



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:30 PM UTC

PDB ID : 5XRQ / pdb_00005xrq
Title : Crystal structure of human monoclonal antibody H3v-47
Authors : Zhang, H.; Willson, I.A.
Deposited on : 2017-06-09
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

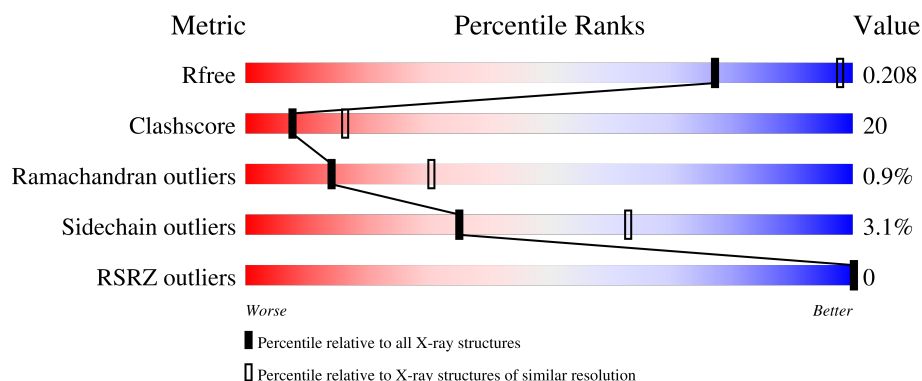
1 Overall quality at a glance

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	A	236	
1	H	236	
2	B	214	
2	L	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6639 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 Fab H3v-47 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1647	1039	275	326	7			
1	A	219	Total	C	N	O	S	0	0	0
			1638	1034	273	324	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	217	HIS	-	expression tag	UNP Q6N089
H	218	HIS	-	expression tag	UNP Q6N089
H	219	HIS	-	expression tag	UNP Q6N089
H	220	HIS	-	expression tag	UNP Q6N089
H	221	HIS	-	expression tag	UNP Q6N089
H	222	HIS	-	expression tag	UNP Q6N089
A	217	HIS	-	expression tag	UNP Q6N089
A	218	HIS	-	expression tag	UNP Q6N089
A	219	HIS	-	expression tag	UNP Q6N089
A	220	HIS	-	expression tag	UNP Q6N089
A	221	HIS	-	expression tag	UNP Q6N089
A	222	HIS	-	expression tag	UNP Q6N089

- Molecule 2 is a protein called Fab H3v-47 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	1	0
			1629	1009	282	333	5			
2	B	212	Total	C	N	O	S	0	1	0
			1619	1003	280	331	5			

- Molecule 3 is water.

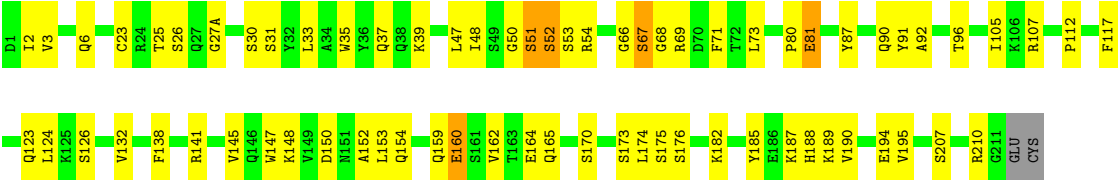
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	17	Total 17	O 17	0	0
3	L	30	Total 30	O 30	0	0
3	A	19	Total 19	O 19	0	0
3	B	40	Total 40	O 40	0	0

Chain B:

66%

30%

..



