



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:01 PM UTC

PDB ID : 2OSL / pdb_00002osl
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

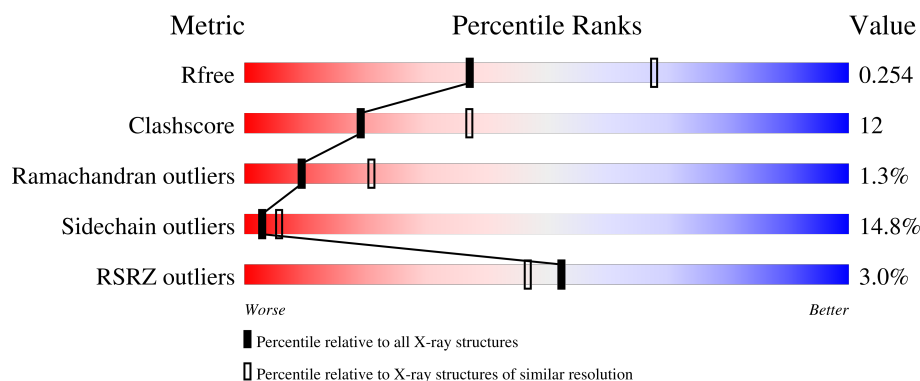
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	B	213	7% 66% 27% 7%
1	L	213	68% 25% 7%
2	A	224	7% 65% 29% ..
2	H	224	3% 67% 25% 7%
3	P	25	4% 64% 16% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	25	4% 56% 32% 12%

2 Entry composition

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, 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, 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	L	51	Total	O	0	0
			51	51		
4	H	61	Total	O	0	0
			61	61		
4	B	47	Total	O	0	0
			47	47		

Continued on next page...

Continued from previous page...

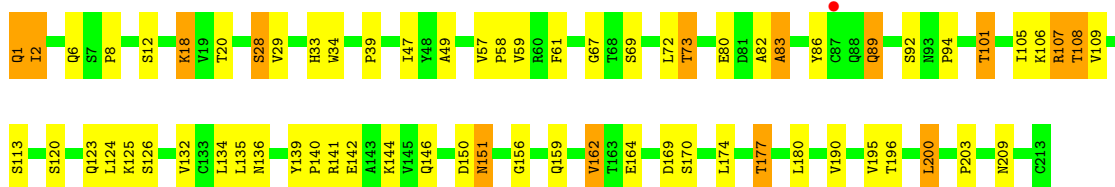
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total 45	O 45	0	0
4	P	3	Total 3	O 3	0	0
4	Q	5	Total 5	O 5	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

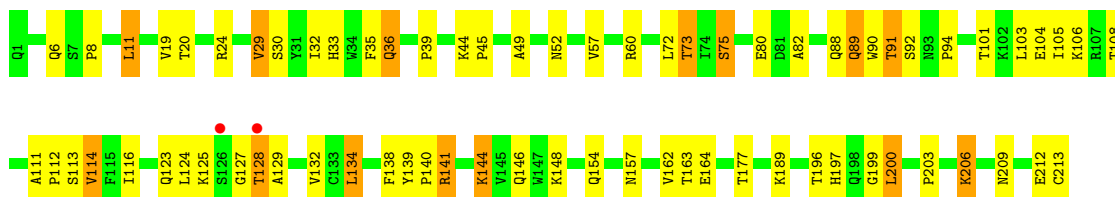
- Molecule 1: light chain of the Rituximab Fab fragment,light chain of the Rituximab Fab fragment

Chain L: 



