Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:50 AM GMT

PDB ID	:	2UYL
Title	:	Crystal structure of a monoclonal antibody directed against an antigenic determinant common to Ogawa and Inaba serotypes of Vibrio cholerae O1
Authors	:	Ahmed, F.; Haouz, A.; Nato, F.; Fournier, J.M.; Alzari, P.M.
Deposited on	:	2007-04-10
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

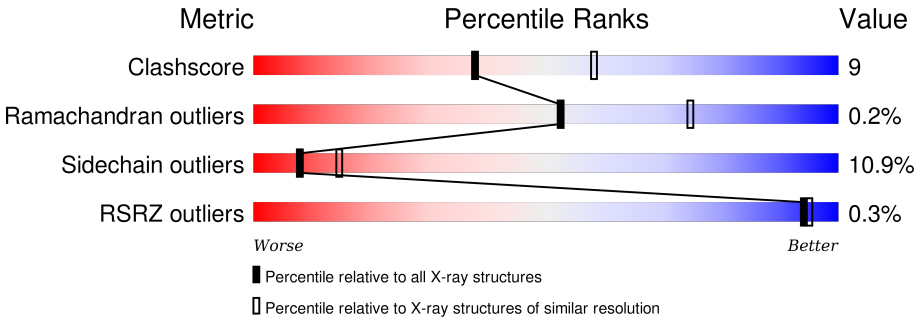
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	219	74% 22%
1	M	219	% 66% 26% 6%
1	V	219	% 74% 20% 5%
1	X	219	66% 30%
2	B	221	73% 19%
2	N	221	79% 13% 5%
2	W	221	81% 14%

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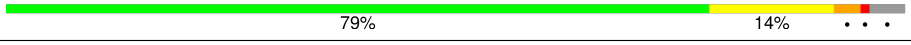
Mol	Chain	Length	Quality of chain
2	Y	221	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13057 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 MONOCLONAL ANTIBODY F-22-30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1676	1046	280	344	6			
1	M	216	Total	C	N	O	S	0	0	0
			1659	1037	277	339	6			
1	V	216	Total	C	N	O	S	0	0	0
			1669	1043	281	339	6			
1	X	216	Total	C	N	O	S	0	0	0
			1669	1043	281	339	6			

- Molecule 2 is a protein called MONOCLONAL ANTIBODY F-22-30.

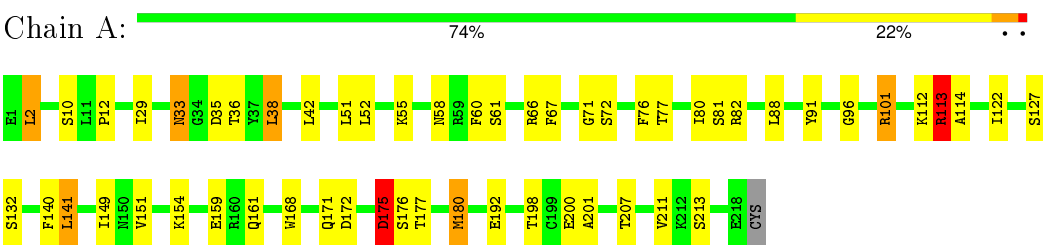
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1596	1007	264	319	6			
2	N	213	Total	C	N	O	S	0	0	0
			1596	1007	264	319	6			
2	W	213	Total	C	N	O	S	0	0	0
			1596	1007	264	319	6			
2	Y	213	Total	C	N	O	S	0	0	0
			1596	1007	264	319	6			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

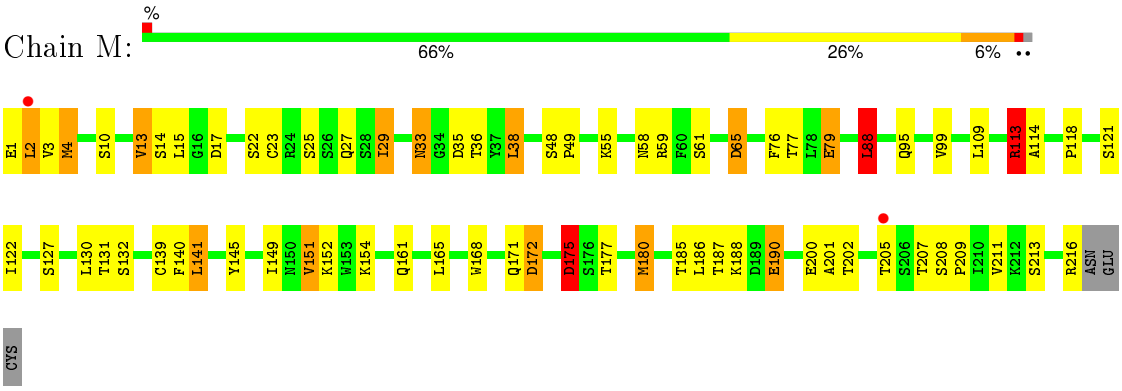
- Molecule 1: MONOCLONAL ANTIBODY F-22-30

Chain A:



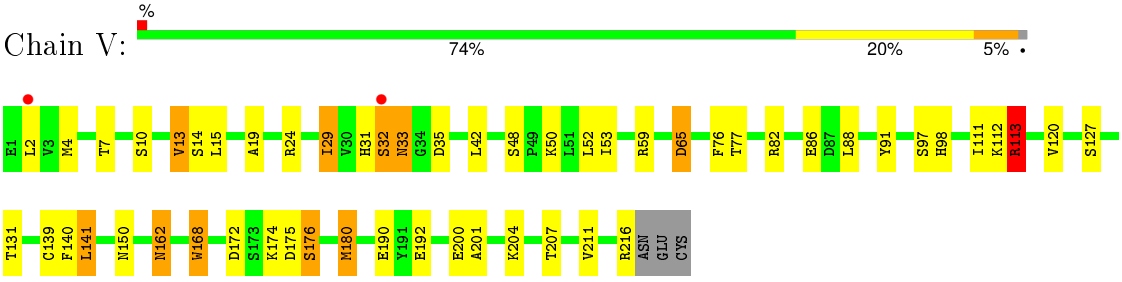
- Molecule 1: MONOCLONAL ANTIBODY F-22-30

