Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:49 pm BST

PDB ID	:	6MQM
Title	:	Vaccine-elicited NHP FP-targeting neutralizing antibody DF1W-a.01 in complex with HIV fusion peptide (residue 512-519)
Authors	:	Xu, K.; Wang, Y.; Kwong, P.D.
Deposited on	:	2018-10-10
Resolution	:	3.48 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 following versions of software and data (see references ⓘ) were used in the production of this report:

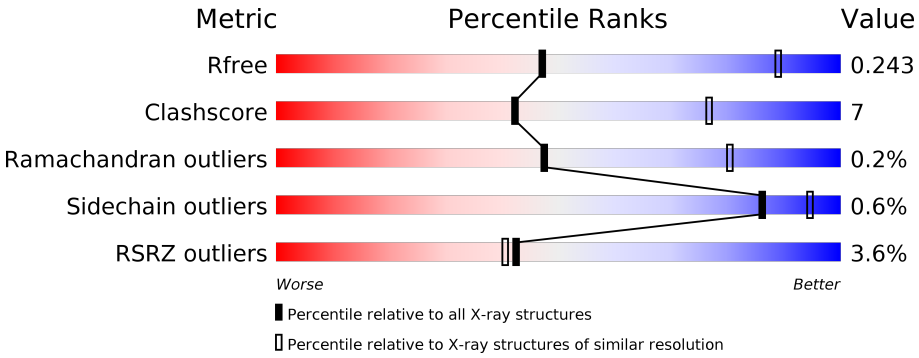
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.48 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}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 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	A	222	5% 83% 17%
1	D	222	5% 88% 12%
1	G	222	4% 82% 17%
1	J	222	4% 82% 18%
2	B	217	2% 79% 20%
2	E	217	81% 18%

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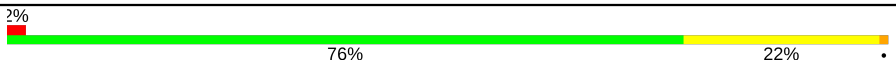
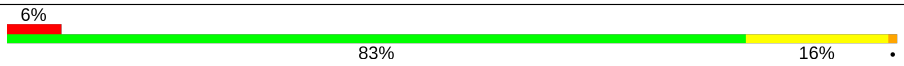
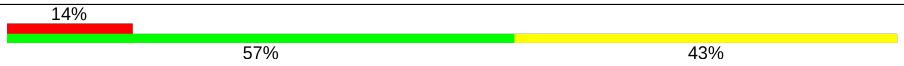
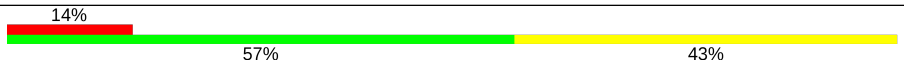
Mol	Chain	Length	Quality of chain
2	H	217	
2	K	217	
3	C	7	
3	F	7	
3	I	7	
3	L	7	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13480 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 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1665	1060	277	323	5			
1	D	222	Total	C	N	O	S	0	0	0
			1665	1060	277	323	5			
1	G	222	Total	C	N	O	S	0	0	0
			1665	1060	277	323	5			
1	J	222	Total	C	N	O	S	0	0	0
			1665	1060	277	323	5			

- Molecule 2 is a protein called antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1665	1043	286	331	5			
2	E	217	Total	C	N	O	S	0	0	0
			1665	1043	286	331	5			
2	H	217	Total	C	N	O	S	0	0	0
			1665	1043	286	331	5			
2	K	217	Total	C	N	O	S	0	0	0
			1665	1043	286	331	5			

- Molecule 3 is a protein called HIV Env fusion peptide residue 512-519.

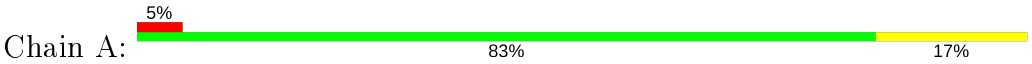
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			40	26	7	7			
3	F	7	Total	C	N	O	0	0	0
			40	26	7	7			
3	I	7	Total	C	N	O	0	0	0
			40	26	7	7			
3	L	7	Total	C	N	O	0	0	0
			40	26	7	7			

