



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:40 AM UTC

PDB ID : 1MAM / pdb_00001mam
Title : CRYSTAL STRUCTURE TO 2.45 Å RESOLUTION OF A MONOCLONAL
FAB SPECIFIC FOR THE BRUCELLA A CELL WALL POLYSACCHARIDE ANTIGEN
Authors : Rose, D.R.
Deposited on : 1992-01-14
Resolution : 2.45 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

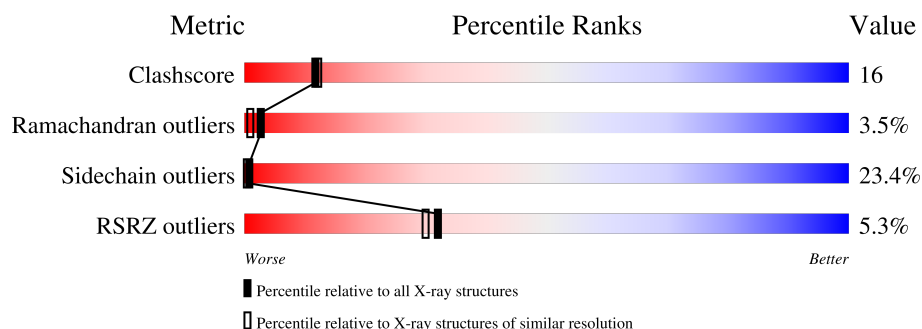
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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))
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	L	214	4% 47% 33% 13% 7%
2	H	217	7% 44% 35% 17% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3296 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 IGG2B-KAPPA YST9.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1668	1032	282	346	8			

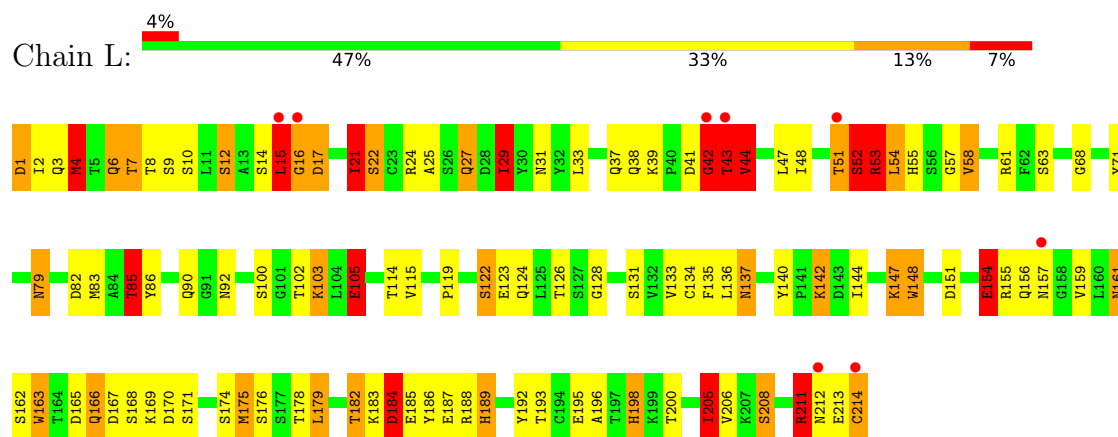
- Molecule 2 is a protein called IGG2B-KAPPA YST9.1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1628	1028	266	326	8			

3 Residue-property plots [i](#)

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: IGG2B-KAPPA YST9.1 FAB (LIGHT CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.73Å 126.82Å 46.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.45 65.02 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.45) 88.4 (65.02-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.45Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.215 , (Not available) 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 97.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3296	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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	L	1.52	15/1702 (0.9%)	2.43	80/2309 (3.5%)
2	H	1.55	15/1671 (0.9%)	2.75	110/2284 (4.8%)
All	All	1.53	30/3373 (0.9%)	2.59	190/4593 (4.1%)