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	135.13Å 135.13Å 78.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.92 – 2.60 46.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.92-2.60) 98.3 (46.92-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.180 , 0.214 0.183 , 0.208	Depositor DCC
R_{free} test set	2460 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.468 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6639	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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	0.46	2/1677 (0.1%)	0.82	8/2287 (0.3%)
1	H	0.48	1/1686 (0.1%)	0.80	6/2299 (0.3%)
2	B	0.42	0/1656	0.77	4/2247 (0.2%)
2	L	0.43	0/1668	0.91	13/2263 (0.6%)
All	All	0.45	3/6687 (0.0%)	0.83	31/9096 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	H	0	1
2	L	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	202	PRO	N-CD	-9.27	1.34	1.47
1	A	76	ARG	NE-CZ	-5.79	1.26	1.33
1	A	76	ARG	CZ-NH1	-5.48	1.25	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	93	THR	N-CA-C	16.20	135.21	108.48
1	A	211	VAL	N-CA-C	-11.96	84.47	109.34
1	H	65	ASP	N-CA-CB	-11.04	95.32	110.67
2	B	52	SER	N-CA-CB	-9.07	97.25	110.40
2	L	52	SER	N-CA-CB	-8.92	98.61	111.54
2	L	93	THR	CB-CA-C	-8.81	98.58	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	52	SER	N-CA-C	8.72	123.60	111.56
1	A	212	GLU	N-CA-C	8.57	134.99	111.00
1	H	144	ASP	N-CA-C	7.82	127.46	110.80
2	B	52	SER	CB-CA-C	7.81	121.44	109.34
1	A	8	GLY	N-CA-C	7.50	124.07	112.60
2	L	189	LYS	N-CA-C	7.10	123.58	114.56
1	H	145	TYR	N-CA-C	7.10	121.17	109.96
2	L	190	VAL	N-CA-CB	6.99	120.61	112.15
1	H	145	TYR	N-CA-CB	-6.81	98.42	110.14
1	H	199	ASN	CB-CA-C	6.71	120.03	110.24
2	L	209	ASN	CB-CA-C	-6.66	98.35	109.27
2	L	189	LYS	CB-CA-C	-6.19	99.47	109.13
1	A	145	TYR	N-CA-C	6.18	119.60	110.46
2	B	92	ALA	N-CA-C	6.16	118.78	111.33
1	A	3	GLN	N-CA-C	5.99	123.56	110.80
2	L	32	TYR	N-CA-C	5.90	119.23	112.57
2	B	51	SER	CB-CA-C	5.45	121.26	110.42
1	A	144	ASP	N-CA-C	5.41	122.31	110.80
1	H	201	LYS	CG-CD-CE	-5.40	98.87	111.30
2	L	209	ASN	N-CA-C	5.40	122.22	114.39
1	A	25	SER	N-CA-C	5.29	118.62	110.42
1	A	145	TYR	N-CA-CB	-5.28	102.27	110.46
2	L	93	THR	CA-C-N	5.28	131.62	122.28
2	L	93	THR	C-N-CA	5.28	131.62	122.28
2	L	183	ALA	N-CA-C	5.17	117.33	111.02

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100(J)	PHE	Peptide
1	A	201	LYS	Mainchain
1	H	100(J)	PHE	Peptide
2	L	93	THR	Peptide

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	1638	0	1598	91	0
1	H	1647	0	1609	74	0
2	B	1619	0	1575	55	1
2	L	1629	0	1586	44	1
3	A	19	0	0	3	0
3	B	40	0	0	4	1
3	H	17	0	0	2	1
3	L	30	0	0	2	0
All	All	6639	0	6368	258	2

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 20.

