



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2022 – 12:04 AM JST

PDB ID : 7WC0  
Title : Crystal structure of Fab region of TAU-2212 neutralizing SARS-CoV-2  
Authors : Xiang, Y.; Li, R.; Ma, B.  
Deposited on : 2021-12-17  
Resolution : 2.71 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.

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)	:	1.13
EDS	:	2.29
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)	:	2.29

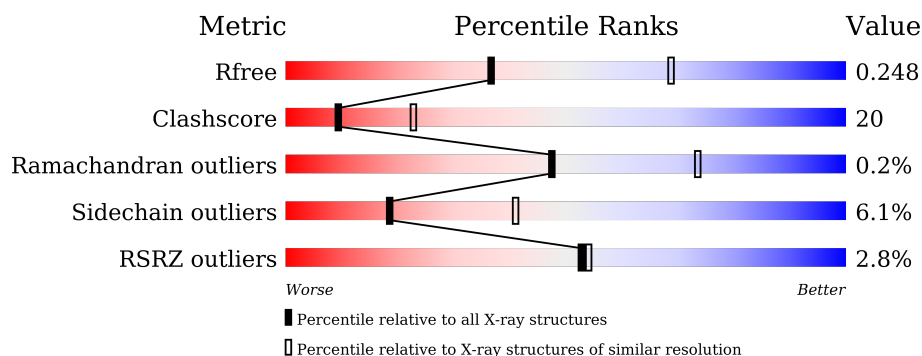
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	252	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>28%</div> <div>•</div> <div>15%</div> </div> </div>
1	H	252	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>25%</div> <div>5%</div> <div>18%</div> </div> </div>
2	B	237	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>•</div> <div>14%</div> </div> </div>
2	L	237	<div> <div>•</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6626 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 TAU-2212 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	206	Total	C	N	O	S	0	0	0
			1592	1016	264	304	8			
1	A	214	Total	C	N	O	S	0	0	0
			1632	1042	268	314	8			

- Molecule 2 is a protein called TAU-2212 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1569	979	262	322	6			
2	B	203	Total	C	N	O	S	0	0	0
			1500	936	251	307	6			

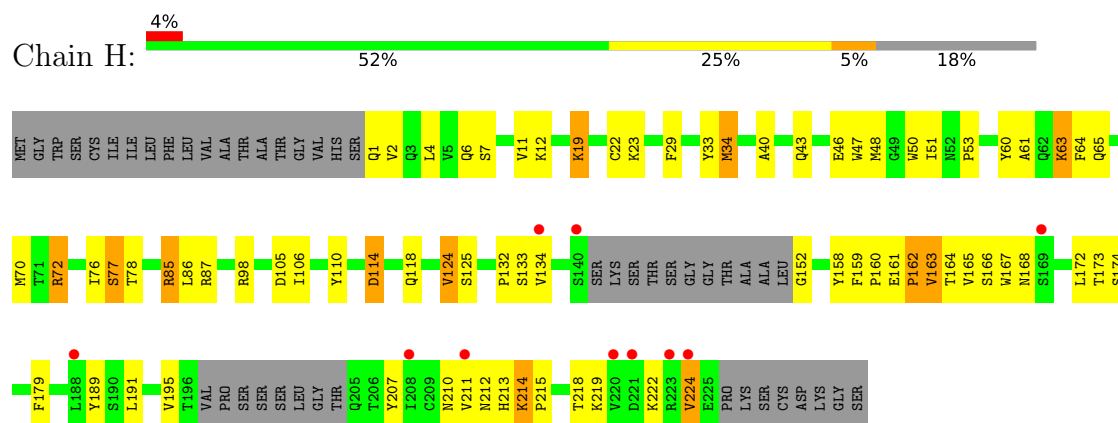
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	91	Total	O	0	0
			91	91		
3	L	75	Total	O	0	0
			75	75		
3	A	86	Total	O	0	0
			86	86		
3	B	81	Total	O	0	0
			81	81		