Chain M:



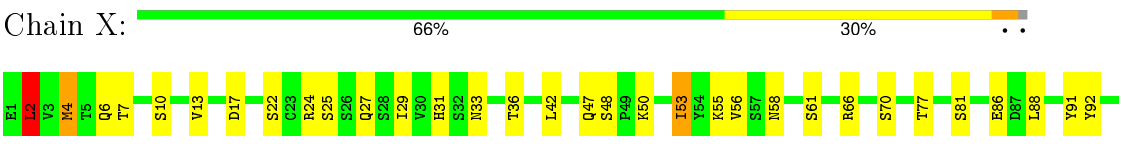
- Molecule 1: MONOCLONAL ANTIBODY F-22-30

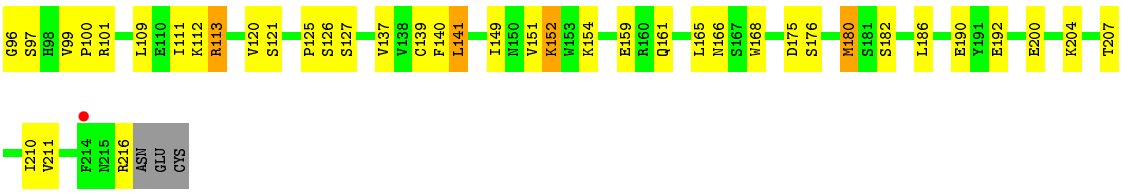
Chain V:



- Molecule 1: MONOCLONAL ANTIBODY F-22-30

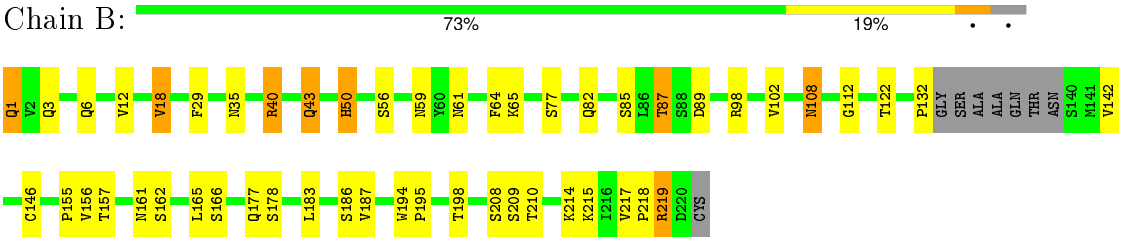
Chain X:





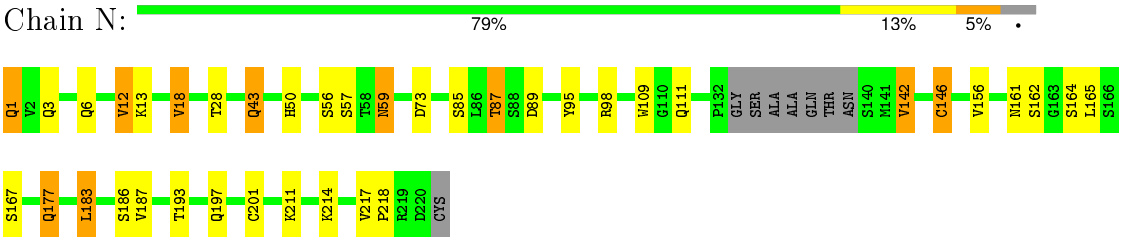
- Molecule 2: MONOCLONAL ANTIBODY F-22-30

Chain B:



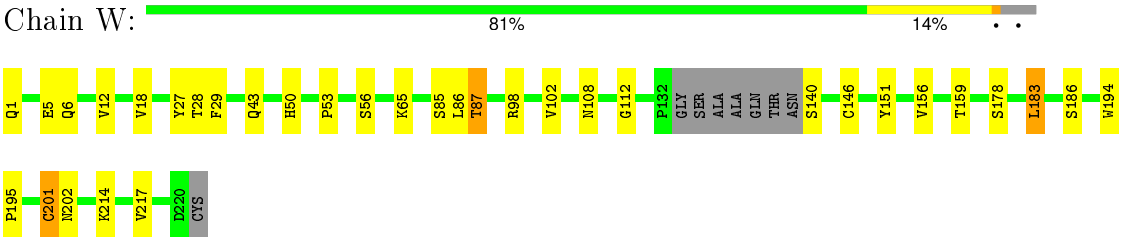
- Molecule 2: MONOCLONAL ANTIBODY F-22-30

Chain N:



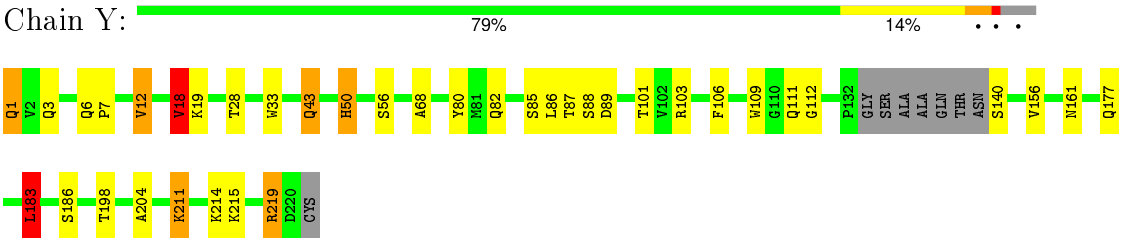
- Molecule 2: MONOCLONAL ANTIBODY F-22-30

