



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 AM GMT

PDB ID : 2OSL  
Title : Crystal structure of Rituximab Fab in complex with an epitope peptide  
Authors : Du, J.; Zhong, C.; Ding, J.  
Deposited on : 2007-02-06  
Resolution : 2.60 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  
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

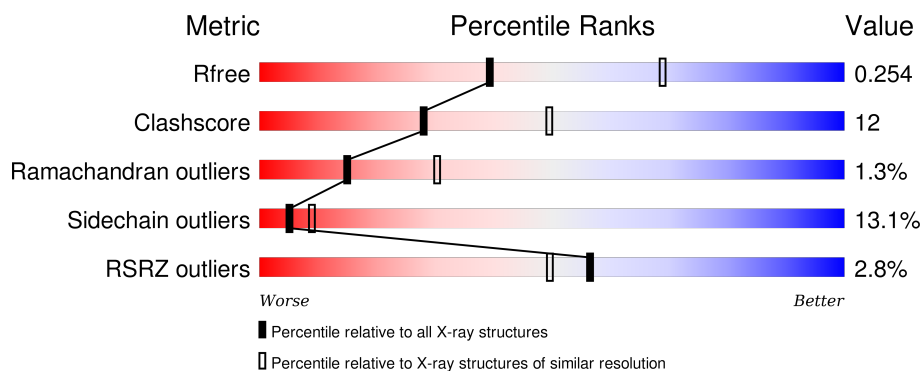
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	B	213	<div> <div>2%</div> <div>67% 28% 5%</div> </div>
1	L	213	<div> <div>72% 23% 5%</div> </div>
2	A	224	<div> <div>7% 67% 29% . .</div> </div>
2	H	224	<div> <div>3% 72% 22% 6%</div> </div>
3	P	25	<div> <div>64% 16% 20%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	25	 A horizontal bar chart showing the quality of chain Q. The bar is divided into three segments: a green segment representing 60%, a yellow segment representing 28%, and a grey segment representing 12%. The percentages are labeled below the corresponding segments.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7100 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 light chain of the Rituximab Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1623	1016	273	328	6			
1	B	213	Total	C	N	O	S	0	0	0
			1623	1016	273	328	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1669	1055	274	332	8			
2	A	221	Total	C	N	O	S	0	0	0
			1647	1043	270	327	7			

- Molecule 3 is a protein called B-lymphocyte antigen CD20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	20	Total	C	N	O	S	0	0	0
			153	93	24	34	2			
3	Q	22	Total	C	N	O	S	0	0	0
			173	106	27	38	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	47	Total	O	0	0
			47	47		
4	H	61	Total	O	0	0
			61	61		
4	L	51	Total	O	0	0
			51	51		

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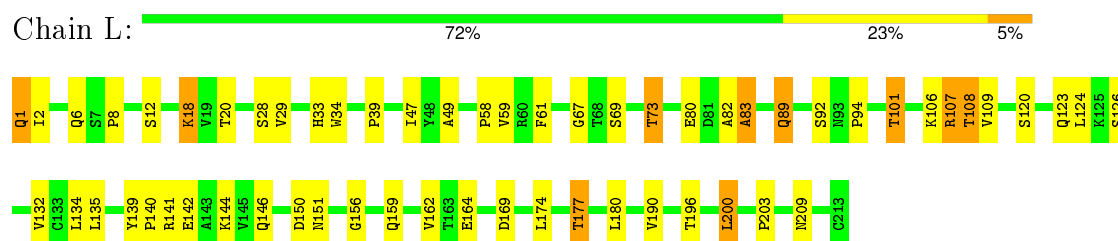
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	3	Total 3	O 3	0	0
4	Q	5	Total 5	O 5	0	0