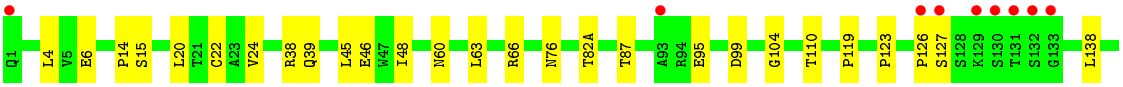
3 Residue-property plots (i)

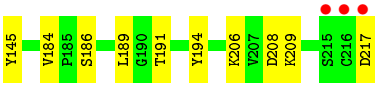
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: antibody Fab heavy chain

Chain A:

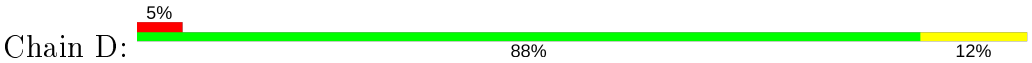






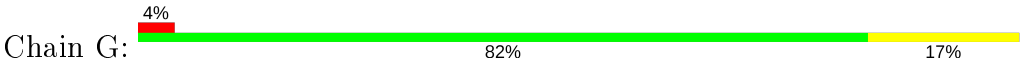
- Molecule 1: antibody Fab heavy chain

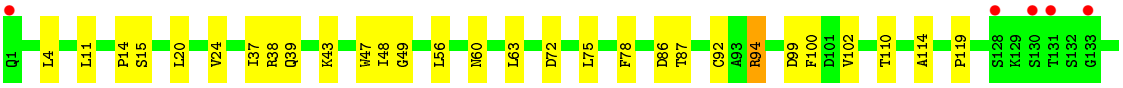
Chain D:

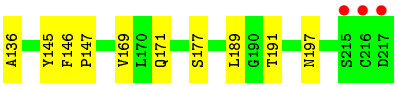


- Molecule 1: antibody Fab heavy chain

Chain G:

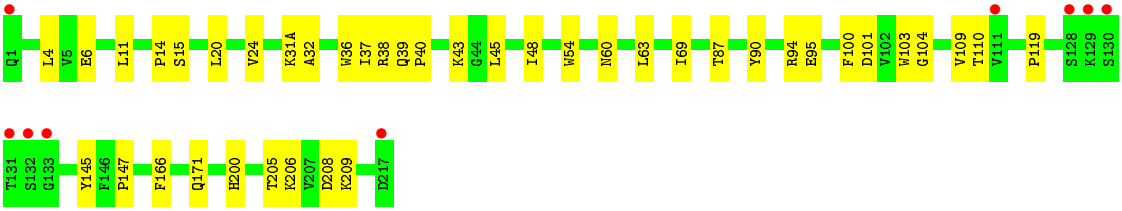






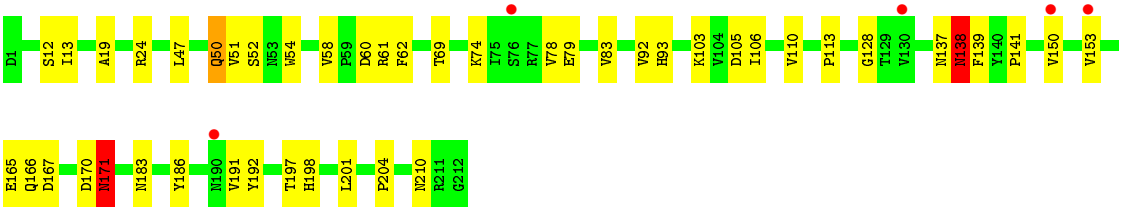
- Molecule 1: antibody Fab heavy chain

Chain J:



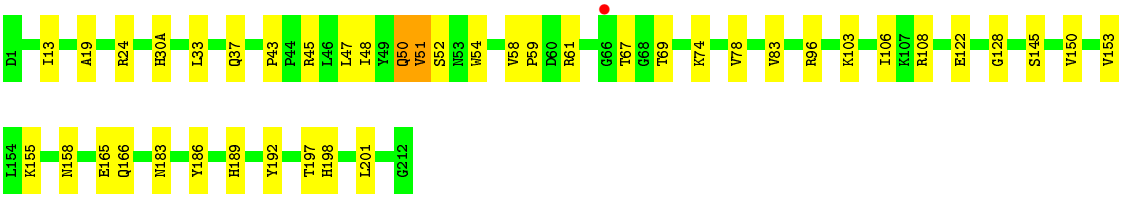
- Molecule 2: antibody Fab light chain

Chain B:



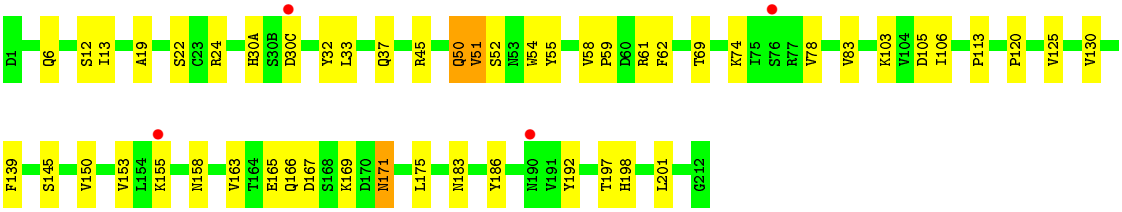
- Molecule 2: antibody Fab light chain

Chain E:



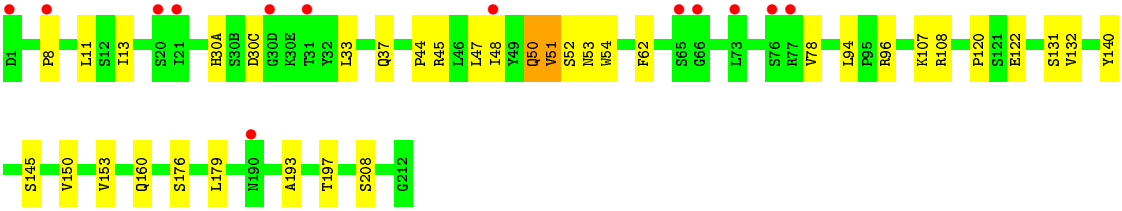
- Molecule 2: antibody Fab light chain

Chain H:



- Molecule 2: antibody Fab light chain

Chain K:



• Molecule 3: HIV Env fusion peptide residue 512-519

Chain C:

• Molecule 3: HIV Env fusion peptide residue 512-519

Chain F:

• Molecule 3: HIV Env fusion peptide residue 512-519

Chain I:

• Molecule 3: HIV Env fusion peptide residue 512-519

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.91Å 147.93Å 102.02Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	43.52 – 3.48 43.52 – 3.48	Depositor EDS
% Data completeness (in resolution range)	95.5 (43.52-3.48) 95.5 (43.52-3.48)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.200 , 0.246 0.200 , 0.243	Depositor DCC
R_{free} test set	1408 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13480	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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	A	0.30	0/1710	0.51	0/2341
1	D	0.30	0/1710	0.53	0/2341
1	G	0.30	0/1710	0.53	0/2341
1	J	0.30	0/1710	0.52	0/2341
2	B	0.32	0/1704	0.76	8/2321 (0.3%)
2	E	0.30	0/1704	0.49	0/2321
2	H	0.30	0/1704	0.87	3/2321 (0.1%)
2	K	0.30	0/1704	0.50	0/2321
3	C	0.31	0/39	0.43	0/52
3	F	0.30	0/39	0.48	0/52
3	I	0.30	0/39	0.47	0/52
3	L	0.30	0/39	0.44	0/52
All	All	0.30	0/13812	0.60	11/18856 (0.1%)

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
2	B	0	3
2	E	0	1
2	H	0	1
2	K	0	1
All	All	0	6

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	171	ASN	CB-CG-OD1	29.13	179.85	121.60
2	H	171	ASN	CB-CG-ND2	-16.32	77.53	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	138	ASN	CB-CG-ND2	-13.46	84.38	116.70
2	B	138	ASN	CB-CG-OD1	13.39	148.38	121.60
2	B	171	ASN	CB-CG-ND2	-11.59	88.88	116.70
2	H	171	ASN	OD1-CG-ND2	-8.49	102.38	121.90
2	B	171	ASN	CB-CG-OD1	7.53	136.66	121.60
2	B	138	ASN	OD1-CG-ND2	-5.92	108.28	121.90
2	B	170	ASP	C-N-CA	5.80	136.21	121.70
2	B	138	ASN	N-CA-CB	-5.64	100.45	110.60
2	B	171	ASN	N-CA-CB	5.62	120.72	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	138	ASN	Sidechain
2	B	171	ASN	Sidechain
2	B	50	GLN	Peptide
2	E	50	GLN	Peptide
2	H	50	GLN	Peptide
2	K	50	GLN	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	A	1665	0	1650	20	1
1	D	1665	0	1650	16	0
1	G	1665	0	1650	24	1
1	J	1665	0	1650	25	0
2	B	1665	0	1623	31	0
2	E	1665	0	1623	25	0
2	H	1665	0	1623	28	0
2	K	1665	0	1623	22	0
3	C	40	0	44	2	0
3	F	40	0	44	1	0
3	I	40	0	44	2	0
3	L	40	0	44	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13480	0	13268	184	1

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 7.