All (258) 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:A:8:GLY:CA	1:A:201:LYS:NZ	1.80	1.44
1:A:8:GLY:HA3	1:A:201:LYS:NZ	1.33	1.42
1:H:201:LYS:HG3	1:H:202:PRO:HD3	1.09	1.07
1:A:8:GLY:HA2	1:A:201:LYS:NZ	1.69	1.04
1:A:100(G):SER:OG	2:B:91:TYR:O	1.79	0.99
1:A:8:GLY:CA	1:A:201:LYS:HZ2	1.57	0.97
1:H:207:VAL:CG1	1:H:209:LYS:HE2	2.01	0.90
1:H:135:THR:HA	1:H:185:PRO:HA	1.50	0.90
1:A:8:GLY:HA3	1:A:201:LYS:HZ2	0.94	0.89
1:A:201:LYS:HG3	1:A:202:PRO:HD3	1.55	0.88
2:B:150:ASP:OD2	2:B:188:HIS:ND1	2.05	0.88
1:A:8:GLY:CA	1:A:201:LYS:HZ1	1.78	0.87
1:A:8:GLY:HA3	1:A:201:LYS:HZ3	1.31	0.86
2:B:123:GLN:O	2:B:126:SER:OG	1.95	0.85
1:H:65:ASP:OD1	1:H:65:ASP:N	2.11	0.84
2:B:148:LYS:NZ	2:B:194:GLU:OE1	2.12	0.83
2:B:150:ASP:HA	2:B:190:VAL:HG23	1.59	0.83
2:B:189:LYS:NZ	2:B:210:ARG:O	2.12	0.82
1:A:26:GLY:O	1:A:27:ASP:HB2	1.79	0.82
1:A:126:PRO:HD3	1:A:211:VAL:CG1	2.10	0.82
1:H:9:ALA:HB3	1:H:201:LYS:HZ2	1.43	0.81
1:H:117:LYS:HD3	1:H:144:ASP:O	1.82	0.80
1:A:9:ALA:N	1:A:201:LYS:NZ	2.30	0.79
1:A:9:ALA:H	1:A:201:LYS:NZ	1.81	0.79
1:H:201:LYS:HG3	1:H:202:PRO:CD	2.04	0.79
1:A:8:GLY:CA	1:A:201:LYS:HZ3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLY:C	1:A:201:LYS:NZ	2.42	0.77
1:A:20:VAL:HG12	1:A:80:MET:HE2	1.67	0.77
1:A:201:LYS:CG	1:A:202:PRO:HD3	2.14	0.77
1:H:201:LYS:CG	1:H:202:PRO:HD3	2.03	0.77
1:H:207:VAL:HG13	1:H:209:LYS:HE2	1.66	0.76
2:L:93:THR:OG1	2:L:94:SER:N	2.18	0.76
2:L:209:ASN:O	2:L:210:ARG:HB2	1.86	0.75
1:A:8:GLY:C	1:A:201:LYS:HZ2	1.94	0.75
1:H:195:ILE:HG12	1:H:210:ARG:HG2	1.68	0.75
1:A:201:LYS:HG3	1:A:202:PRO:CD	2.17	0.74
1:A:8:GLY:HA2	1:A:201:LYS:HZ1	1.34	0.73
1:H:207:VAL:HG12	1:H:209:LYS:HG2	1.71	0.73
1:A:2:VAL:HG13	1:A:25:SER:HB3	1.69	0.73
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.19	0.73
1:A:165:THR:HG1	1:A:180:SER:HG	1.29	0.72
2:B:96:THR:OG1	3:B:301:HOH:O	2.07	0.72
1:A:82(B):SER:O	3:A:301:HOH:O	2.08	0.71
1:A:138:LEU:HD13	1:A:211:VAL:HG21	1.71	0.71
1:H:207:VAL:HG11	1:H:209:LYS:HE2	1.73	0.71
2:B:80:PRO:O	3:B:302:HOH:O	2.09	0.70
1:A:94:ARG:NH1	1:A:101:ASP:OD2	2.22	0.70
1:H:9:ALA:HB1	1:H:108:LEU:O	1.91	0.70
2:L:48:ILE:HG21	2:L:51:SER:O	1.90	0.69
1:H:19:ARG:HB2	1:H:81:GLU:HG3	1.75	0.69
1:H:35:THR:CG2	1:H:47:TRP:HE1	2.06	0.69
