wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:44 PM BST

PDB ID	:	3J30
EMDB ID:	:	EMD-5580
Title	:	Electron Cryo-microscopy of Chikungunya VLP in complex with neutralizing antibody Fab CHK152
Authors	:	Sun, S.; Xiang, Y.; Rossmann, M.G.
Deposited on	:	2013-01-28
Resolution	:	16.00 Å(reported)
Based on PDB ID	:	4GQ8

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

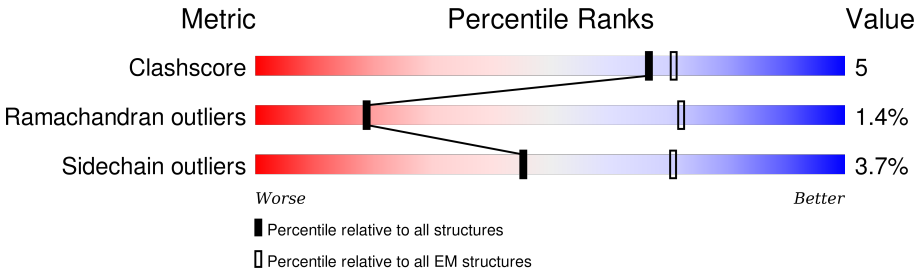
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 16.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	217	85% 13% •
1	C	217	86% 12% •
1	E	217	87% 11% •
1	G	217	86% 12% •
2	B	217	84% 14% •
2	D	217	83% 16% •
2	F	217	83% 15% •
2	H	217	84% 14% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13228 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 CHK152 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	217	Total	C	N	O	S	0	0
			1676	1041	285	344	6		
1	C	217	Total	C	N	O	S	0	0
			1676	1041	285	344	6		
1	E	217	Total	C	N	O	S	0	0
			1676	1041	285	344	6		
1	G	217	Total	C	N	O	S	0	0
			1676	1041	285	344	6		

- Molecule 2 is a protein called CHK152 heavy chain.

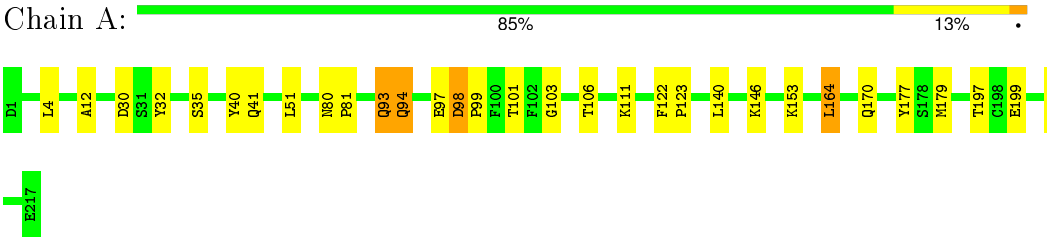
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	217	Total	C	N	O	S	0	0
			1631	1035	263	326	7		
2	D	217	Total	C	N	O	S	0	0
			1631	1035	263	326	7		
2	F	217	Total	C	N	O	S	0	0
			1631	1035	263	326	7		
2	H	217	Total	C	N	O	S	0	0
			1631	1035	263	326	7		

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.

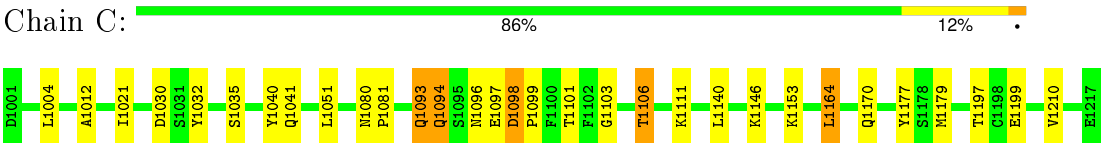
- Molecule 1: CHK152 light chain

Chain A:



