



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:31 PM GMT

PDB ID : 3AAZ
Title : Crystal structure of the humanized recombinant Fab fragment of a murine;
antibody
Authors : Streltsov, V.A.
Deposited on : 2009-11-28
Resolution : 2.20 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>

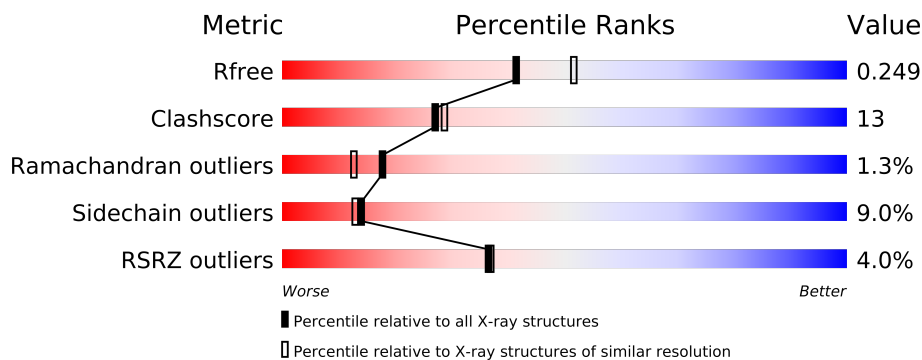
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	A	229	
1	H	229	
2	B	229	
2	L	229	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7401 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 Humanized recombinant Fab fragment of a murine; antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1747	1106	296	338	7			
1	H	229	Total	C	N	O	S	0	0	0
			1751	1108	297	339	7			

- Molecule 2 is a protein called Humanized recombinant Fab fragment of a murine; antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1764	1105	295	358	6			
2	L	228	Total	C	N	O	S	0	0	0
			1756	1101	294	355	6			

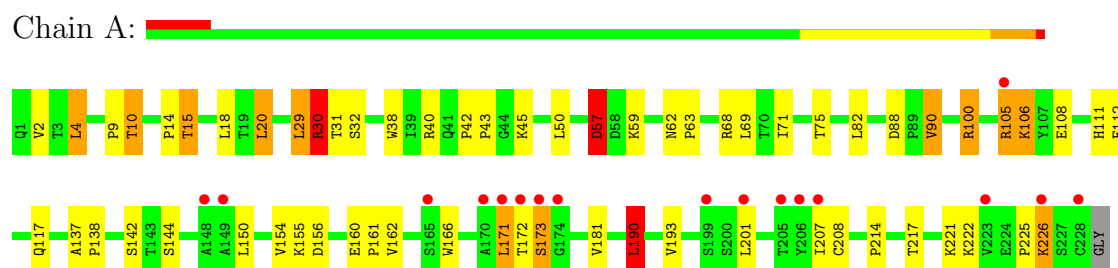
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	77	Total	O	0	0
			77	77		
3	H	125	Total	O	0	0
			125	125		
3	L	76	Total	O	0	0
			76	76		

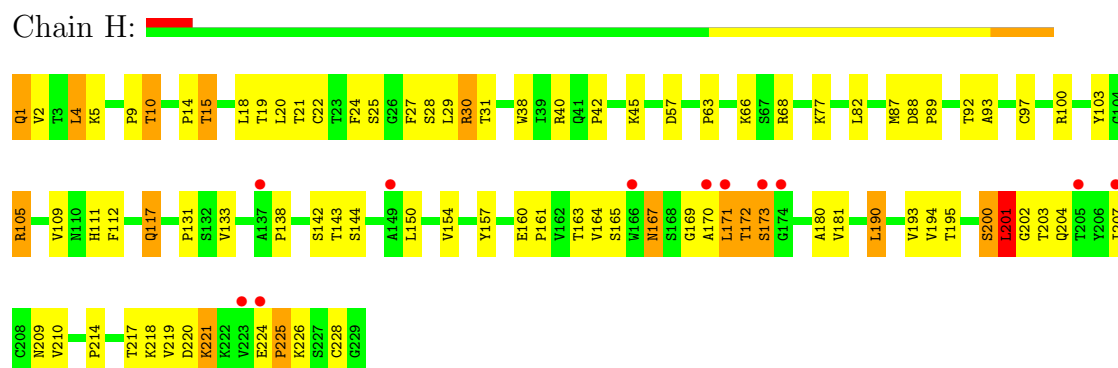
3 Residue-property plots

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.