1:H:85:GLU:OE1	1:H:85:GLU:N	2.22	0.68
2:L:188:HIS:O	2:L:210:ARG:NH1	2.26	0.68
1:H:103:TRP:O	3:H:301:HOH:O	2.12	0.67
2:L:90:GLN:NE2	2:L:93:THR:H	1.93	0.67
1:A:7:SER:OG	1:A:20:VAL:HG23	1.94	0.66
1:A:9:ALA:N	1:A:201:LYS:HZ1	1.92	0.66
1:A:61:GLN:HA	1:A:64:ASP:OD1	1.96	0.66
1:H:31:SER:O	1:H:99:VAL:HG13	1.95	0.66
2:B:37:GLN:HB2	2:B:47:LEU:HD21	1.76	0.66
2:L:90:GLN:HE21	2:L:92:ALA:N	1.95	0.65
2:B:147:TRP:HB2	2:B:154:GLN:HB2	1.79	0.65
1:H:134:GLY:O	1:H:186:SER:N	2.27	0.64
1:A:9:ALA:H	1:A:201:LYS:HZ1	1.44	0.64
1:H:35:THR:HG23	1:H:47:TRP:HE1	1.63	0.63
2:B:150:ASP:HA	2:B:190:VAL:CG2	2.26	0.63
1:A:38:ARG:HH22	1:A:86:ASP:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:119:PRO:HD3	2:L:131:VAL:HG22	1.79	0.62
2:B:2:ILE:O	3:B:301:HOH:O	2.16	0.62
1:A:13:LYS:O	1:A:16:SER:OG	2.17	0.61
2:B:141:ARG:NH2	2:B:162:VAL:HG21	2.15	0.61
1:A:126:PRO:HD3	1:A:211:VAL:HG13	1.81	0.61
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.35	0.61
1:A:31:SER:O	1:A:99:VAL:HG23	2.02	0.59
1:A:125:ALA:HA	1:A:211:VAL:HG13	1.84	0.59
2:B:23:CYS:HB2	2:B:35:TRP:CH2	2.37	0.59
2:L:48:ILE:CG2	2:L:51:SER:O	2.50	0.59
2:L:107:ARG:NH1	2:L:108:THR:O	2.35	0.59
2:B:50:GLY:O	2:B:52:SER:N	2.34	0.59
1:A:119:PRO:HD3	1:A:200:HIS:ND1	2.18	0.58
1:A:126:PRO:HB3	1:A:137:ALA:O	2.03	0.58
1:A:171:GLN:HE21	1:A:175:LEU:C	2.12	0.58
1:H:117:LYS:CD	1:H:144:ASP:O	2.52	0.58
1:A:84:LEU:O	3:A:302:HOH:O	2.17	0.57
1:H:136:ALA:N	1:H:184:VAL:O	2.31	0.57
2:L:47:LEU:HD23	2:L:58:ILE:HD12	1.86	0.57
2:B:39:LYS:HE2	2:B:81:GLU:O	2.05	0.57
2:L:209:ASN:O	2:L:210:ARG:CB	2.51	0.56
2:L:104:GLU:OE2	2:L:172:TYR:OH	2.23	0.56
1:H:9:ALA:HB3	1:H:201:LYS:NZ	2.18	0.55
1:A:124:LEU:HB3	2:B:117:PHE:CD2	2.41	0.55
2:B:105:ILE:O	2:B:165:GLN:NE2	2.32	0.55
1:A:26:GLY:O	1:A:27:ASP:CB	2.54	0.55
2:B:148:LYS:HA	2:B:152:ALA:O	2.06	0.55
1:H:35:THR:CG2	1:H:47:TRP:NE1	2.68	0.55
1:H:207:VAL:CG1	1:H:209:LYS:HG2	2.36	0.55
2:B:124:LEU:HD21	2:B:185:TYR:HD2	1.70	0.55
1:A:38:ARG:HB2	1:A:88:ALA:HB1	1.88	0.55
1:A:195:ILE:HA	1:A:209:LYS:O	2.06	0.55
2:L:189:LYS:HG3	2:L:189:LYS:O	2.06	0.54
2:L:50:GLY:O	2:L:52:SER:N	2.39	0.54
1:A:36:TRP:HB3	1:A:48:MET:HE3	1.88	0.54
2:B:141:ARG:O	2:B:141:ARG:NH1	2.39	0.54
1:H:33:SER:HB3	1:H:52:PHE:CE1	2.43	0.54