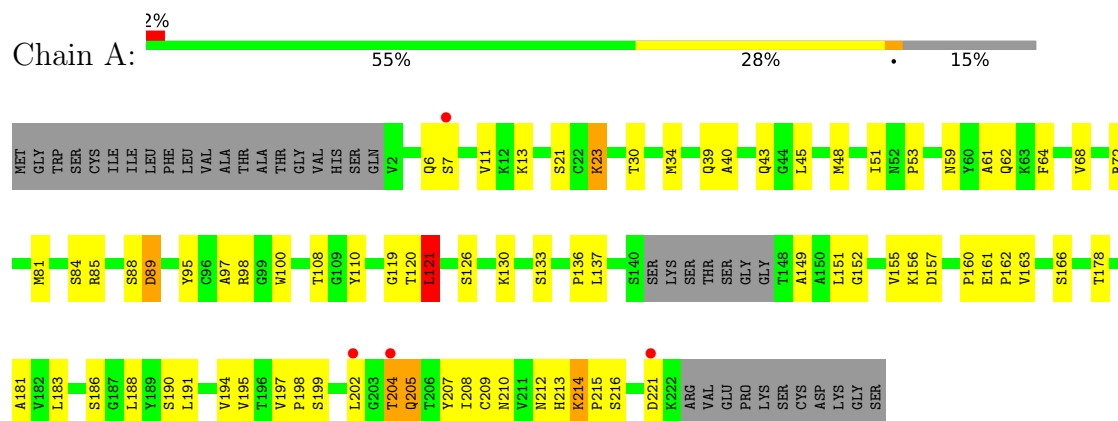
### 3 Residue-property plots [i](#)

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.