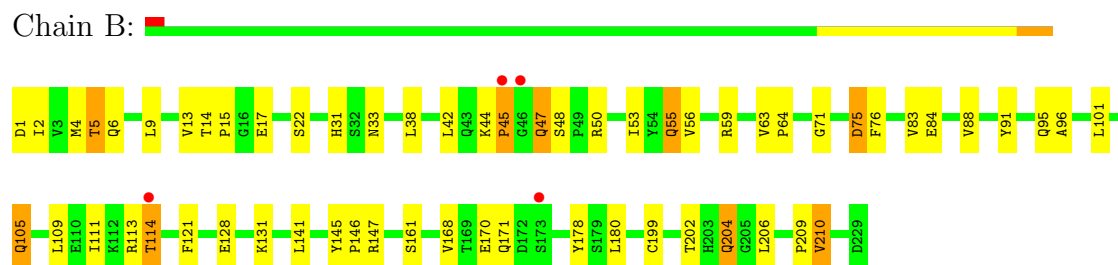
- Molecule 1: Humanized recombinant Fab fragment of a murine; antibody



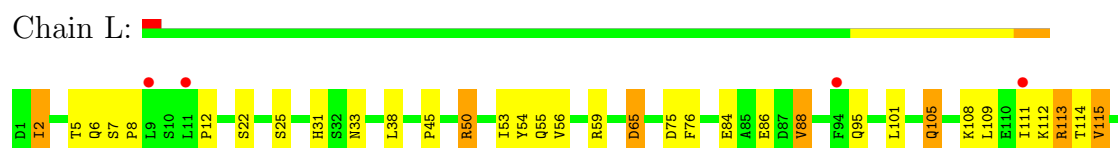
- Molecule 1: Humanized recombinant Fab fragment of a murine; antibody



- Molecule 2: Humanized recombinant Fab fragment of a murine; antibody



- Molecule 2: Humanized recombinant Fab fragment of a murine; antibody





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	106.73Å 106.73Å 90.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.03 – 2.20 46.02 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (46.03-2.20) 92.6 (46.02-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.271 0.224 , 0.249	Depositor DCC
R_{free} test set	2734 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 10.6	EDS
Estimated twinning fraction	0.033 for -h,-k,l 0.477 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54407 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7401	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	0/1792	0.90	7/2445 (0.3%)
1	H	0.84	1/1796 (0.1%)	0.90	7/2450 (0.3%)
2	B	0.72	1/1803 (0.1%)	0.75	0/2450
2	L	0.72	0/1795	0.76	0/2439
All	All	0.77	2/7186 (0.0%)	0.83	14/9784 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	97	CYS	CB-SG	-7.30	1.69	1.82
2	B	199	CYS	CB-SG	-5.16	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	40	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	H	201	LEU	CA-CB-CG	6.67	130.65	115.30
1	A	4	LEU	CA-CB-CG	6.55	130.37	115.30
1	H	4	LEU	CA-CB-CG	6.10	129.33	115.30
1	H	29	LEU	CA-CB-CG	5.88	128.83	115.30
1	H	68	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	H	201	LEU	N-CA-C	-5.83	95.26	111.00
1	A	190	LEU	CA-CB-CG	5.62	128.24	115.30
1	H	68	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	29	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	100	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	171	LEU	CA-CB-CG	-5.25	103.22	115.30
1	A	106	LYS	N-CA-C	-5.09	97.26	111.00
1	A	40	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	A	1747	0	1735	44	0
1	H	1751	0	1739	54	0
2	B	1764	0	1707	44	0
2	L	1756	0	1704	41	0
3	A	105	0	0	6	0
3	B	77	0	0	5	0
3	H	125	0	0	8	0
3	L	76	0	0	7	0
All	All	7401	0	6885	181	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 13.