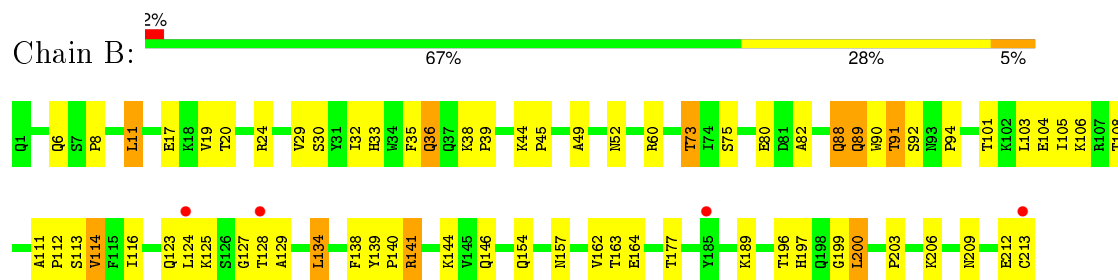
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

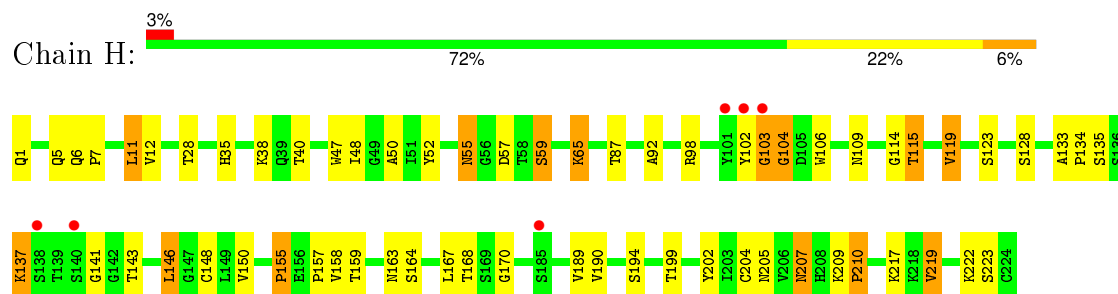
- Molecule 1: light chain of the Rituximab Fab fragment



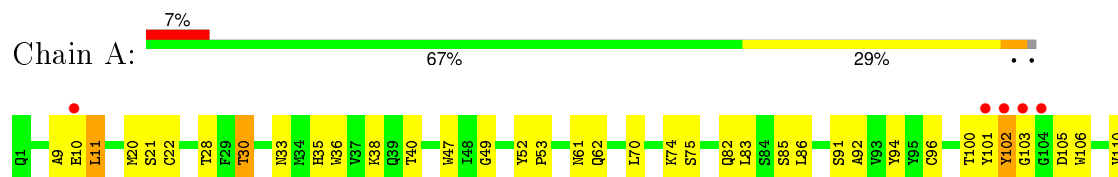
- Molecule 1: light chain of the Rituximab Fab fragment

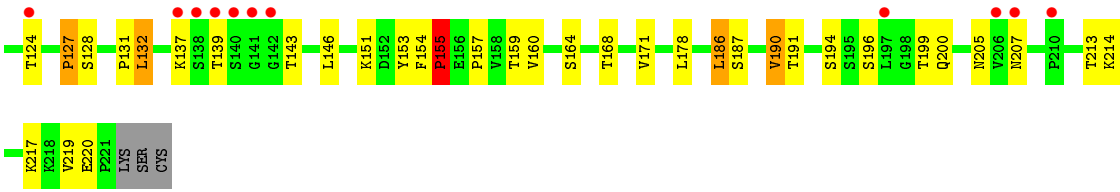


- Molecule 2: heavy chain of the Rituximab Fab fragment



- Molecule 2: heavy chain of the Rituximab Fab fragment





• Molecule 3: B-lymphocyte antigen CD20



• Molecule 3: B-lymphocyte antigen CD20



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.42Å 98.81Å 107.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.97 – 2.60 43.97 – 2.59	Depositor EDS
% Data completeness (in resolution range)	90.6 (43.97-2.60) 90.3 (43.97-2.59)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.296 0.238 , 0.254	Depositor DCC
$R_{free}$ test set	1496 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.7	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 29563 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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	B	0.41	0/1662	0.69	1/2260 (0.0%)
1	L	0.45	0/1662	0.72	0/2260
2	A	0.41	0/1691	0.70	1/2307 (0.0%)
2	H	0.45	0/1713	0.77	1/2334 (0.0%)
3	P	0.50	0/157	0.67	0/214
3	Q	0.43	0/178	0.59	0/243
All	All	0.43	0/7063	0.72	3/9618 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	SER	N-CA-C	-5.55	96.02	111.00
2	H	104	GLY	N-CA-C	-5.45	99.49	113.10
2	A	103	GLY	N-CA-C	-5.12	100.31	113.10