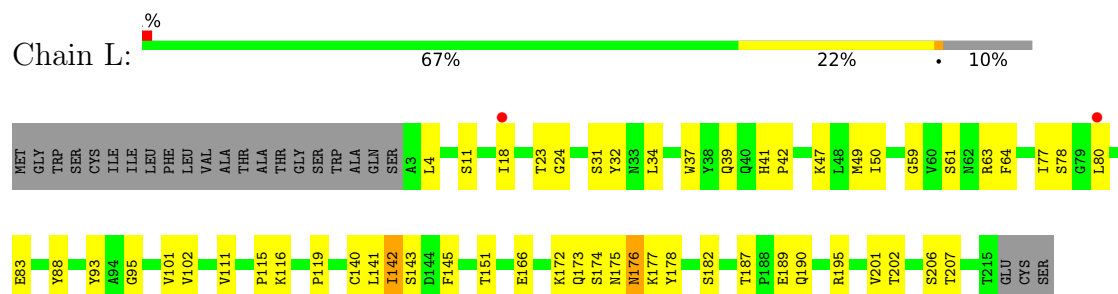
#### • Molecule 1: TAU-2212 Heavy chain



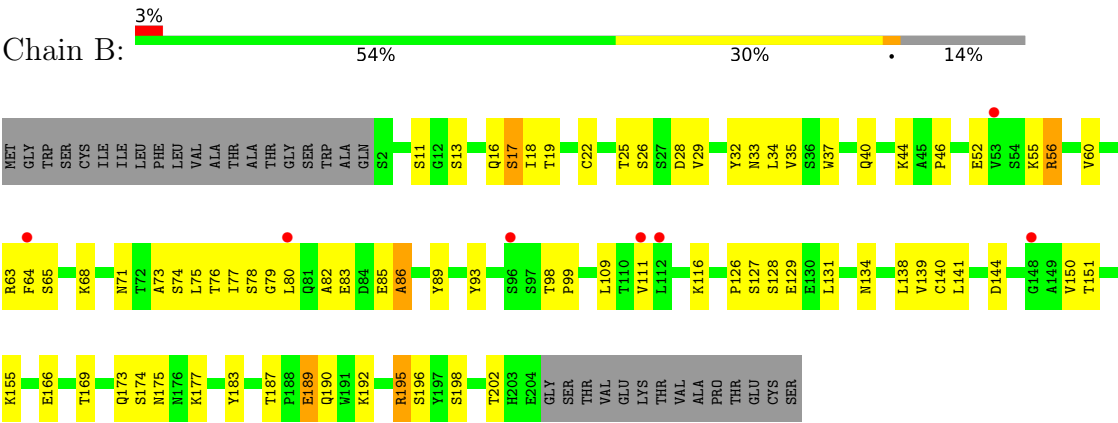
#### • Molecule 1: TAU-2212 Heavy chain



#### • Molecule 2: TAU-2212 Light chain



● Molecule 2: TAU-2212 Light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.98Å 75.98Å 348.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 2.71 29.75 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.75-2.71) 99.8 (29.75-2.71)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.202 , 0.246 0.203 , 0.248	Depositor DCC
$R_{free}$ test set	1554 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.396 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.603 for H, K, L 0.397 for -K, -H, -L	Depositor
Outliers	0 of 30759 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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	0.41	0/1678	0.59	0/2292
1	H	0.41	0/1636	0.57	0/2230
2	B	0.41	0/1537	0.56	0/2096
2	L	0.41	0/1607	0.56	0/2193
All	All	0.41	0/6458	0.57	0/8811

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	A	0	2
1	H	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	LEU	Mainchain
1	A	155	VAL	Peptide
1	H	161	GLU	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	A	1632	0	1574	72	0
1	H	1592	0	1532	73	0
2	B	1500	0	1450	66	0
2	L	1569	0	1523	43	0
3	A	86	0	0	17	0
3	B	81	0	0	21	0
3	H	91	0	0	18	0
3	L	75	0	0	13	0
All	All	6626	0	6079	244	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 20.