All (181) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:105:ARG:HG3	1:H:105:ARG:HH21	1.00	1.10
1:A:105:ARG:HG3	1:A:105:ARG:HH21	1.10	1.09
1:A:29:LEU:O	1:A:30:ARG:HB2	1.52	1.07
2:B:105:GLN:NE2	2:B:105:GLN:H	1.64	0.96
2:L:31:HIS:HD2	2:L:33:ASN:H	1.18	0.90
1:H:105:ARG:HG3	1:H:105:ARG:NH2	1.82	0.89
2:B:105:GLN:HE21	2:B:105:GLN:H	0.93	0.89
1:A:14:PRO:O	1:A:15:THR:HB	1.70	0.89
1:A:105:ARG:NH2	1:A:105:ARG:HG3	1.85	0.88
3:A:235:HOH:O	1:H:15:THR:HG21	1.75	0.86
1:H:209:ASN:HA	3:H:303:HOH:O	1.74	0.86
1:H:105:ARG:HH21	1:H:105:ARG:CG	1.85	0.85
2:B:31:HIS:HD2	2:B:33:ASN:H	1.24	0.83
2:B:31:HIS:CD2	2:B:33:ASN:H	1.99	0.80
1:A:59:LYS:HE3	1:A:71:ILE:O	1.81	0.80
1:A:208:CYS:HA	3:A:286:HOH:O	1.82	0.78
2:L:113:ARG:HD3	2:L:114:THR:O	1.84	0.77
1:A:15:THR:HG21	3:H:266:HOH:O	1.85	0.77
1:H:14:PRO:O	1:H:15:THR:HB	1.84	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:31:HIS:CD2	2:L:33:ASN:H	2.03	0.76
2:B:105:GLN:N	2:B:105:GLN:HE21	1.78	0.76
1:A:30:ARG:HG2	1:A:75:THR:HB	1.68	0.74
2:B:1:ASP:HB2	3:B:293:HOH:O	1.88	0.73
2:L:105:GLN:H	2:L:105:GLN:HE21	1.35	0.73
1:A:154:VAL:HB	1:A:190:LEU:HD22	1.71	0.73
1:H:160:GLU:HG3	1:H:161:PRO:HA	1.70	0.72
2:L:2:ILE:HG22	3:L:240:HOH:O	1.90	0.71
1:H:167:ASN:HB2	1:H:171:LEU:HG	1.71	0.71
1:A:88:ASP:OD1	1:A:90:VAL:HG12	1.89	0.71
1:A:138:PRO:HB2	1:A:201:LEU:HD11	1.73	0.71
1:H:103:TYR:HB2	1:H:109:VAL:HG22	1.72	0.70
2:B:45:PRO:HB3	2:B:170:GLU:HG3	1.73	0.70
2:L:105:GLN:H	2:L:105:GLN:NE2	1.90	0.70
1:A:166:TRP:CE3	3:A:286:HOH:O	2.44	0.69
1:A:105:ARG:CG	1:A:105:ARG:HH21	1.99	0.67
2:L:6:GLN:H	2:L:105:GLN:HE22	1.42	0.67
1:A:111:HIS:HE1	3:B:230:HOH:O	1.78	0.67
1:H:88:ASP:OD2	1:H:89:PRO:HD2	1.95	0.67
1:H:172:THR:OG1	1:H:173:SER:N	2.26	0.67
1:A:111:HIS:HD2	1:A:112:PHE:O	1.78	0.66
1:A:105:ARG:HD3	1:A:106:LYS:NZ	2.11	0.66
1:H:133:VAL:HG21	1:H:210:VAL:HG21	1.78	0.65
1:A:43:PRO:HD2	3:A:231:HOH:O	1.96	0.64
1:H:111:HIS:HD2	1:H:112:PHE:O	1.81	0.62
1:H:10:THR:HG21	1:H:214:PRO:HG3	1.81	0.62
2:L:55:GLN:O	2:L:56:VAL:HB	2.00	0.62
1:H:103:TYR:HB2	1:H:109:VAL:CG2	2.30	0.61
2:L:112:LYS:HD2	2:L:145:TYR:OH	2.00	0.61
1:H:200:SER:O	1:H:201:LEU:HG	2.02	0.60
2:B:38:LEU:HD22	2:B:76:PHE:CG	2.38	0.59
2:L:6:GLN:H	2:L:105:GLN:NE2	1.99	0.59
2:L:88:VAL:HG22	2:L:109:LEU:O	2.02	0.59
2:L:101:LEU:HD23	2:L:101:LEU:N	2.16	0.58
2:B:53:ILE:HD13	2:B:59:ARG:HA	1.85	0.58
2:B:202:THR:HG22	2:B:209:PRO:HG3	1.84	0.58
1:A:30:ARG:HG2	1:A:75:THR:CB	2.34	0.58
2:B:6:GLN:H	2:B:105:GLN:NE2	2.02	0.57
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.39	0.57
2:L:150:LYS:HB3	2:L:202:THR:OG1	2.03	0.57
1:H:24:PHE:CD2	1:H:27:PHE:CZ	2.92	0.56
2:L:206:LEU:HD13	2:L:210:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:LYS:O	1:A:108:GLU:OE2	2.24	0.56
2:L:53:ILE:HD13	2:L:59:ARG:HA	1.87	0.56
2:L:166:GLU:HA	2:L:181:SER:O	2.06	0.56
2:B:180:LEU:C	2:B:180:LEU:HD23	2.26	0.56