Chain W:



- Molecule 2: MONOCLONAL ANTIBODY F-22-30

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.06Å 75.22Å 98.41Å 111.05° 90.39° 106.83°	Depositor
Resolution (Å)	91.29 – 2.50 46.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (91.29-2.50) 84.6 (46.15-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.08 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.257 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 64353 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13057	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.92	1/1715 (0.1%)	1.04	8/2331 (0.3%)
1	M	1.02	9/1698 (0.5%)	1.14	7/2308 (0.3%)
1	V	1.24	8/1708 (0.5%)	0.99	6/2319 (0.3%)
1	X	0.84	3/1708 (0.2%)	0.85	3/2319 (0.1%)
2	B	0.96	1/1637 (0.1%)	0.98	4/2241 (0.2%)
2	N	1.05	4/1637 (0.2%)	1.02	9/2241 (0.4%)
2	W	0.96	2/1637 (0.1%)	0.90	3/2241 (0.1%)
2	Y	0.93	0/1637	0.89	3/2241 (0.1%)
All	All	1.00	28/13377 (0.2%)	0.98	43/18241 (0.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	113	ARG	CZ-NH1	29.33	1.71	1.33
1	V	113	ARG	NE-CZ	13.03	1.50	1.33
1	V	190	GLU	CD-OE2	12.10	1.39	1.25
1	M	113	ARG	NE-CZ	8.01	1.43	1.33
1	V	82	ARG	CZ-NH1	7.48	1.42	1.33
1	V	113	ARG	CD-NE	7.28	1.58	1.46
2	N	13	LYS	CD-CE	7.28	1.69	1.51
2	N	146	CYS	CB-SG	-6.75	1.70	1.82
1	A	113	ARG	NE-CZ	6.55	1.41	1.33
1	M	139	CYS	CB-SG	-6.32	1.71	1.82
1	M	79	GLU	CG-CD	6.15	1.61	1.51
1	V	190	GLU	CD-OE1	5.98	1.32	1.25
1	M	154	LYS	CD-CE	5.86	1.65	1.51
1	V	139	CYS	CB-SG	-5.84	1.72	1.81
2	N	111	GLN	CB-CG	5.82	1.68	1.52
1	M	79	GLU	CB-CG	5.72	1.63	1.52
2	W	5	GLU	CG-CD	5.69	1.60	1.51
1	M	23	CYS	CB-SG	-5.63	1.72	1.81
1	X	139	CYS	CB-SG	-5.63	1.72	1.81
2	N	13	LYS	CE-NZ	5.61	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	174	LYS	CD-CE	5.50	1.65	1.51
1	M	1	GLU	CB-CG	-5.48	1.41	1.52
2	B	146	CYS	CB-SG	-5.42	1.73	1.81
1	M	1	GLU	CG-CD	-5.40	1.43	1.51
2	W	201	CYS	CB-SG	-5.32	1.73	1.81
1	X	154	LYS	CE-NZ	5.25	1.62	1.49
1	M	175	ASP	CB-CG	-5.19	1.40	1.51
1	X	50	LYS	CG-CD	5.11	1.69	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	113	ARG	NE-CZ-NH2	-20.20	110.20	120.30
1	V	113	ARG	NE-CZ-NH2	-17.64	111.48	120.30
1	A	113	ARG	NE-CZ-NH1	16.38	128.49	120.30
1	A	113	ARG	NE-CZ-NH2	-15.85	112.37	120.30
1	M	113	ARG	NE-CZ-NH1	15.01	127.80	120.30
1	M	175	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	M	88	LEU	CB-CG-CD1	-8.44	96.66	111.00
2	N	43	GLN	C-N-CA	-8.12	105.25	122.30
2	B	43	GLN	C-N-CA	-7.51	106.53	122.30
1	X	17	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	A	2	LEU	CA-CB-CG	-7.33	98.45	115.30
1	V	82	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	B	146	CYS	CA-CB-SG	-7.17	101.10	114.00
1	X	50	LYS	CD-CE-NZ	6.68	127.07	111.70
2	N	146	CYS	CA-CB-SG	-6.60	102.11	114.00
1	V	113	ARG	CD-NE-CZ	-6.42	114.62	123.60
1	A	175	ASP	CB-CG-OD1	-6.21	112.72	118.30
2	N	98	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	Y	18	VAL	CB-CA-C	-6.12	99.76	111.40
1	X	2	LEU	CA-CB-CG	-6.12	101.22	115.30
2	N	183	LEU	CA-CB-CG	6.07	129.27	115.30
2	W	43	GLN	C-N-CA	-6.05	109.60	122.30
1	M	4	MET	CG-SD-CE	-6.01	90.58	100.20
2	Y	183	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	101	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	N	142	VAL	CB-CA-C	-5.78	100.43	111.40
2	B	18	VAL	CB-CA-C	-5.71	100.55	111.40
2	W	183	LEU	CA-CB-CG	5.58	128.14	115.30
1	V	82	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	Y	43	GLN	C-N-CA	-5.54	110.67	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	73	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	V	113	ARG	NH1-CZ-NH2	5.51	125.46	119.40
2	N	73	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	101	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	M	151	VAL	CB-CA-C	-5.39	101.17	111.40
1	A	2	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	M	172	ASP	CB-CG-OD2	5.22	123.00	118.30
2	N	43	GLN	O-C-N	-5.19	114.37	123.20
2	B	43	GLN	O-C-N	-5.10	114.53	123.20
2	W	43	GLN	N-CA-C	5.08	124.72	111.00
1	V	168	TRP	CB-CA-C	-5.07	100.27	110.40
2	N	98	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	38	LEU	CA-CB-CG	-5.04	103.70	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	1676	0	1591	36	0
1	M	1659	0	1579	50	0
1	V	1669	0	1601	33	0
1	X	1669	0	1601	44	0
2	B	1596	0	1558	33	0
2	N	1596	0	1558	28	0
2	W	1596	0	1558	14	0
2	Y	1596	0	1558	24	0
All	All	13057	0	12604	236	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 9.