1:A:139:GLY:HA3	1:A:181:VAL:HG12	1.89	0.54
1:A:21:SER:HB3	1:A:79:TYR:CE2	2.43	0.53
2:B:3:VAL:N	2:B:26:SER:OG	2.35	0.53
1:H:35:THR:HG23	1:H:47:TRP:NE1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:NH2	1:A:86:ASP:HA	2.23	0.53
1:A:37:VAL:HG22	1:A:47:TRP:HA	1.90	0.53
1:A:53:ILE:HG23	1:A:54:PHE:CD1	2.45	0.52
1:H:33:SER:HB3	1:H:52:PHE:CZ	2.45	0.52
2:B:30:SER:O	2:B:51:SER:HB3	2.10	0.52
2:B:145:VAL:HG22	2:B:195:VAL:HG22	1.92	0.52
1:H:66:ARG:O	1:H:82(A):THR:N	2.43	0.51
1:A:37:VAL:HG13	1:A:46:GLN:C	2.36	0.51
1:H:100(A):PRO:HA	1:A:54:PHE:CZ	2.45	0.51
1:A:9:ALA:N	1:A:201:LYS:HZ2	2.02	0.51
1:H:100(J):PHE:O	1:H:103:TRP:NE1	2.40	0.51
1:A:195:ILE:HG23	1:A:208:ASP:HB3	1.91	0.51
1:H:6:GLN:HE21	1:H:104:GLY:HA3	1.76	0.51
1:H:28:THR:HG23	1:H:94:ARG:HD3	1.92	0.50
1:H:71:THR:HG22	1:H:78:VAL:HG22	1.92	0.50
2:B:35:TRP:CD2	2:B:73:LEU:HB2	2.46	0.50
2:B:141:ARG:CZ	2:B:162:VAL:HG21	2.41	0.50
2:L:90:GLN:HE21	2:L:92:ALA:H	1.58	0.50
2:L:30:SER:O	2:L:51:SER:HB3	2.11	0.50
1:A:20:VAL:CG1	1:A:80:MET:HE2	2.39	0.50
1:A:211:VAL:HG12	1:A:212:GLU:N	2.26	0.50
1:A:12:LYS:HE2	1:A:17:SER:O	2.12	0.50
2:B:162:VAL:HG13	2:B:173:SER:O	2.12	0.49
2:L:135:LEU:HD21	2:L:195:VAL:HG13	1.94	0.49
1:A:18:VAL:HG13	1:A:82(C):LEU:HD11	1.94	0.49
1:A:112:SER:OG	1:A:113:SER:N	2.43	0.49
2:B:123:GLN:HA	2:B:126:SER:OG	2.12	0.49
2:L:32:TYR:HA	2:L:91:TYR:CE1	2.48	0.49
1:A:139:GLY:HA2	1:A:154:TRP:CH2	2.47	0.49
2:B:112:PRO:HB3	2:B:138:PHE:HB3	1.95	0.49
1:A:197:ASN:ND2	1:A:208:ASP:OD1	2.29	0.48
1:A:23:LYS:HB2	1:A:77:THR:HG22	1.95	0.48
2:L:36:TYR:OH	2:L:89:GLN:OE1	2.12	0.48
2:B:132:VAL:HA	2:B:176:SER:O	2.14	0.48
1:H:53:ILE:HG23	1:H:54:PHE:CD1	2.49	0.48
1:H:6:GLN:NE2	1:H:106:GLY:H	2.12	0.48
1:H:38:ARG:HD3	1:H:90:TYR:CE2	2.49	0.48
1:H:70:THR:O	1:H:79:TYR:N	2.42	0.48
2:B:107:ARG:NH1	2:B:107:ARG:HG2	2.28	0.47
2:L:147:TRP:CD2	2:L:178:LEU:HB2	2.49	0.47
2:B:2:ILE:HB	3:B:301:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HA	2:B:159:GLN:HE22	1.80	0.47
2:B:48:ILE:HG23	2:B:52:SER:O	2.14	0.47
2:B:124:LEU:HD22	2:B:182:LYS:HG3	1.96	0.47
2:L:107:ARG:HG2	2:L:108:THR:O	2.14	0.47
1:A:9:ALA:H	1:A:201:LYS:CE	2.26	0.47
1:A:13:LYS:HA	1:A:112:SER:O	2.15	0.47
2:B:185:TYR:CZ	2:B:210:ARG:HD3	2.50	0.47