1:H:5:LYS:HA	1:H:117:GLN:HE22	1.71	0.56
1:H:221:LYS:HD2	3:H:231:HOH:O	2.06	0.55
1:H:42:PRO:HB2	1:H:45:LYS:HG3	1.88	0.55
1:H:160:GLU:HG3	1:H:161:PRO:CA	2.37	0.55
2:B:171:GLN:HG3	2:B:178:TYR:CZ	2.42	0.55
1:A:160:GLU:HG3	1:A:161:PRO:HA	1.88	0.54
1:A:10:THR:HG21	1:A:214:PRO:HG3	1.89	0.54
1:H:117:GLN:NE2	1:H:117:GLN:H	2.06	0.54
1:H:24:PHE:CD2	1:H:27:PHE:HZ	2.26	0.54
2:B:204:GLN:HG2	2:B:204:GLN:O	2.07	0.54
1:H:142:SER:C	2:L:121:PHE:HD1	2.11	0.53
1:A:42:PRO:HD2	1:A:45:LYS:HB2	1.90	0.53
1:H:14:PRO:O	1:H:15:THR:CB	2.56	0.53
1:H:154:VAL:HB	1:H:190:LEU:HD23	1.90	0.53
2:B:147:ARG:CZ	2:B:168:VAL:HG21	2.39	0.53
2:L:84:GLU:HG2	3:L:285:HOH:O	2.08	0.53
1:A:201:LEU:C	1:A:201:LEU:HD23	2.29	0.52
2:B:1:ASP:CB	3:B:293:HOH:O	2.54	0.52
1:H:221:LYS:HB2	3:H:231:HOH:O	2.10	0.52
2:B:147:ARG:NH2	2:B:168:VAL:HG21	2.25	0.52
2:L:6:GLN:HA	2:L:22:SER:O	2.10	0.52
2:L:180:LEU:C	2:L:180:LEU:HD23	2.31	0.52
2:L:2:ILE:HD11	2:L:25:SER:HB2	1.91	0.51
2:B:128:GLU:O	2:B:131:LYS:HB3	2.10	0.51
2:L:54:TYR:HD1	2:L:55:GLN:HG2	1.76	0.51
1:A:117:GLN:HG2	3:A:236:HOH:O	2.10	0.51
1:A:105:ARG:HD3	1:A:106:LYS:HZ2	1.75	0.51
1:A:105:ARG:HD3	1:A:106:LYS:HZ3	1.76	0.51
2:L:113:ARG:CD	2:L:114:THR:O	2.55	0.51
1:A:138:PRO:HG2	1:A:225:PRO:HB3	1.93	0.51
2:B:6:GLN:H	2:B:105:GLN:HE22	1.59	0.50
2:B:6:GLN:HA	2:B:22:SER:O	2.12	0.50
1:H:138:PRO:HD3	1:H:150:LEU:CB	2.41	0.50
1:H:220:ASP:HA	3:H:303:HOH:O	2.12	0.50
2:L:65:ASP:OD2	2:L:65:ASP:N	2.38	0.49
2:B:206:LEU:HD13	2:B:210:VAL:CG1	2.42	0.49
2:B:13:VAL:HG11	2:B:83:VAL:HG21	1.94	0.49
2:B:50:ARG:HB3	2:B:50:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:THR:HG23	1:A:173:SER:H	1.76	0.49
1:H:170:ALA:HA	1:H:172:THR:HG22	1.95	0.49
1:H:154:VAL:HB	1:H:190:LEU:CD2	2.43	0.49
1:A:190:LEU:C	1:A:190:LEU:HD23	2.33	0.49
2:B:145:TYR:CD1	2:B:146:PRO:HA	2.48	0.49
1:H:202:GLY:H	1:H:204:GLN:HE21	1.61	0.49
1:H:38:TRP:CD1	1:H:82:LEU:HB2	2.48	0.48
1:H:63:PRO:HB2	3:H:251:HOH:O	2.14	0.48
2:B:202:THR:HG23	3:B:295:HOH:O	2.13	0.48
1:A:31:THR:CG2	1:A:31:THR:O	2.61	0.48
1:A:207:ILE:HG22	1:A:222:LYS:HA	1.96	0.48
1:A:155:LYS:HE3	1:A:156:ASP:OD1	2.14	0.48
2:B:14:THR:O	2:B:17:GLU:HB2	2.14	0.48
2:L:129:GLN:HB2	3:L:295:HOH:O	2.14	0.48
2:L:38:LEU:HD22	2:L:76:PHE:CG	2.49	0.47
1:A:142:SER:C	2:B:121:PHE:HD1	2.17	0.47
1:H:171:LEU:N	3:H:334:HOH:O	2.39	0.47
1:H:138:PRO:HD3	1:H:150:LEU:HB3	1.96	0.47
2:L:191:TYR:CZ	2:L:216:ARG:HG3	2.48	0.47
1:H:31:THR:O	1:H:31:THR:HG22	2.13	0.47
1:H:217:THR:HG22	1:H:219:VAL:HG23	1.96	0.47
2:B:113:ARG:HD3	2:B:114:THR:O	2.14	0.47
1:H:167:ASN:HB2	1:H:171:LEU:CG	2.40	0.47
1:A:57:ASP:OD1	1:A:59:LYS:NZ	2.48	0.47
2:B:44:LYS:HA	2:B:45:PRO:HD2	1.50	0.47
1:H:9:PRO:HG2	3:H:269:HOH:O	2.15	0.47
2:B:141:LEU:N	2:B:141:LEU:HD12	2.30	0.47
1:A:29:LEU:O	1:A:30:ARG:CB	2.38	0.47
2:L:202:THR:HG22	2:L:209:PRO:HG3	1.98	0.46
