



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:59 PM UTC

PDB ID : 3AAZ / pdb_00003aaz
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 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

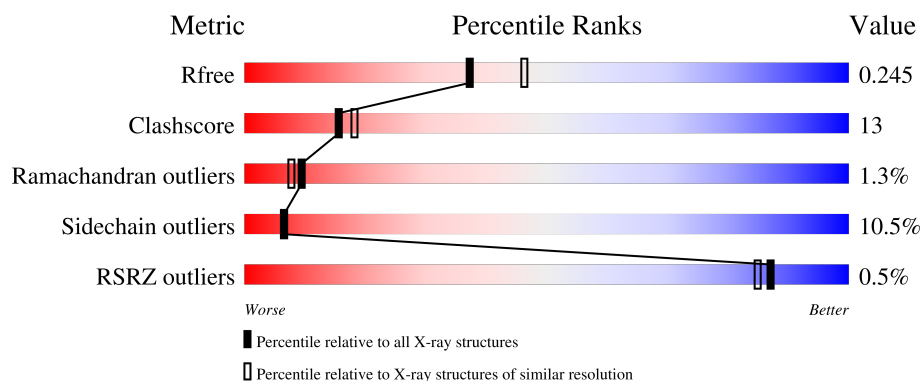
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	A	229	72% 21% 6%
1	H	229	59% 33% 7%
2	B	229	73% 21% 6%
2	L	229	77% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7401 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 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			

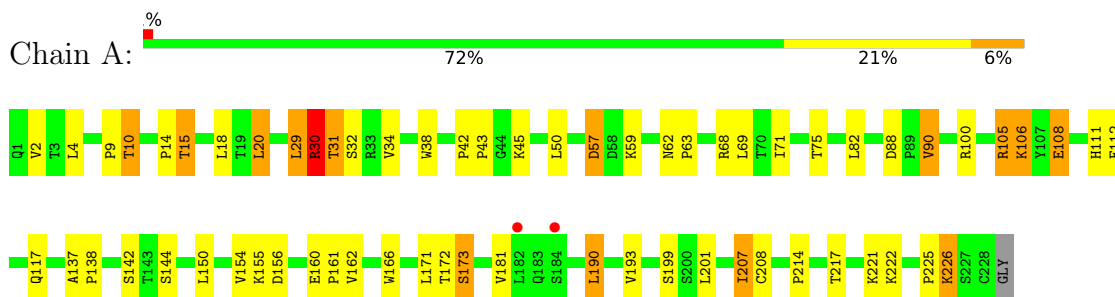
- Molecule 3 is water.

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		

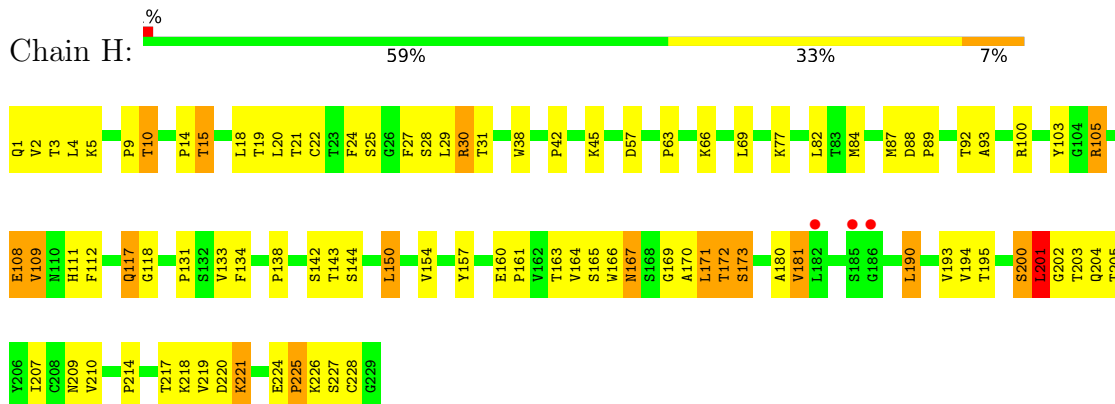
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

