



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 07:23 PM EDT

PDB ID : 3RAJ  
Title : Crystal structure of human CD38 in complex with the Fab fragment of anti-body HB7  
Authors : Zhang, H.; Lee, H.C.; Hao, Q.  
Deposited on : unknown  
Resolution : 3.04 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.

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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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

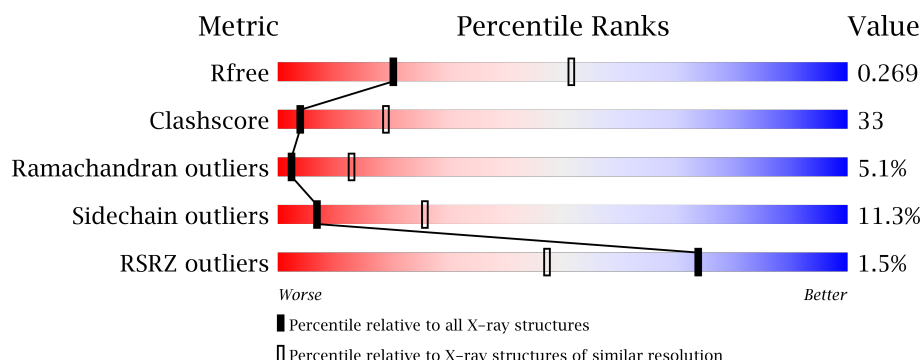
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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))
$R_{free}$	100719	2176 (3.08-3.00)
Clashscore	112137	2542 (3.08-3.00)
Ramachandran outliers	110173	2458 (3.08-3.00)
Sidechain outliers	110143	2461 (3.08-3.00)
RSRZ outliers	101464	2202 (3.08-3.00)

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	257	
2	H	220	
3	L	211	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5034 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 ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1851	1168	318	351	14			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLU	-	EXPRESSION TAG	UNP P28907
A	45	PHE	-	EXPRESSION TAG	UNP P28907
A	49	THR	GLN	ENGINEERED MUTATION	UNP P28907
A	100	ASP	ASN	ENGINEERED MUTATION	UNP P28907
A	164	ASP	ASN	ENGINEERED MUTATION	UNP P28907
A	209	ASP	ASN	ENGINEERED MUTATION	UNP P28907
A	219	ASP	ASN	ENGINEERED MUTATION	UNP P28907

- Molecule 2 is a protein called heavy chain of the Fab fragment of antibody HB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1584	1012	256	309	7			

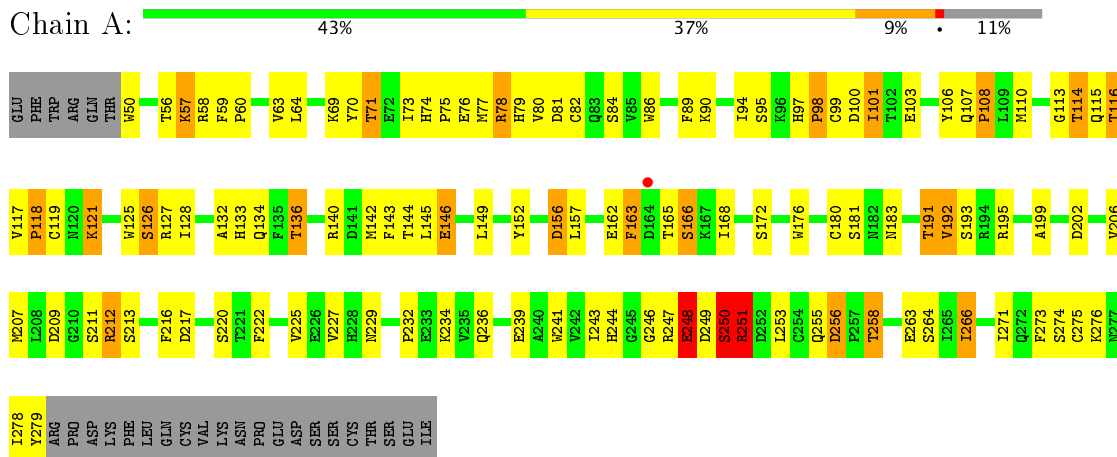
- Molecule 3 is a protein called light chain of the Fab fragment of antibody HB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1599	996	265	332	6			

