Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 02:53 PM EDT

PDB ID	:	1MAM
Title	:	CRYSTAL STRUCTURE TO 2.45 A 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:

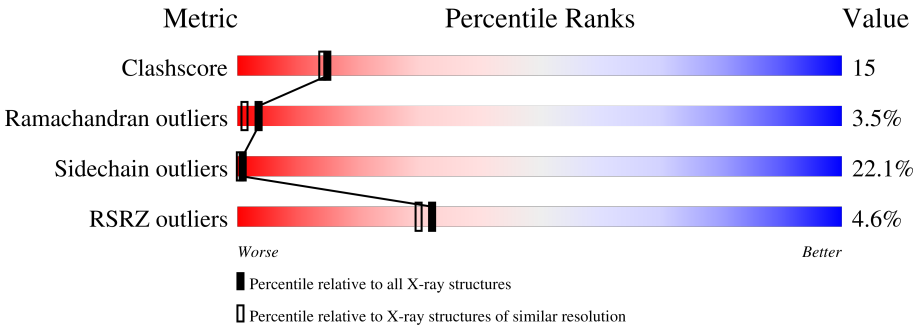
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	3% 53% 34% 8% 5%
2	H	217	6% 48% 35% 13% .

2 Entry composition (i)

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
			Total	C	N	O	S			
1	L	214	1668	1032	282	346	8	0	0	0

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

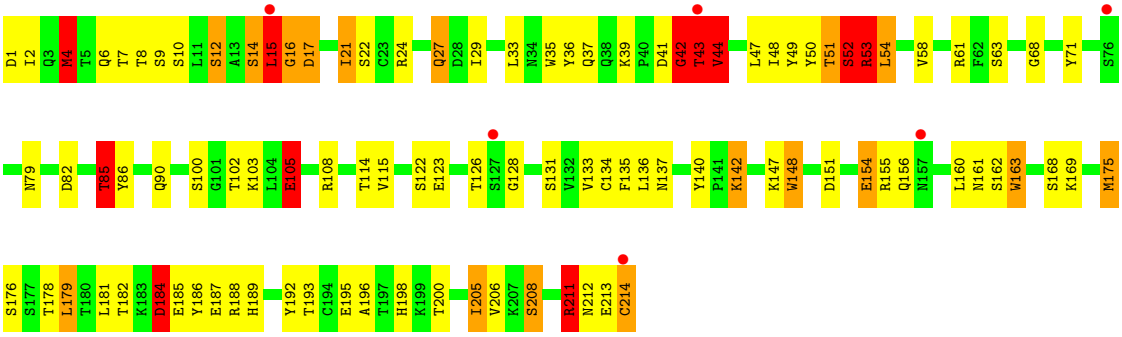
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1628	1028	266	326	8	0	0	0

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.

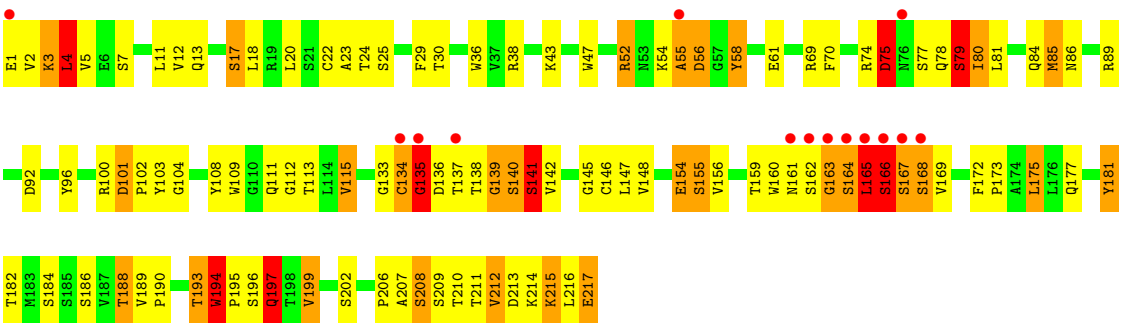
• Molecule 1: IGG2B-KAPPA YST9.1 FAB (LIGHT CHAIN)

Chain L:



• Molecule 2: IGG2B-KAPPA YST9.1 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