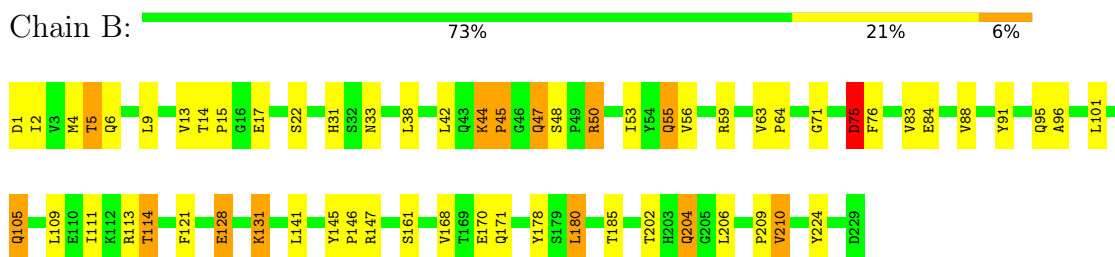
- Molecule 1: Humanized recombinant Fab fragment of a murine; antibody



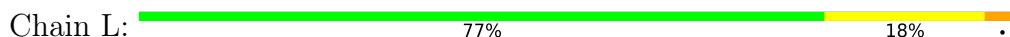
- Molecule 1: Humanized recombinant Fab fragment of a murine; antibody

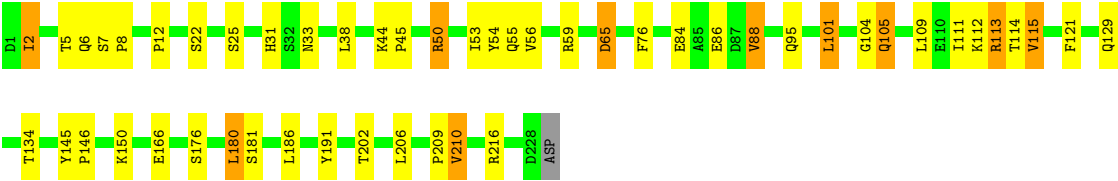


- Molecule 2: Humanized recombinant Fab fragment of a murine; antibody



- 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 46.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (46.03-2.20) 92.6 (46.03-2.20)	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 0.217 , 0.245	Depositor DCC
R_{free} test set	2734 reflections (4.65%)	wwPDB-VP
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 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l 0.477 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	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.

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

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	0.94	0/1792	1.13	4/2445 (0.2%)
1	H	0.98	0/1796	1.15	8/2450 (0.3%)
2	B	0.86	0/1803	1.03	3/2450 (0.1%)
2	L	0.87	0/1795	1.01	3/2439 (0.1%)
All	All	0.92	0/7186	1.08	18/9784 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LYS	N-CA-C	-9.39	97.26	110.50
2	B	44	LYS	CA-C-N	8.57	130.56	119.84
2	B	44	LYS	C-N-CA	8.57	130.56	119.84
1	H	29	LEU	N-CA-C	-7.88	100.13	110.53
1	H	227	SER	N-CA-C	-7.67	105.88	114.62
1	H	201	LEU	N-CA-C	-7.30	95.26	110.80
2	L	44	LYS	CA-C-N	6.81	128.35	119.84
2	L	44	LYS	C-N-CA	6.81	128.35	119.84
1	A	108	GLU	N-CA-C	6.55	120.85	112.34
1	A	29	LEU	N-CA-C	-6.19	101.12	110.28
1	A	34	VAL	N-CA-C	5.98	117.75	109.80
1	H	134	PHE	CA-C-N	5.88	126.08	119.90
1	H	134	PHE	C-N-CA	5.88	126.08	119.90
1	H	118	GLY	N-CA-C	-5.51	106.11	112.29
2	B	75	ASP	N-CA-C	5.36	117.47	108.73
1	H	181	VAL	CB-CA-C	5.26	118.93	110.82
2	L	104	GLY	N-CA-C	-5.22	105.86	112.54
1	H	108	GLU	N-CA-C	5.02	118.50	112.38

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	A	1747	0	1735	44	0
1	H	1751	0	1739	56	0
2	B	1764	0	1707	47	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	186	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 13.

