Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 12:47 PM EST

PDB ID	:	3J2Z
EMDB ID	:	EMD-5579
Title	:	Electron Cryo-microscopy of Chikungunya VLP in complex with neutralizing antibody Fab m10
Authors	:	Sun, S.; Xiang, Y.; Rossmann, M.G.
Deposited on	:	2013-01-28
Resolution	:	16.90 Å(reported)
Based on initial model	:	4GQ9

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

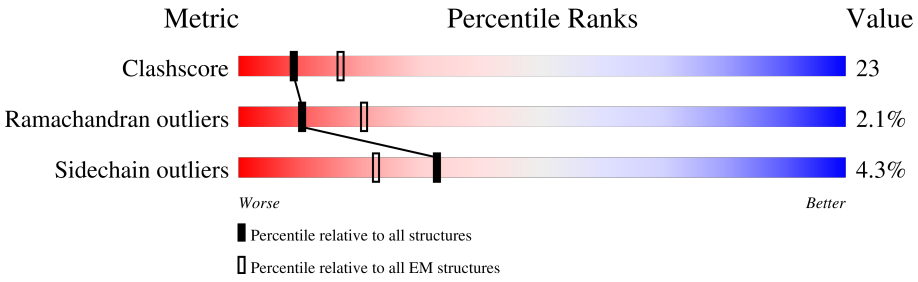
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 16.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	212	83% 15% ·
1	C	212	71% 27% ·
1	E	212	72% 26% ·
1	G	212	73% 25% ·
2	B	218	80% 17% ·
2	D	218	77% 20% ·
2	F	218	76% 21% ·
2	H	218	77% 20% ·

2 Entry composition (i)

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 m10 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 m10 heavy chain.

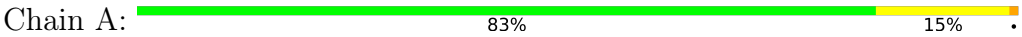
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	D	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	F	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		
2	H	218	Total	C	N	O	S	0	0
			1647	1039	275	326	7		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

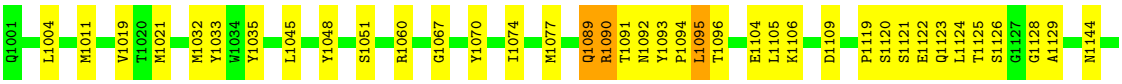
• Molecule 1: m10 light chain

Chain A:



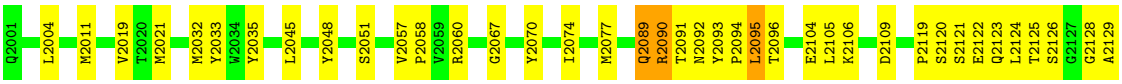
• Molecule 1: m10 light chain

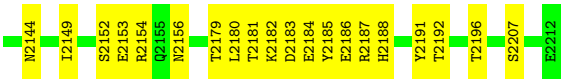
Chain C:



• Molecule 1: m10 light chain

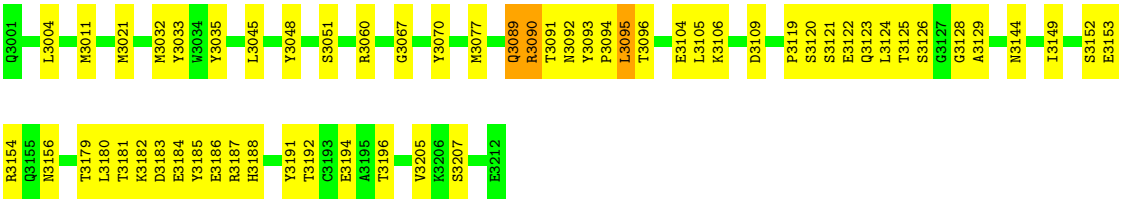
Chain E:





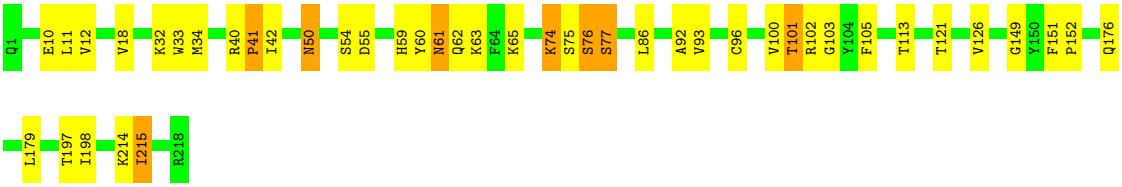
• Molecule 1: m10 light chain

Chain G:



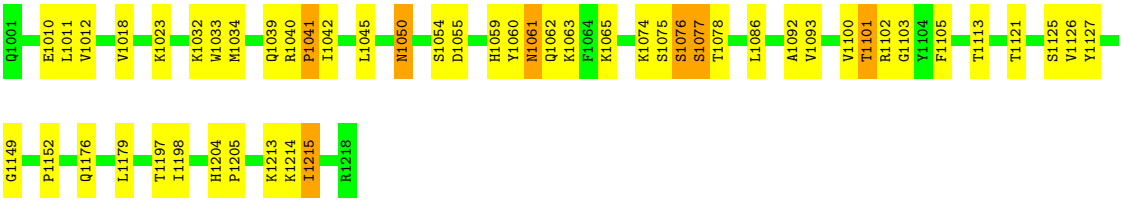
• Molecule 2: m10 heavy chain

Chain B:



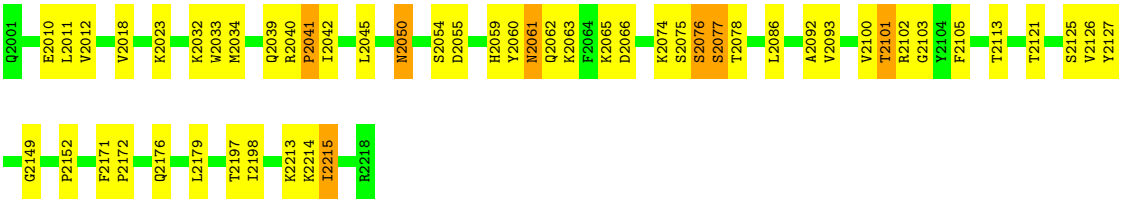
• Molecule 2: m10 heavy chain

Chain D:



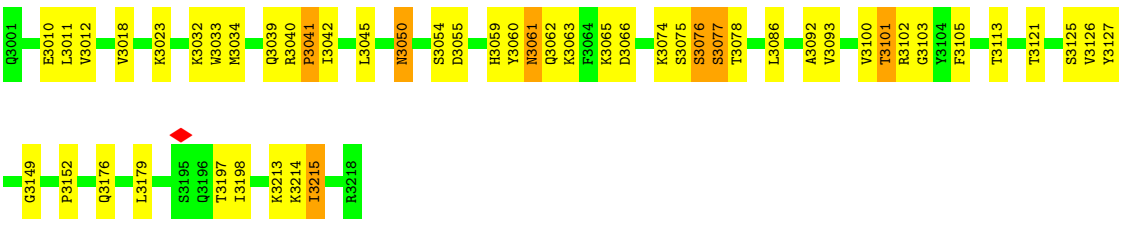
• Molecule 2: m10 heavy chain

Chain F:



• Molecule 2: m10 heavy chain

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1599	Depositor
Resolution determination method	FSC 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	
Maximum defocus (nm)	Not provided	
Magnification	35600	Depositor
Image detector	Not provided	
Maximum map value	6.635	Depositor
Minimum map value	-0.584	Depositor
Average map value	0.559	Depositor
Map value standard deviation	1.194	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	888.0, 888.0, 888.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.22, 2.22, 2.22	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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.34	0/1669	0.48	0/2268
1	C	0.34	0/1669	0.48	0/2268
1	E	0.34	0/1669	0.48	0/2268
1	G	0.34	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

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	19	0
1	C	1633	0	1548	256	0
1	E	1633	0	1548	256	0
1	G	1633	0	1548	256	0
2	B	1647	0	1620	35	0
2	D	1647	0	1615	51	0
2	F	1647	0	1615	52	0
2	H	1647	0	1615	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13120	0	12676	593	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 23.