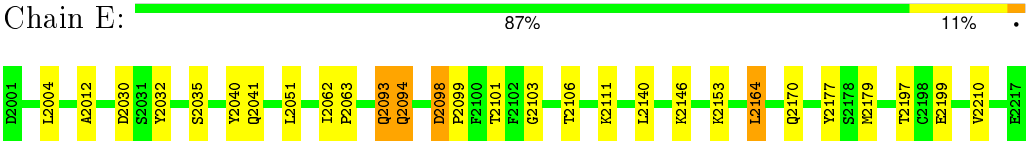
- Molecule 1: CHK152 light chain

Chain C:



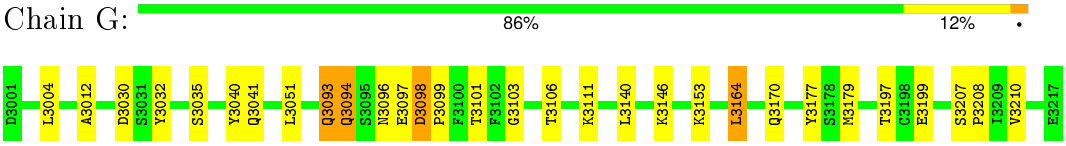
- Molecule 1: CHK152 light chain

Chain E:



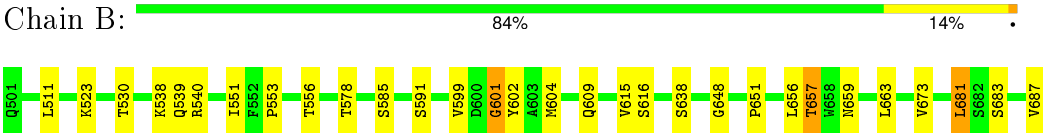
- Molecule 1: CHK152 light chain

Chain G:



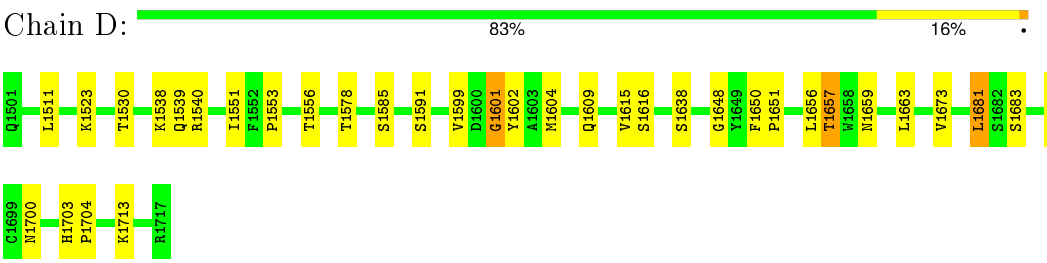
- Molecule 2: CHK152 heavy chain

Chain B:



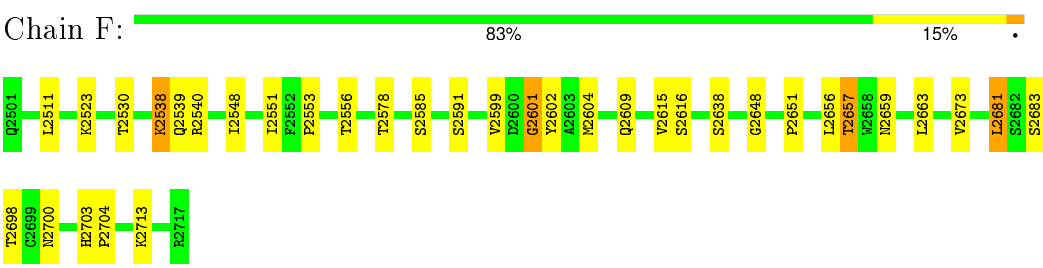
• Molecule 2: CHK152 heavy chain

Chain D:



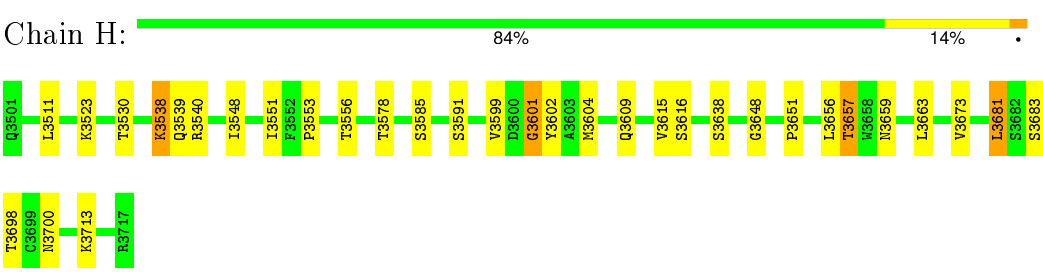
• Molecule 2: CHK152 heavy chain

Chain F:



• Molecule 2: CHK152 heavy chain

Chain H:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	2106	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	35000	Depositor
Image detector	Not provided	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.31	0/1713	0.45	0/2327
1	C	0.31	0/1713	0.45	0/2327
1	E	0.31	0/1713	0.45	0/2327
1	G	0.31	0/1713	0.45	0/2327
2	B	0.31	0/1674	0.48	0/2287
2	D	0.31	0/1674	0.48	0/2287
2	F	0.31	0/1674	0.48	0/2287
2	H	0.31	0/1674	0.48	0/2287
All	All	0.31	0/13548	0.46	0/18456

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

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	1605	17	0
1	C	1676	0	1602	17	0
1	E	1676	0	1602	13	0
1	G	1676	0	1602	15	0
2	B	1631	0	1591	16	0
2	D	1631	0	1591	18	0
2	F	1631	0	1591	18	0
2	H	1631	0	1591	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13228	0	12775	127	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 5.

All (127) 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:F:2656:LEU:HD13	2:F:2683:SER:HB2	1.80	0.64
2:D:1656:LEU:HD13	2:D:1683:SER:HB2	1.80	0.64
2:H:3656:LEU:HD13	2:H:3683:SER:HB2	1.80	0.64
2:B:656:LEU:HD13	2:B:683:SER:HB2	1.80	0.63
1:G:3040:TYR:HE1	1:G:3093:GLN:HG2	1.64	0.63
1:C:1040:TYR:HE1	1:C:1093:GLN:HG2	1.64	0.63
1:A:40:TYR:HE1	1:A:93:GLN:HG2	1.64	0.62
1:E:2098:ASP:HB3	1:E:2099:PRO:HD3	1.81	0.62
1:E:2030:ASP:HA	1:E:2035:SER:HA	1.81	0.62
1:C:1030:ASP:HA	1:C:1035:SER:HA	1.81	0.62
1:E:2040:TYR:HE1	1:E:2093:GLN:HG2	1.64	0.61
1:G:3098:ASP:HB3	1:G:3099:PRO:HD3	1.81	0.61
1:G:3030:ASP:HA	1:G:3035:SER:HA	1.81	0.61
1:A:98:ASP:HB3	1:A:99:PRO:HD3	1.81	0.61
1:A:30:ASP:HA	1:A:35:SER:HA	1.81	0.60
1:C:1098:ASP:HB3	1:C:1099:PRO:HD3	1.81	0.60
2:B:615:VAL:HA	2:B:616:SER:HB2	1.84	0.60
2:H:3615:VAL:HA	2:H:3616:SER:HB2	1.84	0.59
2:F:2615:VAL:HA	2:F:2616:SER:HB2	1.84	0.58
2:D:1615:VAL:HA	2:D:1616:SER:HB2	1.84	0.57
2:F:2591:SER:HB3	2:F:2615:VAL:H	1.76	0.51
2:B:698:THR:HG22	2:B:713:LYS:HG2	1.92	0.51
2:D:1591:SER:HB3	2:D:1615:VAL:H	1.76	0.51
2:F:2698:THR:HG22	2:F:2713:LYS:HG2	1.92	0.51
2:H:3591:SER:HB3	2:H:3615:VAL:H	1.76	0.51
2:H:3698:THR:HG22	2:H:3713:LYS:HG2	1.92	0.50
2:B:615:VAL:CA	2:B:616:SER:HB2	2.42	0.50
1:A:12:ALA:HB1	1:A:111:LYS:HG3	1.94	0.50
2:D:1698:THR:HG22	2:D:1713:LYS:HG2	1.92	0.50
2:B:591:SER:HB3	2:B:615:VAL:H	1.76	0.50
2:H:3615:VAL:CA	2:H:3616:SER:HB2	2.42	0.50
1:G:3012:ALA:HB1	1:G:3111:LYS:HG3	1.94	0.49
1:E:2012:ALA:HB1	1:E:2111:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1615:VAL:CA	2:D:1616:SER:HB2	2.42	0.49
1:C:1012:ALA:HB1	1:C:1111:LYS:HG3	1.94	0.49
1:C:1094:GLN:NE2	1:C:1101:THR:OG1	2.46	0.48
2:F:2615:VAL:CA	2:F:2616:SER:HB2	2.42	0.48
2:H:3530:THR:HA	2:H:3553:PRO:HB2	1.96	0.48
1:A:41:GLN:HB2	1:A:51:LEU:HD11	1.96	0.48
2:F:2530:THR:HA	2:F:2553:PRO:HB2	1.96	0.48
1:E:2041:GLN:HB2	1:E:2051:LEU:HD11	1.96	0.48
2:D:1530:THR:HA	2:D:1553:PRO:HB2	1.96	0.48
2:B:530:THR:HA	2:B:553:PRO:HB2	1.96	0.48
1:E:2094:GLN:NE2	1:E:2101:THR:OG1	2.46	0.47
1:A:4:LEU:HB2	1:A:103:GLY:HA2	1.97	0.47
1:G:3004:LEU:HB2	1:G:3103:GLY:HA2	1.97	0.47
1:G:3041:GLN:HB2	1:G:3051:LEU:HD11	1.96	0.47
1:E:2004:LEU:HB2	1:E:2103:GLY:HA2	1.97	0.47
1:G:3094:GLN:NE2	1:G:3101:THR:OG1	2.46	0.47
1:C:1041:GLN:HB2	1:C:1051:LEU:HD11	1.96	0.47
2:B:601:GLY:HA2	2:B:602:TYR:HA	1.57	0.46
1:C:1004:LEU:HB2	1:C:1103:GLY:HA2	1.97	0.46
2:D:1601:GLY:HA2	2:D:1602:TYR:HA	1.57	0.46
2:D:1656:LEU:HD11	2:D:1681:LEU:HD21	1.98	0.46
2:B:656:LEU:HD11	2:B:681:LEU:HD21	1.98	0.46
2:H:3656:LEU:HD11	2:H:3681:LEU:HD21	1.98	0.46
2:F:2656:LEU:HD11	2:F:2681:LEU:HD21	1.98	0.46
1:G:3140:LEU:HD12	1:G:3179:MET:HB3	1.98	0.45
1:E:2140:LEU:HD12	1:E:2179:MET:HB3	1.98	0.45