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	L	1	2
2	H	1	9
All	All	2	11

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	52	SER	N-CA	23.09	1.75	1.46
2	H	135	GLY	CA-C	21.88	1.82	1.51
2	H	166	SER	C-N	15.51	1.55	1.33
1	L	16	GLY	CA-C	15.25	1.73	1.51
1	L	211	ARG	C-O	14.11	1.44	1.23
2	H	167	SER	N-CA	13.62	1.63	1.46
2	H	101	ASP	C-N	-12.11	1.05	1.33
1	L	15	LEU	C-N	11.98	1.50	1.33
2	H	134	CYS	CA-CB	-10.18	1.37	1.53
1	L	16	GLY	N-CA	9.18	1.58	1.45
2	H	199	VAL	CA-CB	8.85	1.67	1.54
2	H	115	VAL	CA-CB	8.40	1.65	1.54
2	H	156	VAL	N-CA	8.39	1.56	1.46
1	L	44	VAL	N-CA	8.31	1.62	1.46
1	L	198	HIS	CD2-NE2	-7.84	1.29	1.37
1	L	21	ILE	CA-CB	7.59	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	148	VAL	CA-CB	7.41	1.63	1.53
1	L	212	ASN	N-CA	7.15	1.55	1.46
2	H	205	HIS	CD2-NE2	-6.86	1.30	1.37
2	H	207	ALA	CA-C	6.83	1.60	1.53
2	H	137	THR	CA-CB	6.77	1.64	1.53
2	H	170	HIS	CD2-NE2	-6.28	1.30	1.37
1	L	42	GLY	N-CA	6.26	1.54	1.45
1	L	189	HIS	CD2-NE2	-6.06	1.31	1.37
2	H	170	HIS	CG-ND1	-6.01	1.31	1.38
1	L	205	ILE	CA-CB	5.70	1.61	1.54
1	L	85	THR	CA-CB	5.69	1.62	1.53
1	L	55	HIS	CD2-NE2	-5.18	1.32	1.37
2	H	169	VAL	CA-CB	5.17	1.60	1.54
1	L	198	HIS	CG-ND1	-5.05	1.32	1.38