1:H:100:ARG:HA	1:H:112:PHE:HA	1.96	0.46
2:B:15:PRO:HG3	2:B:111:ILE:HG23	1.97	0.46
2:B:55:GLN:O	2:B:56:VAL:HB	2.16	0.46
1:H:42:PRO:HD2	1:H:45:LYS:HB2	1.98	0.46
2:B:71:GLY:HA3	2:B:75:ASP:O	2.14	0.46
2:L:12:PRO:HB2	2:L:112:LYS:HD3	1.97	0.46
2:B:96:ALA:HA	2:B:101:LEU:HD22	1.98	0.46
2:L:145:TYR:CD1	2:L:146:PRO:HA	2.51	0.45
2:L:2:ILE:HD12	2:L:95:GLN:HG2	1.99	0.45
1:H:180:ALA:HA	1:H:190:LEU:HB3	1.98	0.45
1:A:160:GLU:HG3	1:A:161:PRO:CA	2.47	0.45
1:H:143:THR:HG22	1:H:144:SER:N	2.31	0.45
2:B:6:GLN:N	2:B:105:GLN:HE22	2.14	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:1:GLN:H3	1:H:1:GLN:HE21	1.64	0.45
1:A:10:THR:HG21	1:A:214:PRO:HB3	1.98	0.44
2:B:5:THR:HA	2:B:105:GLN:HE22	1.81	0.44
1:A:9:PRO:HG2	3:A:333:HOH:O	2.16	0.44
2:L:50:ARG:HB3	2:L:50:ARG:HH21	1.82	0.44
2:B:2:ILE:O	2:B:2:ILE:HG13	2.16	0.44
1:A:18:LEU:HD11	1:A:20:LEU:HD13	1.99	0.44
2:B:105:GLN:N	2:B:105:GLN:NE2	2.48	0.43
1:A:100:ARG:HA	1:A:112:PHE:HA	1.98	0.43
2:B:63:VAL:HA	2:B:64:PRO:HD3	1.82	0.43
2:B:59:ARG:HD3	2:B:63:VAL:O	2.19	0.43
1:A:62:ASN:HA	1:A:63:PRO:HD2	1.89	0.43
2:L:2:ILE:HD11	2:L:25:SER:CB	2.49	0.43
2:L:113:ARG:O	3:L:279:HOH:O	2.22	0.43
1:H:164:VAL:HA	1:H:209:ASN:O	2.18	0.42
1:H:111:HIS:HE1	3:L:273:HOH:O	2.01	0.42
2:B:4:MET:CE	2:B:95:GLN:HB3	2.48	0.42
1:H:92:THR:O	1:H:93:ALA:HB2	2.20	0.42
1:H:165:SER:HB2	1:H:169:GLY:HA2	2.00	0.42
1:H:131:PRO:HB3	1:H:157:TYR:HB3	2.02	0.42
1:H:21:THR:HG22	1:H:22:CYS:N	2.33	0.42
2:L:86:GLU:HB2	3:L:248:HOH:O	2.19	0.42
1:H:18:LEU:HD22	1:H:87:MET:CE	2.50	0.42
2:L:115:VAL:HG13	3:L:278:HOH:O	2.19	0.42
1:H:150:LEU:O	1:H:194:VAL:HG12	2.20	0.41
1:A:137:ALA:HA	1:A:138:PRO:HD2	1.88	0.41
2:L:112:LYS:HA	2:L:145:TYR:OH	2.21	0.41
2:B:47:GLN:HG3	2:B:48:SER:N	2.35	0.41
1:A:69:LEU:HD22	1:A:82:LEU:HD11	2.03	0.41
2:L:7:SER:HA	2:L:8:PRO:HA	1.75	0.41
3:B:293:HOH:O	2:L:8:PRO:HB2	2.21	0.41
2:B:88:VAL:HG23	2:B:109:LEU:O	2.21	0.40
1:H:224:GLU:HB3	1:H:225:PRO:CD	2.51	0.40
2:L:50:ARG:HB3	2:L:50:ARG:NH2	2.37	0.40
1:A:38:TRP:O	1:A:50:LEU:HB2	2.22	0.40
2:L:111:ILE:HG21	2:L:176:SER:OG	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/229 (99%)	208 (92%)	14 (6%)	4 (2%)	13	7
1	H	227/229 (99%)	209 (92%)	12 (5%)	6 (3%)	8	4
2	B	227/229 (99%)	214 (94%)	12 (5%)	1 (0%)	43	45
2	L	226/229 (99%)	219 (97%)	6 (3%)	1 (0%)	43	45
All	All	906/916 (99%)	850 (94%)	44 (5%)	12 (1%)	18	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	SER
1	H	201	LEU
1	A	30	ARG
1	H	66	LYS
1	H	173	SER
1	H	225	PRO
1	H	228	CYS
1	A	57	ASP
2	B	45	PRO
1	A	226	LYS
1	H	30	ARG
2	L	45	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	202/202 (100%)	181 (90%)	21 (10%)	10	9
1	H	202/202 (100%)	174 (86%)	28 (14%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/202 (100%)	191 (95%)	11 (5%)	31	35
2	L	201/202 (100%)	188 (94%)	13 (6%)	24	25
All	All	807/808 (100%)	734 (91%)	73 (9%)	14	13