1:A:5:VAL:O	1:A:22:CYS:HA	2.14	0.46
1:H:87:THR:HA	1:H:109:VAL:O	2.15	0.46
1:H:103:TRP:CE3	2:L:44:PRO:HD2	2.50	0.46
1:H:35:THR:HG21	1:H:47:TRP:HE1	1.77	0.46
1:H:35:THR:HG21	1:H:47:TRP:NE1	2.30	0.46
1:H:100(B):ALA:HA	1:A:100(B):ALA:HA	1.97	0.46
2:L:33:LEU:C	2:L:33:LEU:HD23	2.40	0.46
1:H:20:VAL:HB	1:H:80:MET:SD	2.56	0.46
1:H:164:HIS:HB2	1:H:181:VAL:HG22	1.98	0.46
1:A:12:LYS:HG3	1:A:18:VAL:CG1	2.46	0.46
1:A:48:MET:HE1	1:A:90:TYR:HD2	1.81	0.46
2:B:37:GLN:OE1	2:B:39:LYS:HE3	2.16	0.46
1:H:20:VAL:HB	1:H:80:MET:HG2	1.99	0.45
1:H:52:PHE:CE2	1:H:100(D):PRO:HB2	2.51	0.45
1:H:195:ILE:HG23	1:H:209:LYS:C	2.41	0.45
1:H:83:ARG:O	1:H:111:VAL:HG11	2.16	0.45
2:L:148:LYS:HG2	2:L:153:LEU:HD23	1.97	0.45
2:L:162:VAL:HG22	2:L:174:LEU:HB2	1.99	0.45
1:A:12:LYS:HG3	1:A:18:VAL:HG12	1.97	0.45
1:A:83:ARG:O	1:A:111:VAL:HG11	2.15	0.45
2:L:4:MET:HE1	2:L:25:THR:HG22	1.97	0.45
2:L:21:LEU:HB3	3:L:309:HOH:O	2.16	0.45
1:A:171:GLN:NE2	1:A:175:LEU:O	2.30	0.45
1:H:31:SER:C	1:H:99:VAL:HG13	2.40	0.45
2:L:148:LYS:HG2	2:L:153:LEU:CD2	2.46	0.45
1:A:87:THR:HG23	1:A:110:THR:HA	1.99	0.45
1:H:29:PHE:CG	1:H:76:ARG:HB3	2.52	0.45
2:L:33:LEU:O	2:L:50:GLY:N	2.50	0.45
1:A:28:THR:O	1:A:32:TYR:HB2	2.16	0.45
2:L:51:SER:OG	2:L:52:SER:N	2.50	0.45
2:B:30:SER:O	2:B:51:SER:CB	2.64	0.45
2:B:187:LYS:HG2	2:B:188:HIS:CD2	2.51	0.45
1:H:9:ALA:CB	1:H:201:LYS:HZ2	2.23	0.45
1:H:35:THR:HG22	1:H:36:TRP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:THR:O	2:B:69:ARG:HD2	2.17	0.44
1:H:96:ALA:N	1:H:100(H):ASP:OD2	2.51	0.44
1:A:21:SER:HB3	1:A:79:TYR:CD2	2.53	0.44
1:A:4:LEU:HD21	1:A:28:THR:HG21	2.00	0.44
2:L:89:GLN:NE2	2:L:91:TYR:HB3	2.33	0.44
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.84	0.44
2:B:27(A):GLY:HA2	2:B:69:ARG:HG2	2.00	0.44
2:L:33:LEU:HD13	2:L:71:PHE:CG	2.52	0.44
2:B:152:ALA:O	2:B:154:GLN:NE2	2.44	0.44
1:H:207:VAL:HG11	1:H:209:LYS:CE	2.46	0.44
2:L:11:LEU:HG	2:L:13:LEU:HD11	1.98	0.44
1:A:152:VAL:HG22	1:A:198:VAL:HG22	1.99	0.44
2:B:165:GLN:HG2	2:B:170:SER:HA	2.00	0.44
2:L:135:LEU:HB3	2:L:138:PHE:CE2	2.53	0.44
2:L:4:MET:SD	2:L:25:THR:HG22	2.58	0.43
1:A:201:LYS:N	1:A:202:PRO:CD	2.81	0.43
2:L:141:ARG:NH1	2:L:162:VAL:HG21	2.33	0.43
1:A:8:GLY:C	1:A:201:LYS:HZ1	2.16	0.43
