



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:44 PM BST

PDB ID : 3J2Y
EMDB ID: : EMD-5578
Title : Electron Cryo-microscopy of Chikungunya VLP in complex with neutralizing antibody Fab 9.8B
Authors : Sun, S.; Xiang, Y.; Rossmann, M.G.
Deposited on : 2013-01-28
Resolution : 14.90 Å(reported)
Based on PDB ID : 4GQ9

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

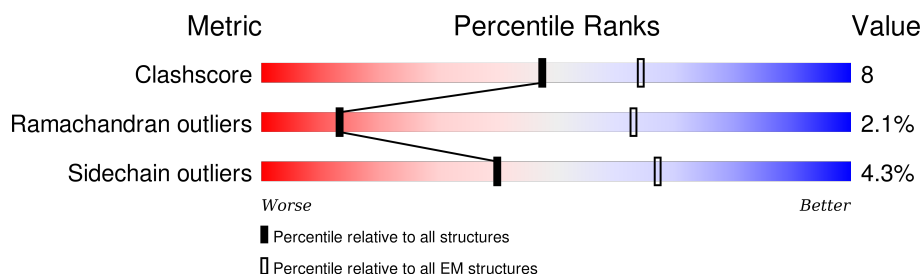
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.90 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	212	83% 16% .
1	C	212	83% 15% .
1	E	212	85% 13% .
1	G	212	85% 14% .
2	B	218	78% 19% .
2	D	218	79% 18% .
2	F	218	79% 17% .
2	H	218	77% 20% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 9.8B light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		
1	C	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		
1	E	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		
1	G	212	Total	C	N	O	S	0	0
			1633	1015	273	336	9		

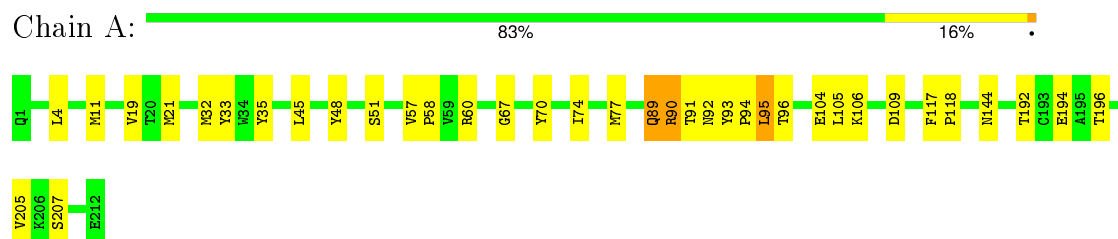
- Molecule 2 is a protein called 9.8B heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	D	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	F	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	H	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		

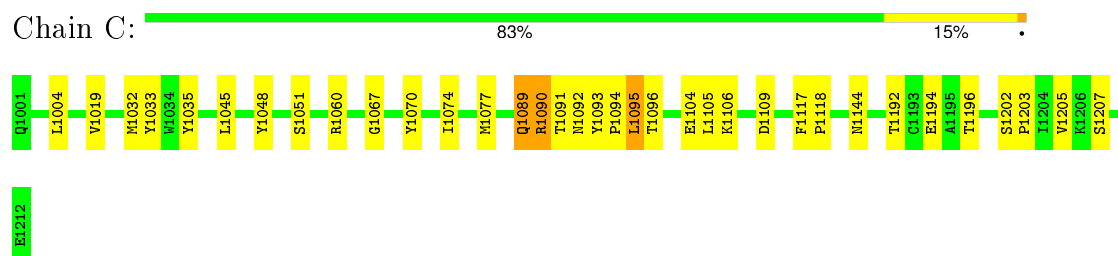
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