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	4	LEU
1	A	10	THR
1	A	15	THR
1	A	20	LEU
1	A	30	ARG
1	A	32	SER
1	A	57	ASP
1	A	68	ARG
1	A	90	VAL
1	A	105	ARG
1	A	144	SER
1	A	150	LEU
1	A	162	VAL
1	A	171	LEU
1	A	181	VAL
1	A	190	LEU
1	A	193	VAL
1	A	217	THR
1	A	221	LYS
1	A	226	LYS
2	B	5	THR
2	B	9	LEU
2	B	47	GLN
2	B	55	GLN
2	B	75	ASP
2	B	84	GLU
2	B	105	GLN
2	B	114	THR
2	B	161	SER
2	B	204	GLN
2	B	210	VAL
1	H	1	GLN
1	H	2	VAL

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Mol	Chain	Res	Type
1	H	4	LEU
1	H	10	THR
1	H	15	THR
1	H	19	THR
1	H	20	LEU
1	H	25	SER
1	H	28	SER
1	H	30	ARG
1	H	57	ASP
1	H	77	LYS
1	H	105	ARG
1	H	117	GLN
1	H	163	THR
1	H	167	ASN
1	H	171	LEU
1	H	172	THR
1	H	181	VAL
1	H	190	LEU
1	H	193	VAL
1	H	195	THR
1	H	200	SER
1	H	203	THR
1	H	207	ILE
1	H	218	LYS
1	H	221	LYS
1	H	226	LYS
2	L	2	ILE
2	L	5	THR
2	L	50	ARG
2	L	65	ASP
2	L	75	ASP
2	L	88	VAL
2	L	105	GLN
2	L	108	LYS
2	L	113	ARG
2	L	115	VAL
2	L	134	THR
2	L	180	LEU
2	L	210	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	111	HIS
1	A	204	GLN
2	B	31	HIS
2	B	35	HIS
2	B	105	GLN
2	B	204	GLN
1	H	1	GLN
1	H	79	GLN
1	H	111	HIS
1	H	117	GLN
1	H	167	ASN
1	H	204	GLN
2	L	31	HIS
2	L	105	GLN
2	L	142	ASN