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 33.72 – 2.44	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.45) 87.2 (33.72-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.45Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.215 , (Not available) 0.224 , (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)	0.45 , 93.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.18	7/1702 (0.4%)	2.02	43/2309 (1.9%)
2	H	1.27	8/1671 (0.5%)	2.27	76/2284 (3.3%)
All	All	1.23	15/3373 (0.4%)	2.15	119/4593 (2.6%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	135	GLY	CA-C	19.30	1.82	1.51
2	H	101	ASP	C-N	-15.13	1.05	1.34
1	L	52	SER	N-CA	14.81	1.75	1.46
1	L	16	GLY	CA-C	13.46	1.73	1.51
1	L	211	ARG	C-O	10.93	1.44	1.23
1	L	15	LEU	C-N	9.97	1.50	1.33
2	H	166	SER	C-N	9.28	1.55	1.34
2	H	167	SER	N-CA	8.70	1.63	1.46
1	L	16	GLY	N-CA	8.43	1.58	1.46
1	L	44	VAL	N-CA	7.84	1.62	1.46
2	H	134	CYS	CA-CB	-7.53	1.37	1.53
2	H	199	VAL	CA-CB	6.03	1.67	1.54
1	L	42	GLY	N-CA	5.60	1.54	1.46
2	H	156	VAL	N-CA	5.17	1.56	1.46
2	H	194	TRP	CD1-NE1	-5.03	1.29	1.38