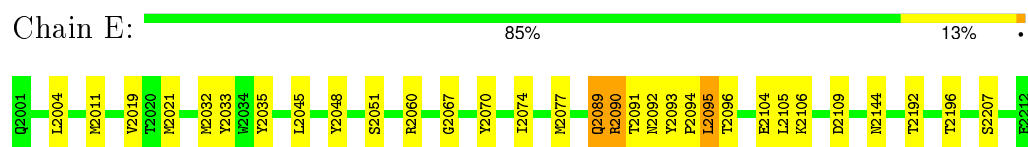
- Molecule 1: 9.8B light chain



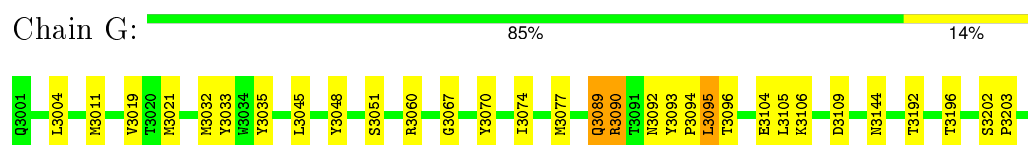
- Molecule 1: 9.8B light chain



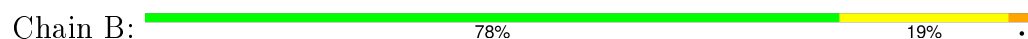
- Molecule 1: 9.8B light chain

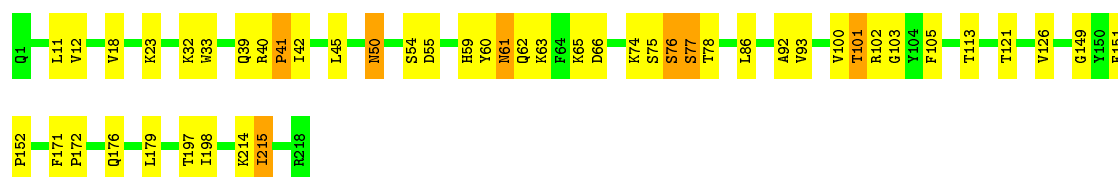


- Molecule 1: 9.8B light chain



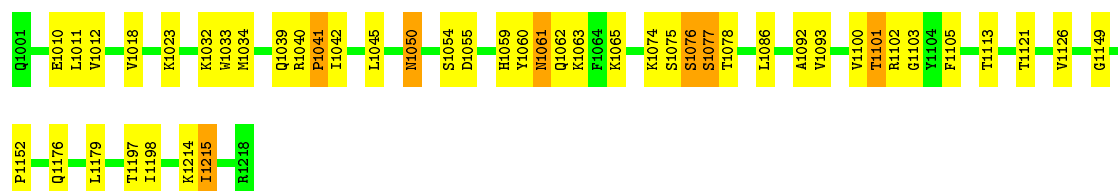
- Molecule 2: 9.8B heavy chain





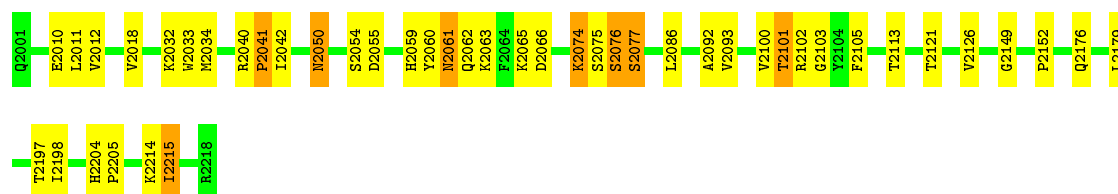
- Molecule 2: 9.8B heavy chain

Chain D: 79% 18% •



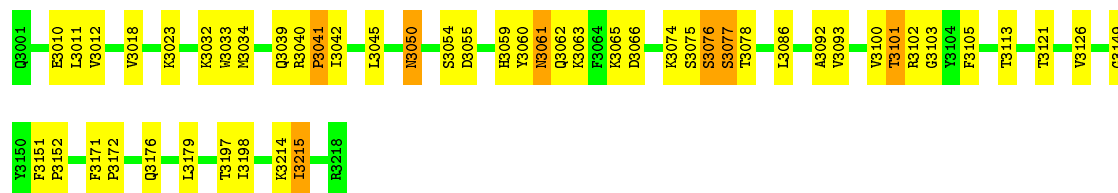
- Molecule 2: 9.8B heavy chain

Chain F: 79% 17% •



- Molecule 2: 9.8B heavy chain

Chain H: 77% 20% •



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	1820	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each Micrograph	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	38000	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 >2	RMSZ	# Z >2
1	A	0.34	0/1669	0.48	0/2268
1	C	0.34	0/1669	0.48	0/2268
1	E	0.33	0/1669	0.48	0/2268
1	G	0.33	0/1669	0.48	0/2268
2	B	0.33	0/1689	0.50	0/2308
2	D	0.33	0/1689	0.50	0/2308
2	F	0.33	0/1689	0.50	0/2308
2	H	0.33	0/1689	0.50	0/2308
All	All	0.33	0/13432	0.49	0/18304

There are no bond length outliers.

There are no bond angle outliers.

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	1633	0	1567	20	0
1	C	1633	0	1564	18	0
1	E	1633	0	1564	16	0
1	G	1633	0	1564	17	0
2	B	1647	0	1620	32	0
2	D	1647	0	1617	30	0
2	F	1647	0	1617	32	0
2	H	1647	0	1617	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13120	0	12730	199	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 8.