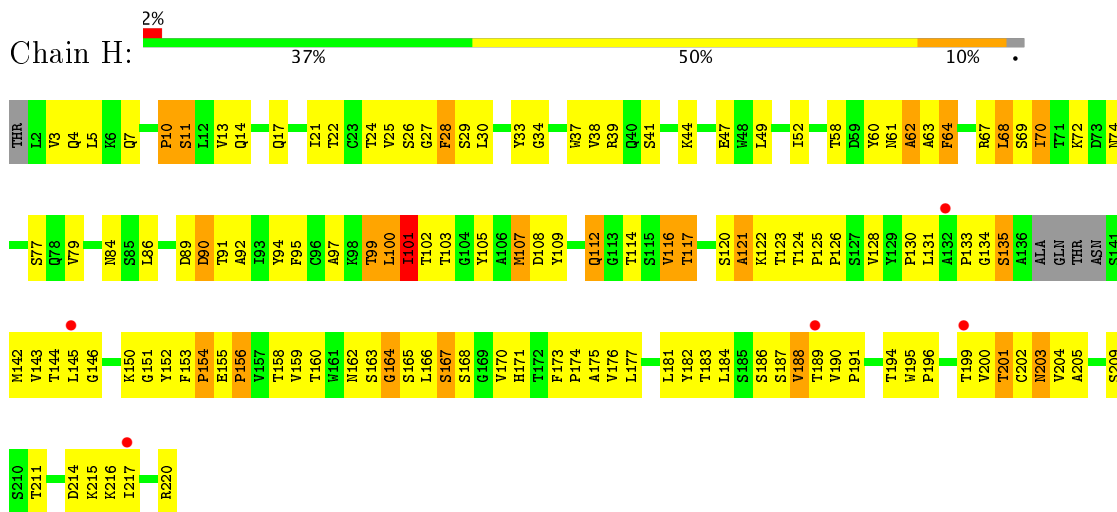
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

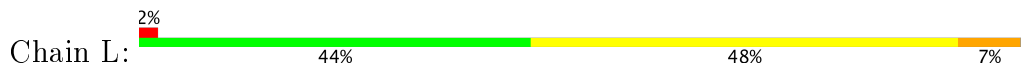
- Molecule 1: ADP-ribosyl cyclase 1

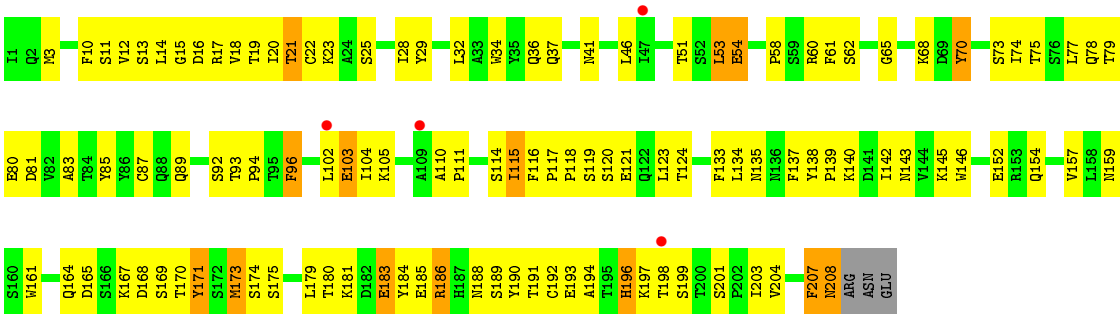


- Molecule 2: heavy chain of the Fab fragment of antibody HB7



- Molecule 3: light chain of the Fab fragment of antibody HB7





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.66Å 271.52Å 136.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 3.04 49.81 – 3.04	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.16-3.04) 90.6 (49.81-3.04)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 3.07Å)	Xtriage
Refinement program	PHENIX dev_378	Depositor
R, $R_{free}$	0.205 , 0.275 0.191 , 0.269	Depositor DCC
$R_{free}$ test set	1000 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.3	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 88.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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

### 5.1 Standard geometry

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	0.63	0/1896	0.77	1/2570 (0.0%)
2	H	0.46	0/1625	0.66	2/2224 (0.1%)
3	L	0.47	0/1634	0.63	0/2221
All	All	0.53	0/5155	0.69	3/7015 (0.0%)

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
3	L	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100	LEU	CA-CB-CG	6.72	130.75	115.30
1	A	192	VAL	CB-CA-C	-5.18	101.56	111.40
2	H	3	VAL	CB-CA-C	-5.04	101.83	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	70	TYR	Peptide

### 5.2 Too-close contacts

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	1851	0	1777	108	0
2	H	1584	0	1518	130	0
3	L	1599	0	1530	100	0
All	All	5034	0	4825	329	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 33.