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	135	GLY	CA-C-O	-27.88	72.06	120.57
1	L	15	LEU	O-C-N	26.13	157.35	122.59
2	H	55	ALA	CA-C-N	25.05	163.87	122.54
2	H	55	ALA	C-N-CA	25.05	163.87	122.54
1	L	43	THR	CA-C-N	24.74	166.23	121.70
1	L	43	THR	C-N-CA	24.74	166.23	121.70
2	H	167	SER	N-CA-CB	-21.53	74.10	110.49
2	H	155	SER	CA-C-N	20.74	150.97	120.69
2	H	155	SER	C-N-CA	20.74	150.97	120.69
2	H	80	ILE	N-CA-C	19.33	137.81	108.23
2	H	208	SER	N-CA-C	18.39	134.90	113.38
2	H	101	ASP	O-C-N	-18.16	100.43	121.32
1	L	211	ARG	O-C-N	-15.52	95.36	122.21
1	L	52	SER	N-CA-CB	15.04	135.91	110.49
2	H	195	PRO	N-CA-C	14.87	150.77	112.10
1	L	212	ASN	N-CA-CB	14.71	135.36	110.49
1	L	212	ASN	N-CA-C	-13.41	82.23	110.80
2	H	141	SER	CA-C-N	13.36	146.02	121.97
2	H	141	SER	C-N-CA	13.36	146.02	121.97
1	L	14	SER	N-CA-C	13.17	127.10	111.82
1	L	15	LEU	CA-C-N	12.29	145.50	121.41
1	L	15	LEU	C-N-CA	12.29	145.50	121.41
2	H	165	LEU	N-CA-C	12.25	128.27	112.34
2	H	136	ASP	N-CA-C	-11.68	99.24	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	ILE	N-CA-CB	-10.97	98.50	111.00
1	L	44	VAL	N-CA-CB	10.96	130.13	111.50
2	H	101	ASP	CA-C-N	10.89	133.46	119.84
2	H	101	ASP	C-N-CA	10.89	133.46	119.84
2	H	154	GLU	O-C-N	10.77	135.13	122.85
1	L	43	THR	N-CA-C	10.74	126.41	110.30
1	L	31	ASN	OD1-CG-ND2	-10.40	112.20	122.60
1	L	184	ASP	CA-CB-CG	-10.35	102.25	112.60
2	H	79	SER	CA-C-N	10.23	135.16	122.37
2	H	79	SER	C-N-CA	10.23	135.16	122.37
1	L	51	THR	CA-C-N	-10.18	102.11	121.54
1	L	51	THR	C-N-CA	-10.18	102.11	121.54
2	H	207	ALA	CA-C-N	9.80	140.18	123.91
2	H	207	ALA	C-N-CA	9.80	140.18	123.91
2	H	156	VAL	N-CA-C	9.55	121.81	109.30
1	L	144	ILE	O-C-N	-9.50	114.70	122.97
1	L	184	ASP	N-CA-C	9.36	121.48	111.28
2	H	161	ASN	CB-CG-ND2	9.09	130.03	116.40
2	H	195	PRO	CA-C-O	9.09	142.00	120.20
2	H	136	ASP	CA-CB-CG	9.01	121.61	112.60
1	L	92	ASN	OD1-CG-ND2	-8.97	113.63	122.60
1	L	17	ASP	O-C-N	8.52	132.65	122.68
2	H	7	SER	O-C-N	-8.46	112.96	121.93
1	L	7	THR	N-CA-C	-8.38	98.08	110.48
1	L	170	ASP	CA-CB-CG	8.22	120.82	112.60
2	H	56	ASP	CA-C-O	8.04	128.75	119.35
2	H	193	THR	CA-CB-OG1	-8.04	97.54	109.60
1	L	53	ARG	CA-CB-CG	7.91	129.92	114.10
2	H	56	ASP	N-CA-CB	7.91	122.19	110.49
2	H	217	GLU	CB-CG-CD	7.88	125.99	112.60
2	H	161	ASN	CA-CB-CG	7.86	120.46	112.60
2	H	152	PHE	O-C-N	-7.63	115.88	121.83
2	H	197	GLN	CA-CB-CG	7.53	129.16	114.10
1	L	3	GLN	OE1-CD-NE2	-7.50	115.10	122.60
2	H	2	VAL	N-CA-C	-7.45	93.84	109.34
2	H	161	ASN	OD1-CG-ND2	-7.33	115.28	122.60
2	H	85	MET	CG-SD-CE	-7.28	84.88	100.90
2	H	182	THR	CA-CB-OG1	-7.25	98.73	109.60
1	L	31	ASN	CB-CG-ND2	7.21	127.22	116.40
2	H	166	SER	N-CA-C	-7.13	95.60	110.80
2	H	164	SER	N-CA-C	7.12	125.97	110.80
2	H	154	GLU	CA-C-N	7.08	135.05	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	154	GLU	C-N-CA	7.08	135.05	121.54