All (593) 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:C:1129:ALA:CB	1:E:2183:ASP:HB3	1.29	1.61
1:C:1183:ASP:HB3	1:G:3129:ALA:CB	1.29	1.60
1:C:1185:TYR:CB	1:G:3182:LYS:CE	1.82	1.57
1:E:2182:LYS:CE	1:G:3185:TYR:CB	1.82	1.57
1:E:2129:ALA:CB	1:G:3183:ASP:HB3	1.29	1.56
1:C:1185:TYR:HB3	1:G:3182:LYS:CE	1.32	1.55
1:C:1182:LYS:CE	1:E:2185:TYR:HB3	1.32	1.54
1:C:1185:TYR:CB	1:G:3182:LYS:NZ	1.71	1.54
1:E:2182:LYS:CE	1:G:3185:TYR:HB3	1.32	1.53
1:C:1182:LYS:CE	1:E:2185:TYR:CB	1.82	1.52
1:C:1185:TYR:CD2	1:G:3182:LYS:CE	1.94	1.51
1:C:1182:LYS:CE	1:E:2185:TYR:CD2	1.94	1.49
1:E:2182:LYS:NZ	1:G:3185:TYR:CB	1.71	1.47
1:E:2182:LYS:CE	1:G:3185:TYR:CD2	1.94	1.46
1:C:1182:LYS:NZ	1:E:2185:TYR:CB	1.71	1.45
1:C:1129:ALA:CB	1:E:2183:ASP:CB	1.94	1.45
1:C:1183:ASP:HA	1:E:2182:LYS:CD	1.14	1.45
1:C:1185:TYR:HB3	1:G:3182:LYS:CD	0.97	1.44
1:C:1183:ASP:CB	1:G:3129:ALA:HB3	1.47	1.44
1:E:2182:LYS:CD	1:G:3185:TYR:HB3	0.96	1.44
1:C:1183:ASP:CB	1:G:3129:ALA:CB	1.94	1.43
1:E:2129:ALA:HB3	1:G:3183:ASP:CB	1.47	1.43
1:C:1182:LYS:CD	1:E:2185:TYR:HB3	0.97	1.42
1:C:1182:LYS:CD	1:G:3183:ASP:HA	1.14	1.42
1:C:1129:ALA:HB3	1:E:2183:ASP:CB	1.47	1.41
1:C:1182:LYS:HD3	1:G:3183:ASP:CA	0.99	1.41
1:C:1183:ASP:CG	1:E:2182:LYS:HD2	1.41	1.41
1:E:2129:ALA:CB	1:G:3183:ASP:CB	1.94	1.41
1:E:2182:LYS:CD	1:G:3185:TYR:CB	1.93	1.41
1:C:1185:TYR:CB	1:G:3182:LYS:HD2	1.49	1.40
1:E:2182:LYS:HD2	1:G:3185:TYR:CB	1.49	1.39
1:E:2183:ASP:CG	1:G:3182:LYS:HD2	1.41	1.39
1:C:1182:LYS:CD	1:E:2185:TYR:CB	1.93	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1182:LYS:HD2	1:G:3183:ASP:CG	1.41	1.36
1:G:3033:TYR:OH	1:G:3090:ARG:NH1	1.58	1.35
1:E:2183:ASP:HA	1:G:3182:LYS:CD	1.14	1.35
1:E:2033:TYR:OH	1:E:2090:ARG:NH1	1.58	1.35
1:A:33:TYR:OH	1:A:90:ARG:NH1	1.58	1.35
1:E:2183:ASP:CA	1:G:3182:LYS:HD3	0.99	1.35
1:C:1182:LYS:HD2	1:E:2185:TYR:CB	1.49	1.34
1:C:1183:ASP:CA	1:E:2182:LYS:HD3	0.99	1.34
1:C:1033:TYR:OH	1:C:1090:ARG:NH1	1.58	1.32
1:C:1156:ASN:CG	2:H:3125:SER:OG	1.70	1.29
1:E:2156:ASN:CG	2:D:1125:SER:OG	1.70	1.28
1:G:3156:ASN:CG	2:F:2125:SER:OG	1.70	1.27
1:E:2182:LYS:HE3	1:G:3185:TYR:C	1.55	1.26
1:C:1182:LYS:HE3	1:E:2185:TYR:C	1.55	1.26
1:C:1185:TYR:C	1:G:3182:LYS:HE3	1.55	1.24
1:C:1185:TYR:CB	1:G:3182:LYS:CD	1.93	1.24
1:C:1182:LYS:HE3	1:E:2186:GLU:N	1.55	1.22
1:G:3156:ASN:OD1	2:F:2125:SER:OG	1.56	1.22
1:E:2156:ASN:OD1	2:D:1125:SER:OG	1.56	1.21
1:C:1186:GLU:N	1:G:3182:LYS:HE3	1.55	1.21
1:C:1185:TYR:CD1	1:G:3182:LYS:NZ	2.09	1.20
1:C:1182:LYS:NZ	1:E:2185:TYR:CD1	2.09	1.19
1:C:1156:ASN:OD1	2:H:3125:SER:OG	1.56	1.19
1:E:2182:LYS:NZ	1:G:3185:TYR:CD1	2.09	1.19
1:E:2182:LYS:HE3	1:G:3186:GLU:N	1.55	1.19
1:C:1182:LYS:CD	1:G:3183:ASP:CA	1.84	1.17
1:C:1129:ALA:HB2	1:E:2183:ASP:CB	1.72	1.17
1:C:1182:LYS:NZ	1:E:2185:TYR:CE2	2.15	1.14
2:F:2076:SER:HA	2:F:2077:SER:HB3	1.16	1.13
1:E:2182:LYS:NZ	1:G:3185:TYR:CE2	2.15	1.12
1:C:1185:TYR:CE2	1:G:3182:LYS:NZ	2.15	1.12
1:C:1183:ASP:CB	1:G:3129:ALA:HB2	1.72	1.11
1:E:2129:ALA:HB2	1:G:3183:ASP:CB	1.72	1.11
1:C:1154:ARG:CZ	2:H:3127:TYR:OH	2.00	1.10
1:C:1191:TYR:CD1	1:G:3125:THR:HG23	1.86	1.10
1:E:2154:ARG:CZ	2:D:1127:TYR:OH	2.00	1.10
1:G:3154:ARG:CZ	2:F:2127:TYR:OH	2.00	1.10
2:B:76:SER:HA	2:B:77:SER:CB	1.82	1.10
2:H:3076:SER:HA	2:H:3077:SER:HB3	1.16	1.10
1:C:1182:LYS:CD	1:G:3183:ASP:OD1	1.75	1.08
2:B:76:SER:HA	2:B:77:SER:HB3	1.16	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1076:SER:HA	2:D:1077:SER:CB	1.82	1.08