All (329) 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:H:162:ASN:HA	2:H:201:THR:HG23	1.42	1.01
2:H:171:HIS:HB2	3:L:135:ASN:HD21	1.23	1.01
2:H:128:VAL:HG21	2:H:204:VAL:HG21	1.47	0.94
1:A:71:THR:HG22	1:A:78:ARG:H	1.35	0.92
2:H:135:SER:HB2	2:H:220:ARG:HB2	1.53	0.91
2:H:131:LEU:HB3	3:L:116:PHE:CD2	2.08	0.89
3:L:117:PRO:HB3	3:L:207:PHE:HE1	1.34	0.88
2:H:209:SER:O	2:H:211:THR:HG23	1.75	0.86
2:H:100:LEU:O	2:H:101:ILE:HG12	1.76	0.85
2:H:60:TYR:HE1	2:H:70:ILE:HG13	1.37	0.85
1:A:250:SER:O	1:A:251:ARG:CB	2.24	0.84
3:L:36:GLN:HB2	3:L:46:LEU:HD11	1.57	0.84
1:A:128:ILE:O	1:A:128:ILE:HG23	1.75	0.83
3:L:77:LEU:HD12	3:L:78:GLN:H	1.46	0.80
2:H:195:TRP:CG	2:H:196:PRO:HA	2.17	0.80
2:H:131:LEU:HB3	3:L:116:PHE:HD2	1.45	0.79
3:L:117:PRO:HB3	3:L:207:PHE:CE1	2.17	0.79
2:H:170:VAL:HG13	2:H:187:SER:O	1.82	0.79
1:A:103:GLU:HG2	1:A:191:THR:OG1	1.81	0.79
3:L:13:SER:O	3:L:16:ASP:HB2	1.83	0.79
1:A:248:GLU:HG2	1:A:249:ASP:N	1.97	0.79
3:L:77:LEU:HD12	3:L:78:GLN:N	1.98	0.79
1:A:60:PRO:HB3	1:A:86:TRP:CZ2	2.20	0.77
3:L:140:LYS:HB3	3:L:171:TYR:CE1	2.21	0.76
2:H:123:THR:HG23	2:H:153:PHE:O	1.86	0.75
3:L:37:GLN:O	3:L:83:ALA:HB1	1.85	0.75
2:H:144:THR:HG22	2:H:189:THR:HG23	1.67	0.75
1:A:132:ALA:C	1:A:134:GLN:H	1.91	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:THR:OG1	2:H:203:ASN:HB2	1.87	0.74
2:H:143:VAL:HG13	2:H:190:VAL:HG23	1.68	0.74
3:L:53:LEU:O	3:L:54:GLU:HB2	1.86	0.74
1:A:250:SER:O	1:A:251:ARG:HB2	1.88	0.73
3:L:14:LEU:HD23	3:L:15:GLY:N	2.03	0.73
3:L:22:CYS:HB2	3:L:34:TRP:CH2	2.24	0.73
1:A:94:ILE:HD12	1:A:94:ILE:O	1.87	0.72
1:A:207:MET:HE2	1:A:241:TRP:HE3	1.53	0.72
1:A:90:LYS:O	1:A:94:ILE:HG13	1.88	0.72
2:H:162:ASN:HB2	2:H:165:SER:HB2	1.72	0.71
3:L:119:SER:O	3:L:123:LEU:HD12	1.90	0.71
1:A:50:TRP:HB2	1:A:172:SER:HB2	1.72	0.71
2:H:38:VAL:HG13	2:H:47:GLU:O	1.91	0.71
2:H:120:SER:O	2:H:121:ALA:HB2	1.89	0.70
3:L:123:LEU:HB3	3:L:181:LYS:HD3	1.74	0.70
2:H:200:VAL:H	2:H:216:LYS:HE3	1.57	0.69
3:L:11:SER:HA	3:L:103:GLU:O	1.92	0.69
3:L:142:ILE:HG12	3:L:143:ASN:H	1.57	0.69
3:L:145:LYS:HB3	3:L:193:GLU:HG3	1.73	0.69
2:H:171:HIS:HB2	3:L:135:ASN:ND2	2.02	0.69
3:L:133:PHE:O	3:L:134:LEU:HD12	1.92	0.69
2:H:145:LEU:HD13	2:H:217:ILE:HG21	1.74	0.68
2:H:7:GLN:HE22	2:H:95:PHE:HA	1.58	0.67
3:L:181:LYS:O	3:L:184:TYR:HB3	1.95	0.67
3:L:190:TYR:HB2	3:L:207:PHE:CE2	2.29	0.67
1:A:69:LYS:HG3	1:A:73:ILE:HD11	1.77	0.67
3:L:115:ILE:O	3:L:115:ILE:HG12	1.94	0.67
2:H:195:TRP:CD1	2:H:196:PRO:HA	2.29	0.67
2:H:170:VAL:HG22	2:H:188:VAL:HA	1.77	0.66
1:A:50:TRP:HB2	1:A:172:SER:CB	2.26	0.66
3:L:190:TYR:HB2	3:L:207:PHE:HE2	1.59	0.66
2:H:68:LEU:HD12	2:H:69:SER:H	1.61	0.65
2:H:190:VAL:HB	2:H:191:PRO:HD2	1.77	0.65
3:L:179:LEU:HD22	3:L:183:GLU:HG3	1.79	0.64
1:A:263:GLU:HG3	1:A:273:PHE:CD2	2.32	0.64
1:A:253:LEU:C	1:A:255:GLN:H	2.00	0.64
1:A:250:SER:O	1:A:251:ARG:HB3	1.97	0.64