All (236) 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:V:113:ARG:NH1	1:V:113:ARG:CZ	1.71	1.53
1:X:4:MET:HE2	1:X:4:MET:CA	1.68	1.22
1:X:4:MET:CE	1:X:4:MET:HA	1.85	1.07
1:X:4:MET:CE	1:X:25:SER:HA	1.84	1.05
1:M:165:LEU:HD11	2:N:177:GLN:NE2	1.78	0.99
2:W:1:GLN:OE1	2:W:1:GLN:N	2.01	0.93
1:X:4:MET:HE3	1:X:25:SER:HA	1.46	0.93
1:X:4:MET:HE2	1:X:4:MET:HA	0.90	0.90
1:M:165:LEU:HD11	2:N:177:GLN:CD	1.93	0.88
1:M:165:LEU:CD1	2:N:177:GLN:NE2	2.39	0.85
1:V:2:LEU:HD21	1:V:98:HIS:HD2	1.42	0.82
1:X:29:ILE:HG22	1:X:29:ILE:O	1.83	0.79
1:M:165:LEU:HD11	2:N:177:GLN:CG	2.14	0.77
1:X:4:MET:HE1	1:X:25:SER:HA	1.67	0.77
1:X:186:LEU:HD22	1:X:190:GLU:HG2	1.68	0.75
1:V:192:GLU:HG2	1:V:216:ARG:NH1	2.03	0.74
1:M:165:LEU:HD11	2:N:177:GLN:HG3	1.69	0.73
1:M:165:LEU:CD1	2:N:177:GLN:HE21	2.00	0.72
1:V:2:LEU:HD12	1:V:2:LEU:N	2.03	0.72
1:M:33:ASN:ND2	1:M:35:ASP:H	1.88	0.71
2:B:40:ARG:HH11	2:B:40:ARG:HG3	1.54	0.71
2:B:1:GLN:H3	2:B:1:GLN:CD	1.94	0.71
1:A:33:ASN:ND2	1:A:35:ASP:H	1.88	0.71
1:X:126:SER:HA	2:Y:219:ARG:HH21	1.57	0.70
1:X:200:GLU:HG2	1:X:211:VAL:HG22	1.75	0.69
2:B:217:VAL:HG23	2:B:218:PRO:HD2	1.73	0.69
1:M:33:ASN:HD21	1:M:35:ASP:HB2	1.57	0.68
1:V:88:LEU:HD21	1:V:111:ILE:CG1	2.23	0.68
1:A:33:ASN:HD21	1:A:35:ASP:HB2	1.56	0.68
1:X:4:MET:CE	1:X:25:SER:CA	2.67	0.68
1:V:88:LEU:HD21	1:V:111:ILE:HG13	1.75	0.67
2:B:1:GLN:CD	2:B:1:GLN:N	2.48	0.67
1:X:4:MET:HE3	1:X:25:SER:CA	2.24	0.67
1:X:192:GLU:HG2	1:X:216:ARG:NH1	2.10	0.67
1:M:141:LEU:HD13	1:M:201:ALA:HB2	1.77	0.66
2:N:165:LEU:HD13	2:N:187:VAL:HG21	1.78	0.64
1:A:67:PHE:CE1	1:A:80:ILE:HD13	2.32	0.64
1:M:165:LEU:CD1	2:N:177:GLN:HG3	2.28	0.64
2:N:164:SER:OG	2:Y:1:GLN:HG3	1.98	0.63
2:B:102:VAL:HG23	2:B:102:VAL:O	1.97	0.63
1:A:129:GLN:O	1:A:132:SER:OG	2.15	0.62
1:M:33:ASN:HD22	1:M:35:ASP:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:HB3	1:A:177:THR:H	1.64	0.62
1:V:33:ASN:ND2	1:V:35:ASP:H	1.98	0.62
2:B:6:GLN:NE2	2:B:112:GLY:H	1.97	0.62
1:X:4:MET:HE1	1:X:25:SER:CA	2.28	0.60
1:A:141:LEU:N	1:A:141:LEU:HD23	2.17	0.60
1:A:140:PHE:CE1	2:B:186:SER:HB3	2.37	0.60
1:A:200:GLU:HG2	1:A:211:VAL:HG22	1.83	0.60
1:V:59:ARG:CZ	1:V:65:ASP:HA	2.32	0.60
1:V:29:ILE:HG22	1:V:97:SER:HB2	1.83	0.59
1:M:2:LEU:HD22	1:M:95:GLN:CD	2.23	0.59
2:N:87:THR:HG22	2:N:89:ASP:H	1.68	0.59
1:M:29:ILE:HG22	1:M:36:THR:HG23	1.85	0.58
2:Y:87:THR:HG22	2:Y:89:ASP:H	1.69	0.58
1:A:66:ARG:HD2	1:A:82:ARG:O	2.02	0.58
1:V:31:HIS:CD2	1:V:32:SER:H	2.21	0.58
1:X:88:LEU:HD21	1:X:111:ILE:CG1	2.32	0.58
2:B:40:ARG:HH11	2:B:40:ARG:CG	2.16	0.58
1:M:113:ARG:HD3	1:M:114:ALA:O	2.04	0.58
2:Y:18:VAL:HG22	2:Y:86:LEU:HD11	1.85	0.58
1:A:88:LEU:CD1	1:A:171:GLN:HB3	2.34	0.57
1:X:2:LEU:HD21	1:X:25:SER:HB2	1.85	0.57
1:A:172:ASP:OD2	1:A:175:ASP:HB2	2.04	0.57
2:N:12:VAL:HG11	2:N:18:VAL:CG1	2.34	0.57
1:X:165:LEU:CD1	2:Y:177:GLN:NE2	2.67	0.57
1:X:88:LEU:CD2	1:X:111:ILE:HG12	2.34	0.56
1:X:88:LEU:HD21	1:X:111:ILE:HG12	1.85	0.56
1:A:29:ILE:HG13	1:A:36:THR:HG23	1.88	0.56
1:M:2:LEU:HD12	1:M:2:LEU:N	2.20	0.56
1:M:99:VAL:HG11	2:N:59:ASN:OD1	2.05	0.56
1:X:29:ILE:O	1:X:29:ILE:CG2	2.53	0.56
1:X:31:HIS:HD2	1:X:97:SER:O	1.89	0.55
1:X:141:LEU:HD12	1:X:149:ILE:HD13	1.88	0.55
1:V:141:LEU:N	1:V:141:LEU:CD2	2.69	0.55
1:V:162:ASN:ND2	1:V:162:ASN:H	2.04	0.55
2:Y:1:GLN:OE1	2:Y:1:GLN:N	2.40	0.55
1:V:141:LEU:CD1	1:V:201:ALA:HB2	2.37	0.55
1:M:33:ASN:C	1:M:33:ASN:HD22	2.09	0.54
2:N:156:VAL:CG2	2:N:183:LEU:HD13	2.37	0.54
1:V:42:LEU:HB2	1:V:52:LEU:HD11	1.89	0.54
2:N:161:ASN:O	2:N:162:SER:HB2	2.06	0.54
2:B:1:GLN:NE2	2:B:1:GLN:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:VAL:CG2	2:B:218:PRO:HD2	2.37	0.53