All (244) 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:A:6:GLN:OE1	1:A:119:GLY:C	1.85	1.13
1:A:194:VAL:HG21	2:B:141:LEU:HD13	1.38	1.06
1:A:161:GLU:HG3	1:A:162:PRO:HA	1.35	1.04
1:H:162:PRO:HD2	1:H:215:PRO:HG2	1.39	1.04
2:B:173:GLN:HG3	2:B:174:SER:H	1.28	0.98
1:A:34:MET:SD	3:A:313:HOH:O	2.26	0.94
2:B:169:THR:HG22	3:B:337:HOH:O	1.68	0.94
1:H:1:GLN:HG2	1:H:2:VAL:H	1.31	0.93
1:A:194:VAL:CG2	2:B:141:LEU:HD13	1.99	0.93
1:A:186:SER:HB2	3:A:302:HOH:O	1.69	0.93
2:B:35:VAL:O	2:B:52:GLU:O	1.92	0.88
2:B:18:ILE:HD11	2:B:80:LEU:HD22	1.55	0.88
1:H:33:TYR:HD1	3:H:304:HOH:O	1.57	0.88
2:B:63:ARG:HD2	2:B:79:GLY:O	1.75	0.86
1:A:186:SER:CB	3:A:302:HOH:O	2.26	0.83
3:H:355:HOH:O	2:L:173:GLN:HG2	1.77	0.82
2:L:95:GLY:HA2	3:L:311:HOH:O	1.80	0.81
1:A:11:VAL:HG11	1:A:160:PRO:HG3	1.60	0.81
1:H:173:THR:O	3:H:301:HOH:O	1.98	0.80
1:H:70:MET:O	3:H:302:HOH:O	1.99	0.79
1:A:6:GLN:OE1	1:A:119:GLY:CA	2.31	0.79
2:B:52:GLU:HG3	2:B:55:LYS:HZ3	1.48	0.79
2:L:116:LYS:O	3:L:301:HOH:O	2.04	0.75
1:A:149:ALA:HB3	1:A:202:LEU:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:THR:CG2	3:B:353:HOH:O	2.37	0.73
1:A:13:LYS:NZ	1:A:126:SER:O	2.22	0.72
1:H:78:THR:HG21	3:H:361:HOH:O	1.89	0.71
2:L:143:SER:O	2:L:173:GLN:NE2	2.21	0.71
1:H:162:PRO:HD2	1:H:215:PRO:CG	2.18	0.71
2:L:111:VAL:O	3:L:302:HOH:O	2.09	0.70
2:L:59:GLY:HA2	3:L:351:HOH:O	1.92	0.70
1:H:212:ASN:HB2	1:H:219:LYS:HE2	1.74	0.69
2:B:173:GLN:HG3	2:B:174:SER:N	2.06	0.69
1:A:186:SER:O	3:A:301:HOH:O	2.09	0.69
2:L:4:LEU:HD12	2:L:24:GLY:HA2	1.76	0.67
1:H:174:SER:N	3:H:305:HOH:O	2.28	0.67
2:B:11:SER:HA	3:B:305:HOH:O	1.95	0.67
2:B:177:LYS:NZ	3:B:304:HOH:O	2.28	0.66
1:A:161:GLU:CG	1:A:162:PRO:HA	2.21	0.66
1:A:6:GLN:OE1	1:A:119:GLY:O	2.14	0.65
1:A:212:ASN:HB2	3:A:379:HOH:O	1.95	0.65
1:A:149:ALA:CB	1:A:202:LEU:HD11	2.27	0.64
1:H:53:PRO:O	1:H:72:ARG:NE	2.19	0.64
1:H:11:VAL:HG11	1:H:160:PRO:HG3	1.79	0.64
2:B:202:THR:HG23	3:B:353:HOH:O	1.95	0.64
1:A:188:LEU:HD22	3:A:302:HOH:O	1.98	0.63
2:L:174:SER:HA	3:L:306:HOH:O	1.97	0.63
1:H:1:GLN:HG2	1:H:2:VAL:N	2.10	0.63
1:A:130:LYS:HD3	1:A:157:ASP:O	1.98	0.63
2:B:18:ILE:HD11	2:B:80:LEU:CD2	2.28	0.62
1:A:208:ILE:HG23	1:A:221:ASP:OD1	1.99	0.62
2:L:42:PRO:HA	3:L:339:HOH:O	2.00	0.62
1:A:214:LYS:N	1:A:215:PRO:CD	2.63	0.61
1:A:160:PRO:HD2	1:A:215:PRO:HB2	1.83	0.61
1:H:158:TYR:OH	1:H:191:LEU:HD23	2.01	0.61
2:L:95:GLY:N	3:L:305:HOH:O	2.34	0.60
2:B:127:SER:HB2	2:B:129:GLU:OE1	2.02	0.60
2:B:187:THR:OG1	2:B:190:GLN:HG3	2.01	0.60
1:H:167:TRP:CZ3	1:H:224:VAL:HG21	2.37	0.59
1:A:181:ALA:HB2	1:A:191:LEU:HD21	1.84	0.59
1:H:160:PRO:CD	1:H:215:PRO:HB2	2.32	0.59
2:L:37:TRP:HB2	2:L:50:ILE:HB	1.82	0.59
1:A:181:ALA:HA	1:A:191:LEU:HD23	1.83	0.59