All (199) 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:G:3033:TYR:OH	1:G:3090:ARG:NH1	1.58	1.36
1:E:2033:TYR:OH	1:E:2090:ARG:NH1	1.58	1.36
1:C:1033:TYR:OH	1:C:1090:ARG:NH1	1.58	1.34
1:A:33:TYR:OH	1:A:90:ARG:NH1	1.58	1.31
2:D:1076:SER:HA	2:D:1077:SER:HB3	1.16	1.14
2:F:2076:SER:HA	2:F:2077:SER:HB3	1.16	1.13
2:H:3076:SER:HA	2:H:3077:SER:HB3	1.16	1.13
2:B:76:SER:HA	2:B:77:SER:HB3	1.16	1.09
2:B:76:SER:HA	2:B:77:SER:CB	1.82	1.09
2:D:1076:SER:HA	2:D:1077:SER:CB	1.82	1.08
2:H:3076:SER:HA	2:H:3077:SER:CB	1.82	1.08
2:F:2076:SER:HA	2:F:2077:SER:CB	1.82	1.07
2:B:54:SER:HB2	2:B:55:ASP:HB3	1.40	1.01
2:D:1054:SER:HB2	2:D:1055:ASP:HB3	1.40	1.01
2:F:2054:SER:HB2	2:F:2055:ASP:HB3	1.40	1.01
2:H:3054:SER:HB2	2:H:3055:ASP:HB3	1.40	1.00
2:H:3076:SER:CA	2:H:3077:SER:HB3	2.01	0.90
2:D:1076:SER:CA	2:D:1077:SER:HB3	2.01	0.90
2:B:76:SER:CA	2:B:77:SER:HB3	2.01	0.90
2:H:3050:ASN:ND2	2:H:3059:HIS:HB2	1.89	0.88
2:F:2076:SER:CA	2:F:2077:SER:HB3	2.01	0.87
2:F:2050:ASN:ND2	2:F:2059:HIS:HB2	1.89	0.87
2:D:1050:ASN:ND2	2:D:1059:HIS:HB2	1.89	0.87
2:B:50:ASN:ND2	2:B:59:HIS:HB2	1.89	0.86
2:D:1050:ASN:HD21	2:D:1059:HIS:HB2	1.48	0.79
2:B:50:ASN:HD21	2:B:59:HIS:HB2	1.48	0.78
2:F:2050:ASN:HD21	2:F:2059:HIS:HB2	1.48	0.78
2:H:3050:ASN:HD21	2:H:3059:HIS:HB2	1.48	0.77
2:F:2075:SER:H	2:F:2076:SER:C	1.89	0.76
2:D:1075:SER:H	2:D:1076:SER:C	1.89	0.75
2:H:3075:SER:H	2:H:3076:SER:C	1.89	0.75
2:B:75:SER:H	2:B:76:SER:C	1.89	0.74
1:A:94:PRO:HA	1:A:95:LEU:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3094:PRO:HA	1:G:3095:LEU:CB	2.23	0.68
1:E:2094:PRO:HA	1:E:2095:LEU:CB	2.23	0.68
1:C:1094:PRO:HA	1:C:1095:LEU:CB	2.23	0.67
2:D:1050:ASN:HD22	2:D:1050:ASN:N	1.95	0.65
2:H:3050:ASN:HD22	2:H:3050:ASN:N	1.95	0.64
2:F:2050:ASN:HD22	2:F:2050:ASN:N	1.95	0.64
2:B:50:ASN:HD22	2:B:50:ASN:N	1.95	0.64
2:D:1062:GLN:HA	2:D:1065:LYS:HE3	1.82	0.62
2:D:1061:ASN:HD22	2:D:1063:LYS:H	1.48	0.61
2:H:3062:GLN:HA	2:H:3065:LYS:HE3	1.82	0.61
2:B:61:ASN:HD22	2:B:63:LYS:H	1.48	0.61
2:F:2062:GLN:HA	2:F:2065:LYS:HE3	1.82	0.61
2:B:62:GLN:HA	2:B:65:LYS:HE3	1.82	0.60
2:F:2061:ASN:HD22	2:F:2063:LYS:H	1.48	0.59
2:H:3061:ASN:HD22	2:H:3063:LYS:H	1.48	0.59
2:B:54:SER:CB	2:B:55:ASP:HB3	2.25	0.59
1:G:3004:LEU:HD11	1:G:3089:GLN:HB3	1.85	0.58