1:M:172:ASP:OD2	1:M:175:ASP:HB2	2.08	0.53
1:X:125:PRO:HD3	1:X:137:VAL:HG22	1.91	0.53
2:B:165:LEU:HD13	2:B:187:VAL:HG21	1.90	0.53
1:A:38:LEU:HD13	1:A:76:PHE:CG	2.44	0.53
1:X:166:ASN:OD1	1:X:182:SER:OG	2.04	0.53
1:V:2:LEU:HD12	1:V:2:LEU:H	1.73	0.53
1:M:2:LEU:N	1:M:2:LEU:CD1	2.72	0.53
1:A:38:LEU:HD13	1:A:76:PHE:CD1	2.44	0.52
1:X:165:LEU:HD11	2:Y:177:GLN:NE2	2.25	0.52
2:Y:6:GLN:NE2	2:Y:112:GLY:H	2.07	0.52
1:A:88:LEU:HD11	1:A:171:GLN:HB3	1.92	0.52
1:X:140:PHE:CE1	2:Y:186:SER:HB3	2.45	0.51
2:B:178:SER:HA	2:W:87:THR:HG21	1.92	0.51
2:N:193:THR:O	2:N:197:GLN:HB2	2.11	0.51
2:W:194:TRP:CG	2:W:195:PRO:HA	2.46	0.51
1:M:48:SER:HB2	2:N:95:TYR:CE2	2.45	0.51
1:V:65:ASP:N	1:V:65:ASP:OD1	2.39	0.51
2:B:161:ASN:O	2:B:162:SER:HB2	2.10	0.51
2:B:178:SER:HA	2:W:87:THR:CG2	2.40	0.51
1:M:118:PRO:HG3	1:M:149:ILE:HD11	1.93	0.51
1:A:113:ARG:HG2	1:A:176:SER:HB2	1.93	0.51
2:N:12:VAL:HG11	2:N:18:VAL:HG13	1.92	0.50
2:N:217:VAL:HG22	2:N:218:PRO:HD2	1.93	0.50
1:M:13:VAL:HG21	1:M:109:LEU:HD11	1.93	0.50
1:M:187:THR:OG1	1:M:190:GLU:HB2	2.10	0.50
1:V:2:LEU:HD21	1:V:98:HIS:CD2	2.34	0.50
2:N:87:THR:HG22	2:N:89:ASP:N	2.27	0.50
2:Y:87:THR:HG22	2:Y:89:ASP:N	2.26	0.50
1:X:13:VAL:HG22	1:X:109:LEU:HD11	1.94	0.49
1:A:168:TRP:CZ2	1:A:180:MET:HE1	2.47	0.49
1:M:140:PHE:CE1	2:N:186:SER:HB3	2.48	0.49
1:V:168:TRP:CE2	1:V:180:MET:HE3	2.48	0.49
1:A:127:SER:O	1:A:131:THR:HG23	2.12	0.49
1:A:96:GLY:HA2	1:A:101:ARG:HD3	1.93	0.49
1:M:127:SER:O	1:M:131:THR:HG23	2.13	0.49
2:Y:33:TRP:CE3	2:Y:50:HIS:CD2	3.01	0.49
2:B:40:ARG:HG3	2:B:40:ARG:NH1	2.27	0.49
1:A:149:ILE:HG23	1:A:180:MET:HE3	1.93	0.48
2:Y:204:ALA:HB2	2:Y:211:LYS:HE3	1.95	0.48
1:M:2:LEU:HD22	1:M:95:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:14:SER:O	1:M:17:ASP:HB2	2.13	0.48
1:V:140:PHE:CE1	2:W:186:SER:HB3	2.49	0.48
1:X:29:ILE:HG22	1:X:36:THR:HG23	1.96	0.48
1:M:185:THR:O	1:M:186:LEU:HD23	2.13	0.48
1:M:165:LEU:HD12	2:N:177:GLN:NE2	2.27	0.48
1:M:113:ARG:HD2	1:M:145:TYR:CG	2.48	0.48
1:V:200:GLU:HG2	1:V:211:VAL:HG22	1.94	0.48
2:B:87:THR:CG2	2:W:178:SER:HA	2.44	0.48
2:B:6:GLN:NE2	2:B:112:GLY:N	2.61	0.47
1:V:42:LEU:HD13	1:V:91:TYR:CZ	2.49	0.47
1:X:2:LEU:CD2	1:X:25:SER:HB2	2.44	0.47
2:Y:19:LYS:HE3	2:Y:80:TYR:CD1	2.50	0.47
2:Y:18:VAL:CG2	2:Y:86:LEU:HD11	2.44	0.47
1:M:152:LYS:HB3	1:M:200:GLU:HB2	1.97	0.47
2:B:64:PHE:O	2:B:65:LYS:C	2.53	0.47
2:W:159:THR:OG1	2:W:202:ASN:HB2	2.14	0.47
1:X:4:MET:CE	1:X:4:MET:CA	2.62	0.47
2:B:87:THR:HG21	2:W:178:SER:HA	1.97	0.47
1:X:53:ILE:HA	1:X:58:ASN:O	2.15	0.47
1:V:2:LEU:N	1:V:2:LEU:CD1	2.74	0.46
2:B:98:ARG:HE	2:B:108:ASN:ND2	2.13	0.46
1:M:141:LEU:HD13	1:M:201:ALA:CB	2.42	0.46
2:N:12:VAL:HG11	2:N:18:VAL:HG11	1.98	0.46
1:X:113:ARG:HG2	1:X:176:SER:HB2	1.97	0.46
1:A:141:LEU:HD13	1:A:201:ALA:HB2	1.98	0.46
1:A:88:LEU:HD13	1:A:171:GLN:HB3	1.98	0.46
1:M:216:ARG:NH1	1:M:216:ARG:HB3	2.30	0.46
1:M:200:GLU:HG2	1:M:211:VAL:HG22	1.96	0.46
1:M:175:ASP:HB3	1:M:177:THR:H	1.80	0.46
1:M:59:ARG:NE	1:M:65:ASP:HA	2.31	0.46
1:M:49:PRO:HG2	2:N:109:TRP:CH2	2.51	0.46
2:Y:156:VAL:CG2	2:Y:183:LEU:HD13	2.45	0.46
1:A:154:LYS:HB2	1:A:198:THR:HB	1.97	0.46
1:M:55:LYS:HB2	1:M:58:ASN:HD22	1.81	0.46
2:Y:106:PHE:HB3	2:Y:109:TRP:CE2	2.51	0.45
2:B:132:PRO:O	2:B:219:ARG:HD2	2.16	0.45
2:B:194:TRP:CG	2:B:195:PRO:HA	2.51	0.45
1:A:12:PRO:HB2	1:A:112:LYS:HD2	1.98	0.45
1:X:6:GLN:OE1	1:X:92:TYR:HA	2.17	0.45
1:A:67:PHE:HE1	1:A:80:ILE:HD13	1.79	0.45
2:W:27:TYR:CZ	2:W:98:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:88:LEU:HA	1:M:88:LEU:HD23	1.74	0.45