2:H:64:PHE:CD2	2:H:64:PHE:N	2.64	0.64
3:L:117:PRO:CB	3:L:207:PHE:HE1	2.09	0.64
2:H:135:SER:H	2:H:220:ARG:HD3	1.63	0.63
2:H:60:TYR:CE1	2:H:70:ILE:HG13	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:HIS:CD2	1:A:253:LEU:HD12	2.33	0.63
3:L:207:PHE:HD2	3:L:207:PHE:H	1.47	0.63
2:H:72:LYS:HB3	2:H:79:VAL:HG22	1.80	0.62
3:L:137:PHE:O	3:L:170:THR:HB	2.00	0.62
2:H:174:PRO:HG2	3:L:161:TRP:O	1.99	0.62
3:L:173:MET:HG3	3:L:174:SER:N	2.15	0.62
1:A:77:MET:O	1:A:79:HIS:N	2.26	0.62
2:H:99:THR:HG23	2:H:101:ILE:O	1.99	0.62
1:A:162:GLU:HG3	1:A:165:THR:OG1	1.99	0.62
3:L:62:SER:HB2	3:L:73:SER:HB2	1.82	0.61
3:L:120:SER:O	3:L:124:THR:HG23	2.01	0.61
3:L:60:ARG:NH2	3:L:81:ASP:OD1	2.29	0.61
3:L:146:TRP:HE1	3:L:175:SER:HB3	1.65	0.61
2:H:25:VAL:CG2	2:H:77:SER:HB3	2.31	0.61
2:H:200:VAL:O	2:H:200:VAL:HG22	2.00	0.60
3:L:118:PRO:HB2	3:L:123:LEU:HD11	1.82	0.60
1:A:128:ILE:O	1:A:128:ILE:CG2	2.49	0.60
2:H:64:PHE:HD2	2:H:64:PHE:H	1.50	0.60
3:L:193:GLU:HB3	3:L:204:VAL:HG22	1.83	0.60
3:L:3:MET:HB2	3:L:96:PHE:O	2.02	0.59
1:A:247:ARG:O	1:A:248:GLU:CB	2.51	0.59
2:H:159:VAL:HG22	2:H:204:VAL:HG12	1.84	0.59
1:A:145:LEU:HD21	1:A:192:VAL:HG23	1.84	0.59
1:A:163:PHE:CD2	1:A:163:PHE:N	2.72	0.58
1:A:126:SER:O	1:A:127:ARG:C	2.42	0.58
2:H:89:ASP:C	2:H:91:THR:H	2.06	0.58
1:A:207:MET:HE2	1:A:241:TRP:CE3	2.36	0.58
1:A:71:THR:HG22	1:A:78:ARG:N	2.12	0.58
1:A:101:ILE:N	1:A:101:ILE:CD1	2.66	0.58
3:L:22:CYS:HB2	3:L:34:TRP:HH2	1.66	0.58
3:L:184:TYR:CE1	3:L:190:TYR:CE2	2.92	0.58
2:H:190:VAL:HB	2:H:194:THR:CG2	2.34	0.57
1:A:132:ALA:O	1:A:134:GLN:N	2.38	0.57
2:H:91:THR:HG23	2:H:117:THR:HA	1.86	0.57
1:A:244:HIS:CD2	1:A:253:LEU:CD1	2.87	0.57
2:H:5:LEU:HD13	2:H:109:TYR:O	2.05	0.57
2:H:10:PRO:O	2:H:11:SER:CB	2.53	0.56
2:H:142:MET:HB3	2:H:190:VAL:O	2.05	0.56
2:H:166:LEU:HD12	2:H:167:SER:H	1.70	0.56
2:H:202:CYS:O	2:H:214:ASP:HA	2.06	0.56
2:H:22:THR:O	2:H:22:THR:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:ASN:C	2:H:164:GLY:H	2.08	0.56
2:H:27:GLY:O	2:H:28:PHE:HB3	2.06	0.56
3:L:96:PHE:CD2	3:L:96:PHE:N	2.74	0.56
3:L:168:ASP:O	3:L:170:THR:HG23	2.06	0.56
2:H:162:ASN:HA	2:H:201:THR:CG2	2.28	0.55
2:H:162:ASN:HB2	2:H:165:SER:CB	2.36	0.55
2:H:37:TRP:CD1	2:H:70:ILE:HD13	2.41	0.55
3:L:171:TYR:CD2	3:L:171:TYR:N	2.73	0.55
1:A:247:ARG:O	1:A:248:GLU:HB3	2.05	0.55
2:H:146:GLY:HA3	2:H:186:SER:O	2.06	0.55
2:H:166:LEU:HD11	2:H:168:SER:OG	2.07	0.55
3:L:138:TYR:CD1	3:L:139:PRO:HA	2.42	0.55
1:A:192:VAL:HG23	1:A:193:SER:N	2.21	0.55
2:H:99:THR:CG2	2:H:101:ILE:O	2.55	0.55
2:H:176:VAL:O	2:H:182:TYR:HA	2.06	0.55
3:L:10:PHE:O	3:L:103:GLU:HG3	2.06	0.55
2:H:28:PHE:CD1	2:H:29:SER:N	2.75	0.55
2:H:158:THR:OG1	2:H:205:ALA:HB3	2.08	0.54
3:L:184:TYR:O	3:L:190:TYR:OH	2.24	0.54
3:L:65:GLY:HA3	3:L:70:TYR:HA	1.90	0.54
2:H:10:PRO:O	2:H:11:SER:HB2	2.07	0.54
1:A:132:ALA:C	1:A:134:GLN:N	2.55	0.54