2:D:1076:SER:HA	2:D:1077:SER:HB3	1.16	1.08
2:H:3076:SER:HA	2:H:3077:SER:CB	1.82	1.06
2:F:2076:SER:HA	2:F:2077:SER:CB	1.82	1.06
1:E:2125:THR:HG23	1:G:3191:TYR:CD1	1.86	1.06
1:C:1125:THR:HG23	1:E:2191:TYR:CD1	1.86	1.05
1:E:2182:LYS:CE	1:G:3185:TYR:CG	2.08	1.05
1:E:2183:ASP:CB	1:G:3182:LYS:CD	2.33	1.05
1:C:1182:LYS:CD	1:G:3183:ASP:CB	2.33	1.05
1:E:2182:LYS:CE	1:G:3185:TYR:HD2	1.48	1.05
1:C:1183:ASP:CB	1:E:2182:LYS:CD	2.33	1.04
1:C:1183:ASP:OD1	1:E:2182:LYS:CD	1.75	1.03
1:C:1183:ASP:HB2	1:G:3129:ALA:CB	1.89	1.03
1:C:1183:ASP:CB	1:E:2182:LYS:HD3	1.88	1.02
1:C:1182:LYS:HD2	1:G:3183:ASP:OD1	0.84	1.02
1:E:2183:ASP:CB	1:G:3182:LYS:HD3	1.88	1.02
2:F:2054:SER:HB2	2:F:2055:ASP:HB3	1.41	1.02
2:H:3054:SER:HB2	2:H:3055:ASP:HB3	1.41	1.01
1:C:1183:ASP:OD1	1:E:2182:LYS:HD2	0.84	1.01
1:E:2182:LYS:NZ	1:G:3185:TYR:CD2	0.84	1.01
2:D:1054:SER:HB2	2:D:1055:ASP:HB3	1.40	1.01
1:E:2183:ASP:OD1	1:G:3182:LYS:HD2	0.84	1.01
1:E:2183:ASP:OD1	1:G:3182:LYS:CD	1.75	1.00
2:B:54:SER:HB2	2:B:55:ASP:HB3	1.40	1.00
1:C:1182:LYS:HD3	1:G:3183:ASP:CB	1.88	0.99
1:C:1129:ALA:CB	1:E:2183:ASP:HB2	1.89	0.99
1:E:2129:ALA:CB	1:G:3183:ASP:HB2	1.89	0.98
1:E:2124:LEU:HD21	1:G:3187:ARG:HG3	1.46	0.98
1:C:1185:TYR:CD2	1:G:3182:LYS:NZ	0.84	0.98
1:C:1182:LYS:NZ	1:E:2185:TYR:CD2	0.84	0.98
1:C:1183:ASP:C	1:G:3129:ALA:HB2	1.84	0.97
1:C:1185:TYR:CG	1:G:3182:LYS:NZ	0.78	0.97
1:C:1182:LYS:NZ	1:E:2185:TYR:CG	0.78	0.97
1:E:2182:LYS:NZ	1:G:3185:TYR:CG	0.78	0.97
1:C:1129:ALA:HB2	1:E:2183:ASP:C	1.84	0.97
1:C:1182:LYS:CE	1:E:2185:TYR:CG	2.08	0.97
1:C:1129:ALA:HB2	1:E:2183:ASP:HB3	1.35	0.97
1:C:1183:ASP:HB3	1:G:3129:ALA:HB3	0.98	0.97
1:E:2129:ALA:HB2	1:G:3183:ASP:C	1.84	0.96
1:C:1187:ARG:HG3	1:G:3124:LEU:HD21	1.46	0.96
1:C:1183:ASP:CB	1:E:2182:LYS:HD2	1.96	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1124:LEU:HD21	1:E:2187:ARG:HG3	1.46	0.95
1:C:1156:ASN:OD1	2:H:3125:SER:CB	2.14	0.95
1:G:3156:ASN:OD1	2:F:2125:SER:CB	2.14	0.95
1:C:1182:LYS:CE	1:E:2185:TYR:HD2	1.48	0.95
1:E:2182:LYS:HE2	1:G:3185:TYR:HD2	1.32	0.95
1:E:2156:ASN:OD1	2:D:1125:SER:CB	2.14	0.95
1:C:1185:TYR:CA	1:G:3182:LYS:HE3	1.97	0.94
1:E:2129:ALA:HB3	1:G:3183:ASP:HB2	1.46	0.94
1:C:1185:TYR:HD2	1:G:3182:LYS:HE2	1.32	0.94
1:E:2183:ASP:CB	1:G:3182:LYS:HD2	1.96	0.94
1:E:2129:ALA:HB3	1:G:3183:ASP:HB3	0.98	0.94
1:E:2182:LYS:HE3	1:G:3185:TYR:CA	1.97	0.94
1:C:1182:LYS:HE3	1:E:2185:TYR:CA	1.97	0.93
1:C:1122:GLU:HA	1:E:2149:ILE:HG21	1.51	0.93
1:C:1125:THR:CG2	1:E:2191:TYR:CD1	2.47	0.93
1:C:1182:LYS:HD2	1:G:3183:ASP:CB	1.96	0.93
1:C:1149:ILE:HD13	1:G:3125:THR:HB	1.51	0.93
1:C:1185:TYR:CB	1:G:3182:LYS:HE3	1.97	0.93
1:E:2125:THR:CG2	1:G:3191:TYR:CD1	2.47	0.93
1:C:1182:LYS:HE2	1:E:2185:TYR:HD2	1.32	0.93
1:E:2122:GLU:HA	1:G:3149:ILE:HG21	1.51	0.93
1:C:1125:THR:HB	1:E:2149:ILE:HD13	1.51	0.92
1:E:2125:THR:HB	1:G:3149:ILE:HD13	1.51	0.92
1:C:1149:ILE:HG21	1:G:3122:GLU:HA	1.51	0.91
1:C:1183:ASP:HB2	1:G:3129:ALA:HB3	1.46	0.91
1:C:1185:TYR:HD2	1:G:3182:LYS:CE	1.48	0.91
1:C:1129:ALA:HB3	1:E:2183:ASP:HB3	0.98	0.91
2:B:76:SER:CA	2:B:77:SER:HB3	2.01	0.91
2:H:3076:SER:CA	2:H:3077:SER:HB3	2.01	0.90
1:E:2182:LYS:HE2	1:G:3186:GLU:HG3	1.54	0.90
2:D:1076:SER:CA	2:D:1077:SER:HB3	2.01	0.90
1:C:1191:TYR:CD1	1:G:3125:THR:CG2	2.47	0.89
1:C:1129:ALA:HB3	1:E:2183:ASP:HB2	1.46	0.89
1:C:1185:TYR:CA	1:G:3182:LYS:CE	2.51	0.89
1:C:1182:LYS:CE	1:E:2185:TYR:CA	2.51	0.89
1:C:1186:GLU:HG3	1:G:3182:LYS:HE2	1.54	0.89
1:E:2153:GLU:N	2:D:1213:LYS:NZ	2.18	0.88