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	A	228/229 (99%)	0.70	17 (7%) 14 13	17, 27, 37, 44	0
1	H	229/229 (100%)	0.59	11 (4%) 29 29	16, 25, 36, 45	0
2	B	229/229 (100%)	0.33	4 (1%) 67 68	13, 30, 36, 42	0
2	L	228/229 (99%)	0.41	5 (2%) 59 59	14, 29, 38, 43	0
All	All	914/916 (99%)	0.50	37 (4%) 36 37	13, 28, 37, 45	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ALA	6.1
1	A	207	ILE	5.2
1	A	171	LEU	5.1
1	A	174	GLY	4.5
1	A	205	THR	4.2
1	A	165	SER	3.8
1	A	173	SER	3.6
1	A	223	VAL	3.5
1	H	170	ALA	3.4
1	H	174	GLY	3.4
2	B	46	GLY	3.1
1	A	206	TYR	2.9
2	B	173	SER	2.9
1	H	223	VAL	2.9
2	B	45	PRO	2.8
1	A	201	LEU	2.7
1	H	207	ILE	2.6
1	H	149	ALA	2.6
1	H	224	GLU	2.6
2	L	11	LEU	2.6
2	L	111	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	226	LYS	2.5
1	H	205	THR	2.4
2	B	114	THR	2.3
1	H	171	LEU	2.3
1	A	105	ARG	2.3
1	A	148	ALA	2.3
1	A	199	SER	2.3
1	H	173	SER	2.3
2	L	94	PHE	2.2
1	A	172	THR	2.2
1	A	228	CYS	2.2
1	A	149	ALA	2.1
2	L	9	LEU	2.1
2	L	122	ILE	2.0
1	H	137	ALA	2.0
1	H	166	TRP	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.