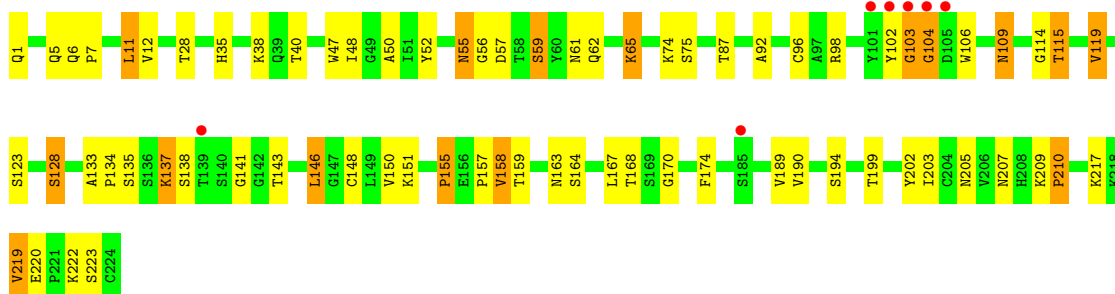
- Molecule 1: light chain of the Rituximab Fab fragment,light chain of the Rituximab Fab fragment

Chain B: 

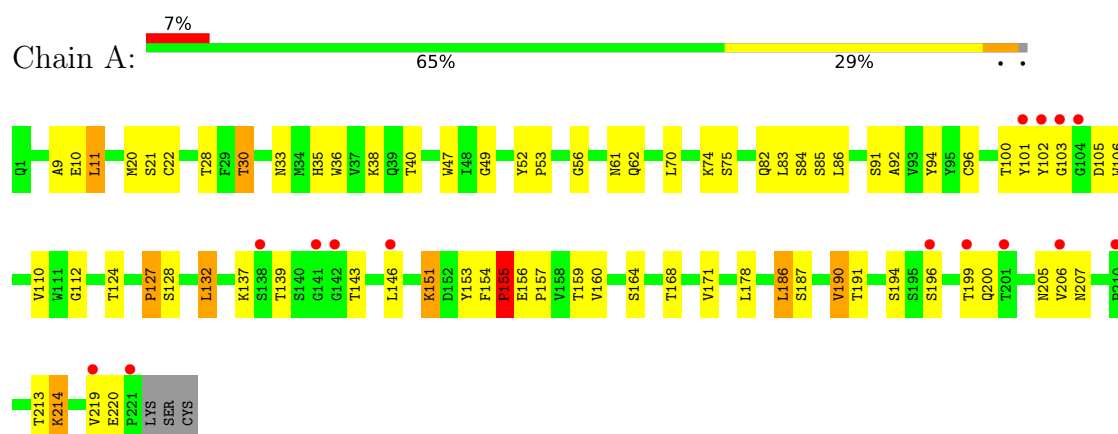


- Molecule 2: heavy chain of the Rituximab Fab fragment,heavy chain of the Rituximab Fab fragment

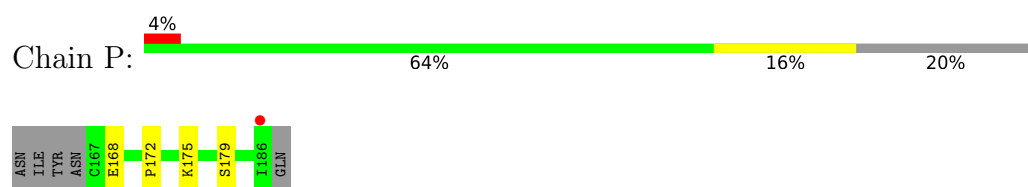
Chain H: 



- Molecule 2: heavy chain of the Rituximab Fab fragment,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, α , β , γ	96.42Å 98.81Å 107.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.97 – 2.60 43.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.6 (43.97-2.60) 90.6 (43.97-2.60)	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	1518 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	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.