2:B:13:SER:O	2:B:16:GLN:HG2	2.03	0.59
1:A:6:GLN:OE1	1:A:120:THR:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ARG:HG2	2:B:60:VAL:HB	1.84	0.59
2:B:134:ASN:HB2	3:B:325:HOH:O	2.03	0.58
1:H:132:PRO:HB3	1:H:158:TYR:HB3	1.85	0.58
2:L:4:LEU:HD21	2:L:102:VAL:HG23	1.85	0.57
1:H:22:CYS:SG	1:H:34:MET:HE3	2.45	0.57
2:L:172:LYS:HE2	2:L:178:TYR:CE1	2.39	0.57
1:H:160:PRO:HD2	1:H:215:PRO:HB2	1.86	0.57
1:H:76:ILE:HD11	3:H:346:HOH:O	2.05	0.57
1:H:162:PRO:CD	1:H:215:PRO:HG2	2.26	0.57
1:H:214:LYS:N	1:H:215:PRO:CD	2.67	0.56
1:A:178:THR:HG22	3:A:364:HOH:O	2.05	0.56
1:H:40:ALA:HB3	1:H:43:GLN:HB2	1.88	0.56
1:H:7:SER:O	3:H:303:HOH:O	2.18	0.56
1:A:166:SER:HB2	1:A:210:ASN:HB2	1.86	0.56
2:B:63:ARG:HD3	2:B:78:SER:O	2.07	0.55
1:A:197:VAL:HG13	1:A:198:PRO:HD2	1.89	0.55
2:B:129:GLU:HG2	3:B:357:HOH:O	2.06	0.55
2:B:202:THR:HG21	3:B:353:HOH:O	2.01	0.55
1:A:97:ALA:C	3:A:313:HOH:O	2.46	0.54
1:H:60:TYR:CE1	1:H:70:MET:HE2	2.43	0.54
1:H:213:HIS:HB3	1:H:218:THR:OG1	2.07	0.54
2:B:155:LYS:HB2	2:B:198:SER:HB3	1.89	0.54
1:H:165:VAL:HG13	1:H:211:VAL:HG22	1.90	0.54
2:L:177:LYS:HE3	3:L:345:HOH:O	2.07	0.53
1:A:137:LEU:HB2	1:A:152:GLY:C	2.28	0.53
2:L:41:HIS:HD2	3:L:309:HOH:O	1.92	0.53
1:H:77:SER:O	1:H:77:SER:OG	2.24	0.53
1:H:162:PRO:HB3	3:H:367:HOH:O	2.08	0.53
2:B:139:VAL:HG13	2:B:183:TYR:CE2	2.44	0.52
1:H:163:VAL:HG23	1:H:213:HIS:CD2	2.44	0.52
2:B:40:GLN:OE1	2:B:46:PRO:HG3	2.10	0.52
2:L:187:THR:HB	2:L:190:GLN:HG3	1.92	0.52
1:A:48:MET:HG2	1:A:64:PHE:CZ	2.45	0.52
1:A:108:THR:CG2	3:A:330:HOH:O	2.57	0.52
1:H:51:ILE:C	3:H:304:HOH:O	2.48	0.52
2:L:49:MET:O	2:L:50:ILE:HD13	2.09	0.52
2:L:47:LYS:HD3	2:L:49:MET:SD	2.50	0.52
1:A:181:ALA:CA	1:A:191:LEU:HD23	2.40	0.51
1:A:59:ASN:OD1	2:B:99:PRO:O	2.28	0.51
2:L:18:ILE:HG13	2:L:80:LEU:HD11	1.92	0.51
2:B:40:GLN:NE2	2:B:44:LYS:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:HG23	3:B:368:HOH:O	2.11	0.51
2:L:172:LYS:NZ	2:L:176:ASN:O	2.29	0.51
1:A:186:SER:OG	3:A:302:HOH:O	2.19	0.51
1:A:133:SER:O	1:A:156:LYS:HB2	2.11	0.50
1:H:19:LYS:N	3:H:312:HOH:O	2.43	0.50
2:B:44:LYS:HE3	3:B:321:HOH:O	2.11	0.50
1:H:106:ILE:HG21	1:H:110:TYR:CE2	2.47	0.50
2:L:31:SER:HB3	2:L:32:TYR:HD1	1.77	0.50
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.94	0.50
1:A:151:LEU:HG	1:A:195:VAL:CG1	2.42	0.50
2:B:76:THR:O	2:B:77:ILE:HD13	2.12	0.50
1:H:162:PRO:CD	1:H:215:PRO:CG	2.86	0.50
1:H:65:GLN:OE1	1:A:126:SER:OG	2.18	0.50
1:H:125:SER:HB2	1:H:159:PHE:CZ	2.47	0.50
2:L:187:THR:HG22	2:L:189:GLU:H	1.77	0.50
2:L:151:THR:OG1	2:L:202:THR:HB	2.12	0.49
1:A:6:GLN:HE22	1:A:95:TYR:HA	1.76	0.49
1:H:166:SER:OG	1:H:210:ASN:HB2	2.12	0.49
2:B:126:PRO:HD3	2:B:138:LEU:HG	1.95	0.49