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	135	GLY	CA-C-O	-26.96	72.06	120.60
2	H	167	SER	N-CA-CB	-24.27	74.10	110.50
1	L	15	LEU	O-C-N	20.09	157.35	123.20
1	L	43	THR	C-N-CA	17.81	166.23	121.70
1	L	15	LEU	CA-C-N	-17.38	81.44	116.20
1	L	211	ARG	O-C-N	-17.09	95.36	122.70
1	L	52	SER	N-CA-CB	16.94	135.91	110.50
2	H	55	ALA	C-N-CA	16.87	163.87	121.70
2	H	195	PRO	N-CA-C	14.87	150.77	112.10
1	L	212	ASN	N-CA-CB	13.76	135.36	110.60
1	L	24	ARG	NE-CZ-NH2	-11.90	114.35	120.30
2	H	155	SER	C-N-CA	11.71	150.97	121.70
1	L	15	LEU	C-N-CA	11.05	145.50	122.30
2	H	101	ASP	O-C-N	-10.88	100.43	121.10
2	H	38	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	L	212	ASN	N-CA-C	-10.65	82.23	111.00
2	H	80	ILE	N-CA-C	9.93	137.81	111.00
1	L	148	TRP	CD1-CG-CD2	9.85	114.18	106.30
2	H	141	SER	C-N-CA	9.73	146.02	121.70
2	H	89	ARG	NE-CZ-NH2	-9.65	115.47	120.30
2	H	85	MET	CG-SD-CE	-9.58	84.88	100.20
2	H	195	PRO	CA-C-N	-9.22	96.93	117.20
2	H	154	GLU	CA-C-N	-9.16	97.05	117.20
2	H	195	PRO	CA-C-O	9.09	142.00	120.20
2	H	208	SER	N-CA-C	8.85	134.90	111.00
1	L	163	TRP	CD1-CG-CD2	8.84	113.38	106.30
2	H	47	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	L	44	VAL	N-CA-CB	8.47	130.13	111.50
1	L	163	TRP	CE2-CD2-CG	-8.43	100.56	107.30
1	L	108	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	H	103	TYR	CB-CG-CD2	-8.01	116.20	121.00
2	H	194	TRP	CD1-CG-CD2	7.98	112.68	106.30
2	H	7	SER	CA-C-N	7.90	132.00	116.20
1	L	51	THR	C-N-CA	-7.84	102.11	121.70
2	H	207	ALA	CA-C-N	-7.77	100.11	117.20
2	H	154	GLU	O-C-N	7.77	135.13	122.70
2	H	194	TRP	CE2-CD2-CG	-7.72	101.13	107.30
2	H	18	LEU	CA-CB-CG	7.64	132.87	115.30
1	L	148	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	L	53	ARG	CA-CB-CG	7.51	129.92	113.40
2	H	207	ALA	C-N-CA	7.39	140.18	121.70
1	L	163	TRP	CB-CG-CD1	-7.23	117.60	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	47	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	H	197	GLN	CA-CB-CG	7.17	129.16	113.40
2	H	109	TRP	CE2-CD2-CG	-7.13	101.59	107.30
2	H	109	TRP	CD1-CG-CD2	7.04	111.93	106.30
2	H	36	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	L	163	TRP	CG-CD2-CE3	6.86	140.08	133.90
1	L	35	TRP	CD1-CG-CD2	6.82	111.76	106.30
1	L	148	TRP	CG-CD1-NE1	-6.71	103.39	110.10
2	H	103	TYR	CB-CG-CD1	6.69	125.01	121.00
2	H	69	ARG	NE-CZ-NH2	-6.67	116.96	120.30
2	H	36	TRP	CD1-CG-CD2	6.65	111.62	106.30
2	H	181	TYR	CB-CG-CD2	-6.57	117.06	121.00
2	H	160	TRP	CD1-CG-CD2	6.56	111.55	106.30
2	H	160	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	L	4	MET	CG-SD-CE	-6.51	89.78	100.20
2	H	56	ASP	N-CA-CB	6.44	122.19	110.60
1	L	181	LEU	CA-CB-CG	6.41	130.03	115.30
2	H	165	LEU	N-CA-C	6.40	128.27	111.00
2	H	2	VAL	N-CA-C	-6.36	93.84	111.00
1	L	17	ASP	O-C-N	6.22	132.65	122.70
2	H	58	TYR	CB-CG-CD2	-6.09	117.35	121.00
2	H	7	SER	O-C-N	-6.02	112.96	123.20
2	H	140	SER	N-CA-CB	6.02	119.53	110.50
1	L	14	SER	N-CA-C	5.96	127.10	111.00
1	L	151	ASP	CB-CG-OD1	5.96	123.66	118.30
2	H	194	TRP	CA-CB-CG	-5.92	102.45	113.70
1	L	35	TRP	CE2-CD2-CG	-5.89	102.59	107.30
1	L	154	GLU	CA-CB-CG	5.88	126.35	113.40
2	H	165	LEU	CB-CG-CD1	-5.87	101.02	111.00
2	H	101	ASP	CA-C-N	5.84	133.44	117.10
2	H	36	TRP	CG-CD2-CE3	5.79	139.11	133.90
2	H	217	GLU	CA-CB-CG	5.76	126.06	113.40
2	H	92	ASP	CB-CG-OD1	5.74	123.46	118.30
1	L	43	THR	N-CA-C	5.71	126.41	111.00
2	H	166	SER	N-CA-C	-5.70	95.60	111.00
1	L	105	GLU	CA-CB-CG	5.69	125.91	113.40
2	H	162	SER	N-CA-CB	-5.66	102.01	110.50
2	H	140	SER	N-CA-C	-5.64	95.76	111.00
1	L	44	VAL	CG1-CB-CG2	5.63	119.91	110.90
2	H	56	ASP	O-C-N	-5.63	113.63	123.20
2	H	75	ASP	CB-CG-OD1	5.59	123.33	118.30
2	H	161	ASN	CB-CG-ND2	5.56	130.03	116.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	164	SER	N-CA-C	5.54	125.97	111.00
2	H	206	PRO	CA-C-N	5.54	129.39	117.20
1	L	185	GLU	CA-CB-CG	-5.46	101.38	113.40
1	L	42	GLY	N-CA-C	5.46	126.76	113.10
2	H	193	THR	CA-CB-OG1	-5.46	97.54	109.00
1	L	50	TYR	CB-CG-CD1	-5.41	117.75	121.00
2	H	2	VAL	CA-CB-CG2	-5.39	102.81	110.90
2	H	194	TRP	CB-CG-CD1	-5.39	119.99	127.00
2	H	79	SER	C-N-CA	5.38	135.16	121.70
1	L	17	ASP	CA-C-N	-5.38	105.37	117.20
1	L	36	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	L	49	TYR	CB-CG-CD1	-5.35	117.79	121.00
2	H	80	ILE	N-CA-CB	-5.35	98.50	110.80
2	H	154	GLU	C-N-CA	5.34	135.05	121.70
2	H	206	PRO	O-C-N	-5.33	114.16	122.70
2	H	4	LEU	CB-CG-CD1	-5.33	101.94	111.00
2	H	52	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	H	89	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	H	38	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	H	194	TRP	CB-CA-C	-5.21	99.98	110.40
2	H	182	THR	CA-CB-CG2	5.19	119.66	112.40
2	H	217	GLU	N-CA-C	-5.16	97.06	111.00
2	H	159	THR	CA-CB-CG2	5.16	119.62	112.40
1	L	128	GLY	N-CA-C	5.16	125.99	113.10
2	H	115	VAL	CG1-CB-CG2	5.16	119.15	110.90
2	H	36	TRP	CB-CG-CD1	-5.11	120.36	127.00
2	H	47	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	L	184	ASP	CA-CB-CG	-5.07	102.25	113.40
2	H	181	TYR	CD1-CG-CD2	5.06	123.47	117.90
1	L	160	LEU	CA-CB-CG	5.03	126.87	115.30
2	H	166	SER	C-N-CA	5.03	134.28	121.70
1	L	163	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	L	211	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	L	85	THR	OG1-CB-CG2	5.01	121.53	110.00
2	H	133	GLY	CA-C-N	-5.00	106.19	117.20