1:H:32:TYR:CG	1:H:94:ARG:HD2	2.53	0.43
1:A:26:GLY:HA3	1:A:76:ARG:CZ	2.49	0.43
2:B:67:SER:OG	2:B:68:GLY:N	2.51	0.43
1:H:35:THR:HG21	1:H:47:TRP:CD1	2.54	0.43
1:A:4:LEU:CD2	1:A:24:ALA:HA	2.49	0.43
2:B:48:ILE:HD13	2:B:54:ARG:HA	2.00	0.43
1:H:12:LYS:HG3	1:H:18:VAL:HB	1.99	0.43
1:H:150:VAL:HG12	1:H:200:HIS:HB2	1.99	0.43
1:H:59:TYR:HB2	1:H:64:ASP:OD1	2.18	0.43
1:H:148:GLU:HA	1:H:149:PRO:HA	1.75	0.43
2:L:99:GLN:H	2:L:99:GLN:CD	2.26	0.43
2:B:107:ARG:HG2	2:B:107:ARG:HH11	1.83	0.43
2:B:124:LEU:HD23	2:B:124:LEU:HA	1.90	0.43
1:H:141:LEU:HD12	1:H:178:LEU:O	2.20	0.42
1:A:6:GLN:HA	1:A:21:SER:O	2.19	0.42
1:H:19:ARG:HA	1:H:80:MET:O	2.19	0.42
1:H:86:ASP:O	1:H:87:THR:C	2.62	0.42
1:H:185:PRO:O	1:H:188:SER:OG	2.35	0.42
2:B:160:GLU:HB3	2:B:174:LEU:HD21	2.01	0.42
1:H:69:ILE:HA	1:H:79:TYR:O	2.19	0.42
1:H:150:VAL:HG22	1:H:178:LEU:HD13	2.02	0.42
2:B:66:GLY:HA3	2:B:71:PHE:HA	2.01	0.42
1:H:164:HIS:HB2	1:H:181:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:CYS:O	1:A:208:ASP:HA	2.20	0.42
2:L:18:ARG:HG3	2:L:76:SER:HA	2.02	0.42
1:H:52:PHE:O	1:H:55:GLY:N	2.53	0.42
2:L:61:ARG:CZ	2:L:79:GLU:HG3	2.50	0.41
1:H:139:GLY:HA2	1:H:154:TRP:CZ2	2.55	0.41
1:H:9:ALA:HB2	3:H:311:HOH:O	2.19	0.41
2:L:139:TYR:CG	2:L:140:PRO:HA	2.54	0.41
1:A:18:VAL:CG2	1:A:82:LEU:HB3	2.51	0.41
1:A:19:ARG:HA	1:A:80:MET:O	2.20	0.41
2:B:124:LEU:HD21	2:B:185:TYR:CD2	2.53	0.41
1:A:148:GLU:O	3:A:303:HOH:O	2.22	0.41
2:B:165:GLN:NE2	2:B:170:SER:HB3	2.35	0.41
1:A:30:SER:O	1:A:53:ILE:HD13	2.21	0.41
1:A:211:VAL:HG12	1:A:212:GLU:H	1.86	0.41
2:L:141:ARG:CZ	2:L:162:VAL:HG21	2.50	0.41
2:L:176:SER:OG	3:L:301:HOH:O	2.22	0.41
1:A:88:ALA:HB3	1:A:90:TYR:CE1	2.56	0.41
2:B:6:GLN:OE1	2:B:87:TYR:HA	2.21	0.41
2:B:124:LEU:HD11	2:B:185:TYR:HE2	1.85	0.41
2:B:153:LEU:HD23	2:B:154:GLN:O	2.21	0.41
2:L:33:LEU:HD13	2:L:71:PHE:CD2	2.55	0.41
2:L:86:TYR:O	2:L:100:GLY:HA2	2.21	0.41
1:A:38:ARG:HB3	1:A:90:TYR:CD2	2.56	0.40
1:A:143:LYS:O	1:A:144:ASP:HB2	2.20	0.40
1:H:124:LEU:HD12	1:H:140:CYS:N	2.37	0.40
1:H:29:PHE:CZ	1:H:76:ARG:HA	2.56	0.40
2:B:2:ILE:HD12	2:B:90:GLN:OE1	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:GLU:OE1	3:B:303:HOH:O[3_454]	2.06	0.14
2:L:107:ARG:NH2	3:H:305:HOH:O[3_564]	2.14	0.06