2:B:50:ASN:ND2	2:B:59:HIS:HB2	1.89	0.88
2:H:3050:ASN:ND2	2:H:3059:HIS:HB2	1.89	0.88
1:C:1182:LYS:HE2	1:E:2186:GLU:HG3	1.54	0.87
1:C:1182:LYS:HE3	1:E:2185:TYR:CB	1.97	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1050:ASN:ND2	2:D:1059:HIS:HB2	1.89	0.87
2:F:2050:ASN:ND2	2:F:2059:HIS:HB2	1.89	0.87
1:E:2182:LYS:CE	1:G:3185:TYR:CA	2.51	0.86
1:G:3153:GLU:N	2:F:2213:LYS:NZ	2.18	0.86
2:F:2076:SER:CA	2:F:2077:SER:HB3	2.01	0.86
1:C:1153:GLU:N	2:H:3213:LYS:NZ	2.18	0.84
1:E:2124:LEU:HB3	1:G:3185:TYR:C	1.98	0.84
1:C:1124:LEU:HB3	1:E:2185:TYR:C	1.98	0.84
1:E:2182:LYS:CE	1:G:3185:TYR:C	2.44	0.83
1:C:1122:GLU:HG3	1:E:2149:ILE:HB	1.61	0.83
1:C:1149:ILE:HB	1:G:3122:GLU:HG3	1.61	0.83
1:C:1125:THR:HB	1:E:2149:ILE:CD1	2.08	0.82
1:C:1149:ILE:CD1	1:G:3125:THR:HB	2.08	0.82
1:C:1185:TYR:C	1:G:3182:LYS:CE	2.44	0.82
1:C:1185:TYR:C	1:G:3124:LEU:HB3	1.98	0.82
1:E:2122:GLU:HG3	1:G:3149:ILE:HB	1.61	0.82
1:E:2125:THR:HB	1:G:3149:ILE:CD1	2.08	0.82
1:C:1182:LYS:HD2	1:E:2185:TYR:HB2	1.62	0.81
1:E:2183:ASP:CA	1:G:3182:LYS:CD	1.84	0.80
1:E:2129:ALA:HB2	1:G:3183:ASP:CA	2.13	0.79
1:E:2182:LYS:HD2	1:G:3185:TYR:HB2	1.62	0.78
1:C:1182:LYS:CE	1:G:3183:ASP:HA	2.13	0.78
1:C:1183:ASP:HA	1:E:2182:LYS:CE	2.13	0.78
1:C:1185:TYR:HB2	1:G:3182:LYS:HD2	1.62	0.78
1:C:1183:ASP:CA	1:G:3129:ALA:HB2	2.13	0.78
1:C:1129:ALA:HB2	1:E:2183:ASP:CA	2.13	0.77
1:C:1182:LYS:CE	1:E:2185:TYR:C	2.44	0.77
2:D:1050:ASN:HD21	2:D:1059:HIS:HB2	1.48	0.77
1:C:1182:LYS:HG2	1:G:3182:LYS:O	1.85	0.76
1:C:1183:ASP:CA	1:E:2182:LYS:CD	1.84	0.76
2:H:3050:ASN:HD21	2:H:3059:HIS:HB2	1.48	0.76
1:C:1149:ILE:CG2	1:G:3122:GLU:HA	2.15	0.76
2:B:50:ASN:HD21	2:B:59:HIS:HB2	1.48	0.76
2:F:2050:ASN:HD21	2:F:2059:HIS:HB2	1.48	0.76
1:E:2122:GLU:HA	1:G:3149:ILE:CG2	2.14	0.76
1:C:1122:GLU:HA	1:E:2149:ILE:CG2	2.15	0.75
2:B:75:SER:H	2:B:76:SER:C	1.89	0.75
1:E:2182:LYS:O	1:G:3182:LYS:HG2	1.85	0.75
2:F:2075:SER:H	2:F:2076:SER:C	1.89	0.75
1:C:1187:ARG:CG	1:G:3124:LEU:HD21	2.17	0.75
1:C:1153:GLU:N	2:H:3213:LYS:HZ3	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1124:LEU:HD21	1:E:2187:ARG:CG	2.17	0.75
1:C:1149:ILE:HG21	1:G:3121:SER:O	1.87	0.75
1:E:2121:SER:O	1:G:3149:ILE:HG21	1.87	0.75
1:E:2129:ALA:HB2	1:G:3183:ASP:HB3	1.35	0.75
2:H:3075:SER:H	2:H:3076:SER:C	1.89	0.74
1:C:1128:GLY:N	1:E:2184:GLU:HB2	1.98	0.74
1:C:1121:SER:O	1:E:2149:ILE:HG21	1.87	0.74
1:C:1182:LYS:O	1:E:2182:LYS:HG2	1.85	0.73
1:E:2124:LEU:HD21	1:G:3187:ARG:CG	2.17	0.73
2:D:1075:SER:H	2:D:1076:SER:C	1.89	0.73
1:E:2128:GLY:N	1:G:3184:GLU:HB2	1.98	0.73
1:E:2125:THR:CB	1:G:3149:ILE:HD13	2.18	0.73
1:E:2183:ASP:HA	1:G:3182:LYS:CE	2.13	0.73
1:C:1125:THR:CB	1:E:2149:ILE:HD13	2.18	0.73
1:C:1149:ILE:HD13	1:G:3125:THR:CB	2.18	0.73
1:C:1182:LYS:NZ	1:E:2185:TYR:HD2	1.27	0.72
1:G:3153:GLU:N	2:F:2213:LYS:HZ3	1.86	0.72
1:C:1185:TYR:CG	1:G:3182:LYS:CE	2.08	0.72
1:C:1182:LYS:CD	1:G:3183:ASP:CG	2.27	0.72
1:E:2182:LYS:NZ	1:G:3185:TYR:HD2	1.27	0.72
1:C:1184:GLU:CB	1:G:3128:GLY:N	2.54	0.71
1:C:1128:GLY:N	1:E:2184:GLU:CB	2.54	0.71
1:E:2153:GLU:N	2:D:1213:LYS:HZ3	1.85	0.71
1:E:2128:GLY:N	1:G:3184:GLU:CB	2.53	0.71
1:C:1124:LEU:CD2	1:E:2187:ARG:HG3	2.20	0.70
1:C:1187:ARG:HG3	1:G:3124:LEU:CD2	2.20	0.70
1:C:1185:TYR:HD2	1:G:3182:LYS:NZ	1.27	0.70
1:C:1123:GLN:HA	1:E:2154:ARG:HH12	1.57	0.69
1:E:2123:GLN:HA	1:G:3154:ARG:HH12	1.57	0.69
1:E:2124:LEU:CD2	1:G:3187:ARG:HG3	2.20	0.69
1:C:1154:ARG:HH12	1:G:3123:GLN:HA	1.57	0.69
1:C:1094:PRO:HA	1:C:1095:LEU:CB	2.24	0.68