2:H:150:LYS:HA	2:H:183:THR:HG23	1.90	0.54
2:H:130:PRO:O	2:H:131:LEU:HD23	2.09	0.53
1:A:101:ILE:N	1:A:101:ILE:HD12	2.23	0.53
2:H:120:SER:O	2:H:121:ALA:CB	2.54	0.53
2:H:199:THR:HA	2:H:216:LYS:NZ	2.23	0.53
3:L:114:SER:O	3:L:115:ILE:HB	2.09	0.53
1:A:98:PRO:O	1:A:183:ASN:HA	2.08	0.52
2:H:152:TYR:CE1	2:H:182:TYR:HB2	2.45	0.52
3:L:110:ALA:HB2	3:L:198:THR:HG21	1.91	0.52
1:A:106:TYR:O	1:A:110:MET:HG2	2.08	0.52
1:A:115:GLN:HG2	1:A:116:THR:H	1.73	0.52
2:H:34:GLY:O	2:H:99:THR:HB	2.08	0.52
2:H:25:VAL:HG22	2:H:77:SER:HB3	1.90	0.52
2:H:130:PRO:HD3	3:L:121:GLU:OE1	2.09	0.52
3:L:104:ILE:CG2	3:L:105:LYS:N	2.73	0.52
1:A:103:GLU:HG2	1:A:191:THR:HG1	1.74	0.52
3:L:189:SER:HA	3:L:207:PHE:O	2.09	0.52
3:L:134:LEU:HD21	3:L:194:ALA:HB2	1.92	0.52
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:CYS:O	1:A:276:LYS:HG3	2.10	0.52
2:H:131:LEU:HB2	2:H:146:GLY:O	2.10	0.52
1:A:94:ILE:O	1:A:95:SER:CB	2.57	0.51
2:H:91:THR:HG23	2:H:116:VAL:O	2.09	0.51
2:H:144:THR:HG22	2:H:189:THR:CG2	2.39	0.51
3:L:207:PHE:N	3:L:207:PHE:HD2	2.07	0.51
1:A:216:PHE:O	1:A:258:THR:HG22	2.10	0.51
1:A:207:MET:CE	1:A:241:TRP:HE3	2.21	0.51
2:H:144:THR:O	2:H:145:LEU:HD23	2.11	0.51
2:H:133:PRO:O	2:H:220:ARG:HD2	2.11	0.51
1:A:107:GLN:HB3	1:A:108:PRO:HD2	1.93	0.51
2:H:103:THR:HG22	2:H:103:THR:O	2.10	0.51
3:L:203:ILE:HD12	3:L:204:VAL:H	1.76	0.51
2:H:39:ARG:HG2	2:H:49:LEU:HD21	1.91	0.51
1:A:253:LEU:C	1:A:255:GLN:N	2.65	0.51
1:A:278:ILE:HG13	1:A:279:TYR:H	1.75	0.51
2:H:34:GLY:H	2:H:99:THR:HG21	1.76	0.51
2:H:52:ILE:HG12	2:H:72:LYS:HG2	1.92	0.51
2:H:72:LYS:HD2	2:H:74:ASN:OD1	2.10	0.51
1:A:136:THR:O	1:A:140:ARG:HB3	2.11	0.51
1:A:165:THR:OG1	1:A:166:SER:N	2.44	0.51
3:L:142:ILE:HG23	3:L:143:ASN:N	2.26	0.50
1:A:107:GLN:OE1	1:A:107:GLN:HA	2.12	0.50
1:A:239:GLU:HA	1:A:274:SER:O	2.12	0.50
1:A:145:LEU:HD21	1:A:192:VAL:CG2	2.42	0.50
2:H:175:ALA:HA	2:H:184:LEU:HB3	1.93	0.50
3:L:207:PHE:CD2	3:L:207:PHE:N	2.77	0.50
3:L:20:ILE:HG22	3:L:21:THR:N	2.26	0.50
1:A:249:ASP:C	1:A:250:SER:O	2.46	0.50
1:A:274:SER:HB2	2:H:101:ILE:HB	1.94	0.50
1:A:100:ASP:CG	1:A:100:ASP:O	2.51	0.49
1:A:202:ASP:HA	1:A:236:GLN:HG2	1.93	0.49
3:L:114:SER:OG	3:L:116:PHE:CE1	2.65	0.49
3:L:186:ARG:HG3	3:L:186:ARG:O	2.11	0.49
1:A:207:MET:CE	1:A:241:TRP:CE3	2.94	0.49
1:A:209:ASP:HB3	1:A:212:ARG:HG3	1.95	0.49
2:H:52:ILE:HD12	2:H:58:THR:CG2	2.42	0.49
3:L:159:ASN:HA	3:L:174:SER:O	2.12	0.49
1:A:81:ASP:O	1:A:84:SER:N	2.46	0.48
3:L:171:TYR:N	3:L:171:TYR:HD2	2.11	0.48
2:H:190:VAL:HB	2:H:191:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:LYS:NZ	2:H:89:ASP:HB2	2.27	0.48
1:A:256:ASP:OD2	1:A:256:ASP:C	2.51	0.48
1:A:279:TYR:CD2	1:A:279:TYR:N	2.81	0.48
2:H:17:GLN:HA	2:H:17:GLN:OE1	2.14	0.48
1:A:222:PHE:O	1:A:227:VAL:HG23	2.13	0.48
2:H:14:GLN:OE1	2:H:120:SER:HA	2.13	0.48
2:H:61:ASN:O	2:H:63:ALA:N	2.47	0.48