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	215/236 (91%)	197 (92%)	15 (7%)	3 (1%)	9	19
1	H	216/236 (92%)	196 (91%)	16 (7%)	4 (2%)	6	13
2	B	211/214 (99%)	196 (93%)	15 (7%)	0	100	100
2	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	46
All	All	854/900 (95%)	792 (93%)	54 (6%)	8 (1%)	14	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	101	ASP
1	A	27	ASP
1	A	44	GLY
1	H	64	ASP
1	H	100(D)	PRO
2	L	51	SER
1	H	149	PRO
1	A	126	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	184/200 (92%)	177 (96%)	7 (4%)	29	56
1	H	185/200 (92%)	181 (98%)	4 (2%)	45	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	185/186 (100%)	177 (96%)	8 (4%)	26	51
2	L	186/186 (100%)	182 (98%)	4 (2%)	45	72
All	All	740/772 (96%)	717 (97%)	23 (3%)	35	63

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	16	SER
1	H	66	ARG
1	H	74	SER
1	H	179	SER
2	L	22	SER
2	L	53	SER
2	L	60	ASP
2	L	130	SER
1	A	21	SER
1	A	30	SER
1	A	31	SER
1	A	35	THR
1	A	43	HIS
1	A	99	VAL
1	A	201	LYS
2	B	31	SER
2	B	33	LEU
2	B	53	SER
2	B	67	SER
2	B	81	GLU
2	B	160	GLU
2	B	175	SER
2	B	207	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	6	GLN
2	L	90	GLN
2	L	136	ASN
1	A	58	ASN
2	B	38	GLN
2	B	146	GLN

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Mol	Chain	Res	Type
2	B	159	GLN
2	B	198	GLN

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	219/236 (92%)	-1.62	0 100 100	37, 64, 99, 117	0
1	H	220/236 (93%)	-1.60	0 100 100	39, 65, 98, 171	0
2	B	212/214 (99%)	-1.74	0 100 100	29, 52, 81, 117	1 (0%)
2	L	213/214 (99%)	-1.69	0 100 100	37, 57, 84, 102	1 (0%)
All	All	864/900 (96%)	-1.66	0 100 100	29, 60, 91, 171	2 (0%)

There are no RSRZ outliers to report.

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.