wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:49 PM BST

PDB ID	:	3J42
EMDB ID:	:	EMD-5674
Title	:	Obstruction of Dengue Virus Maturation by Fab Fragments of the 2H2 Antibody
Authors	:	Wang, Z.; Pennington, J.G.; Jiang, W.; Rossmann, M.G.
Deposited on	:	2013-06-13
Resolution	:	21.00 Å(reported)
Based on PDB ID	:	3C6D, 4KVC

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

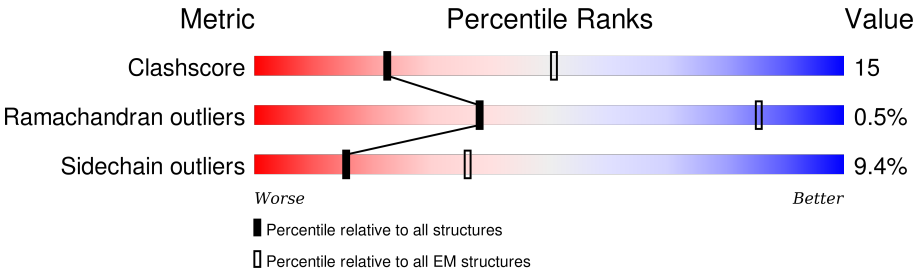
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 21.00 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	390	99% .
1	B	390	99% .
1	C	390	100%
2	D	81	100%
2	E	81	99% .
2	F	81	99% .
3	G	221	76% 19% . .
3	I	221	72% 24% . .
3	K	221	74% 22% . .

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Mol	Chain	Length	Quality of chain
4	H	212	72% 25% •
4	J	212	75% 21% •
4	L	212	75% 21% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11226 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 Envelope protein E.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	390	Total C 390 390	0	390
1	B	390	Total C 390 390	0	390
1	C	390	Total C 390 390	0	390

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ILE	MET	CONFLICT	UNP O11875
A	?	-	GLY	DELETION	UNP O11875
A	?	-	GLY	DELETION	UNP O11875
A	?	-	GLN	DELETION	UNP O11875
A	139	VAL	ILE	CONFLICT	UNP O11875
A	162	VAL	ILE	CONFLICT	UNP O11875
A	?	-	PHE	DELETION	UNP O11875
A	?	-	ASN	DELETION	UNP O11875
A	390	ASP	ASN	CONFLICT	UNP O11875
B	6	ILE	MET	CONFLICT	UNP O11875
B	?	-	GLY	DELETION	UNP O11875
B	?	-	GLY	DELETION	UNP O11875
B	?	-	GLN	DELETION	UNP O11875
B	139	VAL	ILE	CONFLICT	UNP O11875
B	162	VAL	ILE	CONFLICT	UNP O11875
B	?	-	PHE	DELETION	UNP O11875
B	?	-	ASN	DELETION	UNP O11875
B	390	ASP	ASN	CONFLICT	UNP O11875
C	6	ILE	MET	CONFLICT	UNP O11875
C	?	-	GLY	DELETION	UNP O11875
C	?	-	GLY	DELETION	UNP O11875
C	?	-	GLN	DELETION	UNP O11875
C	139	VAL	ILE	CONFLICT	UNP O11875
C	162	VAL	ILE	CONFLICT	UNP O11875

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	DELETION	UNP O11875
C	?	-	ASN	DELETION	UNP O11875
C	390	ASP	ASN	CONFLICT	UNP O11875

- Molecule 2 is a protein called PrM.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	D	81	Total C 81 81	0	81
2	E	81	Total C 81 81	0	81
2	F	81	Total C 81 81	0	81

- Molecule 3 is a protein called Ig heavy chain V region MOPC 21, Igh protein chimera.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	G	216	Total C N O S 1633 1034 274 317 8	0	0
3	I	216	Total C N O S 1633 1034 274 317 8	0	0
3	K	216	Total C N O S 1633 1034 274 317 8	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	104	HIS	-	LINKER	UNP Q6PIP8
G	105	TYR	-	LINKER	UNP Q6PIP8
G	180	GLY	ASP	CONFLICT	UNP Q6PIP8
G	199	THR	SER	CONFLICT	UNP Q6PIP8
I	104	HIS	-	LINKER	UNP Q6PIP8
I	105	TYR	-	LINKER	UNP Q6PIP8
I	180	GLY	ASP	CONFLICT	UNP Q6PIP8
I	199	THR	SER	CONFLICT	UNP Q6PIP8
K	104	HIS	-	LINKER	UNP Q6PIP8
K	105	TYR	-	LINKER	UNP Q6PIP8
K	180	GLY	ASP	CONFLICT	UNP Q6PIP8
K	199	THR	SER	CONFLICT	UNP Q6PIP8

- Molecule 4 is a protein called Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	212	Total	C	N	O	S	0	0
			1638	1017	275	338	8		
4	J	212	Total	C	N	O	S	0	0
			1638	1017	275	338	8		
4	L	212	Total	C	N	O	S	0	0
			1638	1017	275	338	8		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1030	GLY	VAL	CONFLICT	UNP P01634
H	1091	SER	GLY	CONFLICT	UNP P01634
H	1094	THR	TYR	CONFLICT	UNP P01634
J	1030	GLY	VAL	CONFLICT	UNP P01634
J	1091	SER	GLY	CONFLICT	UNP P01634
J	1094	THR	TYR	CONFLICT	UNP P01634
L	1030	GLY	VAL	CONFLICT	UNP P01634
L	1091	SER	GLY	CONFLICT	UNP P01634
L	1094	THR	TYR	CONFLICT	UNP P01634

3 Residue-property plots (i)

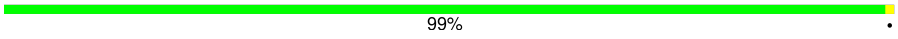
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Envelope protein E

Chain A:

- Molecule 1: Envelope protein E

Chain B:



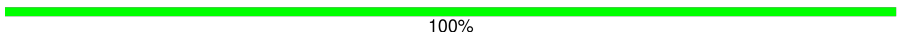
- Molecule 1: Envelope protein E

Chain C:

There are no outlier residues recorded for this chain.