2:B:155:LYS:NZ	3:B:301:HOH:O	2.17	0.49
2:B:83:GLU:OE1	2:B:83:GLU:O	2.30	0.49
2:B:64:PHE:CD1	2:B:77:ILE:HD12	2.47	0.49
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.95	0.49
1:H:167:TRP:HZ3	1:H:224:VAL:HG21	1.78	0.48
1:A:98:ARG:N	3:A:313:HOH:O	2.46	0.48
1:H:23:LYS:HE2	1:H:76:ILE:HG22	1.95	0.48
1:H:47:TRP:CG	2:L:101:VAL:HB	2.48	0.48
2:L:140:CYS:HB3	2:L:182:SER:HB3	1.96	0.48
1:H:134:VAL:HG11	1:H:211:VAL:HG21	1.96	0.48
2:L:11:SER:N	3:L:310:HOH:O	2.46	0.48
2:B:85:GLU:O	2:B:86:ALA:HB2	2.14	0.48
1:A:205:GLN:HB3	1:A:207:TYR:CE1	2.48	0.48
1:H:6:GLN:O	1:H:118:GLN:NE2	2.44	0.48
1:H:179:PHE:CE1	2:L:141:LEU:HD22	2.49	0.48
1:H:98:ARG:NH2	1:H:114:ASP:OD2	2.43	0.48
2:B:18:ILE:HD12	2:B:80:LEU:HD13	1.96	0.48
2:B:19:THR:HB	3:B:363:HOH:O	2.14	0.47
1:A:6:GLN:OE1	1:A:119:GLY:N	2.46	0.47
2:L:201:VAL:O	2:L:207:THR:HA	2.14	0.47
2:B:85:GLU:HA	2:B:109:LEU:HD23	1.96	0.47
2:B:195:ARG:HG3	2:B:196:SER:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ILE:N	3:H:304:HOH:O	2.48	0.47
1:A:204:THR:HG21	3:A:355:HOH:O	2.15	0.47
2:B:98:THR:HA	3:B:306:HOH:O	2.14	0.47
1:H:4:LEU:HD23	1:H:34:MET:HE3	1.97	0.47
1:H:152:GLY:N	3:H:317:HOH:O	2.47	0.47
1:A:62:GLN:HG2	3:A:370:HOH:O	2.14	0.47
1:A:199:SER:O	1:A:202:LEU:HB2	2.14	0.47
2:B:109:LEU:HG	3:B:305:HOH:O	2.14	0.47
1:H:195:VAL:HG23	1:H:195:VAL:O	2.15	0.46
1:H:50:TRP:HB2	3:H:304:HOH:O	2.14	0.46
2:L:4:LEU:HD12	2:L:24:GLY:CA	2.43	0.46
1:H:60:TYR:HE1	1:H:70:MET:HE2	1.79	0.46
2:B:25:THR:O	2:B:28:ASP:OD1	2.33	0.46
1:H:164:THR:OG1	1:H:212:ASN:HB3	2.15	0.46
2:B:63:ARG:HG3	2:B:78:SER:H	1.80	0.46
1:H:158:TYR:CE2	1:H:189:TYR:HB2	2.51	0.46
1:A:51:ILE:O	1:A:53:PRO:HD3	2.16	0.45
1:H:61:ALA:HB3	1:H:64:PHE:HD2	1.82	0.45
1:A:7:SER:HB3	1:A:21:SER:H	1.82	0.45
2:B:99:PRO:HD2	3:B:306:HOH:O	2.16	0.45
2:L:177:LYS:CE	3:L:345:HOH:O	2.64	0.45
1:A:181:ALA:HB2	1:A:191:LEU:CD2	2.47	0.45
2:B:187:THR:OG1	2:B:189:GLU:HG2	2.16	0.45
2:B:192:LYS:CE	3:B:339:HOH:O	2.65	0.45
2:B:28:ASP:OD1	2:B:29:VAL:N	2.47	0.45
2:B:98:THR:HG23	2:B:98:THR:O	2.17	0.45
1:A:48:MET:HE1	1:A:81:MET:SD	2.57	0.45
1:H:85:ARG:HH21	1:A:84:SER:HB3	1.83	0.44
2:L:166:GLU:OE1	2:L:166:GLU:N	2.50	0.44
1:A:89:ASP:OD1	3:A:303:HOH:O	2.20	0.44
2:B:82:ALA:O	2:B:83:GLU:CB	2.65	0.44
1:H:168:ASN:HD22	1:H:172:LEU:HD23	1.82	0.44
1:A:121:LEU:O	1:A:121:LEU:HG	2.17	0.44
1:A:213:HIS:ND1	1:A:216:SER:HB3	2.33	0.44
1:H:12:LYS:O	1:H:124:VAL:HA	2.17	0.44
1:H:207:TYR:O	1:H:224:VAL:HG23	2.17	0.44
1:A:6:GLN:NE2	1:A:95:TYR:HA	2.31	0.44
1:A:194:VAL:HG22	2:B:141:LEU:HD13	1.95	0.44
2:L:119:PRO:HA	2:L:145:PHE:HB3	1.99	0.44
2:B:65:SER:O	2:B:75:LEU:HD12	2.18	0.44
1:A:61:ALA:HB3	1:A:64:PHE:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:GLU:OE2	1:H:63:LYS:HE3	2.18	0.43
