



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:56 PM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

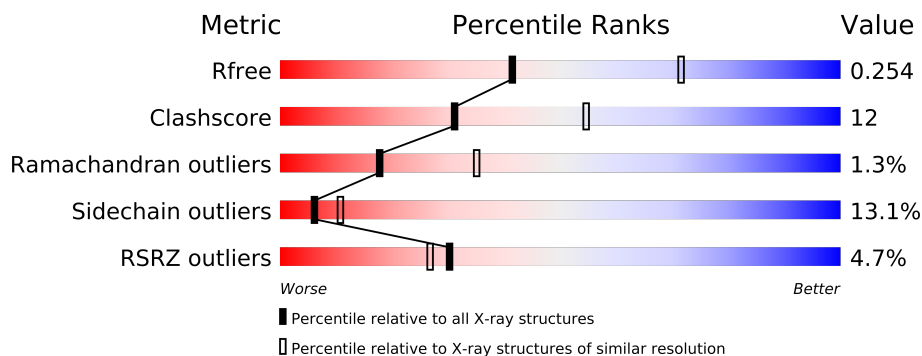
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	213	
1	L	213	
2	A	224	
2	H	224	
3	P	25	
3	Q	25	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7100 atoms, of which 0 are hydrogen and 0 are deuterium.

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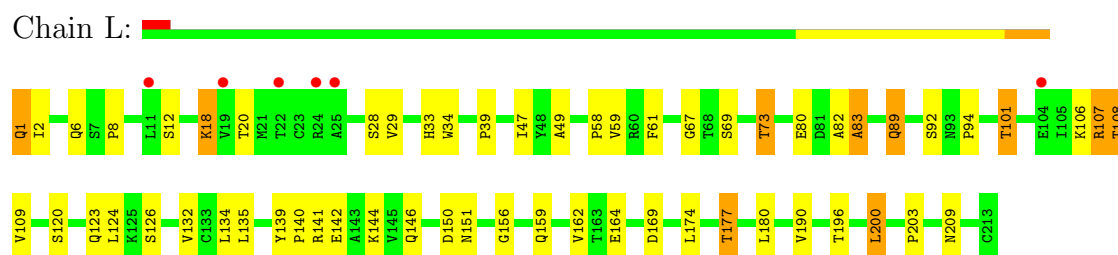
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	3	Total	O	0	0
			3	3		
4	Q	5	Total	O	0	0
			5	5		

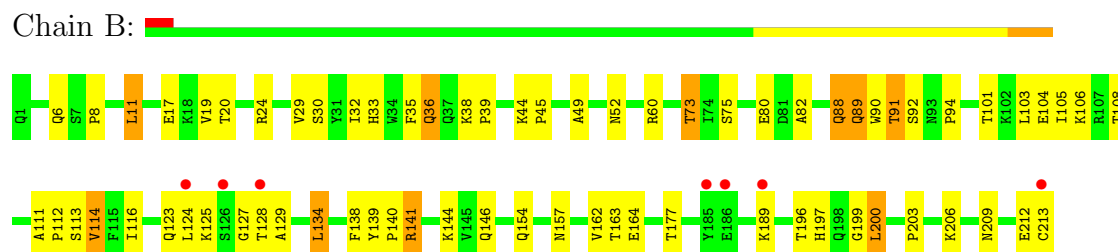
3 Residue-property plots

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.

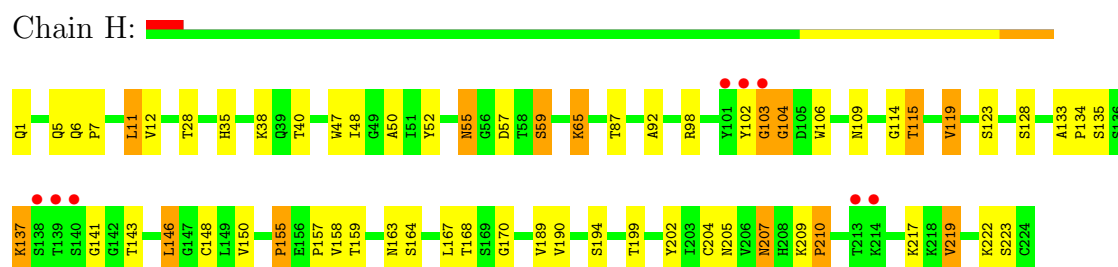
- Molecule 1: light chain of the Rituximab Fab fragment