- Molecule 2: PrM

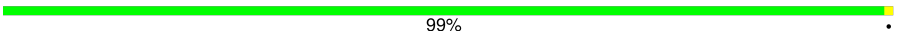
Chain D:



There are no outlier residues recorded for this chain.

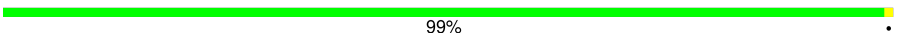
- Molecule 2: PrM

Chain E:



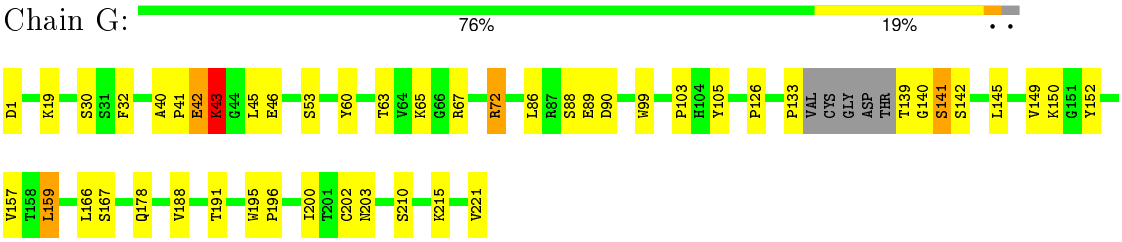
- Molecule 2: PrM

Chain F:



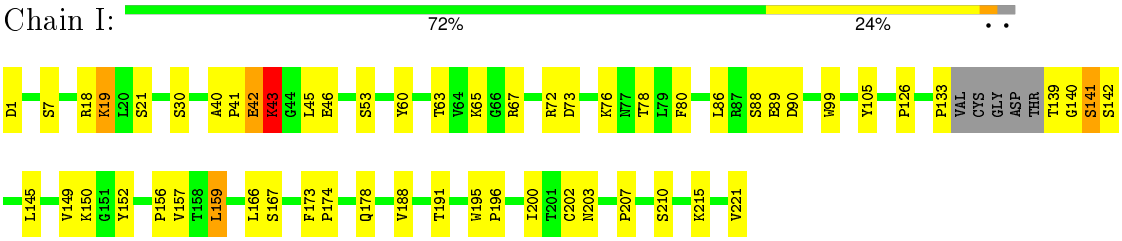
- Molecule 3: Ig heavy chain V region MOPC 21, Igh protein chimera

Chain G:



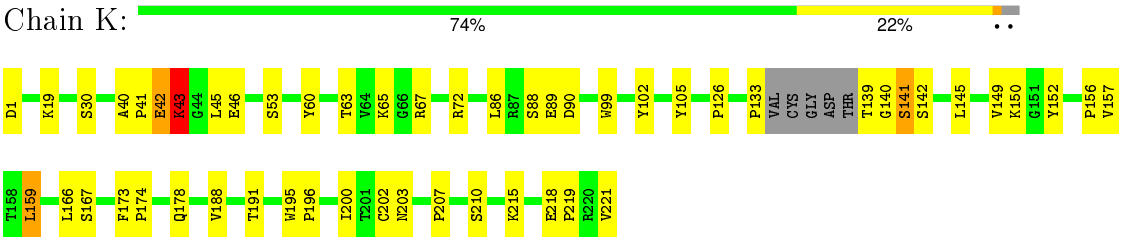
• Molecule 3: Ig heavy chain V region MOPC 21, Igh protein chimera

Chain I:



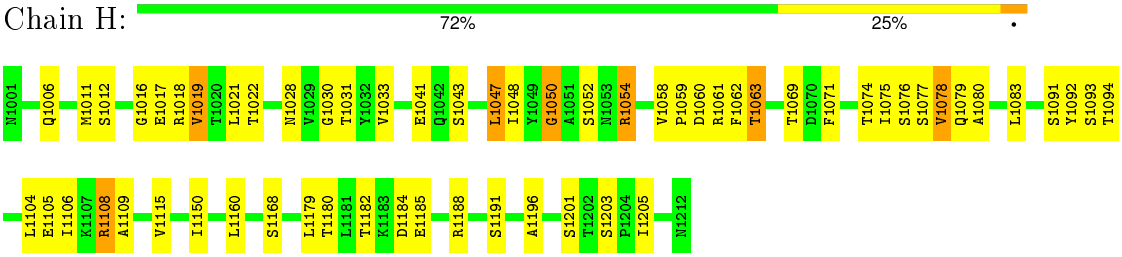
• Molecule 3: Ig heavy chain V region MOPC 21, Igh protein chimera

Chain K:



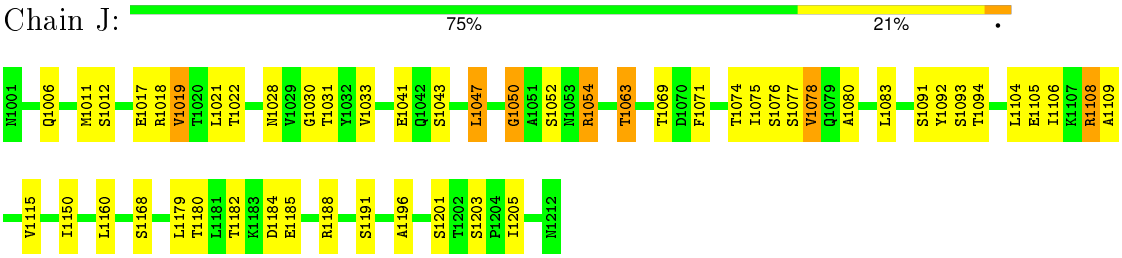
• Molecule 4: Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera

Chain H:



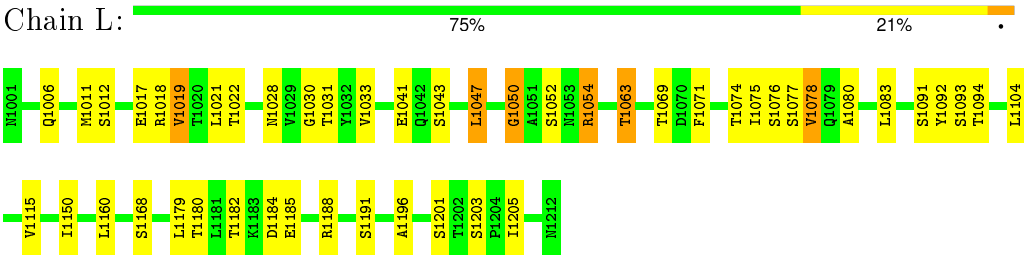
• Molecule 4: Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera

Chain J:



• Molecule 4: Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain chimera

Chain L:


75%
21%
N1001
Q1006
M1011
S1012
E1017
R1018
V1019
T1020
L1021
T1022
N1028
V1029
G1030
T1031
Y1032
V1033
E1041
Q1042
S1043
L1047
G1050
A1051
S1052
N1053
R1054
T1063
T1069
D1070
F1071
T1074
I1075
S1076
S1077
V1078
Q1079
A1080
L1083
S1091
Y1092
S1093
T1094
L1104
E1105
I1106
K1107
R1108
A1109
V1115
I1150
L1160
S1168
L1179
T1180
L1181
T1182
K1183
D1184
E1185
R1188
S1191
A1196
S1201
T1202
S1203
P1204
I1205
N1212

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	378	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Film	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO163 film	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	#$\|Z\|>2$
3	G	0.62	1/1678 (0.1%)	0.65	0/2290
3	I	0.61	1/1678 (0.1%)	0.65	0/2290
3	K	0.61	1/1678 (0.1%)	0.65	0/2290
4	H	0.76	2/1674 (0.1%)	0.68	2/2273 (0.1%)
4	J	0.76	2/1674 (0.1%)	0.68	2/2273 (0.1%)
4	L	0.76	2/1674 (0.1%)	0.68	2/2273 (0.1%)
All	All	0.69	9/10056 (0.1%)	0.67	6/13689 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1092	TYR	CE2-CZ	-6.20	1.30	1.38
4	L	1092	TYR	CE2-CZ	-6.17	1.30	1.38
4	J	1092	TYR	CE2-CZ	-6.16	1.30	1.38
3	K	46	GLU	CD-OE2	-5.11	1.20	1.25
3	G	46	GLU	CD-OE2	-5.08	1.20	1.25
4	H	1092	TYR	CB-CG	-5.05	1.44	1.51
3	I	46	GLU	CD-OE2	-5.04	1.20	1.25
4	L	1092	TYR	CB-CG	-5.04	1.44	1.51
4	J	1092	TYR	CB-CG	-5.04	1.44	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1047	LEU	CA-CB-CG	7.42	132.35	115.30
4	J	1047	LEU	CA-CB-CG	7.38	132.28	115.30
4	L	1047	LEU	CA-CB-CG	7.38	132.28	115.30
4	H	1050	GLY	C-N-CA	-5.27	108.52	121.70
4	L	1050	GLY	C-N-CA	-5.25	108.58	121.70
4	J	1050	GLY	C-N-CA	-5.25	108.58	121.70