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	B	1623	0	1575	44	0
1	L	1623	0	1574	37	0
2	A	1647	0	1602	44	0
2	H	1669	0	1624	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	153	0	134	1	0
3	Q	173	0	149	6	0
4	A	45	0	0	8	0
4	B	47	0	0	6	0
4	H	61	0	0	4	0
4	L	51	0	0	9	0
4	P	3	0	0	0	0
4	Q	5	0	0	0	0
All	All	7100	0	6658	159	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 12.

All (159) 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:A:38:LYS:HE3	4:A:254:HOH:O	1.64	0.97
1:L:20:THR:HG22	1:L:73:THR:HB	1.52	0.89
2:A:100:THR:HG23	2:A:101:TYR:H	1.35	0.89
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.17	0.88
1:L:80:GLU:HG2	4:L:261:HOH:O	1.74	0.87
2:A:96:CYS:HB3	4:A:256:HOH:O	1.75	0.87
2:A:33:ASN:HD21	3:Q:173:SER:H	1.22	0.85
2:A:101:TYR:O	2:A:106:TRP:HA	1.80	0.81
2:H:102:TYR:HD2	2:H:106:TRP:NE1	1.81	0.79
2:H:102:TYR:HD2	2:H:106:TRP:HE1	1.30	0.78
1:L:135:LEU:HD13	4:L:264:HOH:O	1.85	0.77
1:B:197:HIS:CD2	1:B:199:GLY:H	2.04	0.75
2:A:92:ALA:HB3	4:A:254:HOH:O	1.88	0.74
2:H:164:SER:H	2:H:205:ASN:HD21	1.32	0.74
2:A:164:SER:H	2:A:205:ASN:HD21	1.36	0.73
2:A:22:CYS:SG	4:A:256:HOH:O	2.47	0.73
4:L:215:HOH:O	1:B:146:GLN:HG3	1.89	0.72
2:H:102:TYR:HB2	2:H:106:TRP:CZ2	2.24	0.72
2:A:100:THR:HG23	2:A:101:TYR:N	2.05	0.72
1:B:49:ALA:HB3	1:B:52:ASN:HD22	1.55	0.71
1:B:197:HIS:HD2	1:B:199:GLY:H	1.37	0.71
1:B:80:GLU:HB2	4:B:253:HOH:O	1.90	0.71
2:H:59:SER:HB2	3:P:172:PRO:HG3	1.71	0.71
1:L:174:LEU:HD22	4:L:264:HOH:O	1.91	0.70
2:A:146:LEU:HD13	2:A:219:VAL:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:127:PRO:HB3	2:A:153:TYR:HB3	1.72	0.69
1:B:30:SER:H	1:B:91:THR:HG21	1.58	0.67
1:B:197:HIS:HB3	1:B:200:LEU:HD22	1.77	0.67
2:A:137:LYS:HD3	2:A:194:SER:HB2	1.77	0.66
2:H:65:LYS:HB3	4:H:263:HOH:O	1.95	0.66
1:B:128:THR:HA	4:B:250:HOH:O	1.97	0.64
1:B:49:ALA:HB3	1:B:52:ASN:ND2	2.12	0.64
1:L:18:LYS:O	1:L:18:LYS:HG3	1.97	0.64
1:L:8:PRO:O	1:L:101:THR:HB	1.99	0.62