1:A:164:LEU:HD11	2:B:673:VAL:HB	1.98	0.45
1:C:1164:LEU:HD11	2:D:1673:VAL:HB	1.98	0.45
1:C:1140:LEU:HD12	1:C:1179:MET:HB3	1.98	0.45
2:D:1657:THR:HB	2:D:1700:ASN:HB2	1.99	0.45
2:F:2659:ASN:HD21	2:F:2697:ILE:HA	1.82	0.45
1:A:94:GLN:NE2	1:A:101:THR:OG1	2.46	0.45
2:H:3659:ASN:HD21	2:H:3697:ILE:HA	1.82	0.45
1:A:140:LEU:HD12	1:A:179:MET:HB3	1.98	0.45
1:E:2164:LEU:HD11	2:F:2673:VAL:HB	1.98	0.44
1:G:3164:LEU:HD11	2:H:3673:VAL:HB	1.98	0.44
2:D:1659:ASN:HD21	2:D:1697:ILE:HA	1.82	0.44
2:B:657:THR:HB	2:B:700:ASN:HB2	1.99	0.44
1:C:1153:LYS:HB2	1:C:1197:THR:OG1	2.18	0.44
2:H:3601:GLY:HA2	2:H:3602:TYR:HA	1.57	0.44
2:F:2657:THR:HB	2:F:2700:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HB2	1:A:197:THR:OG1	2.18	0.44
1:E:2199:GLU:HG3	1:E:2210:VAL:HG22	2.00	0.44
2:B:659:ASN:HD21	2:B:697:ILE:HA	1.82	0.44
2:B:659:ASN:HD22	2:B:663:LEU:HD12	1.83	0.44
1:A:80:ASN:HA	1:A:81:PRO:HA	1.83	0.44
2:D:1703:HIS:HA	2:D:1704:PRO:HD3	1.84	0.44
1:C:1199:GLU:HG3	1:C:1210:VAL:HG22	2.00	0.44
1:E:2153:LYS:HB2	1:E:2197:THR:OG1	2.18	0.43
1:A:199:GLU:HG3	1:A:210:VAL:HG22	2.00	0.43
2:H:3657:THR:HB	2:H:3700:ASN:HB2	1.99	0.43
1:G:3199:GLU:HG3	1:G:3210:VAL:HG22	2.00	0.43
1:G:3170:GLN:HG3	1:G:3177:TYR:CZ	2.54	0.43
2:F:2511:LEU:HG	2:F:2651:PRO:HG3	2.00	0.43
2:D:1511:LEU:HG	2:D:1651:PRO:HG3	2.00	0.43
2:F:2601:GLY:HA2	2:F:2602:TYR:HA	1.57	0.43
1:A:207:SER:HA	1:A:208:PRO:HD3	1.88	0.43
2:H:3523:LYS:HG2	2:H:3578:THR:HG22	2.01	0.43
1:C:1170:GLN:HG3	1:C:1177:TYR:CZ	2.54	0.43
2:H:3659:ASN:HD22	2:H:3663:LEU:HD12	1.83	0.43
2:F:2599:VAL:HG22	2:F:2604:MET:HA	2.01	0.43
2:F:2659:ASN:HD22	2:F:2663:LEU:HD12	1.83	0.42
1:A:122:PHE:HA	1:A:123:PRO:HD3	1.90	0.42
2:B:511:LEU:HG	2:B:651:PRO:HG3	2.00	0.42
2:D:1523:LYS:HG2	2:D:1578:THR:HG22	2.01	0.42
2:D:1659:ASN:HD22	2:D:1663:LEU:HD12	1.83	0.42
1:G:3153:LYS:HB2	1:G:3197:THR:OG1	2.18	0.42
1:E:2170:GLN:HG3	1:E:2177:TYR:CZ	2.54	0.42
1:G:3097:GLU:HA	1:G:3098:ASP:HA	1.87	0.42
2:B:599:VAL:HG22	2:B:604:MET:HA	2.01	0.42
2:D:1599:VAL:HG22	2:D:1604:MET:HA	2.01	0.42
2:H:3511:LEU:HG	2:H:3651:PRO:HG3	2.00	0.42
2:F:2523:LYS:HG2	2:F:2578:THR:HG22	2.01	0.42
2:B:523:LYS:HG2	2:B:578:THR:HG22	2.01	0.42
1:A:97:GLU:HA	1:A:98:ASP:HA	1.87	0.41
1:C:1098:ASP:HB3	1:C:1099:PRO:CD	2.50	0.41
2:B:599:VAL:HG22	2:B:604:MET:HG2	2.03	0.41
2:H:3599:VAL:HG22	2:H:3604:MET:HA	2.01	0.41
2:D:1599:VAL:HG22	2:D:1604:MET:HG2	2.03	0.41
1:A:170:GLN:HG3	1:A:177:TYR:CZ	2.54	0.41
2:F:2599:VAL:HG22	2:F:2604:MET:HG2	2.02	0.41
1:G:3207:SER:HA	1:G:3208:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2062:ILE:HA	1:E:2063:PRO:HD3	1.94	0.41
1:C:1021:ILE:HG23	1:C:1106:THR:HG21	2.03	0.41
2:D:1650:PHE:HA	2:D:1651:PRO:HA	1.87	0.41
2:F:2538:LYS:HB2	2:F:2548:ILE:HD11	2.03	0.41
1:C:1096:ASN:HB3	1:C:1097:GLU:H	1.71	0.40
2:H:3599:VAL:HG22	2:H:3604:MET:HG2	2.02	0.40
1:C:1097:GLU:HA	1:C:1098:ASP:HA	1.87	0.40
2:H:3538:LYS:HB2	2:H:3548:ILE:HD11	2.03	0.40
1:G:3096:ASN:HB3	1:G:3097:GLU:H	1.71	0.40
2:F:2703:HIS:HA	2:F:2704:PRO:HD3	1.84	0.40
1:A:98:ASP:HB3	1:A:99:PRO:CD	2.50	0.40
1:C:1080:ASN:HA	1:C:1081:PRO:HA	1.83	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	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	34 77
1	C	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	34 77
1	E	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	34 77
1	G	215/217 (99%)	199 (93%)	15 (7%)	1 (0%)	34 77
2	B	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	8 48
2	D	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	8 48
2	F	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	8 48
2	H	215/217 (99%)	194 (90%)	16 (7%)	5 (2%)	8 48
All	All	1720/1736 (99%)	1572 (91%)	124 (7%)	24 (1%)	19 58