1:A:4:LEU:HD11	1:A:89:GLN:HB3	1.85	0.57
1:C:1004:LEU:HD11	1:C:1089:GLN:HB3	1.85	0.57
1:E:2004:LEU:HD11	1:E:2089:GLN:HB3	1.85	0.57
2:F:2033:TRP:CD1	2:F:2101:THR:HA	2.41	0.55
2:H:3033:TRP:CD1	2:H:3101:THR:HA	2.41	0.55
2:B:33:TRP:CD1	2:B:101:THR:HA	2.41	0.55
2:D:1033:TRP:CD1	2:D:1101:THR:HA	2.41	0.55
2:D:1054:SER:CB	2:D:1055:ASP:HB3	2.25	0.55
2:H:3054:SER:CB	2:H:3055:ASP:HB3	2.25	0.54
2:F:2054:SER:CB	2:F:2055:ASP:HB3	2.25	0.54
2:H:3093:VAL:HG22	2:H:3113:THR:HG22	1.91	0.53
2:F:2093:VAL:HG22	2:F:2113:THR:HG22	1.91	0.53
2:B:93:VAL:HG22	2:B:113:THR:HG22	1.91	0.53
2:D:1093:VAL:HG22	2:D:1113:THR:HG22	1.91	0.53
1:A:144:ASN:HB3	1:A:196:THR:HB	1.91	0.53
1:G:3144:ASN:HB3	1:G:3196:THR:HB	1.91	0.53
1:C:1144:ASN:HB3	1:C:1196:THR:HB	1.91	0.52
1:E:2094:PRO:HA	1:E:2095:LEU:HB2	1.91	0.52
1:C:1094:PRO:HA	1:C:1095:LEU:HB2	1.91	0.52
1:A:94:PRO:HA	1:A:95:LEU:HB2	1.91	0.52
2:H:3054:SER:HB2	2:H:3055:ASP:CB	2.28	0.51
1:G:3094:PRO:HA	1:G:3095:LEU:HB2	1.91	0.51
1:E:2144:ASN:HB3	1:E:2196:THR:HB	1.91	0.51
2:D:1054:SER:HB2	2:D:1055:ASP:CB	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1045:LEU:HD11	1:C:1048:TYR:HB3	1.92	0.51
1:E:2045:LEU:HD11	1:E:2048:TYR:HB3	1.92	0.51
1:A:45:LEU:HD11	1:A:48:TYR:HB3	1.92	0.51
1:G:3045:LEU:HD11	1:G:3048:TYR:HB3	1.92	0.50
1:E:2094:PRO:HA	1:E:2095:LEU:HB3	1.94	0.50
1:A:94:PRO:HA	1:A:95:LEU:HB3	1.94	0.50
2:B:121:THR:HG23	2:B:152:PRO:HD3	1.94	0.50
2:D:1121:THR:HG23	2:D:1152:PRO:HD3	1.94	0.49
2:F:2121:THR:HG23	2:F:2152:PRO:HD3	1.94	0.49
2:H:3121:THR:HG23	2:H:3152:PRO:HD3	1.94	0.49
1:G:3094:PRO:HA	1:G:3095:LEU:HB3	1.93	0.49
1:C:1035:TYR:CZ	1:C:1045:LEU:HD23	2.48	0.48
1:C:1094:PRO:HA	1:C:1095:LEU:HB3	1.94	0.48
2:H:3041:PRO:HB2	2:H:3042:ILE:HD12	1.96	0.48
1:E:2094:PRO:HB2	1:E:2096:THR:HG23	1.96	0.48
1:A:94:PRO:HB2	1:A:96:THR:HG23	1.96	0.48
1:A:35:TYR:CZ	1:A:45:LEU:HD23	2.48	0.48
1:E:2035:TYR:CZ	1:E:2045:LEU:HD23	2.49	0.48
1:G:3094:PRO:HB2	1:G:3096:THR:HG23	1.96	0.48
1:E:2089:GLN:HG2	1:E:2090:ARG:N	2.29	0.48
1:G:3089:GLN:HG2	1:G:3090:ARG:N	2.29	0.48
1:A:89:GLN:HG2	1:A:90:ARG:N	2.29	0.48
1:G:3035:TYR:CZ	1:G:3045:LEU:HD23	2.48	0.47
2:F:2054:SER:HB2	2:F:2055:ASP:CB	2.28	0.47
2:D:1041:PRO:HB2	2:D:1042:ILE:HD12	1.96	0.47
2:H:3034:MET:HB3	2:H:3034:MET:HE2	1.74	0.47
1:C:1089:GLN:HG2	1:C:1090:ARG:N	2.29	0.47