2:A:131:PRO:HD3	2:A:217:LYS:HZ3	1.63	0.62
1:B:112:PRO:HB3	1:B:138:PHE:HB3	1.81	0.62
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.07	0.62
1:L:196:THR:HG22	1:L:203:PRO:HB3	1.82	0.62
1:L:82:ALA:O	1:L:83:ALA:HB2	1.99	0.61
1:B:196:THR:HG22	1:B:203:PRO:HB3	1.82	0.61
1:B:111:ALA:HB1	1:B:200:LEU:HD13	1.84	0.60
2:A:33:ASN:ND2	3:Q:173:SER:H	1.98	0.60
2:A:83:LEU:HB3	2:A:86:LEU:HD21	1.84	0.59
1:B:139:TYR:CG	1:B:140:PRO:HA	2.40	0.57
2:H:98:ARG:HD2	4:H:284:HOH:O	2.03	0.57
1:B:35:PHE:HE1	1:B:88:GLN:HE21	1.52	0.57
1:B:141:ARG:NH1	1:B:162:VAL:HG21	2.19	0.57
1:B:8:PRO:O	1:B:101:THR:HG22	2.05	0.56
1:L:1:GLN:N	4:L:259:HOH:O	2.38	0.56
1:L:107:ARG:HD3	1:L:108:THR:O	2.06	0.56
2:H:167:LEU:HD21	2:H:190:VAL:HG11	1.87	0.56
2:H:52:TYR:HD2	2:H:55:ASN:HB2	1.71	0.56
1:B:101:THR:HG21	4:B:256:HOH:O	2.05	0.56
2:A:137:LYS:HD3	2:A:194:SER:CB	2.35	0.55
1:B:36:GLN:O	1:B:36:GLN:HG3	2.07	0.55
2:H:103:GLY:O	2:H:104:GLY:C	2.45	0.54
1:L:2:ILE:HD13	1:L:92:SER:HB3	1.89	0.54
2:H:11:LEU:HG	2:H:155:PRO:HG3	1.88	0.54
2:A:199:THR:O	2:A:199:THR:HG22	2.08	0.54
1:B:89:GLN:NE2	1:B:92:SER:H	2.05	0.54
1:B:20:THR:OG1	1:B:73:THR:HG23	2.09	0.53
1:L:132:VAL:HG22	1:L:177:THR:HB	1.89	0.53
2:A:38:LYS:HG3	4:A:254:HOH:O	2.09	0.53
2:A:102:TYR:CD2	2:A:106:TRP:CZ2	2.97	0.52
2:A:196:SER:O	2:A:200:GLN:HB3	2.09	0.52
1:B:101:THR:CG2	4:B:256:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:VAL:HA	2:A:205:ASN:O	2.09	0.52
2:H:35:HIS:CD2	2:H:50:ALA:HB2	2.45	0.52
1:B:144:LYS:HB3	1:B:196:THR:OG1	2.09	0.51
2:A:100:THR:CG2	2:A:101:TYR:H	2.16	0.51
1:B:11:LEU:HB3	1:B:103:LEU:HD12	1.92	0.51
2:A:47:TRP:CZ2	2:A:49:GLY:HA2	2.46	0.51
1:B:39:PRO:HG3	1:B:164:GLU:HG2	1.93	0.51
2:A:186:LEU:C	2:A:186:LEU:HD23	2.31	0.50
1:B:29:VAL:HG21	1:B:89:GLN:HG3	1.93	0.50
1:B:38:LYS:NZ	4:B:254:HOH:O	2.45	0.50
1:L:135:LEU:HB2	4:L:264:HOH:O	2.12	0.50
2:A:52:TYR:HB2	3:Q:172:PRO:HB2	1.93	0.49
1:B:114:VAL:HG22	1:B:206:LYS:HG3	1.95	0.49