All (184) 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:B:92:VAL:HG13	2:B:93:HIS:HD2	1.29	0.94
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.70	0.73
1:G:99:ASP:OD1	3:I:512:ALA:N	2.21	0.73
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.70	0.72
1:G:39:GLN:NE2	1:G:43:LYS:O	2.20	0.72
1:G:38:ARG:HB3	1:G:48:ILE:HD11	1.73	0.71
1:A:38:ARG:NE	1:A:46:GLU:OE2	2.22	0.70
2:H:13:ILE:HD13	2:H:78:VAL:HG11	1.74	0.69
1:A:60:ASN:HB3	1:A:63:LEU:HD23	1.74	0.69
2:H:33:LEU:HB3	2:H:51:VAL:HG22	1.74	0.68
2:E:33:LEU:HB3	2:E:51:VAL:HG22	1.75	0.68
2:H:30(C):ASP:OD2	2:H:32:TYR:OH	2.10	0.68
1:D:119:PRO:HB3	1:D:145:TYR:HB3	1.74	0.67
2:E:13:ILE:HD13	2:E:78:VAL:HG11	1.75	0.67
1:J:171:GLN:NE2	2:K:160:GLN:OE1	2.26	0.67
2:B:92:VAL:HG13	2:B:93:HIS:CD2	2.21	0.66
1:J:95:GLU:OE2	2:K:96:ARG:NH1	2.26	0.65
1:J:38:ARG:HB3	1:J:48:ILE:HD11	1.77	0.65
1:A:87:THR:HG23	1:A:110:THR:HA	1.78	0.65
2:B:54:TRP:NE1	2:B:62:PHE:O	2.28	0.65
1:D:66:ARG:NH2	1:D:82(B):SER:O	2.31	0.64
2:B:166:GLN:NE2	2:B:171:ASN:HB3	2.13	0.64
2:H:155:LYS:NZ	2:H:158:ASN:OD1	2.30	0.64
1:G:87:THR:HG23	1:G:110:THR:HA	1.80	0.64
1:J:119:PRO:HB3	1:J:145:TYR:HB3	1.79	0.64
2:E:50:GLN:O	2:E:52:SER:N	2.30	0.63
2:B:106:ILE:HG13	2:B:171:ASN:OD1	1.99	0.63
1:J:40:PRO:HG2	1:J:43:LYS:HE3	1.79	0.63
2:K:50:GLN:O	2:K:52:SER:N	2.31	0.63
2:B:50:GLN:O	2:B:52:SER:N	2.33	0.62
1:D:60:ASN:HB3	1:D:63:LEU:HD23	1.81	0.62
2:H:50:GLN:O	2:H:52:SER:N	2.33	0.62
1:G:4:LEU:HG	1:G:24:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HB3	1:A:48:ILE:HD11	1.82	0.61
1:A:95:GLU:OE2	3:C:512:ALA:N	2.34	0.60
1:A:24:VAL:O	1:A:76:ASN:ND2	2.35	0.60
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.85	0.59
1:D:87:THR:HG23	1:D:110:THR:HA	1.86	0.58
1:G:11:LEU:HD12	1:G:147:PRO:HD3	1.85	0.57
1:J:87:THR:HG23	1:J:110:THR:HA	1.84	0.57
2:K:13:ILE:HD12	2:K:78:VAL:HG11	1.87	0.57
1:J:95:GLU:OE2	3:L:512:ALA:N	2.37	0.57
1:J:4:LEU:HG	1:J:24:VAL:HG22	1.87	0.56
2:H:54:TRP:NE1	2:H:62:PHE:O	2.32	0.56
1:A:6:GLU:OE2	1:A:104:GLY:HA3	2.04	0.55
1:J:6:GLU:OE2	1:J:104:GLY:HA3	2.05	0.55
1:D:39:GLN:HB2	1:D:45:LEU:HD23	1.89	0.55
2:H:198:HIS:HB3	2:H:201:LEU:HD12	1.88	0.55
1:A:76:ASN:O	1:A:76:ASN:ND2	2.39	0.54
1:J:60:ASN:HB3	1:J:63:LEU:HD23	1.89	0.54
2:B:60:ASP:N	2:B:60:ASP:OD2	2.40	0.54
2:H:19:ALA:O	2:H:74:LYS:HA	2.08	0.54
2:B:186:TYR:O	2:B:192:TYR:OH	2.25	0.53
1:J:11:LEU:HG	1:J:147:PRO:HG3	1.90	0.53
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.90	0.53
2:B:13:ILE:HG21	2:B:78:VAL:HG11	1.91	0.53
2:B:166:GLN:HE21	2:B:171:ASN:HB3	1.73	0.52
1:A:127:SER:HA	1:A:217:ASP:OD2	2.08	0.52
2:E:155:LYS:NZ	2:E:158:ASN:OD1	2.37	0.52
1:G:169:VAL:HG13	1:G:171:GLN:HE22	1.74	0.52