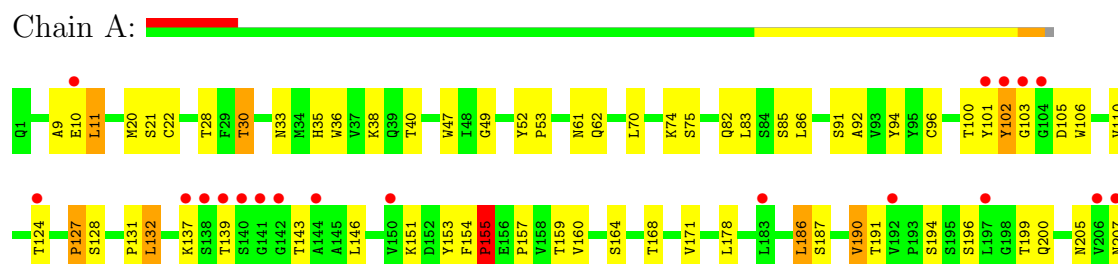
- Molecule 1: light chain of the Rituximab Fab fragment

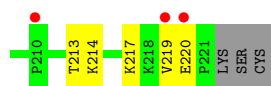


- Molecule 2: heavy chain of the Rituximab Fab fragment



- Molecule 2: heavy chain of the Rituximab Fab fragment





- Molecule 3: B-lymphocyte antigen CD20

Chain P:



- Molecule 3: B-lymphocyte antigen CD20

Chain Q:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	49.9	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.5	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1647	0	1602	44	0
2	H	1669	0	1624	34	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (159) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
2:A:160:VAL:HA	2:A:205:ASN:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	B	211/213 (99%)	199 (94%)	11 (5%)	1 (0%)	38	67
1	L	211/213 (99%)	201 (95%)	7 (3%)	3 (1%)	16	32
2	A	219/224 (98%)	202 (92%)	14 (6%)	3 (1%)	16	32
2	H	222/224 (99%)	205 (92%)	13 (6%)	4 (2%)	13	25
3	P	18/25 (72%)	16 (89%)	1 (6%)	1 (6%)	3	3
3	Q	20/25 (80%)	17 (85%)	3 (15%)	0	100	100
All	All	901/924 (98%)	840 (93%)	49 (5%)	12 (1%)	18	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	103	GLY
1	B	129	ALA
2	A	62	GLN
1	L	83	ALA
2	H	137	LYS
2	A	85	SER
3	P	175	LYS

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Mol	Chain	Res	Type
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%)	6	10
1	L	185/185 (100%)	165 (89%)	20 (11%)	9	17
2	A	183/186 (98%)	156 (85%)	27 (15%)	4	8
2	H	186/186 (100%)	159 (86%)	27 (14%)	5	8
3	P	19/24 (79%)	17 (90%)	2 (10%)	10	18
3	Q	21/24 (88%)	20 (95%)	1 (5%)	35	64
All	All	779/790 (99%)	677 (87%)	102 (13%)	6	11

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	B	213/213 (100%)	0.10	7 (3%)	44	41	24, 44, 78, 121	0
1	L	213/213 (100%)	0.01	6 (2%)	50	48	24, 40, 64, 90	0
2	A	221/224 (98%)	0.49	22 (9%)	8	5	30, 57, 97, 156	0
2	H	224/224 (100%)	0.03	8 (3%)	41	37	23, 41, 73, 127	0
3	P	20/25 (80%)	0.03	0	100	100	36, 53, 83, 100	0
3	Q	22/25 (88%)	-0.05	0	100	100	34, 49, 62, 66	0
All	All	913/924 (98%)	0.15	43 (4%)	30	27	23, 45, 82, 156	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	140	SER	9.4
2	A	102	TYR	7.7
2	A	141	GLY	7.5
2	A	104	GLY	4.7
2	H	140	SER	4.7
2	H	103	GLY	4.6
2	H	138	SER	4.6
2	A	139	THR	4.5
2	A	206	VAL	4.5
2	H	102	TYR	4.1
1	B	124	LEU	3.7
2	A	138	SER	3.6
2	A	103	GLY	3.6
2	A	101	TYR	3.5
1	B	213	CYS	3.3
2	A	142	GLY	3.2
2	A	207	ASN	2.9
1	B	128	THR	2.8
1	B	126	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	139	THR	2.8
1	B	186	GLU	2.7
1	B	185	TYR	2.7
2	H	101	TYR	2.6
2	H	214	LYS	2.6
2	A	137	LYS	2.6
2	H	213	THR	2.6
1	L	11	LEU	2.5
2	A	197	LEU	2.5
1	L	19	VAL	2.5
2	A	124	THR	2.4
2	A	150	VAL	2.4
1	L	24	ARG	2.3
2	A	219	VAL	2.3
2	A	10	GLU	2.3
2	A	210	PRO	2.3
1	L	25	ALA	2.2
2	A	144	ALA	2.1
2	A	192	VAL	2.1
2	A	220	GLU	2.1
1	L	22	THR	2.0
2	A	183	LEU	2.0
1	L	104	GLU	2.0
1	B	189	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.