2:F:2041:PRO:HB2	2:F:2042:ILE:HD12	1.96	0.47
2:B:54:SER:HB2	2:B:55:ASP:CB	2.28	0.47
2:F:2060:TYR:HB2	2:F:2065:LYS:HE2	1.96	0.47
2:F:2034:MET:HB3	2:F:2034:MET:HE2	1.73	0.47
2:B:41:PRO:HB2	2:B:42:ILE:HD12	1.96	0.47
1:C:1094:PRO:HB2	1:C:1096:THR:HG23	1.96	0.47
2:D:1060:TYR:HB2	2:D:1065:LYS:HE2	1.96	0.46
2:D:1040:ARG:HG2	2:D:1092:ALA:HB2	1.96	0.46
2:F:2040:ARG:HG2	2:F:2092:ALA:HB2	1.96	0.46
2:H:3060:TYR:HB2	2:H:3065:LYS:HE2	1.96	0.46
2:B:198:ILE:HG22	2:B:215:ILE:HD11	1.98	0.46
2:B:60:TYR:HB2	2:B:65:LYS:HE2	1.96	0.46
2:H:3040:ARG:HG2	2:H:3092:ALA:HB2	1.96	0.46
2:H:3065:LYS:HA	2:H:3066:ASP:HA	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2198:ILE:HG22	2:F:2215:ILE:HD11	1.98	0.46
2:B:40:ARG:HG2	2:B:92:ALA:HB2	1.96	0.46
2:D:1198:ILE:HG22	2:D:1215:ILE:HD11	1.98	0.45
2:B:65:LYS:HA	2:B:66:ASP:HA	1.66	0.45
2:F:2075:SER:N	2:F:2076:SER:C	2.66	0.45
2:F:2102:ARG:HA	2:F:2103:GLY:HA2	1.68	0.45
2:H:3198:ILE:HG22	2:H:3215:ILE:HD11	1.98	0.45
1:G:3089:GLN:NE2	1:G:3092:ASN:HB3	2.32	0.45
1:A:89:GLN:NE2	1:A:92:ASN:HB3	2.32	0.45
2:H:3075:SER:N	2:H:3076:SER:C	2.66	0.45
2:H:3102:ARG:HA	2:H:3103:GLY:HA2	1.68	0.45
1:C:1089:GLN:NE2	1:C:1092:ASN:HB3	2.32	0.45
1:C:1090:ARG:HB2	1:C:1091:THR:H	1.47	0.45
1:E:2090:ARG:HB2	1:E:2091:THR:H	1.47	0.44
1:E:2089:GLN:NE2	1:E:2092:ASN:HB3	2.32	0.44
2:H:3197:THR:HG23	2:H:3214:LYS:HE3	1.99	0.44
2:H:3076:SER:N	2:H:3077:SER:HB3	2.33	0.44
1:E:2192:THR:HG23	1:E:2207:SER:HB2	2.00	0.44
2:F:2065:LYS:HA	2:F:2066:ASP:HA	1.66	0.44
2:D:1076:SER:N	2:D:1077:SER:HB3	2.33	0.44
1:G:3192:THR:HG23	1:G:3207:SER:HB2	2.00	0.44
1:G:3202:SER:HA	1:G:3203:PRO:HD3	1.88	0.44
2:F:2197:THR:HG23	2:F:2214:LYS:HE3	1.99	0.44
2:F:2149:GLY:HA2	2:F:2179:LEU:HB3	2.00	0.44
2:B:197:THR:HG23	2:B:214:LYS:HE3	1.99	0.44
2:B:149:GLY:HA2	2:B:179:LEU:HB3	2.00	0.44
2:D:1197:THR:HG23	2:D:1214:LYS:HE3	2.00	0.43
2:H:3032:LYS:HD3	2:H:3100:VAL:HG22	2.01	0.43
2:H:3149:GLY:HA2	2:H:3179:LEU:HB3	2.00	0.43
2:D:1149:GLY:HA2	2:D:1179:LEU:HB3	2.00	0.43
1:A:192:THR:HG23	1:A:207:SER:HB2	2.00	0.43
1:C:1192:THR:HG23	1:C:1207:SER:HB2	2.00	0.43
2:D:1032:LYS:HD3	2:D:1100:VAL:HG22	2.01	0.43
2:B:151:PHE:HA	2:B:152:PRO:HA	1.89	0.43
2:B:75:SER:N	2:B:76:SER:C	2.66	0.43
1:G:3032:MET:HG3	1:G:3070:TYR:CG	2.54	0.43