1:E:2124:LEU:HG	1:G:3187:ARG:HD3	1.76	0.68
1:C:1182:LYS:HE2	1:E:2185:TYR:CD2	2.11	0.68
1:A:94:PRO:HA	1:A:95:LEU:CB	2.23	0.68
1:E:2156:ASN:OD1	2:D:1125:SER:HB3	1.94	0.68
1:G:3094:PRO:HA	1:G:3095:LEU:CB	2.23	0.68
1:C:1149:ILE:HD13	1:G:3122:GLU:O	1.94	0.68
1:E:2125:THR:CB	1:G:3149:ILE:CD1	2.72	0.67
1:E:2094:PRO:HA	1:E:2095:LEU:CB	2.23	0.67
1:C:1122:GLU:O	1:E:2149:ILE:HD13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1125:THR:CB	1:E:2149:ILE:CD1	2.72	0.67
1:E:2124:LEU:HD23	1:G:3184:GLU:CA	2.14	0.67
1:E:2182:LYS:CE	1:G:3186:GLU:N	2.48	0.67
1:G:3156:ASN:OD1	2:F:2125:SER:HB3	1.94	0.67
1:E:2122:GLU:O	1:G:3149:ILE:HD13	1.94	0.66
1:C:1180:LEU:HD22	1:G:3123:GLN:O	1.95	0.66
1:C:1183:ASP:HB3	1:G:3129:ALA:HB2	1.35	0.66
1:E:2123:GLN:O	1:G:3180:LEU:HD22	1.95	0.66
1:C:1187:ARG:HD3	1:G:3124:LEU:HG	1.76	0.66
1:C:1123:GLN:O	1:E:2180:LEU:HD22	1.96	0.66
1:C:1124:LEU:HG	1:E:2187:ARG:HD3	1.76	0.66
1:C:1149:ILE:CD1	1:G:3125:THR:CB	2.72	0.65
1:C:1184:GLU:CA	1:G:3124:LEU:HD23	2.14	0.65
2:H:3050:ASN:N	2:H:3050:ASN:HD22	1.95	0.65
1:C:1184:GLU:HB2	1:G:3128:GLY:N	1.98	0.65
1:C:1156:ASN:OD1	2:H:3125:SER:HB3	1.95	0.64
2:B:50:ASN:N	2:B:50:ASN:HD22	1.95	0.64
1:E:2124:LEU:CD2	1:G:3187:ARG:CG	2.76	0.64
1:C:1149:ILE:HG21	1:G:3122:GLU:CA	2.28	0.64
2:F:2050:ASN:N	2:F:2050:ASN:HD22	1.95	0.64
1:E:2124:LEU:CD2	1:G:3187:ARG:N	2.59	0.63
1:C:1124:LEU:CD2	1:E:2187:ARG:CG	2.76	0.63
1:C:1122:GLU:CA	1:E:2149:ILE:HG21	2.28	0.63
1:C:1187:ARG:CG	1:G:3124:LEU:CD2	2.76	0.63
1:C:1187:ARG:CG	1:G:3124:LEU:CG	2.57	0.63
2:D:1050:ASN:N	2:D:1050:ASN:HD22	1.95	0.62
1:C:1124:LEU:CG	1:E:2187:ARG:CG	2.57	0.62
2:B:62:GLN:HA	2:B:65:LYS:HE3	1.82	0.62
2:H:3062:GLN:HA	2:H:3065:LYS:HE3	1.82	0.62
1:E:2124:LEU:CG	1:G:3187:ARG:CG	2.57	0.62
2:D:1062:GLN:HA	2:D:1065:LYS:HE3	1.82	0.61
1:C:1154:ARG:NH1	2:H:3127:TYR:OH	2.33	0.61
1:E:2154:ARG:NH1	2:D:1127:TYR:OH	2.33	0.61
2:D:1061:ASN:HD22	2:D:1063:LYS:H	1.48	0.61
2:F:2062:GLN:HA	2:F:2065:LYS:HE3	1.82	0.61
1:C:1185:TYR:CE2	1:G:3182:LYS:HZ3	1.58	0.61
2:H:3061:ASN:HD22	2:H:3063:LYS:H	1.48	0.61
1:C:1187:ARG:N	1:G:3124:LEU:CD2	2.59	0.61
1:C:1124:LEU:CD2	1:E:2187:ARG:N	2.59	0.61
1:C:1156:ASN:ND2	2:H:3125:SER:OG	2.33	0.61
1:C:1187:ARG:N	1:G:3124:LEU:HD22	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2061:ASN:HD22	2:F:2063:LYS:H	1.48	0.61
1:C:1182:LYS:CE	1:E:2186:GLU:N	2.48	0.60
1:C:1186:GLU:N	1:G:3182:LYS:CE	2.48	0.60
1:E:2122:GLU:O	1:G:3149:ILE:CD1	2.50	0.60
1:G:3154:ARG:NH1	2:F:2127:TYR:OH	2.33	0.60
1:G:3156:ASN:ND2	2:F:2125:SER:OG	2.33	0.60
2:B:61:ASN:HD22	2:B:63:LYS:H	1.48	0.60
1:C:1122:GLU:O	1:E:2149:ILE:CD1	2.50	0.60
2:D:1054:SER:CB	2:D:1055:ASP:HB3	2.25	0.60
1:E:2124:LEU:HD22	1:G:3187:ARG:N	2.16	0.60
1:E:2122:GLU:CA	1:G:3149:ILE:HG21	2.27	0.59
1:C:1149:ILE:CD1	1:G:3122:GLU:O	2.50	0.59
1:C:1124:LEU:HD22	1:E:2187:ARG:N	2.16	0.59
1:E:2181:THR:HA	1:G:3181:THR:HB	1.85	0.59
1:C:1181:THR:HB	1:G:3181:THR:HA	1.85	0.59
1:E:2129:ALA:HB1	1:G:3183:ASP:HB3	1.68	0.58
2:H:3054:SER:CB	2:H:3055:ASP:HB3	2.25	0.58
1:C:1004:LEU:HD11	1:C:1089:GLN:HB3	1.86	0.58
1:C:1181:THR:HA	1:E:2181:THR:HB	1.85	0.58
1:C:1185:TYR:CD2	1:G:3182:LYS:HE2	2.11	0.58
1:A:4:LEU:HD11	1:A:89:GLN:HB3	1.85	0.58
1:C:1153:GLU:H	2:H:3213:LYS:HZ3	1.52	0.58
1:G:3004:LEU:HD11	1:G:3089:GLN:HB3	1.86	0.58
1:C:1154:ARG:NH1	2:H:3127:TYR:CE1	2.72	0.58
1:E:2004:LEU:HD11	1:E:2089:GLN:HB3	1.85	0.57
1:E:2154:ARG:NH1	2:D:1127:TYR:CE1	2.72	0.57