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	390	0	0	1	0
1	B	390	0	0	1	0
1	C	390	0	0	0	0
2	D	81	0	0	0	0
2	E	81	0	0	3	0
2	F	81	0	0	1	0
3	G	1633	0	1585	53	0
3	I	1633	0	1584	115	0
3	K	1633	0	1585	54	0
4	H	1638	0	1564	94	0
4	J	1638	0	1565	31	0
4	L	1638	0	1565	31	0
All	All	11226	0	9448	307	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (307) 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)
3:I:42:GLU:HA	3:I:43:LYS:CG	1.43	1.48
3:G:42:GLU:HA	3:G:43:LYS:CG	1.43	1.47
3:K:42:GLU:CA	3:K:43:LYS:HG2	1.46	1.46
3:G:42:GLU:CA	3:G:43:LYS:HG2	1.46	1.46
3:K:42:GLU:HA	3:K:43:LYS:CG	1.43	1.45
3:I:42:GLU:CA	3:I:43:LYS:HG2	1.46	1.44
4:H:1076:SER:O	3:I:19:LYS:HE3	1.19	1.34
4:H:1060:ASP:OD1	3:I:73:ASP:CB	1.74	1.32
4:H:1060:ASP:C	3:I:80:PHE:HZ	1.38	1.26
4:H:1060:ASP:O	3:I:80:PHE:HZ	1.11	1.23
4:H:1060:ASP:O	3:I:80:PHE:CZ	1.90	1.23
4:H:1058:VAL:CG1	3:I:76:LYS:HE3	1.69	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1058:VAL:CG1	3:I:76:LYS:CE	2.27	1.11
4:H:1060:ASP:OD1	3:I:73:ASP:HB3	0.92	1.09
3:K:139:THR:N	3:K:140:GLY:HA3	1.61	1.09
3:G:139:THR:N	3:G:140:GLY:HA3	1.61	1.08
3:I:139:THR:N	3:I:140:GLY:HA3	1.61	1.06
4:H:1060:ASP:C	3:I:80:PHE:CZ	2.28	1.02
4:H:1077:SER:OG	3:I:19:LYS:O	1.80	0.99
3:I:42:GLU:HA	3:I:43:LYS:CB	1.93	0.99
4:H:1058:VAL:HG11	3:I:76:LYS:CE	1.92	0.98
3:G:42:GLU:HA	3:G:43:LYS:CB	1.93	0.98
4:H:1058:VAL:HG12	3:I:76:LYS:HE3	1.44	0.98
4:H:1076:SER:O	3:I:19:LYS:CE	2.12	0.98
4:H:1061:ARG:HA	3:I:80:PHE:CE1	1.97	0.97
3:K:42:GLU:HA	3:K:43:LYS:CB	1.93	0.97
4:H:1058:VAL:HG12	3:I:76:LYS:CE	1.92	0.95
4:H:1061:ARG:HG2	3:I:21:SER:OG	1.67	0.94
3:K:139:THR:N	3:K:140:GLY:CA	2.29	0.94
3:I:139:THR:N	3:I:140:GLY:CA	2.29	0.94
4:H:1076:SER:C	3:I:19:LYS:HG2	1.88	0.94
4:H:1054:ARG:NE	3:I:73:ASP:OD2	2.02	0.92
3:G:139:THR:N	3:G:140:GLY:CA	2.29	0.91
4:H:1054:ARG:HA	3:I:76:LYS:HZ1	1.32	0.91
4:L:1083:LEU:HD21	4:L:1106:ILE:HG13	1.55	0.89
4:H:1076:SER:C	3:I:19:LYS:HE3	1.93	0.89
4:J:1083:LEU:HD21	4:J:1106:ILE:HG13	1.55	0.88
3:K:42:GLU:HA	3:K:43:LYS:HG2	0.88	0.88
4:H:1079:GLN:NE2	3:I:7:SER:OG	2.06	0.87
3:G:42:GLU:HA	3:G:43:LYS:HG2	0.88	0.87
3:I:42:GLU:HA	3:I:43:LYS:HG2	0.88	0.87
4:H:1054:ARG:HA	3:I:76:LYS:NZ	1.87	0.86
4:H:1083:LEU:HD21	4:H:1106:ILE:HG13	1.55	0.86
4:L:1054:ARG:HH21	4:L:1063:THR:HA	1.41	0.85
4:H:1054:ARG:HH21	4:H:1063:THR:HA	1.41	0.84
3:I:140:GLY:O	3:I:141:SER:HB3	1.76	0.84
3:K:41:PRO:O	3:K:43:LYS:HE2	1.79	0.83
3:K:140:GLY:O	3:K:141:SER:HB3	1.76	0.83
3:G:140:GLY:O	3:G:141:SER:HB3	1.76	0.83
3:I:41:PRO:O	3:I:43:LYS:HE2	1.79	0.83
3:G:41:PRO:O	3:G:43:LYS:HE2	1.79	0.82
3:G:42:GLU:C	3:G:43:LYS:HG2	2.00	0.82
3:K:42:GLU:C	3:K:43:LYS:HG2	2.00	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1058:VAL:CG1	3:I:76:LYS:HE2	2.07	0.82
3:K:42:GLU:CB	3:K:43:LYS:HE2	2.10	0.82
4:J:1054:ARG:HH21	4:J:1063:THR:HA	1.42	0.82
3:I:42:GLU:C	3:I:43:LYS:HG2	2.00	0.81
3:G:42:GLU:CB	3:G:43:LYS:HE2	2.10	0.81
3:I:42:GLU:CB	3:I:43:LYS:HE2	2.10	0.80
4:H:1016:GLY:HA3	3:I:18:ARG:CZ	2.11	0.80
3:K:41:PRO:O	3:K:43:LYS:CE	2.30	0.79
3:I:41:PRO:O	3:I:43:LYS:CE	2.30	0.79
3:G:41:PRO:O	3:G:43:LYS:CE	2.30	0.79
4:H:1077:SER:N	3:I:19:LYS:HG2	1.99	0.78
3:I:140:GLY:O	3:I:141:SER:CB	2.30	0.77
3:G:67:ARG:NH2	3:G:90:ASP:OD2	2.17	0.77
3:K:67:ARG:NH2	3:K:90:ASP:OD2	2.17	0.77
2:E:27:THR:CA	3:G:103:PRO:CD	2.63	0.77
3:I:42:GLU:HB2	3:I:43:LYS:HE2	1.67	0.76
3:I:67:ARG:NH2	3:I:90:ASP:OD2	2.17	0.76
3:G:42:GLU:HB2	3:G:43:LYS:HE2	1.67	0.76
4:H:1033:VAL:O	4:H:1050:GLY:O	2.04	0.75
4:H:1058:VAL:CB	3:I:76:LYS:HE3	2.16	0.75
3:I:42:GLU:CB	3:I:43:LYS:HG2	2.17	0.75
4:J:1033:VAL:O	4:J:1050:GLY:O	2.04	0.75
3:K:42:GLU:HB2	3:K:43:LYS:HE2	1.67	0.75
4:L:1033:VAL:O	4:L:1050:GLY:O	2.04	0.75
4:H:1060:ASP:CG	3:I:73:ASP:HB3	2.04	0.75
3:G:42:GLU:CB	3:G:43:LYS:HG2	2.17	0.74
3:K:42:GLU:CB	3:K:43:LYS:HG2	2.17	0.73
2:E:27:THR:CA	3:G:103:PRO:HD2	2.18	0.73
4:H:1077:SER:CB	3:I:19:LYS:O	2.38	0.71
3:I:42:GLU:CA	3:I:43:LYS:HE2	2.21	0.71
3:G:42:GLU:CA	3:G:43:LYS:HE2	2.21	0.71
4:H:1061:ARG:HA	3:I:80:PHE:CZ	2.26	0.71
3:G:42:GLU:CA	3:G:43:LYS:CG	2.29	0.70
4:H:1061:ARG:HA	3:I:80:PHE:HE1	1.55	0.70
3:K:42:GLU:CA	3:K:43:LYS:HE2	2.21	0.70
4:J:1115:VAL:HG21	4:J:1205:ILE:HD13	1.74	0.69
4:H:1115:VAL:HG21	4:H:1205:ILE:HD13	1.75	0.69
3:G:133:PRO:HD3	3:G:145:LEU:HD23	1.75	0.69
3:K:133:PRO:HD3	3:K:145:LEU:HD23	1.75	0.68
3:I:133:PRO:HD3	3:I:145:LEU:HD23	1.75	0.68
4:L:1115:VAL:HG21	4:L:1205:ILE:HD13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:140:GLY:O	3:G:141:SER:CB	2.30	0.68
3:K:140:GLY:O	3:K:141:SER:CB	2.30	0.67
4:H:1058:VAL:HG11	3:I:76:LYS:HE2	1.69	0.67
4:H:1054:ARG:CD	3:I:73:ASP:OD2	2.43	0.67
3:I:42:GLU:HG2	3:I:43:LYS:HG2	1.76	0.67
3:G:42:GLU:HG2	3:G:43:LYS:HG2	1.76	0.67
4:L:1080:ALA:HA	4:L:1106:ILE:HD11	1.77	0.67