2:H:109:ASN:OD1	4:H:284:HOH:O	2.20	0.49
1:L:150:ASP:O	1:L:151:ASN:HB2	2.11	0.49
1:L:80:GLU:CG	4:L:261:HOH:O	2.47	0.49
1:B:60:ARG:NH2	4:B:253:HOH:O	2.46	0.48
2:H:55:ASN:HB3	2:H:57:ASP:H	1.79	0.48
1:L:124:LEU:C	1:L:126:SER:H	2.17	0.48
1:L:20:THR:HG22	1:L:73:THR:CB	2.34	0.48
2:H:35:HIS:HD2	2:H:47:TRP:NE1	2.00	0.48
1:B:123:GLN:HG3	1:B:127:GLY:HA3	1.95	0.47
1:L:139:TYR:CG	1:L:140:PRO:HA	2.50	0.47
3:Q:177:SER:O	3:Q:181:GLN:HG2	2.15	0.47
2:H:7:PRO:O	2:H:115:THR:HB	2.14	0.47
1:B:29:VAL:CG2	1:B:89:GLN:HG3	2.44	0.46
1:L:6:GLN:NE2	1:L:101:THR:HG23	2.30	0.46
2:A:171:VAL:HG22	2:A:190:VAL:HG13	1.97	0.46
2:A:96:CYS:CB	4:A:256:HOH:O	2.47	0.46
2:A:9:ALA:HB2	2:A:157:PRO:HD3	1.96	0.46
2:A:20:MET:HE1	2:A:83:LEU:HD22	1.98	0.46
2:A:164:SER:H	2:A:205:ASN:ND2	2.10	0.46
1:L:82:ALA:O	1:L:83:ALA:CB	2.64	0.46
1:B:197:HIS:HB3	1:B:200:LEU:CD2	2.45	0.45
2:H:40:THR:HG22	2:H:92:ALA:HB2	1.98	0.45
1:L:141:ARG:NH1	1:L:162:VAL:HG21	2.31	0.45
1:B:89:GLN:HE22	1:B:92:SER:HB2	1.82	0.45
1:L:190:VAL:HG22	1:L:209:ASN:ND2	2.32	0.45
1:L:141:ARG:HH12	1:L:162:VAL:HG21	1.82	0.44
1:L:33:HIS:CE1	1:L:49:ALA:H	2.34	0.44
1:B:196:THR:CG2	1:B:203:PRO:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.98	0.44
1:B:33:HIS:HE1	2:A:105:ASP:OD2	2.00	0.44
2:H:103:GLY:O	2:H:104:GLY:O	2.36	0.44
3:Q:180:THR:HG22	3:Q:184:TYR:CE1	2.53	0.44
2:A:30:THR:HA	2:A:53:PRO:HB2	2.00	0.44
2:H:87:THR:HG23	4:H:250:HOH:O	2.16	0.44
2:A:124:THR:O	2:A:124:THR:HG23	2.17	0.44
1:L:6:GLN:HE21	1:L:101:THR:HG23	1.83	0.44
2:H:163:ASN:O	2:H:164:SER:HB2	2.18	0.44
2:H:12:VAL:O	2:H:119:VAL:HA	2.18	0.44
2:H:219:VAL:O	2:H:219:VAL:HG22	2.17	0.44
2:H:146:LEU:HD21	2:H:202:TYR:HB2	2.00	0.43
2:A:33:ASN:HD21	3:Q:173:SER:N	2.04	0.43
1:B:140:PRO:O	1:B:197:HIS:HE1	2.02	0.43
2:H:133:ALA:HA	2:H:134:PRO:HD3	1.71	0.43
2:A:154:PHE:HA	2:A:155:PRO:HA	1.81	0.43
1:L:29:VAL:HG11	1:L:89:GLN:HG3	2.00	0.43
1:L:169:ASP:C	1:L:169:ASP:OD2	2.56	0.43