2:B:138:ASN:ND2	2:B:138:ASN:N	2.56	0.52
2:B:171:ASN:N	2:B:171:ASN:HD22	2.06	0.51
2:E:19:ALA:O	2:E:74:LYS:HA	2.10	0.51
2:H:186:TYR:O	2:H:192:TYR:OH	2.23	0.51
1:D:38:ARG:HB3	1:D:48:ILE:HD11	1.93	0.51
2:K:33:LEU:HB3	2:K:51:VAL:HG22	1.93	0.51
2:H:167:ASP:O	2:H:171:ASN:HA	2.11	0.50
2:E:24:ARG:HA	2:E:69:THR:O	2.12	0.50
2:E:59:PRO:HB2	2:E:61:ARG:HG2	1.93	0.50
1:D:6:GLU:OE2	1:D:104:GLY:HA3	2.11	0.50
1:D:95:GLU:OE2	2:E:96:ARG:NH1	2.38	0.50
1:A:186:SER:O	1:A:189:LEU:HB2	2.12	0.50
2:E:37:GLN:O	2:E:45:ARG:N	2.39	0.49
1:G:60:ASN:HB3	1:G:63:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TRP:CE2	1:J:31(A):LYS:HG3	2.48	0.48
2:K:54:TRP:NE1	2:K:62:PHE:O	2.45	0.48
1:D:11:LEU:HD12	1:D:147:PRO:HD3	1.94	0.48
1:A:4:LEU:HB3	1:A:22:CYS:SG	2.53	0.48
2:H:13:ILE:HD11	2:H:106:ILE:HG12	1.95	0.48
2:H:59:PRO:HB2	2:H:61:ARG:HG2	1.96	0.48
2:H:103:LYS:NZ	2:H:165:GLU:OE2	2.47	0.48
2:K:107:LYS:HA	2:K:140:TYR:OH	2.14	0.48
1:G:78:PHE:CZ	1:G:92:CYS:HB2	2.49	0.48
2:H:150:VAL:O	2:H:153:VAL:HG22	2.14	0.48
1:J:39:GLN:HB2	1:J:45:LEU:HD23	1.96	0.47
2:H:163:VAL:HG22	2:H:175:LEU:HD12	1.96	0.47
2:B:167:ASP:O	2:B:171:ASN:HA	2.14	0.47
2:H:83:VAL:HG12	2:H:106:ILE:HG13	1.95	0.47
2:H:24:ARG:HA	2:H:69:THR:O	2.15	0.47
1:A:184:VAL:HG21	1:A:194:TYR:CZ	2.49	0.47
2:B:47:LEU:HA	2:B:58:VAL:HG21	1.96	0.47
1:D:4:LEU:HB3	1:D:92:CYS:SG	2.56	0.46
1:G:171:GLN:NE2	1:G:177:SER:HB2	2.30	0.46
1:J:206:LYS:HE3	1:J:208:ASP:OD2	2.15	0.46
1:G:37:ILE:HD11	1:G:100:PHE:CZ	2.51	0.46
2:K:48:ILE:HG21	2:K:51:VAL:O	2.16	0.46
2:B:128:GLY:CA	2:B:183:ASN:HD21	2.29	0.46
3:C:516:GLY:H	3:C:518:VAL:HG22	1.81	0.46
2:E:83:VAL:HG12	2:E:106:ILE:HG12	1.98	0.46
2:K:8:PRO:HG2	2:K:11:LEU:HB2	1.98	0.46
1:A:126:PRO:HD3	1:A:138:LEU:HB3	1.97	0.46
2:B:137:ASN:CG	2:B:138:ASN:HD22	2.19	0.46
1:J:37:ILE:HD11	1:J:100:PHE:CE2	2.50	0.45
2:K:131:SER:HA	2:K:179:LEU:O	2.15	0.45
2:H:30(A):HIS:HE1	3:I:518:VAL:HG21	1.81	0.45
1:A:123:PRO:HD3	1:A:209:LYS:HE2	1.98	0.45
2:K:37:GLN:O	2:K:45:ARG:N	2.39	0.45
2:B:83:VAL:HG12	2:B:106:ILE:HG12	1.99	0.45
2:K:150:VAL:O	2:K:153:VAL:HG22	2.18	0.44
1:A:206:LYS:HE3	1:A:208:ASP:OD2	2.17	0.44
2:H:37:GLN:O	2:H:45:ARG:N	2.43	0.44
1:A:66:ARG:HD2	1:A:82(A):THR:O	2.17	0.44
2:E:67:THR:HG21	1:G:114:ALA:HB2	1.99	0.44
2:H:120:PRO:HG3	2:H:130:VAL:HG13	2.00	0.44
1:J:36:TRP:HD1	1:J:69:ILE:HD13	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:37:GLN:HB2	2:K:47:LEU:HD11	2.00	0.44
1:J:166:PHE:CE2	2:K:176:SER:HB3	2.53	0.44
2:B:138:ASN:HD22	2:B:138:ASN:N	2.15	0.44
1:D:184:VAL:HG21	1:D:194:TYR:OH	2.17	0.44
1:G:72:ASP:OD2	1:G:75:LEU:HD13	2.17	0.44
2:E:150:VAL:O	2:E:153:VAL:HG22	2.17	0.44