4:J:1196:ALA:HB3	4:J:1205:ILE:HD11	1.77	0.66
3:I:42:GLU:CA	3:I:43:LYS:CB	2.70	0.66
3:K:42:GLU:HG2	3:K:43:LYS:HG2	1.76	0.66
3:G:42:GLU:HA	3:G:43:LYS:CD	2.25	0.66
4:H:1196:ALA:HB3	4:H:1205:ILE:HD11	1.77	0.66
3:K:42:GLU:HA	3:K:43:LYS:CD	2.24	0.66
4:H:1060:ASP:CG	3:I:80:PHE:CE2	2.69	0.66
4:L:1196:ALA:HB3	4:L:1205:ILE:HD11	1.77	0.66
4:J:1080:ALA:HA	4:J:1106:ILE:HD11	1.77	0.66
4:H:1080:ALA:HA	4:H:1106:ILE:HD11	1.77	0.65
4:L:1052:SER:O	4:L:1054:ARG:NH1	2.29	0.65
3:I:41:PRO:O	3:I:43:LYS:NZ	2.30	0.65
4:H:1054:ARG:CA	3:I:76:LYS:NZ	2.59	0.65
4:J:1052:SER:O	4:J:1054:ARG:NH1	2.29	0.65
3:K:140:GLY:O	3:K:142:SER:N	2.30	0.65
3:K:41:PRO:O	3:K:43:LYS:NZ	2.30	0.64
3:I:140:GLY:O	3:I:142:SER:N	2.30	0.64
3:G:42:GLU:CA	3:G:43:LYS:CB	2.70	0.64
4:H:1052:SER:O	4:H:1054:ARG:NH1	2.29	0.64
4:H:1054:ARG:CZ	3:I:73:ASP:OD2	2.46	0.64
3:G:41:PRO:O	3:G:43:LYS:NZ	2.30	0.64
4:H:1061:ARG:CA	3:I:80:PHE:CE1	2.79	0.63
4:H:1060:ASP:N	3:I:78:THR:OG1	2.26	0.63
3:K:42:GLU:CA	3:K:43:LYS:CB	2.70	0.63
4:H:1060:ASP:OD1	3:I:73:ASP:HB2	1.92	0.63
3:G:140:GLY:O	3:G:142:SER:N	2.30	0.62
3:I:42:GLU:HA	3:I:43:LYS:CD	2.25	0.62
3:G:42:GLU:CG	3:G:43:LYS:HG2	2.30	0.61
3:K:42:GLU:CG	3:K:43:LYS:HG2	2.30	0.61
4:H:1054:ARG:CA	3:I:76:LYS:HZ1	2.09	0.61
4:L:1182:THR:OG1	4:L:1184:ASP:OD1	2.12	0.61
3:I:42:GLU:CG	3:I:43:LYS:HG2	2.30	0.60
3:K:42:GLU:CA	3:K:43:LYS:CG	2.29	0.59
4:H:1060:ASP:O	3:I:80:PHE:CE2	2.53	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1061:ARG:N	3:I:80:PHE:CZ	2.71	0.59
4:H:1076:SER:C	3:I:19:LYS:CE	2.58	0.58
3:K:42:GLU:HA	3:K:43:LYS:HE2	1.85	0.58
4:H:1182:THR:OG1	4:H:1184:ASP:OD1	2.12	0.58
4:J:1019:VAL:HG11	4:J:1104:LEU:HD11	1.86	0.57
4:H:1058:VAL:HB	3:I:76:LYS:HE3	1.84	0.57
3:G:42:GLU:HG2	3:G:43:LYS:CG	2.35	0.57
3:G:42:GLU:HA	3:G:43:LYS:HE2	1.85	0.56
4:J:1182:THR:OG1	4:J:1184:ASP:OD1	2.13	0.56
4:H:1058:VAL:HG12	3:I:76:LYS:HE2	1.72	0.56
4:H:1019:VAL:HG11	4:H:1104:LEU:HD11	1.86	0.56
4:H:1077:SER:HB3	3:I:19:LYS:HB3	1.88	0.56
4:L:1019:VAL:HG11	4:L:1104:LEU:HD11	1.86	0.56
3:K:42:GLU:HG2	3:K:43:LYS:CG	2.35	0.55
4:H:1076:SER:O	3:I:19:LYS:HG2	2.06	0.55
3:I:42:GLU:CA	3:I:43:LYS:CG	2.29	0.55
3:I:42:GLU:HG2	3:I:43:LYS:CG	2.35	0.55
4:H:1061:ARG:CA	3:I:80:PHE:CZ	2.89	0.55
4:H:1061:ARG:N	3:I:80:PHE:HZ	1.99	0.55
4:H:1062:PHE:HB2	3:I:76:LYS:HE2	1.89	0.54
3:I:40:ALA:HB1	3:I:41:PRO:HD2	1.90	0.54
3:K:40:ALA:HB1	3:K:41:PRO:HD2	1.90	0.54
4:L:1006:GLN:HG2	4:L:1021:LEU:HD21	1.90	0.53
4:H:1006:GLN:HG2	4:H:1021:LEU:HD21	1.91	0.53
3:G:166:LEU:HD11	3:G:200:ILE:HD12	1.91	0.53
4:H:1048:ILE:CD1	3:I:76:LYS:HZ3	2.22	0.52
3:K:99:TRP:CZ2	3:K:105:TYR:HB3	2.45	0.52
2:E:27:THR:CA	3:G:103:PRO:CG	2.88	0.52
3:K:166:LEU:HD11	3:K:200:ILE:HD12	1.91	0.52
4:J:1006:GLN:HG2	4:J:1021:LEU:HD21	1.91	0.52
3:G:40:ALA:HB1	3:G:41:PRO:HD2	1.90	0.52
3:G:99:TRP:CZ2	3:G:105:TYR:HB3	2.45	0.52
3:I:42:GLU:HA	3:I:43:LYS:HE2	1.85	0.51
4:H:1108:ARG:HD3	4:H:1109:ALA:O	2.10	0.51
4:L:1108:ARG:HD3	4:L:1109:ALA:O	2.10	0.51
3:K:42:GLU:C	3:K:43:LYS:CG	2.71	0.51
3:I:166:LEU:HD11	3:I:200:ILE:HD12	1.91	0.51
4:H:1062:PHE:O	3:I:76:LYS:HD2	2.10	0.51
3:I:99:TRP:CZ2	3:I:105:TYR:HB3	2.45	0.51
4:H:1077:SER:HB3	3:I:19:LYS:O	2.10	0.51
4:J:1108:ARG:HD3	4:J:1109:ALA:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:210:SER:OG	3:I:210:SER:O	2.29	0.51
4:H:1019:VAL:HG23	4:H:1075:ILE:HB	1.93	0.51
4:J:1019:VAL:HG23	4:J:1075:ILE:HB	1.93	0.51
3:I:221:VAL:CG1	3:I:221:VAL:O	2.59	0.51
3:G:210:SER:O	3:G:210:SER:OG	2.29	0.50
4:L:1019:VAL:HG23	4:L:1075:ILE:HB	1.93	0.50
3:G:126:PRO:HB3	3:G:152:TYR:HB3	1.94	0.50
3:G:221:VAL:O	3:G:221:VAL:CG1	2.59	0.50
3:I:42:GLU:O	3:I:42:GLU:OE2	2.30	0.50
4:J:1201:SER:OG	4:J:1203:SER:O	2.24	0.50
3:K:221:VAL:CG1	3:K:221:VAL:O	2.59	0.50
4:L:1017:GLU:O	4:L:1078:VAL:HG12	2.12	0.50
4:J:1017:GLU:O	4:J:1078:VAL:HG12	2.12	0.49
3:K:210:SER:OG	3:K:210:SER:O	2.29	0.49
4:H:1017:GLU:O	4:H:1078:VAL:HG12	2.12	0.49
3:I:42:GLU:C	3:I:43:LYS:CG	2.71	0.49
4:L:1083:LEU:HD22	4:L:1105:GLU:HA	1.94	0.49
3:G:42:GLU:OE2	3:G:42:GLU:O	2.30	0.49
3:I:126:PRO:HB3	3:I:152:TYR:HB3	1.94	0.49
3:K:126:PRO:HB3	3:K:152:TYR:HB3	1.94	0.49
3:I:42:GLU:HA	3:I:43:LYS:CE	2.43	0.49
3:K:195:TRP:CD1	3:K:196:PRO:HA	2.48	0.49
3:G:42:GLU:C	3:G:43:LYS:CG	2.71	0.49
3:K:42:GLU:HA	3:K:43:LYS:CE	2.43	0.49
3:G:195:TRP:CD1	3:G:196:PRO:HA	2.48	0.48
3:K:42:GLU:O	3:K:42:GLU:OE2	2.30	0.48
4:H:1184:ASP:OD1	4:H:1185:GLU:N	2.47	0.48
4:J:1184:ASP:OD1	4:J:1185:GLU:N	2.46	0.48
4:H:1083:LEU:HD22	4:H:1105:GLU:HA	1.94	0.48
3:I:195:TRP:CD1	3:I:196:PRO:HA	2.48	0.48
4:J:1083:LEU:HD22	4:J:1105:GLU:HA	1.94	0.48
4:L:1184:ASP:OD1	4:L:1185:GLU:N	2.47	0.48
3:K:63:THR:O	3:K:67:ARG:NH1	2.47	0.48
4:H:1059:PRO:O	3:I:76:LYS:HD3	2.14	0.48
3:G:42:GLU:HA	3:G:43:LYS:CE	2.43	0.48
2:F:26:LYS:CA	3:K:102:TYR:O	2.62	0.47