2	H	140	SER	N-CA-C	-7.06	95.76	110.80
1	L	205	ILE	CB-CA-C	7.03	121.30	110.83
1	L	137	ASN	N-CA-C	7.00	121.25	109.76
2	H	56	ASP	O-C-N	-6.97	113.63	122.34
1	L	171	SER	N-CA-C	6.79	120.87	112.58
2	H	32	TYR	N-CA-C	6.79	120.75	109.95
2	H	166	SER	CA-C-N	6.67	134.28	121.54
2	H	166	SER	C-N-CA	6.67	134.28	121.54
1	L	29	ILE	N-CA-CB	-6.62	103.72	112.26
2	H	203	VAL	O-C-N	6.58	130.17	123.20
2	H	118	SER	CA-C-O	6.52	128.06	120.89
1	L	157	ASN	CA-CB-CG	6.46	119.06	112.60
2	H	205	HIS	CA-CB-CG	6.39	120.19	113.80
1	L	183	LYS	N-CA-C	-6.36	103.48	111.11
1	L	185	GLU	CA-CB-CG	-6.36	101.38	114.10
1	L	6	GLN	CA-C-O	6.35	127.25	120.46
2	H	209	SER	N-CA-C	6.31	119.82	109.72
2	H	213	ASP	CA-CB-CG	-6.31	106.29	112.60
2	H	206	PRO	O-C-N	-6.28	114.16	122.64
1	L	122	SER	N-CA-C	-6.27	104.45	111.28
1	L	163	TRP	CB-CG-CD1	-6.20	117.60	126.90
1	L	163	TRP	CG-CD2-CE3	6.18	140.08	133.90
2	H	7	SER	N-CA-C	6.18	124.03	114.64
2	H	13	GLN	OE1-CD-NE2	-6.16	116.44	122.60
2	H	166	SER	CA-C-O	6.15	129.31	120.51
2	H	172	PHE	CA-CB-CG	-6.15	107.65	113.80
1	L	154	GLU	CA-CB-CG	6.12	126.35	114.10
1	L	85	THR	OG1-CB-CG2	6.12	121.53	109.30
1	L	38	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	L	167	ASP	CA-C-O	6.04	127.76	120.81
1	L	198	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	L	52	SER	N-CA-C	-6.03	97.97	110.80
2	H	135	GLY	O-C-N	5.99	130.49	122.70
2	H	217	GLU	CA-CB-CG	5.98	126.06	114.10
2	H	62	TYR	O-C-N	-5.98	116.34	123.27
1	L	205	ILE	CA-C-O	5.98	126.81	120.48
1	L	151	ASP	CA-CB-CG	5.93	118.53	112.60
1	L	42	GLY	CA-C-N	5.93	130.69	121.26
1	L	42	GLY	C-N-CA	5.93	130.69	121.26
1	L	105	GLU	CA-CB-CG	5.91	125.91	114.10
2	H	159	THR	CA-CB-OG1	-5.90	100.75	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	182	THR	N-CA-C	5.89	119.11	108.69
2	H	194	TRP	CA-CB-CG	-5.87	102.45	113.60
1	L	124	GLN	OE1-CD-NE2	-5.86	116.74	122.60
2	H	208	SER	N-CA-CB	-5.82	103.88	112.78
2	H	65	SER	N-CA-C	5.81	118.40	111.71
2	H	162	SER	N-CA-CB	-5.81	102.01	110.84
1	L	103	LYS	CG-CD-CE	5.81	124.67	111.30
2	H	164	SER	CA-C-N	5.76	129.91	120.63
2	H	164	SER	C-N-CA	5.76	129.91	120.63
2	H	52	ARG	CA-CB-CG	-5.75	102.61	114.10
1	L	42	GLY	N-CA-C	5.73	126.76	113.18
1	L	16	GLY	O-C-N	-5.72	115.27	122.70
2	H	216	LEU	CA-C-N	5.68	131.92	121.70
2	H	216	LEU	C-N-CA	5.68	131.92	121.70
1	L	182	THR	CA-CB-OG1	-5.64	101.14	109.60
2	H	114	LEU	N-CA-C	5.63	117.91	108.96
2	H	13	GLN	CB-CG-CD	5.62	122.16	112.60
1	L	198	HIS	CB-CG-ND1	5.61	131.12	122.70
2	H	205	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	L	159	VAL	N-CA-C	5.55	116.09	107.99
1	L	163	TRP	CE2-CD2-CG	-5.54	100.56	107.20
2	H	187	VAL	N-CA-C	-5.53	100.23	108.46
2	H	162	SER	CB-CA-C	5.49	118.91	110.62
1	L	57	GLY	N-CA-C	-5.49	107.12	114.25