2:E:186:TYR:O	2:E:192:TYR:OH	2.27	0.44
2:B:61:ARG:NH1	2:B:79:GLU:HG3	2.33	0.43
1:G:47:TRP:CZ2	1:G:49:GLY:HA2	2.52	0.43
1:J:14:PRO:O	1:J:15:SER:OG	2.34	0.43
2:B:12:SER:HA	2:B:105:ASP:O	2.18	0.43
1:D:31(A):LYS:HG3	1:J:54:TRP:CE2	2.54	0.43
1:G:38:ARG:NH2	1:G:86:ASP:OD1	2.43	0.43
2:E:13:ILE:HD11	2:E:106:ILE:HG23	1.99	0.43
1:G:94:ARG:HG2	1:G:102:VAL:HG22	2.00	0.43
2:E:128:GLY:CA	2:E:183:ASN:HD21	2.32	0.43
3:L:516:GLY:H	3:L:518:VAL:HG22	1.83	0.43
2:B:198:HIS:HB3	2:B:201:LEU:HD12	2.01	0.43
2:H:166:GLN:NE2	2:H:171:ASN:HB3	2.34	0.43
1:J:103:TRP:CE3	2:K:44:PRO:HD2	2.53	0.43
2:E:198:HIS:HB3	2:E:201:LEU:HD12	2.00	0.43
1:G:20:LEU:HA	1:G:20:LEU:HD23	1.90	0.43
2:H:113:PRO:HB3	2:H:139:PHE:HB3	2.01	0.43
2:B:103:LYS:NZ	2:B:165:GLU:OE2	2.48	0.42
1:J:20:LEU:HA	1:J:20:LEU:HD23	1.90	0.42
1:J:200:HIS:HB3	1:J:205:THR:OG1	2.19	0.42
2:K:48:ILE:HG23	2:K:53:ASN:O	2.20	0.42
2:B:113:PRO:HB3	2:B:139:PHE:HB3	2.01	0.42
1:J:90:TYR:HE1	1:J:109:VAL:HB	1.85	0.42
1:G:136:ALA:HB3	1:G:189:LEU:HD11	2.02	0.42
2:B:110:VAL:HG22	2:B:141:PRO:HD3	2.02	0.42
1:G:4:LEU:HB3	1:G:92:CYS:SG	2.59	0.42
2:K:122:GLU:HG2	2:K:122:GLU:H	1.60	0.42
2:H:167:ASP:OD2	2:H:169:LYS:N	2.39	0.42
2:B:150:VAL:O	2:B:153:VAL:HG22	2.19	0.42
2:K:145:SER:HB3	2:K:197:THR:OG1	2.20	0.42
2:E:145:SER:HB3	2:E:197:THR:OG1	2.19	0.41
2:E:30(A):HIS:HE1	3:F:518:VAL:HG21	1.84	0.41
2:E:47:LEU:HA	2:E:58:VAL:HG21	2.01	0.41
2:K:30(A):HIS:HB3	2:K:30(C):ASP:OD1	2.20	0.41
2:B:137:ASN:ND2	2:B:138:ASN:ND2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.21	0.41
1:D:78:PHE:CZ	1:D:92:CYS:HB2	2.56	0.41
2:E:106:ILE:N	2:E:166:GLN:OE1	2.45	0.41
1:G:146:PHE:HA	1:G:147:PRO:HA	1.84	0.41
2:H:12:SER:HA	2:H:105:ASP:OD2	2.21	0.41
2:H:125:VAL:O	2:H:183:ASN:ND2	2.53	0.41
2:H:55:TYR:O	2:H:58:VAL:HG23	2.21	0.41
2:B:24:ARG:HA	2:B:69:THR:O	2.21	0.41
2:E:47:LEU:HB3	2:E:48:ILE:HD12	2.01	0.41
2:H:6:GLN:HA	2:H:22:SER:O	2.20	0.41
2:H:145:SER:HB3	2:H:197:THR:OG1	2.21	0.41
2:B:197:THR:HG22	2:B:204:PRO:HB3	2.03	0.41
1:D:47:TRP:CZ2	1:D:49:GLY:HA2	2.56	0.41
2:E:122:GLU:HG2	2:E:122:GLU:H	1.60	0.41
2:E:150:VAL:HG11	2:E:189:HIS:CD2	2.56	0.41
1:G:169:VAL:O	1:G:171:GLN:NE2	2.53	0.41
1:A:14:PRO:O	1:A:15:SER:OG	2.32	0.40
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.90	0.40
2:B:61:ARG:CZ	2:B:79:GLU:HG3	2.51	0.40
2:E:103:LYS:NZ	2:E:165:GLU:OE2	2.36	0.40
1:J:32:ALA:HB1	1:J:94:ARG:HG3	2.02	0.40
1:G:72:ASP:OD2	1:G:75:LEU:HB2	2.22	0.40
2:K:193:ALA:HB2	2:K:208:SER:HB3	2.03	0.40
2:K:94:LEU:HD23	2:K:96:ARG:HD3	2.02	0.40
2:B:19:ALA:O	2:B:74:LYS:HA	2.21	0.40
1:G:14:PRO:O	1:G:15:SER:OG	2.31	0.40
1:J:94:ARG:HG2	1:J:94:ARG:HH21	1.86	0.40
1:D:104:GLY:O	2:E:43:PRO:HB3	2.22	0.40