1:A:199:SER:HA	1:A:202:LEU:HG	2.00	0.43
2:B:40:GLN:O	2:B:86:ALA:HB1	2.18	0.43
1:H:4:LEU:HD12	1:H:4:LEU:H	1.84	0.43
1:H:29:PHE:CE2	1:H:53:PRO:HB3	2.54	0.43
2:L:32:TYR:HD2	2:L:34:LEU:HD12	1.81	0.43
1:A:163:VAL:HG23	1:A:213:HIS:HD2	1.82	0.43
2:B:37:TRP:NE1	3:B:311:HOH:O	2.50	0.43
1:A:156:LYS:O	1:A:190:SER:OG	2.30	0.43
1:H:47:TRP:CD2	2:L:101:VAL:HB	2.53	0.43
1:H:86:LEU:HB3	1:H:124:VAL:HG11	2.00	0.43
1:H:48:MET:HB3	1:H:48:MET:HE2	1.88	0.43
1:H:166:SER:HA	3:H:376:HOH:O	2.19	0.43
1:A:68:VAL:CG1	1:A:81:MET:HE2	2.49	0.43
1:A:214:LYS:N	1:A:215:PRO:HD3	2.33	0.43
1:H:212:ASN:CB	1:H:219:LYS:HE2	2.47	0.42
2:L:173:GLN:HB3	3:L:332:HOH:O	2.18	0.42
1:A:136:PRO:HG3	3:B:357:HOH:O	2.18	0.42
1:A:197:VAL:HG13	1:A:198:PRO:CD	2.49	0.42
1:H:50:TRP:CD1	1:H:50:TRP:C	2.93	0.42
1:H:133:SER:HA	3:H:365:HOH:O	2.20	0.42
2:L:202:THR:HA	2:L:206:SER:O	2.20	0.42
2:B:76:THR:C	2:B:77:ILE:HD13	2.40	0.42
1:H:72:ARG:HG3	3:H:338:HOH:O	2.20	0.42
1:H:11:VAL:HG23	1:H:11:VAL:O	2.19	0.42
2:L:39:GLN:HB2	2:L:88:TYR:CE1	2.55	0.42
2:B:151:THR:HG21	3:B:377:HOH:O	2.20	0.41
1:H:4:LEU:HD12	1:H:4:LEU:N	2.34	0.41
2:L:63:ARG:HB3	2:L:78:SER:O	2.19	0.41
2:B:18:ILE:HD12	2:B:109:LEU:HD11	2.02	0.41
2:B:32:TYR:CD2	2:B:93:TYR:HD2	2.38	0.41
1:H:87:ARG:O	1:H:124:VAL:HG21	2.20	0.41
1:A:23:LYS:HG3	3:A:350:HOH:O	2.19	0.41
1:A:62:GLN:HG3	3:A:351:HOH:O	2.19	0.41
1:A:157:ASP:HB3	1:A:188:LEU:HD23	2.02	0.41
2:B:22:CYS:HB3	2:B:73:ALA:HB3	2.03	0.41
2:L:31:SER:HB3	2:L:32:TYR:CD1	2.55	0.41
2:L:64:PHE:CE2	2:L:77:ILE:HD13	2.55	0.41
2:B:116:LYS:N	3:B:309:HOH:O	2.53	0.41
1:H:76:ILE:HG22	1:H:76:ILE:O	2.20	0.41
1:H:106:ILE:HD13	3:H:318:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:O	1:A:11:VAL:HG23	2.20	0.41
2:L:32:TYR:CE2	2:L:93:TYR:HD2	2.38	0.41
2:B:17:SER:HA	2:B:77:ILE:O	2.21	0.41
1:A:100:TRP:CE3	1:A:110:TYR:HB3	2.56	0.41
2:B:29:VAL:HG13	2:B:71:ASN:HA	2.02	0.41
2:B:82:ALA:O	2:B:83:GLU:HB2	2.21	0.41
2:B:111:VAL:HG13	3:B:327:HOH:O	2.19	0.41
1:A:23:LYS:HE2	1:A:23:LYS:HB3	1.74	0.41
2:B:128:SER:HA	2:B:131:LEU:HD12	2.03	0.41
2:L:119:PRO:HB2	2:L:142:ILE:CG2	2.52	0.40
1:A:183:LEU:HD11	3:A:314:HOH:O	2.21	0.40
2:B:33:ASN:C	2:B:34:LEU:HD23	2.41	0.40
1:H:23:LYS:HA	1:H:78:THR:HG22	2.03	0.40
2:L:115:PRO:HD2	3:L:345:HOH:O	2.20	0.40
1:A:110:TYR:HB2	2:B:52:GLU:OE1	2.21	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	210/252 (83%)	204 (97%)	6 (3%)	0	100	100
1	H	200/252 (79%)	192 (96%)	7 (4%)	1 (0%)	29	54
2	B	201/237 (85%)	188 (94%)	12 (6%)	1 (0%)	29	54
2	L	211/237 (89%)	199 (94%)	12 (6%)	0	100	100
All	All	822/978 (84%)	783 (95%)	37 (4%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	ALA
1	H	162	PRO