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	601	GLY
2	D	1601	GLY
2	F	2601	GLY
2	H	3601	GLY
2	B	556	THR
2	B	585	SER
2	B	638	SER
2	D	1556	THR
2	D	1585	SER
2	D	1638	SER
2	F	2556	THR
2	F	2585	SER
2	F	2638	SER
2	H	3556	THR
2	H	3585	SER
2	H	3638	SER
1	A	98	ASP
1	C	1098	ASP
1	E	2098	ASP
1	G	3098	ASP
2	B	648	GLY
2	D	1648	GLY
2	F	2648	GLY
2	H	3648	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 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	191/191 (100%)	185 (97%)	6 (3%)	47 77
1	C	191/191 (100%)	185 (97%)	6 (3%)	47 77
1	E	191/191 (100%)	185 (97%)	6 (3%)	47 77
1	G	191/191 (100%)	185 (97%)	6 (3%)	47 77
2	B	187/187 (100%)	179 (96%)	8 (4%)	35 70
2	D	187/187 (100%)	179 (96%)	8 (4%)	35 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	187/187 (100%)	179 (96%)	8 (4%)	35 70
2	H	187/187 (100%)	179 (96%)	8 (4%)	35 70
All	All	1512/1512 (100%)	1456 (96%)	56 (4%)	45 73