All (1) 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)
1:A:191:THR:OG1	1:G:191:THR:OG1[2_544]	2.01	0.19

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	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
1	D	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
1	G	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
1	J	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
2	B	215/217 (99%)	209 (97%)	5 (2%)	1 (0%)	29	66
2	E	215/217 (99%)	209 (97%)	5 (2%)	1 (0%)	29	66
2	H	215/217 (99%)	209 (97%)	5 (2%)	1 (0%)	29	66
2	K	215/217 (99%)	208 (97%)	6 (3%)	1 (0%)	29	66
3	C	5/7 (71%)	5 (100%)	0	0	100	100
3	F	5/7 (71%)	5 (100%)	0	0	100	100
3	I	5/7 (71%)	5 (100%)	0	0	100	100
3	L	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1760/1784 (99%)	1716 (98%)	40 (2%)	4 (0%)	47	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	E	51	VAL
2	H	51	VAL
2	K	51	VAL

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	190/190 (100%)	189 (100%)	1 (0%)	88 95
1	D	190/190 (100%)	189 (100%)	1 (0%)	88 95
1	G	190/190 (100%)	187 (98%)	3 (2%)	62 82
1	J	190/190 (100%)	188 (99%)	2 (1%)	73 88
2	B	193/193 (100%)	193 (100%)	0	100 100
2	E	193/193 (100%)	191 (99%)	2 (1%)	76 89
2	H	193/193 (100%)	193 (100%)	0	100 100
2	K	193/193 (100%)	192 (100%)	1 (0%)	88 95
3	C	3/3 (100%)	3 (100%)	0	100 100
3	F	3/3 (100%)	3 (100%)	0	100 100
3	I	3/3 (100%)	3 (100%)	0	100 100
3	L	3/3 (100%)	3 (100%)	0	100 100
All	All	1544/1544 (100%)	1534 (99%)	10 (1%)	86 94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	D	197	ASN
2	E	54	TRP
2	E	108	ARG
1	G	56	LEU
1	G	94	ARG
1	G	197	ASN
1	J	101	ASP
1	J	209	LYS
2	K	108	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
2	B	93	HIS
2	B	137	ASN
2	B	138	ASN
2	E	30(A)	HIS