1	L	79	ASN	OD1-CG-ND2	-5.48	117.12	122.60
2	H	137	THR	CA-C-N	5.48	132.00	121.54
2	H	137	THR	C-N-CA	5.48	132.00	121.54
1	L	58	VAL	N-CA-C	5.48	114.32	108.95
2	H	165	LEU	CA-C-N	5.47	131.99	121.54
2	H	165	LEU	C-N-CA	5.47	131.99	121.54
2	H	166	SER	O-C-N	-5.45	115.34	122.59
1	L	85	THR	CB-CA-C	5.45	119.15	109.72
2	H	170	HIS	CA-CB-CG	-5.42	108.38	113.80
1	L	22	SER	N-CA-C	5.41	118.93	110.32
2	H	140	SER	O-C-N	5.41	129.78	122.59
1	L	128	GLY	N-CA-C	5.41	125.99	113.18
2	H	182	THR	CA-CB-CG2	5.39	119.66	110.50
1	L	24	ARG	NE-CZ-NH2	-5.39	114.35	119.20
2	H	139	GLY	CA-C-N	5.38	131.82	121.54
2	H	139	GLY	C-N-CA	5.38	131.82	121.54
2	H	165	LEU	O-C-N	5.37	129.31	122.33
2	H	159	THR	CA-CB-CG2	5.37	119.62	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	142	VAL	N-CA-CB	5.35	120.06	111.23
2	H	140	SER	N-CA-CB	5.35	119.53	110.49
2	H	107	ALA	N-CA-C	5.34	118.09	110.24
2	H	216	LEU	N-CA-C	-5.32	101.48	109.95
2	H	75	ASP	N-CA-C	-5.32	99.78	108.76
1	L	7	THR	CA-CB-OG1	-5.31	101.63	109.60
1	L	1	ASP	CA-CB-CG	-5.31	107.29	112.60
2	H	13	GLN	CG-CD-NE2	5.31	124.36	116.40
2	H	51	ILE	N-CA-CB	-5.31	104.08	111.41
1	L	189	HIS	CB-CG-CD2	-5.30	124.32	131.20
1	L	43	THR	CA-CB-OG1	-5.28	101.68	109.60
1	L	137	ASN	O-C-N	5.25	129.33	123.19
1	L	148	TRP	CG-CD1-NE1	-5.23	103.39	110.20
1	L	29	ILE	CA-CB-CG2	5.22	119.38	110.50
1	L	166	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	H	148	VAL	CA-C-O	5.22	127.47	120.69
2	H	161	ASN	N-CA-C	-5.21	99.69	110.80
2	H	36	TRP	CG-CD2-CE3	5.21	139.11	133.90
1	L	185	GLU	O-C-N	5.20	128.08	122.15
2	H	95	THR	N-CA-C	-5.18	100.87	109.46
2	H	148	VAL	CB-CA-C	5.17	117.58	111.32
2	H	194	TRP	CB-CA-C	-5.17	99.98	110.17
2	H	133	GLY	O-C-N	5.17	129.42	122.70
1	L	161	ASN	OD1-CG-ND2	-5.17	117.43	122.60
2	H	110	GLY	O-C-N	-5.17	118.22	122.92
2	H	81	LEU	O-C-N	-5.16	117.17	123.16
1	L	42	GLY	O-C-N	5.16	129.41	122.70
2	H	95	THR	CB-CA-C	5.13	118.22	109.80
2	H	78	GLN	CG-CD-NE2	5.11	124.07	116.40
1	L	25	ALA	O-C-N	-5.10	117.23	123.10
1	L	119	PRO	CA-C-N	5.08	125.07	119.89
1	L	119	PRO	C-N-CA	5.08	125.07	119.89
2	H	78	GLN	O-C-N	5.08	128.51	122.27
1	L	31	ASN	N-CA-C	5.07	119.32	113.38
2	H	78	GLN	OE1-CD-NE2	-5.06	117.54	122.60
2	H	194	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	L	165	ASP	N-CA-C	-5.06	103.37	110.35
1	L	4	MET	CG-SD-CE	-5.05	89.78	100.90
2	H	111	GLN	O-C-N	5.04	128.33	122.24
1	L	174	SER	N-CA-C	-5.01	101.75	109.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L	44	VAL	CA
2	H	195	PRO	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	104	GLY	Peptide
2	H	135	GLY	Peptide,Mainchain
2	H	141	SER	Peptide
2	H	155	SER	Peptide
2	H	166	SER	Peptide,Mainchain
2	H	181	TYR	Sidechain
2	H	79	SER	Peptide
1	L	211	ARG	Mainchain
1	L	43	THR	Peptide