1:E:2124:LEU:HB3	1:G:3186:GLU:N	2.20	0.56
1:G:3154:ARG:NH1	2:F:2127:TYR:CE1	2.72	0.56
1:C:1124:LEU:HB3	1:E:2186:GLU:N	2.20	0.56
1:E:2125:THR:CG2	1:G:3191:TYR:HD1	2.15	0.56
1:E:2156:ASN:ND2	2:D:1125:SER:OG	2.33	0.56
1:C:1186:GLU:N	1:G:3124:LEU:HB3	2.20	0.56
1:E:2183:ASP:CG	1:G:3182:LYS:CD	2.27	0.56
2:H:3033:TRP:CD1	2:H:3101:THR:HA	2.41	0.56
2:F:2033:TRP:CD1	2:F:2101:THR:HA	2.42	0.55
1:C:1124:LEU:HD23	1:E:2184:GLU:CA	2.14	0.55
2:B:54:SER:CB	2:B:55:ASP:HB3	2.26	0.55
2:D:1033:TRP:CD1	2:D:1101:THR:HA	2.42	0.55
1:E:2182:LYS:CE	1:G:3186:GLU:HG3	2.32	0.55
1:C:1186:GLU:HG3	1:G:3182:LYS:CE	2.32	0.54
2:B:33:TRP:CD1	2:B:101:THR:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1122:GLU:HA	1:E:2149:ILE:CB	2.38	0.54
1:C:1182:LYS:CE	1:E:2186:GLU:HG3	2.32	0.54
1:E:2183:ASP:OD1	1:G:3182:LYS:CG	2.51	0.54
2:F:2054:SER:CB	2:F:2055:ASP:HB3	2.25	0.54
1:C:1191:TYR:HD1	1:G:3125:THR:CG2	2.15	0.54
1:C:1149:ILE:HG12	1:G:3125:THR:HG21	1.90	0.53
1:C:1182:LYS:CG	1:G:3183:ASP:OD1	2.51	0.53
1:C:1183:ASP:OD1	1:E:2182:LYS:CG	2.51	0.53
1:C:1149:ILE:CB	1:G:3122:GLU:HA	2.38	0.53
1:E:2122:GLU:HA	1:G:3149:ILE:CB	2.38	0.53
1:E:2144:ASN:HB3	1:E:2196:THR:HB	1.91	0.53
2:F:2093:VAL:HG22	2:F:2113:THR:HG22	1.91	0.53
2:H:3093:VAL:HG22	2:H:3113:THR:HG22	1.91	0.53
1:C:1125:THR:OG1	1:E:2149:ILE:CG2	2.57	0.52
1:G:3094:PRO:HA	1:G:3095:LEU:HB2	1.91	0.52
1:A:144:ASN:HB3	1:A:196:THR:HB	1.91	0.52
1:C:1183:ASP:CG	1:E:2182:LYS:CD	2.27	0.52
1:G:3144:ASN:HB3	1:G:3196:THR:HB	1.91	0.52
1:E:2125:THR:OG1	1:G:3149:ILE:CG2	2.57	0.52
1:A:45:LEU:HD11	1:A:48:TYR:HB3	1.92	0.52
1:G:3154:ARG:NH2	2:F:2127:TYR:OH	2.42	0.52
2:B:93:VAL:HG22	2:B:113:THR:HG22	1.91	0.52
1:C:1125:THR:HA	1:E:2191:TYR:CZ	2.44	0.52
1:C:1149:ILE:CG2	1:G:3125:THR:OG1	2.57	0.52
1:E:2121:SER:HA	1:G:3188:HIS:N	2.23	0.52
1:C:1125:THR:HG21	1:E:2149:ILE:HG12	1.90	0.52
1:E:2125:THR:HG21	1:G:3149:ILE:HG12	1.90	0.52
1:C:1045:LEU:HD11	1:C:1048:TYR:HB3	1.92	0.52
1:E:2182:LYS:HE2	1:G:3185:TYR:CD2	2.11	0.52
1:C:1184:GLU:CA	1:G:3124:LEU:N	2.39	0.52
1:A:94:PRO:HA	1:A:95:LEU:HB2	1.91	0.51
1:C:1125:THR:CG2	1:E:2191:TYR:HD1	2.15	0.51
1:C:1121:SER:HA	1:E:2188:HIS:N	2.23	0.51
1:C:1191:TYR:CZ	1:G:3125:THR:HA	2.44	0.51
1:E:2094:PRO:HA	1:E:2095:LEU:HB2	1.91	0.51
1:E:2125:THR:HA	1:G:3191:TYR:CZ	2.44	0.51
1:G:3045:LEU:HD11	1:G:3048:TYR:HB3	1.91	0.51
1:E:2128:GLY:N	1:G:3184:GLU:HB3	2.24	0.51
2:D:1093:VAL:HG22	2:D:1113:THR:HG22	1.91	0.51
1:C:1094:PRO:HA	1:C:1095:LEU:HB2	1.91	0.51
1:C:1144:ASN:HB3	1:C:1196:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1128:GLY:N	1:E:2184:GLU:HB3	2.25	0.51
1:C:1179:THR:O	1:G:3126:SER:HB3	2.11	0.51
1:C:1154:ARG:NH2	2:H:3127:TYR:OH	2.42	0.51
1:E:2122:GLU:OE2	1:G:3152:SER:HB2	2.11	0.51
1:E:2126:SER:HB3	1:G:3179:THR:O	2.11	0.51
1:C:1122:GLU:OE2	1:E:2152:SER:HB2	2.11	0.50
1:C:1126:SER:HB3	1:E:2179:THR:O	2.11	0.50
1:A:94:PRO:HA	1:A:95:LEU:HB3	1.93	0.50
1:C:1149:ILE:HG21	1:G:3121:SER:C	2.32	0.50
1:C:1184:GLU:HB3	1:G:3128:GLY:N	2.24	0.50
1:C:1152:SER:HB2	1:G:3122:GLU:OE2	2.11	0.50
1:C:1184:GLU:CB	1:G:3128:GLY:H	2.23	0.50
1:E:2045:LEU:HD11	1:E:2048:TYR:HB3	1.92	0.50
2:D:1121:THR:HG23	2:D:1152:PRO:HD3	1.94	0.50
1:E:2094:PRO:HA	1:E:2095:LEU:HB3	1.94	0.50
1:E:2153:GLU:H	2:D:1213:LYS:NZ	2.04	0.50
2:B:121:THR:HG23	2:B:152:PRO:HD3	1.94	0.50
1:C:1124:LEU:N	1:E:2184:GLU:HA	2.26	0.50
1:E:2124:LEU:N	1:G:3184:GLU:CA	2.39	0.50
1:E:2182:LYS:CD	1:G:3185:TYR:CA	2.84	0.50
1:G:3154:ARG:NE	2:F:2127:TYR:OH	2.44	0.50