3:L:104:ILE:HB	3:L:164:GLN:NE2	2.28	0.48
1:A:211:SER:O	1:A:212:ARG:C	2.52	0.48
1:A:81:ASP:HB3	1:A:84:SER:HB2	1.96	0.48
2:H:126:PRO:HB3	2:H:152:TYR:CD2	2.49	0.48
3:L:104:ILE:HB	3:L:164:GLN:HE22	1.79	0.47
2:H:128:VAL:CG2	2:H:204:VAL:HG21	2.33	0.47
2:H:63:ALA:HB3	2:H:64:PHE:CD2	2.50	0.47
1:A:57:LYS:H	1:A:57:LYS:HD2	1.79	0.47
1:A:70:TYR:O	1:A:74:HIS:HB2	2.14	0.47
2:H:97:ALA:HB1	2:H:107:MET:HB2	1.96	0.47
1:A:225:VAL:O	1:A:229:ASN:ND2	2.40	0.47
1:A:278:ILE:CG1	1:A:279:TYR:N	2.78	0.47
2:H:14:GLN:O	2:H:17:GLN:HG2	2.14	0.47
3:L:53:LEU:O	3:L:54:GLU:CB	2.57	0.47
1:A:97:HIS:CE1	1:A:99:CYS:HB2	2.50	0.47
2:H:91:THR:O	2:H:92:ALA:HB2	2.14	0.47
1:A:255:GLN:O	1:A:256:ASP:C	2.52	0.47
2:H:13:VAL:HG11	2:H:86:LEU:CD1	2.45	0.47
1:A:114:THR:HA	1:A:195:ARG:HH12	1.80	0.47
2:H:124:THR:HG22	2:H:125:PRO:O	2.14	0.47
1:A:57:LYS:N	1:A:57:LYS:HD2	2.29	0.46
2:H:99:THR:HG22	2:H:99:THR:O	2.14	0.46
2:H:61:ASN:O	2:H:62:ALA:C	2.54	0.46
2:H:67:ARG:HB2	2:H:84:ASN:H	1.80	0.46
1:A:94:ILE:O	1:A:95:SER:HB2	2.15	0.46
2:H:146:GLY:CA	2:H:186:SER:O	2.63	0.46
2:H:162:ASN:HD22	2:H:165:SER:HB2	1.81	0.46
1:A:113:GLY:O	1:A:114:THR:C	2.54	0.46
1:A:192:VAL:CG2	1:A:193:SER:N	2.79	0.46
1:A:75:PRO:HD2	1:A:76:GLU:H	1.81	0.46
3:L:167:LYS:C	3:L:169:SER:H	2.19	0.46
3:L:199:SER:C	3:L:201:SER:H	2.18	0.46
2:H:216:LYS:HG2	2:H:217:ILE:N	2.31	0.46
3:L:110:ALA:HB1	3:L:111:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:CD2	1:A:149:LEU:HD13	2.51	0.46
3:L:196:HIS:CG	3:L:197:LYS:H	2.34	0.46
3:L:154:GLN:N	3:L:154:GLN:OE1	2.49	0.45
3:L:23:LYS:HA	3:L:68:LYS:O	2.16	0.45
2:H:72:LYS:NZ	2:H:74:ASN:HD21	2.14	0.45
1:A:117:VAL:HG12	1:A:143:PHE:CE2	2.51	0.45
2:H:4:GLN:HB2	2:H:26:SER:OG	2.17	0.45
3:L:89:GLN:O	3:L:94:PRO:HA	2.16	0.45
3:L:179:LEU:HD22	3:L:183:GLU:CG	2.46	0.45
2:H:200:VAL:N	2:H:216:LYS:HE3	2.28	0.45
1:A:57:LYS:O	1:A:58:ARG:C	2.55	0.45
1:A:232:PRO:C	1:A:234:LYS:H	2.20	0.45
1:A:75:PRO:C	1:A:77:MET:H	2.20	0.45
3:L:165:ASP:O	3:L:169:SER:HA	2.17	0.45
1:A:125:TRP:HZ3	1:A:146:GLU:OE1	2.00	0.45
1:A:216:PHE:O	1:A:258:THR:CG2	2.65	0.45
2:H:30:LEU:HB2	2:H:74:ASN:OD1	2.17	0.45
1:A:100:ASP:C	1:A:101:ILE:HD12	2.37	0.45
2:H:105:TYR:O	2:H:107:MET:HG2	2.17	0.45
3:L:115:ILE:O	3:L:115:ILE:CG1	2.65	0.44
3:L:168:ASP:N	3:L:168:ASP:OD1	2.50	0.44
1:A:115:GLN:CG	1:A:116:THR:H	2.30	0.44
2:H:126:PRO:CA	2:H:152:TYR:HB3	2.47	0.44
2:H:144:THR:CG2	2:H:189:THR:HG23	2.43	0.44
3:L:58:PRO:HG2	3:L:61:PHE:CD1	2.51	0.44
1:A:50:TRP:HB2	1:A:172:SER:OG	2.16	0.44
2:H:153:PHE:HA	2:H:154:PRO:HA	1.66	0.44
2:H:215:LYS:HE2	2:H:215:LYS:HB2	1.87	0.44
2:H:39:ARG:HD3	2:H:94:TYR:CZ	2.53	0.44
1:A:119:CYS:HB2	1:A:199:ALA:O	2.18	0.44
1:A:246:GLY:C	1:A:247:ARG:O	2.51	0.44
1:A:73:ILE:HG13	1:A:73:ILE:H	1.51	0.44
3:L:28:ILE:O	3:L:29:TYR:C	2.55	0.44
1:A:207:MET:SD	1:A:243:ILE:HD11	2.58	0.44
2:H:134:GLY:O	2:H:135:SER:C	2.57	0.44