5.2 Too-close contacts [i](#)

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	L	1668	0	1593	56	0
2	H	1628	0	1578	48	0
All	All	3296	0	3171	103	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 16.

All (103) 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:H:135:GLY:CA	2:H:135:GLY:C	1.82	1.52
1:L:52:SER:N	1:L:52:SER:CA	1.76	1.44
2:H:135:GLY:CA	2:H:135:GLY:O	1.87	1.22
2:H:166:SER:OG	2:H:188:THR:O	1.64	1.11
2:H:166:SER:HB2	2:H:190:PRO:HD3	1.26	1.11
1:L:15:LEU:O	1:L:15:LEU:HG	1.48	1.06
1:L:214:CYS:SG	2:H:134:CYS:SG	2.55	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:THR:C	1:L:52:SER:CA	2.41	0.92
2:H:166:SER:CB	2:H:190:PRO:HD3	2.02	0.88
1:L:41:ASP:OD2	1:L:43:THR:HG23	1.76	0.86
2:H:134:CYS:HB3	2:H:217:GLU:OE2	1.79	0.83
2:H:166:SER:HB2	2:H:190:PRO:CD	2.09	0.82
1:L:189:HIS:O	1:L:211:ARG:NH1	2.20	0.75
2:H:134:CYS:SG	2:H:134:CYS:O	2.47	0.73
1:L:2:ILE:HD13	1:L:29:ILE:HD11	1.73	0.71
1:L:186:TYR:CZ	1:L:211:ARG:HD2	2.26	0.70
1:L:2:ILE:HG12	1:L:27:GLN:HB2	1.74	0.70
2:H:163:GLY:O	2:H:165:LEU:HD22	1.92	0.69
1:L:51:THR:O	1:L:52:SER:CA	2.40	0.69
1:L:52:SER:N	1:L:52:SER:C	2.50	0.68
1:L:51:THR:O	1:L:52:SER:HA	1.94	0.68
1:L:182:THR:HG22	1:L:184:ASP:H	1.60	0.67
2:H:166:SER:OG	2:H:189:VAL:HA	1.95	0.65
2:H:4:LEU:HG	2:H:108:TYR:CD1	2.33	0.64
2:H:193:THR:OG1	2:H:197:GLN:HG2	1.99	0.63
2:H:3:LYS:O	2:H:24:THR:HA	1.98	0.62
1:L:4:MET:HE1	1:L:90:GLN:HG2	1.80	0.62
2:H:215:LYS:HB3	2:H:215:LYS:HZ3	1.65	0.62
1:L:135:PHE:HB3	1:L:137:ASN:HD21	1.65	0.61
1:L:6:GLN:HE21	1:L:21:ILE:HD11	1.66	0.61
2:H:165:LEU:HG	2:H:190:PRO:HG3	1.81	0.61
1:L:2:ILE:HD13	1:L:29:ILE:CD1	2.30	0.61
1:L:193:THR:HG23	1:L:206:VAL:HG13	1.83	0.59
2:H:166:SER:OG	2:H:188:THR:C	2.45	0.59
1:L:186:TYR:CE2	1:L:211:ARG:HD2	2.38	0.59
2:H:169:VAL:HA	2:H:186:SER:O	2.06	0.56
2:H:4:LEU:HG	2:H:108:TYR:HD1	1.67	0.56
1:L:4:MET:N	1:L:4:MET:HE2	2.21	0.55
2:H:166:SER:CB	2:H:189:VAL:HA	2.37	0.55
2:H:96:TYR:O	2:H:112:GLY:HA2	2.06	0.55
2:H:4:LEU:HA	2:H:23:ALA:O	2.07	0.54
2:H:135:GLY:C	2:H:135:GLY:N	2.62	0.54
2:H:168:SER:HB2	2:H:188:THR:HG23	1.89	0.54
1:L:182:THR:HG22	1:L:184:ASP:N	2.24	0.53
2:H:145:GLY:O	2:H:215:LYS:HE3	2.08	0.53
2:H:52:ARG:O	2:H:74:ARG:NH1	2.43	0.52
1:L:51:THR:O	1:L:51:THR:HG22	2.10	0.51
1:L:123:GLU:O	1:L:126:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ASP:OD2	2:H:78:GLN:HB2	2.10	0.51
1:L:195:GLU:HG3	1:L:206:VAL:HG22	1.93	0.51
1:L:140:TYR:O	1:L:198:HIS:HE1	1.94	0.51