2:H:170:GLY:O	2:H:190:VAL:HA	2.18	0.43
2:H:146:LEU:O	2:H:189:VAL:HA	2.19	0.43
1:B:116:ILE:O	1:B:116:ILE:HG23	2.18	0.43
2:A:132:LEU:HD12	2:A:132:LEU:HA	1.81	0.43
1:L:6:GLN:HB3	1:L:101:THR:HG22	1.99	0.43
2:A:213:THR:HA	4:A:245:HOH:O	2.18	0.43
1:B:139:TYR:CD1	1:B:140:PRO:HA	2.53	0.43
2:A:11:LEU:HG	2:A:155:PRO:HG3	2.00	0.43
1:B:212:GLU:O	1:B:213:CYS:HB2	2.19	0.43
1:L:39:PRO:HG3	1:L:164:GLU:HG2	2.01	0.42
1:L:58:PRO:HG2	1:L:61:PHE:HD1	1.83	0.42
1:B:6:GLN:HB3	1:B:101:THR:HG23	2.01	0.42
2:H:209:LYS:N	2:H:210:PRO:HD2	2.34	0.42
1:B:90:TRP:HH2	2:A:35:HIS:CE1	2.37	0.42
1:L:59:VAL:O	1:L:59:VAL:HG12	2.20	0.42
2:H:150:VAL:HG11	2:H:158:VAL:HG11	2.02	0.41
1:L:200:LEU:H	1:L:200:LEU:HG	1.70	0.41
2:A:207:ASN:ND2	2:A:214:LYS:HG3	2.35	0.41
1:L:174:LEU:CD2	4:L:264:HOH:O	2.62	0.41
2:A:101:TYR:HD2	4:A:230:HOH:O	2.03	0.41
2:A:47:TRP:CZ3	2:A:61:ASN:HB3	2.55	0.41
1:L:34:TRP:HB2	1:L:47:ILE:HB	2.02	0.41
2:H:52:TYR:CD2	2:H:55:ASN:HB2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:GLN:NE2	2:H:114:GLY:H	2.19	0.41
1:L:120:SER:OG	1:L:123:GLN:HB2	2.21	0.41
2:A:83:LEU:HD21	2:A:94:TYR:CZ	2.56	0.41
1:B:114:VAL:HA	1:B:134:LEU:O	2.21	0.41
1:L:141:ARG:NH1	4:L:230:HOH:O	2.45	0.41
2:H:159:THR:HB	2:H:207:ASN:HB3	2.03	0.41
2:A:36:TRP:CD1	2:A:70:LEU:HD22	2.56	0.41
1:B:82:ALA:HB2	1:B:105:ILE:HG12	2.03	0.40
1:B:154:GLN:HG3	1:B:157:ASN:HD21	1.87	0.40
1:L:180:LEU:HD23	1:L:180:LEU:N	2.36	0.40
1:B:44:LYS:HA	1:B:45:PRO:HD3	1.86	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	B	211/213 (99%)	199 (94%)	11 (5%)	1 (0%)	34	60
1	L	211/213 (99%)	201 (95%)	7 (3%)	3 (1%)	14	28
2	A	219/224 (98%)	202 (92%)	14 (6%)	3 (1%)	14	28
2	H	222/224 (99%)	205 (92%)	13 (6%)	4 (2%)	11	21
3	P	18/25 (72%)	16 (89%)	1 (6%)	1 (6%)	2	2
3	Q	20/25 (80%)	17 (85%)	3 (15%)	0	100	100
All	All	901/924 (98%)	840 (93%)	49 (5%)	12 (1%)	15	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	103	GLY