²Theoretical 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	B	0.50	0/1662	1.00	6/2260 (0.3%)
1	L	0.54	0/1662	1.05	8/2260 (0.4%)
2	A	0.49	0/1691	0.99	5/2307 (0.2%)
2	H	0.54	0/1713	1.10	10/2334 (0.4%)
3	P	0.57	0/157	1.05	0/214
3	Q	0.48	0/178	1.09	2/243 (0.8%)
All	All	0.52	0/7063	1.04	31/9618 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	SER	N-CA-C	-8.11	96.02	109.24
2	A	56	GLY	N-CA-C	-7.90	104.41	115.32
2	H	56	GLY	N-CA-C	-7.56	104.06	114.64
1	L	113	SER	N-CA-C	-6.78	97.68	108.73
2	H	61	ASN	N-CA-C	-6.71	98.68	109.96
1	L	28	SER	N-CA-C	6.59	119.53	110.24
1	L	136	ASN	N-CA-C	6.47	119.49	109.07
2	H	128	SER	N-CA-C	-6.42	99.23	109.76
2	H	138	SER	N-CA-C	-6.24	104.36	112.23
3	Q	171	ASN	CA-C-N	6.08	127.44	119.84
3	Q	171	ASN	C-N-CA	6.08	127.44	119.84
1	B	57	VAL	CA-C-N	6.04	126.39	119.92
1	B	57	VAL	C-N-CA	6.04	126.39	119.92
2	A	151	LYS	N-CA-C	6.03	119.32	109.06
2	H	174	PHE	N-CA-C	5.99	118.35	110.08
2	H	96	CYS	N-CA-C	-5.94	99.71	109.40
1	L	57	VAL	CA-C-N	5.92	125.88	119.78
1	L	57	VAL	C-N-CA	5.92	125.88	119.78
2	H	151	LYS	N-CA-C	5.89	119.16	109.85
2	H	104	GLY	N-CA-C	-5.78	99.49	113.18
1	B	132	VAL	N-CA-C	5.68	116.07	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	SER	N-CA-C	5.66	117.25	111.14
2	A	84	SER	N-CA-C	5.62	118.97	109.76
2	A	103	GLY	N-CA-C	-5.43	100.31	113.18
1	L	86	TYR	N-CA-C	5.36	118.22	109.59
2	H	75	SER	N-CA-C	5.27	117.02	111.28
2	A	112	GLY	N-CA-C	-5.21	104.67	112.89
1	B	128	THR	N-CA-C	5.13	118.81	112.24
1	L	170	SER	N-CA-C	5.13	118.80	112.24
1	L	195	VAL	N-CA-C	5.08	115.44	108.12
2	H	109	ASN	N-CA-C	5.06	119.09	113.02

There are no chirality outliers.

There are no planarity outliers.