2:H:199:THR:HA	2:H:216:LYS:HE3	1.99	0.44
3:L:18:VAL:HG12	3:L:19:THR:N	2.33	0.44
2:H:145:LEU:HD13	2:H:217:ILE:CG2	2.46	0.44
2:H:155:GLU:OE2	2:H:156:PRO:HA	2.18	0.44
1:A:69:LYS:O	1:A:73:ILE:HG13	2.17	0.43
2:H:142:MET:SD	2:H:191:PRO:HA	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PRO:HB2	1:A:121:LYS:HB2	1.99	0.43
1:A:149:LEU:O	1:A:152:TYR:HB3	2.18	0.43
1:A:217:ASP:O	1:A:220:SER:OG	2.29	0.43
2:H:13:VAL:HG11	2:H:86:LEU:HD11	2.01	0.43
1:A:56:THR:O	1:A:59:PHE:HB2	2.18	0.43
3:L:146:TRP:NE1	3:L:175:SER:HB3	2.33	0.43
2:H:151:GLY:C	2:H:181:LEU:HD22	2.39	0.43
2:H:41:SER:OG	2:H:44:LYS:HE3	2.18	0.43
3:L:14:LEU:CD1	3:L:79:THR:HG22	2.49	0.43
1:A:266:ILE:HG22	1:A:271:ILE:O	2.18	0.43
2:H:97:ALA:HB1	2:H:107:MET:CB	2.49	0.43
2:H:89:ASP:C	2:H:91:THR:N	2.71	0.43
1:A:248:GLU:HG2	1:A:249:ASP:H	1.79	0.43
1:A:263:GLU:HG3	1:A:273:PHE:HD2	1.82	0.43
1:A:63:VAL:HG12	1:A:63:VAL:O	2.19	0.43
2:H:173:PHE:HE1	3:L:173:MET:CA	2.32	0.43
3:L:188:ASN:O	3:L:208:ASN:HB3	2.19	0.43
3:L:17:ARG:HG2	3:L:74:ILE:O	2.18	0.43
3:L:164:GLN:HB2	3:L:171:TYR:CZ	2.53	0.42
3:L:37:GLN:C	3:L:83:ALA:HB1	2.39	0.42
1:A:59:PHE:HB3	1:A:60:PRO:HD3	2.01	0.42
1:A:78:ARG:C	1:A:80:VAL:H	2.23	0.42
2:H:152:TYR:OH	2:H:184:LEU:HD23	2.20	0.42
2:H:7:GLN:HB2	2:H:112:GLN:HE21	1.83	0.42
2:H:199:THR:HA	2:H:216:LYS:CE	2.50	0.42
3:L:80:GLU:H	3:L:80:GLU:CD	2.22	0.42
1:A:191:THR:HG22	1:A:192:VAL:N	2.34	0.42
1:A:156:ASP:C	1:A:157:LEU:HD23	2.40	0.42
1:A:273:PHE:O	2:H:102:THR:HB	2.19	0.42
3:L:96:PHE:N	3:L:96:PHE:HD2	2.18	0.42
3:L:145:LYS:HE3	3:L:152:GLU:OE2	2.20	0.41
1:A:163:PHE:N	1:A:163:PHE:HD2	2.16	0.41
3:L:21:THR:HB	3:L:23:LYS:NZ	2.36	0.41
2:H:11:SER:O	2:H:116:VAL:HA	2.20	0.41
2:H:37:TRP:HE1	2:H:79:VAL:HG11	1.85	0.41
2:H:68:LEU:HD12	2:H:69:SER:N	2.31	0.41
1:A:216:PHE:H	1:A:258:THR:HB	1.85	0.41
3:L:54:GLU:HA	3:L:54:GLU:OE1	2.21	0.41
3:L:165:ASP:C	3:L:167:LYS:H	2.23	0.41
3:L:17:ARG:HD3	3:L:17:ARG:O	2.21	0.41
3:L:22:CYS:C	3:L:23:LYS:HG3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:HIS:CD2	1:A:253:LEU:HD11	2.56	0.41
3:L:92:SER:OG	3:L:93:THR:N	2.54	0.41
2:H:191:PRO:HD2	2:H:194:THR:CG2	2.51	0.41
3:L:123:LEU:HD12	3:L:123:LEU:H	1.85	0.41
3:L:142:ILE:HG12	3:L:143:ASN:N	2.32	0.41
1:A:278:ILE:CG1	1:A:279:TYR:H	2.34	0.40
2:H:33:TYR:HB3	2:H:99:THR:HG22	2.03	0.40
1:A:266:ILE:HD13	1:A:266:ILE:HA	1.66	0.40
1:A:75:PRO:C	1:A:77:MET:N	2.75	0.40
3:L:21:THR:HB	3:L:23:LYS:HZ1	1.86	0.40
3:L:3:MET:HB2	3:L:96:PHE:C	2.41	0.40
2:H:143:VAL:CG1	2:H:190:VAL:HG23	2.44	0.40
3:L:36:GLN:HG3	3:L:85:TYR:CZ	2.56	0.40
2:H:52:ILE:HG23	2:H:52:ILE:O	2.21	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	228/257 (89%)	184 (81%)	30 (13%)	14 (6%)	2	9
2	H	211/220 (96%)	169 (80%)	28 (13%)	14 (7%)	1	7
3	L	206/211 (98%)	163 (79%)	38 (18%)	5 (2%)	7	31
All	All	645/688 (94%)	516 (80%)	96 (15%)	33 (5%)	2	13