All (186) 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)
1:H:105:ARG:HG3	1:H:105:ARG:HH21	1.00	1.10
1:A:105:ARG:HH21	1:A:105:ARG:HG3	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:H	2:B:105:GLN:HE21	0.93	0.89
1:A:14:PRO:O	1:A:15:THR:HB	1.70	0.89
1:A:105:ARG:HG3	1:A:105:ARG:NH2	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
1:A:59:LYS:HE3	1:A:71:ILE:O	1.81	0.80
2:B:31:HIS:CD2	2:B:33:ASN:H	1.99	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	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:HIS:CD2	2:L:33:ASN:H	2.03	0.76
2:B:105:GLN:HE21	2:B:105:GLN:N	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
1:A:154:VAL:HB	1:A:190:LEU:HD22	1.71	0.73
2:L:105:GLN:HE21	2:L:105:GLN:H	1.35	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:HH21	1:A:105:ARG:CG	1.99	0.67
1:H:18:LEU:HD22	1:H:87:MET:HE2	1.77	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: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
1:H:172:THR:OG1	1:H:173:SER:N	2.26	0.61
2:L:112:LYS:HD2	2:L:145:TYR:OH	2.00	0.61
2:B:180:LEU:C	2:B:180:LEU:HD23	2.26	0.60
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:B:53:ILE:HD13	2:B:59:ARG:HA	1.85	0.58
2:L:101:LEU:HD23	2:L:101:LEU:N	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:SER:C	2:L:121:PHE:HD1	2.11	0.57
1:A:201:LEU:C	1:A:201:LEU:HD23	2.29	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:180:LEU:C	2:L:180:LEU:HD23	2.31	0.56
2:L:206:LEU:HD13	2:L:210:VAL:HG12	1.87	0.56
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
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:O	2:B:204:GLN:HG2	2.07	0.54
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:A:190:LEU:C	1:A:190:LEU:HD23	2.33	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
2:B:4:MET:HE2	2:B:95:GLN:HB3	1.90	0.52
1:A:142:SER:C	2:B:121:PHE:HD1	2.17	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: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
1:A:117:GLN:HG2	3:A:236:HOH:O	2.10	0.51
2:L:54:TYR:HD1	2:L:55:GLN:HG2	1.76	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
1:A:138:PRO:HG2	1:A:225:PRO:HB3	1.93	0.51
2:L:113:ARG:CD	2:L:114:THR:O	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:206:LEU:HD13	2:B:210:VAL:CG1	2.42	0.49
2:L:65:ASP:OD2	2:L:65:ASP:N	2.38	0.49
2:B:13:VAL:HG11	2:B:83:VAL:HG21	1.94	0.49
1:A:172:THR:HG23	1:A:173:SER:H	1.76	0.49
2:B:50:ARG:HH21	2:B:50:ARG:HB3	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
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:O	1:A:31:THR:CG2	2.61	0.48
1:A:155:LYS:HE3	1:A:156:ASP:OD1	2.14	0.48
1:A:207:ILE:HG22	1:A:222:LYS:HA	1.96	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:H:138:PRO:HD3	1:H:150:LEU:HB3	1.96	0.47
1:H:171:LEU:N	3:H:334:HOH:O	2.39	0.47
2:L:191:TYR:CZ	2:L:216:ARG:HG3	2.48	0.47
1:H:31:THR:HG22	1:H:31:THR:O	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:HD12	2:B:141:LEU:N	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:69:LEU:HD21	1:H:84:MET:HE3	1.97	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
2:B:71:GLY:HA3	2:B:75:ASP:O	2.14	0.46
1:H:42:PRO:HD2	1:H:45:LYS:HB2	1.98	0.46
2:B:96:ALA:HA	2:B:101:LEU:HD22	1.98	0.46
2:L:12:PRO:HB2	2:L:112:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:145:TYR:CD1	2:L:146:PRO:HA	2.51	0.45
1:H:180:ALA:HA	1:H:190:LEU:HB3	1.98	0.45
2:L:2:ILE:HD12	2:L:95:GLN:HG2	1.99	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
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:HH21	2:L:50:ARG:HB3	1.82	0.44
1:A:18:LEU:HD11	1:A:20:LEU:HD13	1.99	0.44
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:105:GLN:NE2	2:B:105:GLN:N	2.48	0.43
2:B:31:HIS:CD2	2:B:33:ASN:CG	2.96	0.43
1:A:62:ASN:HA	1:A:63:PRO:HD2	1.89	0.43
2:B:59:ARG:HD3	2:B:63:VAL:O	2.19	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
2:B:4:MET:CE	2:B:95:GLN:HB3	2.48	0.42
1:H:111:HIS:HE1	3:L:273:HOH:O	2.01	0.42
1:H:164:VAL:HA	1:H:209:ASN:O	2.18	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:166:TRP:C	1:H:167:ASN:HD22	2.28	0.42
1:H:21:THR:HG22	1:H:22:CYS:N	2.33	0.42
1:H:131:PRO:HB3	1:H:157:TYR:HB3	2.02	0.42
2:L:86:GLU:HB2	3:L:248:HOH:O	2.19	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:B:2:ILE:O	2:B:2:ILE:HG13	2.16	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:B:224:TYR:CD1	2:B:224:TYR:C	2.98	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
1:H:202:GLY:C	1:H:204:GLN:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TRP:O	1:A:50:LEU:HB2	2.22	0.40
2:L:50:ARG:HB3	2:L:50:ARG:NH2	2.37	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 [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	226/229 (99%)	208 (92%)	14 (6%)	4 (2%)	6	4
1	H	227/229 (99%)	209 (92%)	12 (5%)	6 (3%)	4	2
2	B	227/229 (99%)	214 (94%)	12 (5%)	1 (0%)	30	34
2	L	226/229 (99%)	219 (97%)	6 (3%)	1 (0%)	30	34
All	All	906/916 (99%)	850 (94%)	44 (5%)	12 (1%)	9	8