1:X:168:TRP:CZ2	1:X:180:MET:HE1	2.52	0.45
2:N:1:GLN:HG2	2:Y:161:ASN:HB3	1.99	0.45
1:M:2:LEU:HD23	1:M:29:ILE:HD11	1.98	0.44
1:V:141:LEU:N	1:V:141:LEU:HD22	2.32	0.44
1:X:152:LYS:HD3	1:X:159:GLU:HG3	1.99	0.44
1:M:2:LEU:HD23	1:M:29:ILE:CG1	2.47	0.44
2:Y:87:THR:HG22	2:Y:88:SER:N	2.33	0.44
1:X:210:ILE:HD12	1:X:210:ILE:N	2.33	0.44
1:X:99:VAL:HG13	1:X:100:PRO:HA	1.98	0.44
1:A:51:LEU:HD23	1:A:60:PHE:CD1	2.53	0.43
1:V:2:LEU:CD2	1:V:29:ILE:HG23	2.48	0.43
1:V:168:TRP:CE2	1:V:180:MET:CE	3.01	0.43
2:W:86:LEU:HD23	2:W:86:LEU:N	2.33	0.43
2:W:29:PHE:CE2	2:W:53:PRO:HB3	2.54	0.43
2:B:177:GLN:HG2	2:B:178:SER:N	2.34	0.43
1:M:38:LEU:HD13	1:M:76:PHE:CG	2.53	0.43
1:A:168:TRP:CZ2	1:A:180:MET:CE	3.01	0.43
2:W:6:GLN:NE2	2:W:112:GLY:H	2.17	0.43
2:Y:87:THR:CG2	2:Y:88:SER:N	2.82	0.43
1:A:113:ARG:HD3	1:A:114:ALA:O	2.17	0.43
2:W:151:TYR:CE1	2:W:156:VAL:HG13	2.54	0.43
2:B:156:VAL:CG2	2:B:183:LEU:HD13	2.48	0.43
2:B:40:ARG:O	2:B:43:GLN:HB3	2.19	0.42
1:A:42:LEU:HD13	1:A:91:TYR:CZ	2.54	0.42
1:X:120:VAL:HA	1:X:140:PHE:O	2.18	0.42
1:V:168:TRP:CZ2	1:V:180:MET:HE1	2.54	0.42
2:B:87:THR:HG22	2:B:89:ASP:H	1.84	0.42
1:A:42:LEU:HB2	1:A:52:LEU:HD11	2.01	0.42
1:X:96:GLY:HA2	1:X:101:ARG:HG2	2.00	0.42
1:M:2:LEU:HB3	1:M:4:MET:HE3	2.01	0.42
1:V:29:ILE:HD11	1:V:76:PHE:CE1	2.55	0.42
2:B:87:THR:HG22	2:B:89:ASP:N	2.35	0.42
1:M:208:SER:HA	1:M:209:PRO:HD3	1.81	0.42
1:A:71:GLY:O	1:A:72:SER:HB3	2.19	0.42
1:M:4:MET:HE1	1:M:25:SER:HA	2.02	0.41
1:X:66:ARG:HA	1:X:81:SER:OG	2.19	0.41
2:B:29:PHE:CD2	2:B:77:SER:HA	2.55	0.41
2:Y:198:THR:HG23	2:Y:215:LYS:HE3	2.01	0.41
2:Y:68:ALA:HA	2:Y:82:GLN:O	2.20	0.41
1:V:120:VAL:HA	1:V:140:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:C	1:A:33:ASN:HD22	2.24	0.41
1:M:130:LEU:HD22	1:M:188:LYS:HG3	2.03	0.41
2:N:6:GLN:HE22	2:N:95:TYR:HA	1.85	0.41
1:V:2:LEU:HB3	1:V:4:MET:CE	2.51	0.41
1:X:168:TRP:CZ2	1:X:180:MET:CE	3.04	0.41
2:B:35:ASN:OD1	2:B:50:HIS:HB3	2.21	0.41
2:N:43:GLN:HG3	2:N:43:GLN:O	2.21	0.41
1:M:88:LEU:HD11	1:M:171:GLN:HB3	2.03	0.41
2:B:122:THR:CG2	2:B:208:SER:HB3	2.51	0.41
2:W:27:TYR:CE1	2:W:98:ARG:HD2	2.56	0.41
1:V:13:VAL:HG11	1:V:19:ALA:HB2	2.03	0.41
2:B:198:THR:HG23	2:B:215:LYS:HE3	2.03	0.41
2:B:61:ASN:C	2:B:61:ASN:OD1	2.59	0.41
1:V:127:SER:O	1:V:131:THR:HG23	2.20	0.41
1:X:55:LYS:O	1:X:56:VAL:HB	2.21	0.40
1:M:168:TRP:CZ2	1:M:180:MET:HE2	2.55	0.40
1:A:151:VAL:HA	1:A:200:GLU:O	2.21	0.40
2:Y:12:VAL:CG2	2:Y:86:LEU:HD12	2.51	0.40
1:X:42:LEU:HD13	1:X:91:TYR:CZ	2.56	0.40
1:A:122:ILE:HD13	1:A:213:SER:HA	2.02	0.40
2:N:164:SER:OG	2:Y:1:GLN:CG	2.67	0.40
1:M:165:LEU:CD1	2:N:177:GLN:CG	2.91	0.40
1:V:113:ARG:HG2	1:V:176:SER:HB2	2.03	0.40
1:X:4:MET:HE3	1:X:25:SER:CB	2.52	0.40
1:V:192:GLU:HG2	1:V:216:ARG:CZ	2.52	0.40
2:B:1:GLN:OE1	2:B:1:GLN:N	2.54	0.40
2:Y:211:LYS:HE2	2:Y:211:LYS:HB3	1.92	0.40
1:A:51:LEU:HD23	1:A:60:PHE:CG	2.57	0.40
1:M:130:LEU:HD23	1:M:130:LEU:HA	1.93	0.40
1:A:55:LYS:HB2	1:A:58:ASN:HD22	1.87	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	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
1	M	214/219 (98%)	206 (96%)	8 (4%)	0	100	100
1	V	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
1	X	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
2	B	209/221 (95%)	201 (96%)	7 (3%)	1 (0%)	34	55
2	N	209/221 (95%)	202 (97%)	6 (3%)	1 (0%)	34	55
2	W	209/221 (95%)	203 (97%)	5 (2%)	1 (0%)	34	55
2	Y	209/221 (95%)	201 (96%)	7 (3%)	1 (0%)	34	55
All	All	1694/1760 (96%)	1636 (97%)	54 (3%)	4 (0%)	52	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	SER
2	N	85	SER
2	W	85	SER
2	Y	85	SER