2:H:3171:PHE:HA	2:H:3172:PRO:HD3	1.94	0.42
1:E:2011:MET:HE3	1:E:2021:MET:HG2	2.01	0.42
2:F:2032:LYS:HD3	2:F:2100:VAL:HG22	2.01	0.42
1:E:2032:MET:HG3	1:E:2070:TYR:CG	2.54	0.42
2:B:102:ARG:HA	2:B:103:GLY:HA2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1032:MET:HG3	1:C:1070:TYR:CG	2.54	0.42
2:D:1102:ARG:HA	2:D:1103:GLY:HA2	1.68	0.42
1:A:57:VAL:HA	1:A:58:PRO:HD3	1.94	0.42
2:B:32:LYS:HD3	2:B:100:VAL:HG22	2.01	0.42
2:B:12:VAL:HG21	2:B:18:VAL:HG22	2.02	0.42
2:F:2076:SER:N	2:F:2077:SER:HB3	2.33	0.42
1:A:32:MET:HG3	1:A:70:TYR:CG	2.54	0.42
1:C:1117:PHE:HA	1:C:1118:PRO:HD3	1.93	0.42
1:A:33:TYR:CZ	1:A:90:ARG:NH1	2.74	0.42
2:H:3050:ASN:ND2	2:H:3050:ASN:N	2.67	0.42
2:B:50:ASN:HD22	2:B:50:ASN:H	1.66	0.42
2:F:2012:VAL:HG21	2:F:2018:VAL:HG22	2.02	0.42
2:F:2204:HIS:HA	2:F:2205:PRO:HD3	1.88	0.42
1:A:117:PHE:HA	1:A:118:PRO:HD3	1.93	0.41
1:G:3019:VAL:HB	1:G:3074:ILE:HB	2.02	0.41
1:G:3033:TYR:CZ	1:G:3090:ARG:NH1	2.74	0.41
2:D:1034:MET:HB3	2:D:1034:MET:HE2	1.75	0.41
2:D:1012:VAL:HG21	2:D:1018:VAL:HG22	2.02	0.41
2:B:39:GLN:HB2	2:B:45:LEU:HD23	2.03	0.41
2:H:3012:VAL:HG21	2:H:3018:VAL:HG22	2.02	0.41
2:H:3151:PHE:HA	2:H:3152:PRO:HA	1.88	0.41
2:D:1023:LYS:HA	2:D:1078:THR:HG22	2.03	0.41
1:E:2019:VAL:HB	1:E:2074:ILE:HB	2.02	0.41
2:B:23:LYS:HA	2:B:78:THR:HG22	2.03	0.41
2:D:1010:GLU:HG2	2:D:1018:VAL:HG13	2.03	0.41
2:F:2010:GLU:HG2	2:F:2018:VAL:HG13	2.03	0.41
1:A:11:MET:HE3	1:A:21:MET:HG2	2.03	0.41
2:D:1039:GLN:HB2	2:D:1045:LEU:HD23	2.03	0.41
1:A:90:ARG:HB2	1:A:91:THR:H	1.47	0.41
2:H:3023:LYS:HA	2:H:3078:THR:HG22	2.03	0.41
2:F:2074:LYS:H	2:F:2074:LYS:HE3	1.87	0.40
1:G:3011:MET:HE3	1:G:3021:MET:HG2	2.02	0.40
1:A:19:VAL:HB	1:A:74:ILE:HB	2.02	0.40
2:B:76:SER:N	2:B:77:SER:HB3	2.33	0.40
2:D:1100:VAL:O	2:D:1101:THR:HG22	2.21	0.40
1:A:194:GLU:HG2	1:A:205:VAL:HG22	2.04	0.40
1:C:1019:VAL:HB	1:C:1074:ILE:HB	2.02	0.40
1:C:1194:GLU:HG2	1:C:1205:VAL:HG22	2.04	0.40
2:H:3039:GLN:HB2	2:H:3045:LEU:HD23	2.03	0.40
2:B:171:PHE:HA	2:B:172:PRO:HD3	1.94	0.40
2:F:2050:ASN:N	2:F:2050:ASN:ND2	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3010:GLU:HG2	2:H:3018:VAL:HG13	2.03	0.40
1:C:1202:SER:HA	1:C:1203:PRO:HD3	1.88	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 PDB entries followed by that with respect to all EM entries.