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%)	179 (89%)	23 (11%)	5	5
1	H	202/202 (100%)	169 (84%)	33 (16%)	2	2
2	B	202/202 (100%)	186 (92%)	16 (8%)	11	13
2	L	201/202 (100%)	188 (94%)	13 (6%)	15	18
All	All	807/808 (100%)	722 (90%)	85 (10%)	6	6

All (85) 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	31	THR
1	A	32	SER
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	199	SER
1	A	207	ILE
1	A	217	THR
1	A	221	LYS
1	A	226	LYS
2	B	5	THR

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Mol	Chain	Res	Type
2	B	9	LEU
2	B	47	GLN
2	B	50	ARG
2	B	55	GLN
2	B	75	ASP
2	B	84	GLU
2	B	105	GLN
2	B	114	THR
2	B	128	GLU
2	B	131	LYS
2	B	161	SER
2	B	180	LEU
2	B	185	THR
2	B	204	GLN
2	B	210	VAL
1	H	1	GLN
1	H	2	VAL
1	H	3	THR
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	108	GLU
1	H	109	VAL
1	H	117	GLN
1	H	150	LEU
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

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Mol	Chain	Res	Type
1	H	203	THR
1	H	205	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	88	VAL
2	L	101	LEU
2	L	105	GLN
2	L	113	ARG
2	L	115	VAL
2	L	134	THR
2	L	180	LEU
2	L	186	LEU
2	L	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	86	ASN
1	A	111	HIS
1	A	183	GLN
1	A	204	GLN
2	B	27	GLN
2	B	31	HIS
2	B	35	HIS
2	B	105	GLN
2	B	142	ASN
2	B	165	GLN
2	B	204	GLN
1	H	1	GLN
1	H	86	ASN
1	H	111	HIS
1	H	117	GLN
1	H	167	ASN
1	H	176	HIS
1	H	204	GLN

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Mol	Chain	Res	Type
2	L	27	GLN
2	L	31	HIS
2	L	105	GLN
2	L	142	ASN
2	L	194	HIS

5.3.3 RNA [i](#)

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 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 [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, 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%)	-0.95	2 (0%) 81 79	17, 27, 37, 44	0
1	H	229/229 (100%)	-0.93	3 (1%) 75 73	16, 25, 36, 45	0
2	B	229/229 (100%)	-1.18	0 100 100	13, 30, 36, 42	0
2	L	228/229 (99%)	-1.20	0 100 100	14, 29, 38, 43	0
All	All	914/916 (99%)	-1.06	5 (0%) 87 85	13, 28, 37, 45	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	182	LEU	4.1
1	A	184	SER	3.5
1	H	185	SER	2.6
1	A	182	LEU	2.6
1	H	186	GLY	2.1

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.