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	A	192/196 (98%)	178 (93%)	14 (7%)	17	32
1	M	190/196 (97%)	161 (85%)	29 (15%)	3	6
1	V	192/196 (98%)	166 (86%)	26 (14%)	5	9
1	X	192/196 (98%)	165 (86%)	27 (14%)	4	7
2	B	184/190 (97%)	165 (90%)	19 (10%)	9	17
2	N	184/190 (97%)	167 (91%)	17 (9%)	11	21
2	W	184/190 (97%)	169 (92%)	15 (8%)	14	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Y	184/190 (97%)	167 (91%)	17 (9%)	11 21
All	All	1502/1544 (97%)	1338 (89%)	164 (11%)	8 15

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	10	SER
1	A	33	ASN
1	A	61	SER
1	A	77	THR
1	A	81	SER
1	A	113	ARG
1	A	141	LEU
1	A	159	GLU
1	A	161	GLN
1	A	175	ASP
1	A	180	MET
1	A	192	GLU
1	A	207	THR
2	B	1	GLN
2	B	3	GLN
2	B	12	VAL
2	B	18	VAL
2	B	40	ARG
2	B	50	HIS
2	B	56	SER
2	B	59	ASN
2	B	82	GLN
2	B	87	THR
2	B	108	ASN
2	B	142	VAL
2	B	155	PRO
2	B	157	THR
2	B	166	SER
2	B	209	SER
2	B	210	THR
2	B	214	LYS
2	B	219	ARG
1	M	2	LEU
1	M	3	VAL
1	M	10	SER