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	B	1623	0	1575	43	0
1	L	1623	0	1574	38	0
2	A	1647	0	1602	43	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	5	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	158	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 (158) 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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:GLY:O	2:H:104:GLY:C	2.45	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: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:186:LEU:C	2:A:186:LEU:HD23	2.31	0.56
2:A:137:LYS:HD3	2:A:194:SER:CB	2.35	0.55
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:HG22	2:A:199:THR:O	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
1:L:124:LEU:C	1:L:126:SER:H	2.17	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:20:MET:HE1	2:A:83:LEU:HD22	1.90	0.52
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
1:L:1:GLN:N	4:L:259:HOH:O	2.38	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
1:B:29:VAL:HG21	1:B:89:GLN:HG3	1.93	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
1:L:150:ASP:O	1:L:151:ASN:HB2	2.11	0.49
2:H:109:ASN:OD1	4:H:284:HOH:O	2.20	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
1:L:169:ASP:OD2	1:L:169:ASP:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLN:O	1:B:36:GLN:HG3	2.07	0.48
2:H:55:ASN:HB3	2:H:57:ASP:H	1.79	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: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:L:141:ARG:NH1	1:L:162:VAL:HG21	2.31	0.45
2:H:40:THR:HG22	2:H:92:ALA:HB2	1.98	0.45
1:B:197:HIS:HB3	1:B:200:LEU:CD2	2.45	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:33:HIS:CE1	1:L:49:ALA:H	2.34	0.44
1:L:141:ARG:HH12	1:L:162:VAL:HG21	1.82	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
1:B:196:THR:CG2	1:B:203:PRO:HB3	2.48	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
1:L:6:GLN:HE21	1:L:101:THR:HG23	1.83	0.44
2:H:12:VAL:O	2:H:119:VAL:HA	2.18	0.44
2:H:219:VAL:HG22	2:H:219:VAL:O	2.17	0.44
2:A:124:THR:O	2:A:124:THR:HG23	2.17	0.44
2:H:146:LEU:HD21	2:H:202:TYR:HB2	2.00	0.43
1:L:29:VAL:HG11	1:L:89:GLN:HG3	2.00	0.43
2:H:133:ALA:HA	2:H:134:PRO:HD3	1.71	0.43
2:H:163:ASN:O	2:H:164:SER:HB2	2.18	0.43
1:B:140:PRO:O	1:B:197:HIS:HE1	2.02	0.43
2:A:33:ASN:HD21	3:Q:173:SER:N	2.04	0.43
2:A:154:PHE:HA	2:A:155:PRO:HA	1.81	0.43
2:H:170:GLY:O	2:H:190:VAL:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:LEU:O	2:H:189:VAL:HA	2.19	0.43
1:L:72:LEU:C	1:L:72:LEU:HD23	2.44	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
1:B:212:GLU:O	1:B:213:CYS:HB2	2.19	0.43
2:A:11:LEU:HG	2:A:155:PRO:HG3	2.00	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
2:H:209:LYS:N	2:H:210:PRO:HD2	2.34	0.42
1:B:6:GLN:HB3	1:B:101:THR:HG23	2.01	0.42
1:B:90:TRP:HH2	2:A:35:HIS:CE1	2.37	0.42
1:L:59:VAL:HG12	1:L:59:VAL:O	2.20	0.42
1:L:200:LEU:H	1:L:200:LEU:HG	1.70	0.41
2:H:150:VAL:HG11	2:H:158:VAL:HG11	2.02	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
1:L:34:TRP:HB2	1:L:47:ILE:HB	2.02	0.41
2:A:47:TRP:CZ3	2:A:61:ASN:HB3	2.55	0.41
2:A:101:TYR:HD2	4:A:230:HOH:O	2.03	0.41
2:H:6:GLN:NE2	2:H:114:GLY:H	2.19	0.41
2:H:52:TYR:CD2	2:H:55:ASN:HB2	2.52	0.41
1:L:120:SER:OG	1:L:123:GLN:HB2	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
1:B:114:VAL:HA	1:B:134:LEU:O	2.21	0.41
2:A:36:TRP:CD1	2:A:70:LEU:HD22	2.56	0.41
2:A:83:LEU:HD21	2:A:94:TYR:CZ	2.56	0.41
1:B:82:ALA:HB2	1:B:105:ILE:HG12	2.03	0.40
1:L:180:LEU:HD23	1:L:180:LEU:N	2.36	0.40
1:B:154:GLN:HG3	1:B:157:ASN:HD21	1.87	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%)	24	46
1	L	211/213 (99%)	201 (95%)	7 (3%)	3 (1%)	9	19
2	A	219/224 (98%)	202 (92%)	14 (6%)	3 (1%)	9	19
2	H	222/224 (99%)	205 (92%)	13 (6%)	4 (2%)	6	14
3	P	18/25 (72%)	16 (89%)	1 (6%)	1 (6%)	1	1
3	Q	20/25 (80%)	17 (85%)	3 (15%)	0	100	100
All	All	901/924 (98%)	840 (93%)	49 (5%)	12 (1%)	9	21

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
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%)	157 (85%)	28 (15%)	3	5
1	L	185/185 (100%)	160 (86%)	25 (14%)	4	7
2	A	183/186 (98%)	154 (84%)	29 (16%)	2	4
2	H	186/186 (100%)	156 (84%)	30 (16%)	2	4
3	P	19/24 (79%)	17 (90%)	2 (10%)	6	14
3	Q	21/24 (88%)	20 (95%)	1 (5%)	23	47
All	All	779/790 (99%)	664 (85%)	115 (15%)	3	6