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	Mainchain,Peptide
2	H	141	SER	Peptide
2	H	155	SER	Peptide
2	H	166	SER	Mainchain,Peptide
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	53	0
2	H	1628	0	1576	46	0
All	All	3296	0	3169	98	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 15.

All (98) 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	1.47
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
2:H:166:SER:CB	2:H:190:PRO:HD3	2.02	0.88
1:L:51:THR:C	1:L:52:SER:CA	2.41	0.87
1:L:41:ASP:OD2	1:L:43:THR:HG23	1.76	0.86
1:L:4:MET:HE1	1:L:90:GLN:HG2	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:L:52:SER:N	1:L:52:SER:C	2.50	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
2:H:215:LYS:HB3	2:H:215:LYS:HZ3	1.64	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
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
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: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
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:4:MET:N	1:L:4:MET:HE2	2.25	0.50
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:3:LYS:HZ2	2:H:3:LYS:HB2	1.77	0.49
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
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:20:LEU:HD13	2:H:85:MET:HE1	1.95	0.48
2:H:166:SER:OG	2:H:188:THR:C	2.45	0.48
1:L:142:LYS:HZ3	1:L:142:LYS:HB3	1.80	0.47
2:H:138:THR:HG22	2:H:139:GLY:H	1.79	0.47
2:H:175:LEU:N	2:H:175:LEU:HD12	2.30	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:135:GLY:C	2:H:135:GLY:N	2.62	0.45
1:L:39:LYS:HB2	1:L:43:THR:O	2.16	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
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
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
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
2:H:135:GLY:CA	2:H:136:ASP:N	2.70	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
2:H:215:LYS:HZ3	2:H:215:LYS:CB	2.32	0.41
1:L:61:ARG:NH1	1:L:82:ASP:OD1	2.52	0.41
1:L:4:MET:HE1	1:L:90:GLN:CG	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:41:ASP:O	1:L:42:GLY:C	2.60	0.40
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
2:H:101:ASP:O	2:H:102:PRO:C	2.55	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%)	4	1
2	H	215/217 (99%)	185 (86%)	22 (10%)	8 (4%)	3	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	163	GLY
1	L	16	GLY

5.3.2 Protein sidechains (i)

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%)	140 (76%)	43 (24%)	1	0
All	All	376/376 (100%)	293 (78%)	83 (22%)	1	0

All (83) 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	14	SER
1	L	15	LEU
1	L	17	ASP
1	L	21	ILE
1	L	27	GLN
1	L	33	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	25	SER
2	H	30	THR
2	H	56	ASP
2	H	61	GLU
2	H	75	ASP
2	H	77	SER
2	H	79	SER
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	147	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	208	SER
2	H	209	SER
2	H	210	THR
2	H	211	THR
2	H	212	VAL
2	H	213	ASP
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	137	ASN
1	L	161	ASN
1	L	190	ASN
2	H	76	ASN

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 monosaccharides 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

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, 95^{th} 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%)	0.05	6 (2%)	53	49	2, 9, 20, 31	0
2	H	217/217 (100%)	0.23	14 (6%)	18	15	3, 10, 27, 38	0
All	All	431/431 (100%)	0.14	20 (4%)	32	30	2, 10, 25, 38	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	166	SER	11.2
2	H	164	SER	7.5
2	H	165	LEU	5.8
2	H	134	CYS	5.6
1	L	15	LEU	4.3
2	H	167	SER	4.2
2	H	135	GLY	4.1
2	H	55	ALA	4.0
2	H	163	GLY	3.9
2	H	162	SER	3.5
1	L	76	SER	2.7
2	H	168	SER	2.6
1	L	157	ASN	2.5
1	L	127	SER	2.3
1	L	43	THR	2.3
2	H	1	GLU	2.2
2	H	161	ASN	2.1
2	H	137	THR	2.1
2	H	76	ASN	2.1
1	L	214	CYS	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 monosaccharides 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.