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	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	14	58
1	C	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	14	58
1	E	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	14	58
1	G	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	14	58
2	B	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	44
2	D	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	44
2	F	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	44
2	H	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	6	44
All	All	1704/1720 (99%)	1532 (90%)	136 (8%)	36 (2%)	13	50

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	77	SER
2	D	1077	SER
2	F	2077	SER
2	H	3077	SER
1	A	93	TYR
1	C	1093	TYR
1	E	2093	TYR
1	G	3093	TYR

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Mol	Chain	Res	Type
2	B	101	THR
2	D	1101	THR
2	F	2101	THR
2	H	3101	THR
1	A	60	ARG
1	C	1060	ARG
1	E	2060	ARG
1	G	3060	ARG
2	B	76	SER
2	B	86	LEU
2	B	126	VAL
2	D	1076	SER
2	D	1086	LEU
2	D	1126	VAL
2	F	2076	SER
2	F	2086	LEU
2	F	2126	VAL
2	H	3076	SER
2	H	3086	LEU
2	H	3126	VAL
2	B	41	PRO
2	D	1041	PRO
2	F	2041	PRO
2	H	3041	PRO
1	A	67	GLY
1	C	1067	GLY
1	E	2067	GLY
1	G	3067	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 PDB entries followed by that with respect to all EM entries.