2:H:54:LYS:HB2	2:H:58:TYR:OH	2.11	0.51
1:L:12:SER:HA	1:L:105:GLU:O	2.11	0.51
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.92	0.50
1:L:187:GLU:O	1:L:211:ARG:NH2	2.45	0.50
1:L:85:THR:HA	1:L:102:THR:O	2.11	0.50
1:L:135:PHE:HB3	1:L:137:ASN:ND2	2.25	0.50
1:L:133:VAL:HG22	1:L:178:THR:HG23	1.93	0.49
1:L:155:ARG:HG2	1:L:179:LEU:HD21	1.94	0.48
2:H:29:PHE:HD1	2:H:34:MET:HE3	1.77	0.48
1:L:21:ILE:HD12	1:L:22:SER:N	2.29	0.48
2:H:29:PHE:CZ	2:H:74:ARG:HG3	2.49	0.48
1:L:131:SER:HA	1:L:179:LEU:O	2.14	0.48
1:L:184:ASP:OD2	1:L:188:ARG:NH1	2.47	0.48
2:H:29:PHE:CD1	2:H:34:MET:HE3	2.49	0.47
2:H:138:THR:HG22	2:H:139:GLY:H	1.79	0.47
2:H:20:LEU:HD13	2:H:85:MET:HE1	1.97	0.47
1:L:83:MET:HE1	1:L:166:GLN:O	2.14	0.47
1:L:2:ILE:HG22	1:L:4:MET:HE1	1.96	0.47
1:L:4:MET:CE	1:L:90:GLN:HG2	2.44	0.46
2:H:175:LEU:N	2:H:175:LEU:HD12	2.30	0.46
1:L:147:LYS:HZ3	1:L:154:GLU:CD	2.23	0.46
2:H:22:CYS:HB3	2:H:81:LEU:HB3	1.98	0.46
1:L:29:ILE:HG22	1:L:71:TYR:OH	2.15	0.46
1:L:51:THR:O	1:L:51:THR:CG2	2.64	0.45
2:H:101:ASP:O	2:H:102:PRO:C	2.55	0.45
1:L:41:ASP:O	1:L:42:GLY:C	2.60	0.45
1:L:39:LYS:HB2	1:L:43:THR:O	2.16	0.45
1:L:142:LYS:HZ3	1:L:142:LYS:HB3	1.82	0.45
2:H:166:SER:CB	2:H:190:PRO:CD	2.85	0.44
2:H:172:PHE:HA	2:H:173:PRO:HD2	1.70	0.44
2:H:202:SER:OG	2:H:212:VAL:HG12	2.17	0.44
1:L:37:GLN:HG3	1:L:86:TYR:CE1	2.53	0.44
2:H:3:LYS:C	2:H:4:LEU:HD23	2.43	0.44
1:L:162:SER:O	1:L:175:MET:HA	2.18	0.43
1:L:192:TYR:O	1:L:208:SER:HA	2.18	0.43
2:H:80:ILE:H	2:H:80:ILE:HG13	1.56	0.43
2:H:141:SER:HA	2:H:189:VAL:O	2.19	0.42
1:L:48:ILE:HG12	1:L:54:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:SER:HB3	2:H:86:ASN:HA	2.01	0.42
2:H:146:CYS:O	2:H:184:SER:HA	2.19	0.42
2:H:183:MET:HE2	2:H:183:MET:HB2	1.86	0.42
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.55	0.41
2:H:70:PHE:HA	2:H:84:GLN:O	2.20	0.41
1:L:48:ILE:HG23	1:L:53:ARG:O	2.20	0.41
2:H:138:THR:HG22	2:H:139:GLY:N	2.34	0.41
1:L:61:ARG:NH1	1:L:82:ASP:OD1	2.52	0.41
2:H:215:LYS:HZ3	2:H:215:LYS:CB	2.31	0.41
1:L:161:ASN:HA	1:L:176:SER:O	2.21	0.41
1:L:21:ILE:HD13	1:L:102:THR:OG1	2.21	0.41
1:L:136:LEU:CD2	1:L:196:ALA:HB2	2.52	0.40
1:L:195:GLU:HG3	1:L:206:VAL:CG2	2.51	0.40
1:L:115:VAL:HG21	1:L:205:ILE:CD1	2.52	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	L	212/214 (99%)	191 (90%)	14 (7%)	7 (3%)	3	1
2	H	215/217 (99%)	185 (86%)	22 (10%)	8 (4%)	2	1
All	All	427/431 (99%)	376 (88%)	36 (8%)	15 (4%)	3	1