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Mol	Chain	Res	Type
1	M	13	VAL
1	M	15	LEU
1	M	22	SER
1	M	27	GLN
1	M	29	ILE
1	M	33	ASN
1	M	38	LEU
1	M	61	SER
1	M	65	ASP
1	M	77	THR
1	M	79	GLU
1	M	88	LEU
1	M	113	ARG
1	M	121	SER
1	M	122	ILE
1	M	132	SER
1	M	141	LEU
1	M	151	VAL
1	M	161	GLN
1	M	175	ASP
1	M	180	MET
1	M	190	GLU
1	M	202	THR
1	M	205	THR
1	M	207	THR
1	M	213	SER
2	N	1	GLN
2	N	3	GLN
2	N	12	VAL
2	N	18	VAL
2	N	28	THR
2	N	50	HIS
2	N	56	SER
2	N	57	SER
2	N	59	ASN
2	N	87	THR
2	N	142	VAL
2	N	146	CYS
2	N	167	SER
2	N	177	GLN
2	N	201	CYS
2	N	211	LYS

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Mol	Chain	Res	Type
2	N	214	LYS
1	V	7	THR
1	V	10	SER
1	V	13	VAL
1	V	14	SER
1	V	15	LEU
1	V	24	ARG
1	V	29	ILE
1	V	32	SER
1	V	33	ASN
1	V	48	SER
1	V	50	LYS
1	V	53	ILE
1	V	65	ASP
1	V	77	THR
1	V	86	GLU
1	V	112	LYS
1	V	113	ARG
1	V	141	LEU
1	V	150	ASN
1	V	162	ASN
1	V	172	ASP
1	V	175	ASP
1	V	176	SER
1	V	180	MET
1	V	204	LYS
1	V	207	THR
2	W	12	VAL
2	W	18	VAL
2	W	28	THR
2	W	50	HIS
2	W	56	SER
2	W	65	LYS
2	W	87	THR
2	W	102	VAL
2	W	108	ASN
2	W	140	SER
2	W	146	CYS
2	W	183	LEU
2	W	201	CYS
2	W	214	LYS
2	W	217	VAL

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Mol	Chain	Res	Type
1	X	2	LEU
1	X	4	MET
1	X	7	THR
1	X	10	SER
1	X	22	SER
1	X	24	ARG
1	X	27	GLN
1	X	33	ASN
1	X	47	GLN
1	X	48	SER
1	X	53	ILE
1	X	61	SER
1	X	70	SER
1	X	77	THR
1	X	86	GLU
1	X	112	LYS
1	X	113	ARG
1	X	121	SER
1	X	127	SER
1	X	141	LEU
1	X	151	VAL
1	X	152	LYS
1	X	161	GLN
1	X	175	ASP
1	X	180	MET
1	X	204	LYS
1	X	207	THR
2	Y	1	GLN
2	Y	3	GLN
2	Y	7	PRO
2	Y	12	VAL
2	Y	18	VAL
2	Y	28	THR
2	Y	43	GLN
2	Y	50	HIS
2	Y	56	SER
2	Y	101	THR
2	Y	103	ARG
2	Y	111	GLN
2	Y	140	SER
2	Y	183	LEU
2	Y	211	LYS

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Mol	Chain	Res	Type
2	Y	214	LYS
2	Y	219	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	58	ASN
1	A	142	ASN
1	A	161	GLN
1	A	217	ASN
2	B	6	GLN
2	B	32	ASN
2	B	108	ASN
2	B	170	HIS
2	B	177	GLN
1	M	18	GLN
1	M	31	HIS
1	M	33	ASN
1	M	43	GLN
1	M	58	ASN
1	M	142	ASN
2	N	6	GLN
2	N	32	ASN
2	N	39	GLN
2	N	43	GLN
2	N	170	HIS
2	N	177	GLN
1	V	31	HIS
1	V	33	ASN
1	V	98	HIS
1	V	142	ASN
1	V	161	GLN
1	V	162	ASN
2	W	6	GLN
2	W	32	ASN
2	W	170	HIS
1	X	31	HIS
1	X	33	ASN
1	X	142	ASN
1	X	161	GLN
2	Y	6	GLN

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Mol	Chain	Res	Type
2	Y	32	ASN
2	Y	170	HIS
2	Y	177	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	218/219 (99%)	-0.09	0 100 100	29, 34, 38, 45	0
1	M	216/219 (98%)	-0.08	2 (0%) 85 88	28, 33, 38, 42	0
1	V	216/219 (98%)	0.16	2 (0%) 85 88	29, 33, 38, 42	0
1	X	216/219 (98%)	0.10	1 (0%) 91 92	26, 33, 37, 41	0
2	B	213/221 (96%)	-0.14	0 100 100	25, 33, 39, 44	0
2	N	213/221 (96%)	-0.12	0 100 100	25, 32, 39, 45	0
2	W	213/221 (96%)	-0.06	0 100 100	26, 33, 39, 43	0
2	Y	213/221 (96%)	-0.11	0 100 100	27, 32, 37, 45	0
All	All	1718/1760 (97%)	-0.04	5 (0%) 94 95	25, 33, 38, 45	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	2	LEU	2.5
1	V	32	SER	2.4
1	M	2	LEU	2.2
1	X	214	PHE	2.1
1	M	205	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.