4:H:1188:ARG:HA	4:H:1188:ARG:HD3	1.68	0.47
4:L:1188:ARG:HA	4:L:1188:ARG:HD3	1.68	0.47
3:K:60:TYR:HB2	3:K:65:LYS:HG3	1.96	0.47
3:G:60:TYR:HB2	3:G:65:LYS:HG3	1.96	0.47
3:K:42:GLU:CB	3:K:43:LYS:CE	2.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:99:TRP:HH2	4:J:1091:SER:HB2	1.79	0.47
3:I:63:THR:O	3:I:67:ARG:NH1	2.47	0.47
4:J:1196:ALA:HB3	4:J:1205:ILE:CD1	2.44	0.47
3:K:99:TRP:HH2	4:L:1091:SER:HB2	1.79	0.47
3:I:60:TYR:HB2	3:I:65:LYS:HG3	1.96	0.47
4:H:1196:ALA:HB3	4:H:1205:ILE:CD1	2.44	0.46
4:H:1061:ARG:CA	3:I:80:PHE:HE1	2.23	0.46
4:H:1006:GLN:HE21	4:H:1021:LEU:HD21	1.81	0.46
4:J:1006:GLN:HE21	4:J:1021:LEU:HD21	1.81	0.46
3:G:99:TRP:HH2	4:H:1091:SER:HB2	1.79	0.46
4:H:1201:SER:OG	4:H:1203:SER:O	2.24	0.46
3:K:149:VAL:HG21	3:K:159:LEU:HD21	1.97	0.46
4:H:1060:ASP:HA	3:I:76:LYS:HB2	1.98	0.46
4:L:1076:SER:HA	4:L:1077:SER:HA	1.71	0.46
4:H:1060:ASP:OD2	3:I:80:PHE:CE2	2.69	0.46
3:I:149:VAL:HG21	3:I:159:LEU:HD21	1.97	0.46
3:G:166:LEU:HD13	3:G:188:VAL:HG21	1.97	0.46
3:I:166:LEU:HD13	3:I:188:VAL:HG21	1.97	0.46
4:J:1076:SER:HA	4:J:1077:SER:HA	1.71	0.46
3:G:63:THR:O	3:G:67:ARG:NH1	2.47	0.45
4:L:1006:GLN:HE21	4:L:1021:LEU:HD21	1.81	0.45
3:K:166:LEU:HD13	3:K:188:VAL:HG21	1.97	0.45
3:G:149:VAL:HG21	3:G:159:LEU:HD21	1.97	0.45
4:H:1054:ARG:HD3	3:I:73:ASP:OD2	2.16	0.45
3:K:42:GLU:HA	3:K:43:LYS:HB3	1.94	0.45
4:H:1060:ASP:OD1	3:I:80:PHE:CE2	2.70	0.45
3:K:139:THR:HG23	3:K:139:THR:O	2.15	0.45
3:I:139:THR:O	3:I:139:THR:HG23	2.16	0.45
3:I:221:VAL:O	3:I:221:VAL:HG13	2.17	0.45
3:G:42:GLU:CB	3:G:43:LYS:CE	2.90	0.44
3:G:139:THR:HG23	3:G:139:THR:O	2.16	0.44
4:L:1196:ALA:HB3	4:L:1205:ILE:CD1	2.44	0.44
3:K:40:ALA:O	3:K:43:LYS:HA	2.18	0.44
4:H:1019:VAL:HG11	4:H:1104:LEU:CD1	2.47	0.44
3:G:30:SER:O	3:G:53:SER:HB2	2.17	0.44
4:J:1188:ARG:HD3	4:J:1188:ARG:HA	1.68	0.44
3:I:40:ALA:O	3:I:43:LYS:HA	2.18	0.44
3:G:150:LYS:HZ1	4:H:1180:THR:HG23	1.83	0.44
4:H:1019:VAL:O	4:H:1074:THR:HA	2.18	0.44
3:K:30:SER:O	3:K:53:SER:HB2	2.17	0.43
4:H:1063:THR:HG23	4:H:1074:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:221:VAL:HG13	3:K:221:VAL:O	2.17	0.43
4:H:1061:ARG:CG	3:I:21:SER:OG	2.53	0.43
4:L:1063:THR:HG23	4:L:1074:THR:OG1	2.19	0.43
4:J:1063:THR:HG23	4:J:1074:THR:OG1	2.19	0.43
4:L:1201:SER:OG	4:L:1203:SER:O	2.24	0.43
4:L:1019:VAL:HG11	4:L:1104:LEU:CD1	2.47	0.43
3:I:173:PHE:HA	3:I:174:PRO:HD3	1.92	0.43
3:I:30:SER:O	3:I:53:SER:HB2	2.17	0.43
4:H:1058:VAL:HG11	3:I:76:LYS:HE3	1.63	0.43
4:J:1019:VAL:HG11	4:J:1104:LEU:CD1	2.47	0.43
3:G:40:ALA:O	3:G:43:LYS:HA	2.18	0.43
3:G:221:VAL:HG13	3:G:221:VAL:O	2.17	0.43
4:H:1060:ASP:CG	3:I:80:PHE:CZ	2.92	0.42
3:I:150:LYS:HZ1	4:J:1180:THR:HG23	1.84	0.42
3:K:218:GLU:HA	3:K:219:PRO:HD3	1.89	0.42
4:H:1071:PHE:CD1	4:H:1071:PHE:N	2.87	0.42
4:L:1071:PHE:N	4:L:1071:PHE:CD1	2.87	0.42
3:I:178:GLN:HB3	4:J:1160:LEU:HD21	2.01	0.42
4:H:1054:ARG:HA	3:I:76:LYS:HZ2	1.77	0.42
4:L:1019:VAL:O	4:L:1074:THR:HA	2.18	0.42
4:J:1019:VAL:O	4:J:1074:THR:HA	2.18	0.42
3:K:178:GLN:HB3	4:L:1160:LEU:HD21	2.01	0.42
3:K:150:LYS:HZ1	4:L:1180:THR:HG23	1.85	0.42
4:J:1071:PHE:N	4:J:1071:PHE:CD1	2.87	0.42
3:G:40:ALA:HB1	3:G:41:PRO:CD	2.50	0.42
4:L:1012:SER:HA	4:L:1105:GLU:HG2	2.02	0.42
3:K:40:ALA:HB1	3:K:41:PRO:CD	2.50	0.42
4:H:1012:SER:HA	4:H:1105:GLU:HG2	2.02	0.42
3:G:178:GLN:HB3	4:H:1160:LEU:HD21	2.01	0.42
3:I:40:ALA:HB1	3:I:41:PRO:CD	2.50	0.42
4:H:1060:ASP:OD1	3:I:80:PHE:HE2	2.02	0.42
4:H:1150:ILE:HD11	4:H:1179:LEU:HD21	2.03	0.41
4:L:1150:ILE:HD11	4:L:1179:LEU:HD21	2.03	0.41
4:H:1076:SER:HA	4:H:1077:SER:HA	1.71	0.41
4:J:1012:SER:HA	4:J:1105:GLU:HG2	2.02	0.41
4:J:1115:VAL:HG21	4:J:1205:ILE:CD1	2.48	0.41
3:G:32:PHE:O	3:G:72:ARG:NH2	2.45	0.41
4:L:1019:VAL:CG2	4:L:1075:ILE:HB	2.51	0.41
4:H:1016:GLY:O	3:I:18:ARG:HG3	2.20	0.41
3:I:42:GLU:CB	3:I:43:LYS:CE	2.90	0.41
4:J:1019:VAL:CG2	4:J:1075:ILE:HB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:156:PRO:O	3:I:207:PRO:HD2	2.21	0.41
4:J:1150:ILE:HD11	4:J:1179:LEU:HD21	2.03	0.41
3:K:173:PHE:HA	3:K:174:PRO:HD3	1.92	0.41
1:A:331:SER:CA	1:A:332:PRO:CA	2.99	0.41
1:B:331:SER:CA	1:B:332:PRO:CA	2.99	0.40
4:L:1033:VAL:HG11	4:L:1071:PHE:CD2	2.57	0.40
4:H:1019:VAL:CG2	4:H:1075:ILE:HB	2.51	0.40
3:K:156:PRO:O	3:K:207:PRO:HD2	2.21	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	
3	G	212/221 (96%)	205 (97%)	6 (3%)	1 (0%)	34	77
3	I	212/221 (96%)	205 (97%)	6 (3%)	1 (0%)	34	77
3	K	212/221 (96%)	205 (97%)	6 (3%)	1 (0%)	34	77
4	H	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	34	77
4	J	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	34	77
4	L	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	34	77
All	All	1266/1299 (98%)	1227 (97%)	33 (3%)	6 (0%)	38	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	43	LYS
3	I	43	LYS
3	K	43	LYS
4	H	1030	GLY