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	164	SER
2	H	167	SER
1	L	42	GLY
1	L	52	SER

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Mol	Chain	Res	Type
1	L	68	GLY
2	H	55	ALA
2	H	43	LYS
1	L	15	LEU
2	H	141	SER
1	L	8	THR
1	L	44	VAL
2	H	139	GLY
2	H	194	TRP
2	H	163	GLY
1	L	16	GLY

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	L	193/193 (100%)	153 (79%)	40 (21%)	1	0
2	H	183/183 (100%)	135 (74%)	48 (26%)	0	0
All	All	376/376 (100%)	288 (77%)	88 (23%)	1	0

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	4	MET
1	L	7	THR
1	L	9	SER
1	L	10	SER
1	L	12	SER
1	L	15	LEU
1	L	17	ASP
1	L	21	ILE
1	L	27	GLN
1	L	29	ILE
1	L	33	LEU

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Mol	Chain	Res	Type
1	L	43	THR
1	L	44	VAL
1	L	52	SER
1	L	53	ARG
1	L	54	LEU
1	L	63	SER
1	L	79	ASN
1	L	85	THR
1	L	100	SER
1	L	103	LYS
1	L	105	GLU
1	L	114	THR
1	L	122	SER
1	L	142	LYS
1	L	147	LYS
1	L	154	GLU
1	L	156	GLN
1	L	163	TRP
1	L	168	SER
1	L	169	LYS
1	L	175	MET
1	L	179	LEU
1	L	184	ASP
1	L	200	THR
1	L	205	ILE
1	L	208	SER
1	L	213	GLU
1	L	214	CYS
2	H	1	GLU
2	H	2	VAL
2	H	3	LYS
2	H	4	LEU
2	H	5	VAL
2	H	11	LEU
2	H	12	VAL
2	H	13	GLN
2	H	17	SER
2	H	20	LEU
2	H	25	SER
2	H	30	THR
2	H	41	PRO
2	H	56	ASP

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Mol	Chain	Res	Type
2	H	60	THR
2	H	61	GLU
2	H	75	ASP
2	H	77	SER
2	H	78	GLN
2	H	79	SER
2	H	80	ILE
2	H	100	ARG
2	H	111	GLN
2	H	113	THR
2	H	115	VAL
2	H	137	THR
2	H	140	SER
2	H	142	VAL
2	H	144	LEU
2	H	147	LEU
2	H	148	VAL
2	H	154	GLU
2	H	165	LEU
2	H	168	SER
2	H	175	LEU
2	H	177	GLN
2	H	188	THR
2	H	194	TRP
2	H	196	SER
2	H	197	GLN
2	H	199	VAL
2	H	209	SER
2	H	210	THR
2	H	211	THR
2	H	212	VAL
2	H	214	LYS
2	H	215	LYS
2	H	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	92	ASN
1	L	137	ASN
1	L	138	ASN

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Mol	Chain	Res	Type
1	L	161	ASN
1	L	190	ASN
2	H	197	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	101:ASP	C	102:PRO	N	1.05

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	L	214/214 (100%)	0.19	8 (3%) 45 45	2, 9, 20, 31	0
2	H	217/217 (100%)	0.45	15 (6%) 23 20	3, 10, 27, 38	0
All	All	431/431 (100%)	0.32	23 (5%) 32 30	2, 10, 25, 38	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	166	SER	9.3
2	H	135	GLY	6.2
2	H	164	SER	6.2
2	H	134	CYS	5.7
2	H	55	ALA	5.6
1	L	43	THR	4.8
1	L	15	LEU	4.7
2	H	165	LEU	4.4
2	H	161	ASN	4.0
2	H	167	SER	3.2
2	H	137	THR	3.0
1	L	16	GLY	2.8
2	H	56	ASP	2.7
2	H	163	GLY	2.6
2	H	195	PRO	2.5
1	L	42	GLY	2.4
1	L	212	ASN	2.2
2	H	136	ASP	2.2
1	L	214	CYS	2.1
1	L	51	THR	2.1
2	H	207	ALA	2.1
2	H	101	ASP	2.1
1	L	157	ASN	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.