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Mol	Chain	Res	Type
1	G	171	GLN
2	H	30(A)	HIS
2	H	183	ASN
2	K	53	ASN

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	222/222 (100%)	0.21	12 (5%) 25 25	35, 50, 92, 116	0
1	D	222/222 (100%)	0.10	10 (4%) 33 31	31, 51, 82, 139	0
1	G	222/222 (100%)	0.09	8 (3%) 42 40	36, 53, 88, 146	0
1	J	222/222 (100%)	0.32	9 (4%) 37 35	42, 65, 94, 123	0
2	B	217/217 (100%)	0.26	5 (2%) 60 56	39, 57, 80, 95	0
2	E	217/217 (100%)	0.24	1 (0%) 91 88	37, 59, 74, 97	0
2	H	217/217 (100%)	0.25	4 (1%) 68 64	34, 62, 82, 93	0
2	K	217/217 (100%)	0.51	13 (5%) 21 21	47, 73, 97, 117	0
3	C	7/7 (100%)	0.61	1 (14%) 2 3	52, 58, 74, 103	0
3	F	7/7 (100%)	0.47	0 100 100	54, 59, 72, 98	0
3	I	7/7 (100%)	0.46	0 100 100	51, 61, 77, 94	0
3	L	7/7 (100%)	0.97	1 (14%) 2 3	65, 75, 93, 94	0
All	All	1784/1784 (100%)	0.25	64 (3%) 42 40	31, 59, 89, 146	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	ASP	6.2
1	G	217	ASP	6.0
1	J	130	SER	5.7
1	D	132	SER	4.7
1	A	130	SER	4.6
1	A	1	GLN	4.5
1	A	129	LYS	4.4
1	D	1	GLN	4.4
3	C	518	VAL	4.0
2	K	76	SER	4.0
2	H	190	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	130	SER	3.6
1	A	132	SER	3.6
1	J	128	SER	3.4
1	J	132	SER	3.4
1	J	1	GLN	3.4
1	G	130	SER	3.2
1	J	131	THR	3.2
2	K	65	SER	3.1
1	J	133	GLY	3.1
1	D	131	THR	3.0
2	B	150	VAL	2.9
2	K	20	SER	2.9
2	B	153	VAL	2.8
3	L	518	VAL	2.8
1	A	133	GLY	2.8
1	J	217	ASP	2.7
1	D	216	CYS	2.7
1	G	131	THR	2.7
1	A	93	ALA	2.7
1	A	215	SER	2.6
1	G	128	SER	2.6
2	K	30(D)	GLY	2.6
1	D	215	SER	2.6
2	K	66	GLY	2.6
2	H	76	SER	2.6
1	G	215	SER	2.6
1	D	128	SER	2.5
1	A	131	THR	2.5
1	G	1	GLN	2.4
2	K	190	ASN	2.4
2	K	21	ILE	2.4
2	H	155	LYS	2.4
1	J	129	LYS	2.4
1	D	133	GLY	2.3
1	G	216	CYS	2.3
2	K	73	LEU	2.3
2	H	30(C)	ASP	2.3
2	B	190	ASN	2.2
1	A	126	PRO	2.2
2	B	76	SER	2.2
2	K	8	PRO	2.2
1	A	216	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	217	ASP	2.2
2	K	48	ILE	2.2
1	A	127	SER	2.1
2	B	130	VAL	2.1
2	E	66	GLY	2.1
2	K	31	THR	2.1
1	G	133	GLY	2.1
2	K	1	ASP	2.1
1	D	2	VAL	2.0
1	J	111	VAL	2.0
2	K	77	ARG	2.0

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.