### 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	179/210 (85%)	168 (94%)	11 (6%)	18	41
1	H	174/210 (83%)	161 (92%)	13 (8%)	13	31
2	B	170/197 (86%)	158 (93%)	12 (7%)	14	34
2	L	178/197 (90%)	171 (96%)	7 (4%)	32	61
All	All	701/814 (86%)	658 (94%)	43 (6%)	18	41

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	19	LYS
1	H	34	MET
1	H	63	LYS
1	H	72	ARG
1	H	77	SER
1	H	85	ARG
1	H	105	ASP
1	H	114	ASP
1	H	124	VAL
1	H	163	VAL
1	H	214	LYS
1	H	222	LYS
1	H	224	VAL
2	L	23	THR
2	L	61	SER
2	L	83	GLU
2	L	142	ILE
2	L	175	ASN
2	L	176	ASN
2	L	195	ARG

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Mol	Chain	Res	Type
1	A	23	LYS
1	A	30	THR
1	A	72	ARG
1	A	85	ARG
1	A	88	SER
1	A	89	ASP
1	A	121	LEU
1	A	204	THR
1	A	205	GLN
1	A	209	CYS
1	A	214	LYS
2	B	17	SER
2	B	26	SER
2	B	56	ARG
2	B	68	LYS
2	B	74	SER
2	B	89	TYR
2	B	140	CYS
2	B	144	ASP
2	B	166	GLU
2	B	175	ASN
2	B	189	GLU
2	B	195	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	59	ASN
1	A	3	GLN
1	A	59	ASN
1	A	205	GLN
2	B	114	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	214/252 (84%)	0.24	4 (1%) 66 69	64, 88, 129, 165	0
1	H	206/252 (81%)	0.39	10 (4%) 29 28	68, 94, 147, 187	0
2	B	203/237 (85%)	0.35	7 (3%) 45 45	72, 99, 143, 158	0
2	L	213/237 (89%)	0.15	2 (0%) 84 85	49, 88, 120, 133	0
All	All	836/978 (85%)	0.28	23 (2%) 53 54	49, 92, 133, 187	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	208	ILE	6.4
2	B	80	LEU	3.6
1	A	221	ASP	3.6
1	H	188	LEU	3.6
1	H	223	ARG	3.3
1	H	211	VAL	3.0
2	B	112	LEU	3.0
1	A	202	LEU	2.9
1	A	204	THR	2.9
1	A	7	SER	2.8
1	H	220	VAL	2.8
1	H	169	SER	2.7
2	L	80	LEU	2.7
1	H	134	VAL	2.4
1	H	140	SER	2.4
2	B	64	PHE	2.3
2	B	96	SER	2.3
1	H	224	VAL	2.2
1	H	221	ASP	2.1
2	B	111	VAL	2.1
2	L	18	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	53	VAL	2.0
2	B	148	GLY	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.