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	2	ILE
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	105	ILE
1	L	106	LYS
1	L	107	ARG
1	L	108	THR
1	L	109	VAL
1	L	125	LYS
1	L	134	LEU
1	L	142	GLU
1	L	144	LYS
1	L	146	GLN
1	L	151	ASN
1	L	159	GLN
1	L	162	VAL
1	L	177	THR
1	L	200	LEU
2	H	1	GLN
2	H	5	GLN
2	H	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	28	THR
2	H	55	ASN
2	H	59	SER
2	H	62	GLN
2	H	65	LYS
2	H	74	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	158	VAL
2	H	168	THR
2	H	194	SER
2	H	199	THR
2	H	203	ILE
2	H	217	LYS
2	H	219	VAL
2	H	220	GLU
2	H	222	LYS
2	H	223	SER
1	B	11	LEU
1	B	19	VAL
1	B	24	ARG
1	B	29	VAL
1	B	32	ILE
1	B	36	GLN
1	B	72	LEU
1	B	73	THR
1	B	75	SER
1	B	89	GLN
1	B	91	THR
1	B	94	PRO
1	B	104	GLU
1	B	106	LYS
1	B	108	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	114	VAL
1	B	124	LEU
1	B	125	LYS
1	B	134	LEU
1	B	141	ARG
1	B	144	LYS
1	B	148	LYS
1	B	163	THR
1	B	177	THR
1	B	189	LYS
1	B	200	LEU
1	B	206	LYS
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	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	156	GLU
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	206	VAL
2	A	214	LYS
2	A	220	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	168	GLU
3	P	179	SER
3	Q	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	52	ASN
1	L	136	ASN
1	L	146	GLN
1	L	159	GLN
1	L	209	ASN
2	H	6	GLN
2	H	35	HIS
2	H	39	GLN
2	H	55	ASN
2	H	172	HIS
2	H	205	ASN
2	H	207	ASN
1	B	36	GLN
1	B	52	ASN
1	B	88	GLN
1	B	89	GLN
1	B	197	HIS
1	B	198	GLN
2	A	33	ASN
2	A	179	GLN
2	A	205	ASN
2	A	207	ASN
3	Q	176	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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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%)	0.16	2 (0%) 81 78	24, 44, 78, 121	0
1	L	213/213 (100%)	-0.10	1 (0%) 87 85	24, 40, 64, 90	0
2	A	221/224 (98%)	0.53	15 (6%) 23 19	30, 57, 97, 156	0
2	H	224/224 (100%)	0.05	7 (3%) 51 45	23, 41, 73, 127	0
3	P	20/25 (80%)	0.54	1 (5%) 34 28	36, 53, 83, 100	0
3	Q	22/25 (88%)	0.01	1 (4%) 38 32	34, 49, 62, 66	0
All	All	913/924 (98%)	0.17	27 (2%) 52 47	23, 45, 82, 156	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	103	GLY	7.5
2	A	102	TYR	6.9
2	H	102	TYR	6.0
2	A	104	GLY	4.6
2	A	101	TYR	4.5
2	A	219	VAL	4.4
2	H	104	GLY	3.8
3	P	186	ILE	3.8
2	A	141	GLY	3.6
2	H	101	TYR	3.5
2	H	139	THR	3.2
2	A	221	PRO	2.7
1	B	126	SER	2.7
2	A	103	GLY	2.7
3	Q	186	ILE	2.7
2	A	210	PRO	2.6
2	A	196	SER	2.4
2	A	138	SER	2.2
2	A	199	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	142	GLY	2.2
2	A	146	LEU	2.2
2	H	185	SER	2.1
1	B	128	THR	2.1
2	H	105	ASP	2.1
2	A	206	VAL	2.1
2	A	201	THR	2.1
1	L	87	CYS	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 oligosaccharides 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.