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	251	ARG
2	H	10	PRO

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Mol	Chain	Res	Type
2	H	11	SER
2	H	101	ILE
2	H	121	ALA
3	L	75	THR
3	L	115	ILE
1	A	248	GLU
2	H	62	ALA
2	H	164	GLY
3	L	53	LEU
3	L	54	GLU
1	A	78	ARG
1	A	82	CYS
2	H	90	ASP
2	H	122	LYS
1	A	114	THR
1	A	133	HIS
1	A	212	ARG
2	H	135	SER
2	H	167	SER
1	A	98	PRO
1	A	250	SER
1	A	108	PRO
1	A	180	CYS
2	H	163	SER
3	L	183	GLU
1	A	168	ILE
1	A	118	PRO
2	H	188	VAL
2	H	154	PRO
2	H	156	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	208/238 (87%)	182 (88%)	26 (12%)	5 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	174/191 (91%)	157 (90%)	17 (10%)	9	33
3	L	183/187 (98%)	162 (88%)	21 (12%)	6	25
All	All	565/616 (92%)	501 (89%)	64 (11%)	7	26

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	64	LEU
1	A	71	THR
1	A	89	PHE
1	A	101	ILE
1	A	116	THR
1	A	121	LYS
1	A	126	SER
1	A	136	THR
1	A	142	MET
1	A	144	THR
1	A	146	GLU
1	A	156	ASP
1	A	163	PHE
1	A	176	TRP
1	A	181	SER
1	A	191	THR
1	A	206	VAL
1	A	213	SER
1	A	248	GLU
1	A	250	SER
1	A	251	ARG
1	A	256	ASP
1	A	258	THR
1	A	264	SER
1	A	266	ILE
2	H	21	ILE
2	H	24	THR
2	H	28	PHE
2	H	64	PHE
2	H	68	LEU
2	H	70	ILE
2	H	99	THR
2	H	101	ILE

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Mol	Chain	Res	Type
2	H	107	MET
2	H	108	ASP
2	H	112	GLN
2	H	114	THR
2	H	116	VAL
2	H	117	THR
2	H	177	LEU
2	H	201	THR
2	H	203	ASN
3	L	12	VAL
3	L	21	THR
3	L	25	SER
3	L	32	LEU
3	L	41	ASN
3	L	51	THR
3	L	87	CYS
3	L	96	PHE
3	L	102	LEU
3	L	103	GLU
3	L	157	VAL
3	L	171	TYR
3	L	173	MET
3	L	180	THR
3	L	185	GLU
3	L	186	ARG
3	L	191	THR
3	L	192	CYS
3	L	196	HIS
3	L	207	PHE
3	L	208	ASN

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

### 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 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 [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	230/257 (89%)	-0.11	1 (0%) 92 78	47, 74, 112, 139	0
2	H	215/220 (97%)	-0.04	5 (2%) 61 31	58, 102, 182, 204	0
3	L	208/211 (98%)	0.03	4 (1%) 67 38	70, 112, 150, 160	0
All	All	653/688 (94%)	-0.04	10 (1%) 74 47	47, 94, 159, 204	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	217	ILE	3.8
3	L	102	LEU	2.8
2	H	189	THR	2.8
3	L	109	ALA	2.7
2	H	132	ALA	2.7
2	H	199	THR	2.4
3	L	198	THR	2.3
1	A	164	ASP	2.2
3	L	47	ILE	2.2
2	H	145	LEU	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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.