CYS	6.6
2	L	104	LEU	6.4
2	B	104	LEU	6.2
1	A	42	GLY	6.1
2	B	208	SER	6.0
2	B	163	TRP	6.0
1	H	42	GLY	6.0
2	L	163	TRP	5.9
2	L	194	CYS	5.8
2	B	201	SER	5.6
1	A	199	SER	5.5
1	H	145	VAL	5.5
1	A	201	THR	5.4
1	A	219	ILE	5.3
2	B	187	GLU	5.3
1	A	163	TRP	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	200	GLU	5.3
1	A	203	THR	5.2
1	A	144	MET	5.2
2	B	128	GLY	5.2
2	B	122	SER	5.1
1	A	211	SER	5.1
2	B	130	ALA	5.0
1	A	220	VAL	5.0
1	H	196	THR	4.7
2	B	10	SER	4.7
2	B	159	VAL	4.7
2	B	191	SER	4.6
1	A	44	GLY	4.6
2	B	175	MET	4.5
2	B	181	LEU	4.5
1	A	88	THR	4.4
2	B	183	LYS	4.4
2	B	152	GLY	4.3
1	A	193	PRO	4.3
2	B	189	HIS	4.3
2	B	210	ASN	4.3
2	B	184	ASP	4.1
2	B	155	ARG	4.0
2	B	185	GLU	4.0
2	B	149	LYS	4.0
1	H	141	THR	3.9
2	B	188	ARG	3.9
1	A	197	TRP	3.9
2	L	175	MET	3.9
2	B	156	GLN	3.8
2	B	20	SER	3.8
1	H	17	SER	3.8
2	B	186	TYR	3.8
2	B	118	PHE	3.7
2	B	148	TRP	3.7
2	B	209	PHE	3.7
2	L	69	SER	3.5
1	A	187	SER	3.4
2	B	202	THR	3.4
2	B	127	SER	3.4
2	L	10	SER	3.4
1	H	41	PRO	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	192	VAL	3.3
1	A	73	ASP	3.3
2	B	112	ALA	3.3
2	B	121	SER	3.3
2	B	120	PRO	3.3
1	A	183	LEU	3.3
1	A	204	CYS	3.3
2	L	214	CYS	3.2
2	B	143	ASP	3.2
1	H	43	HIS	3.1
1	A	16	ALA	3.1
1	H	59	ASN	3.1
1	A	75	SER	3.1
2	B	190	ASN	3.1
2	L	20	SER	3.1
1	H	140	GLN	3.1
1	H	171	GLY	3.1
1	H	204	CYS	3.1
1	A	170	SER	3.1
1	H	142	ASN	3.0
2	B	117	ILE	3.0
1	A	217	LYS	3.0
2	B	157	ASN	3.0
1	A	132	PRO	3.0
2	B	31	SER	2.9
1	A	148	GLY	2.9
1	A	17	SER	2.9
1	A	43	HIS	2.9
2	B	125	LEU	2.9
1	H	224	CYS	2.8
1	A	180	GLN	2.8
2	B	111	ALA	2.8
2	B	203	SER	2.8
1	A	154	TYR	2.8
1	H	136	GLY	2.8
1	A	41	PRO	2.7
1	A	145	VAL	2.7
2	L	143	ASP	2.7
2	L	127	SER	2.7
2	B	194	CYS	2.7
1	A	76	SER	2.6
2	L	129	GLY	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	88	THR	2.6
1	H	193	PRO	2.6
1	A	167	SER	2.6
2	B	195	GLU	2.6
1	A	202	VAL	2.6
1	A	164	ASN	2.5
2	B	205	ILE	2.5
1	H	167	SER	2.5
1	H	199	SER	2.5
1	A	208	HIS	2.5
1	A	13	LYS	2.5
1	H	139	ALA	2.4
2	L	213	GLU	2.4
1	H	75	SER	2.4
1	A	11	LEU	2.4
1	H	74	THR	2.4
1	A	127	PRO	2.4
1	A	184	TYR	2.4
2	B	146	VAL	2.4
2	B	134	CYS	2.4
2	B	200	THR	2.4
2	B	123	GLU	2.4
1	A	190	VAL	2.3
1	A	45	LEU	2.3
2	B	206	VAL	2.3
2	B	150	ILE	2.3
2	L	94	SER	2.3
2	L	106	ILE	2.3
1	H	170	SER	2.3
1	A	191	THR	2.3
2	L	202	THR	2.2
2	L	68	GLY	2.2
2	B	17	GLU	2.2
1	A	196	THR	2.2
1	A	62	GLU	2.2
1	H	187	SER	2.2
1	A	182	ASP	2.2
2	B	151	ASP	2.2
1	A	221	PRO	2.1
1	A	74	THR	2.1
1	A	116	THR	2.1
2	B	89	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1	GLN	2.1
1	H	137	SER	2.1
2	B	197	THR	2.1
1	A	14	PRO	2.1
2	B	87	TYR	2.1
1	A	135	PRO	2.1
1	A	165	SER	2.1
2	B	180	THR	2.0
2	B	182	THR	2.0
2	L	30	GLY	2.0
1	A	215	VAL	2.0
2	B	94	SER	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 carbohydrates 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.