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	93	GLN
1	A	94	GLN
1	A	106	THR
1	A	146	LYS
1	A	164	LEU
2	B	538	LYS
2	B	539	GLN
2	B	540	ARG
2	B	551	ILE
2	B	609	GLN
2	B	657	THR
2	B	681	LEU
2	B	687	VAL
1	C	1032	TYR
1	C	1093	GLN
1	C	1094	GLN
1	C	1106	THR
1	C	1146	LYS
1	C	1164	LEU
2	D	1538	LYS
2	D	1539	GLN
2	D	1540	ARG
2	D	1551	ILE
2	D	1609	GLN
2	D	1657	THR
2	D	1681	LEU
2	D	1687	VAL
1	E	2032	TYR
1	E	2093	GLN
1	E	2094	GLN
1	E	2106	THR
1	E	2146	LYS
1	E	2164	LEU

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Mol	Chain	Res	Type
2	F	2538	LYS
2	F	2539	GLN
2	F	2540	ARG
2	F	2551	ILE
2	F	2609	GLN
2	F	2657	THR
2	F	2681	LEU
2	F	2687	VAL
1	G	3032	TYR
1	G	3093	GLN
1	G	3094	GLN
1	G	3106	THR
1	G	3146	LYS
1	G	3164	LEU
2	H	3538	LYS
2	H	3539	GLN
2	H	3540	ARG
2	H	3551	ILE
2	H	3609	GLN
2	H	3657	THR
2	H	3681	LEU
2	H	3687	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	96	ASN
2	B	539	GLN
1	C	1042	GLN
1	C	1094	GLN
1	C	1096	ASN
2	D	1539	GLN
1	E	2042	GLN
1	E	2096	ASN
2	F	2539	GLN
1	G	3042	GLN
1	G	3094	GLN
1	G	3096	ASN
2	H	3539	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.