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Mol	Chain	Res	Type
4	J	1030	GLY
4	L	1030	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	
3	G	183/187 (98%)	166 (91%)	17 (9%)	11	42
3	I	183/187 (98%)	166 (91%)	17 (9%)	11	42
3	K	183/187 (98%)	166 (91%)	17 (9%)	11	42
4	H	188/188 (100%)	170 (90%)	18 (10%)	10	40
4	J	188/188 (100%)	170 (90%)	18 (10%)	10	40
4	L	188/188 (100%)	170 (90%)	18 (10%)	10	40
All	All	1113/1125 (99%)	1008 (91%)	105 (9%)	15	42

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	1	ASP
3	G	19	LYS
3	G	42	GLU
3	G	43	LYS
3	G	45	LEU
3	G	72	ARG
3	G	86	LEU
3	G	88	SER
3	G	89	GLU
3	G	141	SER
3	G	157	VAL
3	G	159	LEU
3	G	167	SER
3	G	191	THR
3	G	202	CYS
3	G	203	ASN

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Mol	Chain	Res	Type
3	G	215	LYS
4	H	1011	MET
4	H	1018	ARG
4	H	1019	VAL
4	H	1022	THR
4	H	1028	ASN
4	H	1031	THR
4	H	1041	GLU
4	H	1043	SER
4	H	1047	LEU
4	H	1054	ARG
4	H	1063	THR
4	H	1069	THR
4	H	1078	VAL
4	H	1093	SER
4	H	1094	THR
4	H	1108	ARG
4	H	1168	SER
4	H	1191	SER
3	I	1	ASP
3	I	19	LYS
3	I	42	GLU
3	I	43	LYS
3	I	45	LEU
3	I	72	ARG
3	I	86	LEU
3	I	88	SER
3	I	89	GLU
3	I	141	SER
3	I	157	VAL
3	I	159	LEU
3	I	167	SER
3	I	191	THR
3	I	202	CYS
3	I	203	ASN
3	I	215	LYS
4	J	1011	MET
4	J	1018	ARG
4	J	1019	VAL
4	J	1022	THR
4	J	1028	ASN
4	J	1031	THR