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Mol	Chain	Res	Type
1	B	129	ALA
2	A	62	GLN
1	L	83	ALA
2	H	137	LYS
2	A	85	SER
3	P	175	LYS
2	H	210	PRO
1	L	67	GLY
1	L	156	GLY
2	H	141	GLY
2	A	155	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	B	185/185 (100%)	160 (86%)	25 (14%)	5	8
1	L	185/185 (100%)	165 (89%)	20 (11%)	8	15
2	A	183/186 (98%)	156 (85%)	27 (15%)	4	6
2	H	186/186 (100%)	159 (86%)	27 (14%)	4	6
3	P	19/24 (79%)	17 (90%)	2 (10%)	8	16
3	Q	21/24 (88%)	20 (95%)	1 (5%)	31	58
All	All	779/790 (99%)	677 (87%)	102 (13%)	5	9

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	12	SER
1	L	18	LYS
1	L	28	SER
1	L	69	SER
1	L	73	THR
1	L	89	GLN

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Mol	Chain	Res	Type
1	L	94	PRO
1	L	101	THR
1	L	106	LYS
1	L	107	ARG
1	L	108	THR
1	L	109	VAL
1	L	134	LEU
1	L	142	GLU
1	L	144	LYS
1	L	146	GLN
1	L	159	GLN
1	L	177	THR
1	L	200	LEU
2	H	1	GLN
2	H	5	GLN
2	H	11	LEU
2	H	28	THR
2	H	55	ASN
2	H	59	SER
2	H	65	LYS
2	H	115	THR
2	H	119	VAL
2	H	123	SER
2	H	128	SER
2	H	135	SER
2	H	137	LYS
2	H	143	THR
2	H	146	LEU
2	H	148	CYS
2	H	155	PRO
2	H	157	PRO
2	H	168	THR
2	H	194	SER
2	H	199	THR
2	H	204	CYS
2	H	207	ASN
2	H	217	LYS
2	H	219	VAL
2	H	222	LYS
2	H	223	SER
1	B	11	LEU
1	B	17	GLU

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Mol	Chain	Res	Type
1	B	19	VAL
1	B	24	ARG
1	B	32	ILE
1	B	36	GLN
1	B	73	THR
1	B	75	SER
1	B	88	GLN
1	B	89	GLN
1	B	91	THR
1	B	94	PRO
1	B	104	GLU
1	B	106	LYS
1	B	108	THR
1	B	114	VAL
1	B	124	LEU
1	B	125	LYS
1	B	134	LEU
1	B	141	ARG
1	B	163	THR
1	B	177	THR
1	B	189	LYS
1	B	200	LEU
1	B	209	ASN
2	A	10	GLU
2	A	11	LEU
2	A	21	SER
2	A	28	THR
2	A	30	THR
2	A	40	THR
2	A	74	LYS
2	A	75	SER
2	A	82	GLN
2	A	91	SER
2	A	102	TYR
2	A	110	VAL
2	A	127	PRO
2	A	128	SER
2	A	132	LEU
2	A	139	THR
2	A	143	THR
2	A	151	LYS
2	A	155	PRO

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Mol	Chain	Res	Type
2	A	159	THR
2	A	168	THR
2	A	178	LEU
2	A	186	LEU
2	A	187	SER
2	A	190	VAL
2	A	191	THR
2	A	220	GLU
3	P	168	GLU
3	P	179	SER
3	Q	168	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	52	ASN
1	L	146	GLN
1	L	159	GLN
1	L	209	ASN
2	H	6	GLN
2	H	35	HIS
2	H	55	ASN
2	H	205	ASN
2	H	207	ASN
1	B	33	HIS
1	B	36	GLN
1	B	52	ASN
1	B	88	GLN
1	B	89	GLN
1	B	197	HIS
2	A	33	ASN
2	A	205	ASN
2	A	207	ASN
3	Q	181	GLN

### 5.3.3 RNA ⓘ

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	B	213/213 (100%)	-0.10	4 (1%) 70 64	24, 44, 78, 121	0
1	L	213/213 (100%)	-0.13	0 100 100	24, 40, 64, 90	0
2	A	221/224 (98%)	0.41	16 (7%) 18 13	30, 57, 97, 156	0
2	H	224/224 (100%)	-0.05	6 (2%) 58 51	23, 41, 73, 127	0
3	P	20/25 (80%)	0.09	0 100 100	36, 53, 83, 100	0
3	Q	22/25 (88%)	-0.17	0 100 100	34, 49, 62, 66	0
All	All	913/924 (98%)	0.03	26 (2%) 56 49	23, 45, 82, 156	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	140	SER	8.7
2	A	102	TYR	7.2
2	A	141	GLY	5.9
2	H	103	GLY	4.8
2	A	104	GLY	4.4
2	H	102	TYR	3.9
2	A	139	THR	3.8
2	A	206	VAL	3.5
2	A	103	GLY	3.4
2	H	138	SER	3.4
2	A	137	LYS	3.3
2	A	101	TYR	3.2
2	A	138	SER	3.1
1	B	213	CYS	3.0
2	A	142	GLY	3.0
2	A	210	PRO	2.9
2	H	140	SER	2.8
2	A	197	LEU	2.5
2	A	124	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	124	LEU	2.4
2	H	101	TYR	2.3
1	B	128	THR	2.3
2	A	207	ASN	2.2
2	A	10	GLU	2.2
2	H	185	SER	2.1
1	B	185	TYR	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.