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	187/187 (100%)	178 (95%)	9 (5%)	31	67
1	C	187/187 (100%)	178 (95%)	9 (5%)	31	67
1	E	187/187 (100%)	178 (95%)	9 (5%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	187/187 (100%)	178 (95%)	9 (5%)	31	67
2	B	189/189 (100%)	182 (96%)	7 (4%)	41	73
2	D	189/189 (100%)	182 (96%)	7 (4%)	41	73
2	F	189/189 (100%)	182 (96%)	7 (4%)	41	73
2	H	189/189 (100%)	182 (96%)	7 (4%)	41	73
All	All	1504/1504 (100%)	1440 (96%)	64 (4%)	40	70

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	77	MET
1	A	89	GLN
1	A	90	ARG
1	A	95	LEU
1	A	104	GLU
1	A	105	LEU
1	A	106	LYS
1	A	109	ASP
1	C	1051	SER
1	C	1077	MET
1	C	1089	GLN
1	C	1090	ARG
1	C	1095	LEU
1	C	1104	GLU
1	C	1105	LEU
1	C	1106	LYS
1	C	1109	ASP
1	E	2051	SER
1	E	2077	MET
1	E	2089	GLN
1	E	2090	ARG
1	E	2095	LEU
1	E	2104	GLU
1	E	2105	LEU
1	E	2106	LYS
1	E	2109	ASP
1	G	3051	SER
1	G	3077	MET
1	G	3089	GLN

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Mol	Chain	Res	Type
1	G	3090	ARG
1	G	3095	LEU
1	G	3104	GLU
1	G	3105	LEU
1	G	3106	LYS
1	G	3109	ASP
2	B	11	LEU
2	B	50	ASN
2	B	61	ASN
2	B	74	LYS
2	B	105	PHE
2	B	176	GLN
2	B	215	ILE
2	D	1011	LEU
2	D	1050	ASN
2	D	1061	ASN
2	D	1074	LYS
2	D	1105	PHE
2	D	1176	GLN
2	D	1215	ILE
2	F	2011	LEU
2	F	2050	ASN
2	F	2061	ASN
2	F	2074	LYS
2	F	2105	PHE
2	F	2176	GLN
2	F	2215	ILE
2	H	3011	LEU
2	H	3050	ASN
2	H	3061	ASN
2	H	3074	LYS
2	H	3105	PHE
2	H	3176	GLN
2	H	3215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	88	GLN
1	C	1037	GLN
1	C	1088	GLN

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Mol	Chain	Res	Type
1	E	2037	GLN
1	E	2088	GLN
1	G	3037	GLN
1	G	3088	GLN
2	B	35	HIS
2	B	39	GLN
2	B	50	ASN
2	B	61	ASN
2	D	1035	HIS
2	D	1039	GLN
2	D	1050	ASN
2	D	1061	ASN
2	F	2035	HIS
2	F	2039	GLN
2	F	2050	ASN
2	F	2061	ASN
2	H	3035	HIS
2	H	3039	GLN
2	H	3050	ASN
2	H	3061	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.