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Mol	Chain	Res	Type
4	J	1041	GLU
4	J	1043	SER
4	J	1047	LEU
4	J	1054	ARG
4	J	1063	THR
4	J	1069	THR
4	J	1078	VAL
4	J	1093	SER
4	J	1094	THR
4	J	1108	ARG
4	J	1168	SER
4	J	1191	SER
3	K	1	ASP
3	K	19	LYS
3	K	42	GLU
3	K	43	LYS
3	K	45	LEU
3	K	72	ARG
3	K	86	LEU
3	K	88	SER
3	K	89	GLU
3	K	141	SER
3	K	157	VAL
3	K	159	LEU
3	K	167	SER
3	K	191	THR
3	K	202	CYS
3	K	203	ASN
3	K	215	LYS
4	L	1011	MET
4	L	1018	ARG
4	L	1019	VAL
4	L	1022	THR
4	L	1028	ASN
4	L	1031	THR
4	L	1041	GLU
4	L	1043	SER
4	L	1047	LEU
4	L	1054	ARG
4	L	1063	THR
4	L	1069	THR
4	L	1078	VAL

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Mol	Chain	Res	Type
4	L	1093	SER
4	L	1094	THR
4	L	1108	ARG
4	L	1168	SER
4	L	1191	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	H	1079	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.