2:H:3121:THR:HG23	2:H:3152:PRO:HD3	1.94	0.50
1:C:1154:ARG:CZ	1:G:3126:SER:OG	2.60	0.49
1:E:2123:GLN:HA	1:G:3154:ARG:NH1	2.26	0.49
1:C:1154:ARG:NH1	1:G:3123:GLN:HA	2.26	0.49
1:E:2126:SER:OG	1:G:3154:ARG:CZ	2.61	0.49
2:F:2121:THR:HG23	2:F:2152:PRO:HD3	1.94	0.49
1:C:1128:GLY:H	1:E:2184:GLU:CB	2.23	0.49
1:E:2121:SER:C	1:G:3149:ILE:HG21	2.32	0.49
1:C:1121:SER:C	1:E:2149:ILE:HG21	2.32	0.49
1:C:1154:ARG:NH1	2:H:3127:TYR:CZ	2.81	0.49
1:E:2128:GLY:H	1:G:3184:GLU:CB	2.23	0.49
1:G:3094:PRO:HA	1:G:3095:LEU:HB3	1.93	0.49
1:C:1188:HIS:N	1:G:3121:SER:HA	2.24	0.49
1:G:3154:ARG:NH1	2:F:2127:TYR:CZ	2.81	0.49
2:H:3054:SER:HB2	2:H:3055:ASP:CB	2.29	0.49
1:C:1128:GLY:O	1:E:2184:GLU:OE1	2.31	0.49
1:C:1124:LEU:N	1:E:2184:GLU:CA	2.39	0.48
1:G:3094:PRO:HB2	1:G:3096:THR:HG23	1.96	0.48
1:A:35:TYR:CZ	1:A:45:LEU:HD23	2.48	0.48
1:C:1094:PRO:HB2	1:C:1096:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1035:TYR:CZ	1:C:1045:LEU:HD23	2.48	0.48
1:E:2154:ARG:NH1	2:D:1127:TYR:CZ	2.81	0.48
1:E:2154:ARG:NH2	2:D:1127:TYR:OH	2.42	0.48
1:C:1126:SER:OG	1:E:2154:ARG:CZ	2.60	0.48
1:C:1094:PRO:HA	1:C:1095:LEU:HB3	1.94	0.48
1:A:94:PRO:HB2	1:A:96:THR:HG23	1.96	0.48
2:H:3040:ARG:HG2	2:H:3092:ALA:HB2	1.96	0.48
1:C:1089:GLN:HG2	1:C:1090:ARG:N	2.29	0.48
1:C:1149:ILE:CG2	1:G:3121:SER:O	2.60	0.47
1:E:2154:ARG:CZ	2:D:1127:TYR:HH	2.24	0.47
2:F:2040:ARG:HG2	2:F:2092:ALA:HB2	1.96	0.47
1:E:2035:TYR:CZ	1:E:2045:LEU:HD23	2.48	0.47
2:D:1040:ARG:HG2	2:D:1092:ALA:HB2	1.96	0.47
1:C:1123:GLN:HA	1:E:2154:ARG:NH1	2.26	0.47
1:C:1184:GLU:OE1	1:G:3128:GLY:O	2.31	0.47
1:E:2094:PRO:HB2	1:E:2096:THR:HG23	1.96	0.47
1:E:2153:GLU:H	2:D:1213:LYS:HZ3	1.56	0.47
2:F:2041:PRO:HB2	2:F:2042:ILE:HD12	1.96	0.47
1:E:2089:GLN:HG2	1:E:2090:ARG:N	2.29	0.47
1:G:3035:TYR:CZ	1:G:3045:LEU:HD23	2.48	0.47
1:E:2120:SER:HB2	1:G:3188:HIS:HE1	1.80	0.47
1:E:2124:LEU:N	1:G:3184:GLU:HA	2.25	0.47
2:B:40:ARG:HG2	2:B:92:ALA:HB2	1.96	0.47
2:D:1041:PRO:HB2	2:D:1042:ILE:HD12	1.96	0.47
2:H:3041:PRO:HB2	2:H:3042:ILE:HD12	1.95	0.47
2:B:41:PRO:HB2	2:B:42:ILE:HD12	1.96	0.47
1:E:2128:GLY:O	1:G:3184:GLU:OE1	2.31	0.47
2:D:1034:MET:HE3	2:D:1034:MET:HB3	1.74	0.47
2:F:2054:SER:HB2	2:F:2055:ASP:CB	2.29	0.47
1:C:1154:ARG:NE	2:H:3127:TYR:OH	2.44	0.46
2:D:1060:TYR:HB2	2:D:1065:LYS:HE2	1.96	0.46
1:A:89:GLN:HG2	1:A:90:ARG:N	2.29	0.46
1:G:3089:GLN:HG2	1:G:3090:ARG:N	2.29	0.46
1:C:1188:HIS:HE1	1:G:3120:SER:HB2	1.79	0.46
1:E:2090:ARG:HB2	1:E:2091:THR:H	1.47	0.46
2:H:3034:MET:HE2	2:H:3034:MET:HB3	1.73	0.46
2:H:3060:TYR:HB2	2:H:3065:LYS:HE2	1.96	0.46
1:A:90:ARG:HB2	1:A:91:THR:H	1.47	0.46
2:B:102:ARG:HA	2:B:103:GLY:HA2	1.68	0.46
1:C:1125:THR:HB	1:E:2149:ILE:HD11	1.97	0.46
1:G:3153:GLU:H	2:F:2213:LYS:HZ3	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1181:THR:HB	1:G:3182:LYS:H	1.81	0.46
2:B:198:ILE:HG22	2:B:215:ILE:HD11	1.98	0.46
1:G:3153:GLU:H	2:F:2213:LYS:NZ	2.04	0.46
2:F:2198:ILE:HG22	2:F:2215:ILE:HD11	1.98	0.46
1:E:2121:SER:O	1:G:3149:ILE:CG2	2.60	0.46
2:D:1198:ILE:HG22	2:D:1215:ILE:HD11	1.98	0.46
2:F:2060:TYR:HB2	2:F:2065:LYS:HE2	1.96	0.46
1:C:1122:GLU:HA	1:E:2149:ILE:CD1	2.46	0.46
1:C:1182:LYS:H	1:E:2181:THR:HB	1.81	0.46
1:C:1120:SER:HB2	1:E:2188:HIS:HE1	1.79	0.45
1:C:1129:ALA:HB1	1:E:2183:ASP:HB3	1.68	0.45
1:E:2122:GLU:HA	1:G:3149:ILE:CD1	2.46	0.45
2:B:75:SER:N	2:B:76:SER:C	2.66	0.45
1:E:2125:THR:HG21	1:G:3191:TYR:CD1	2.47	0.45
1:E:2182:LYS:H	1:G:3181:THR:HB	1.80	0.45
2:B:60:TYR:HB2	2:B:65:LYS:HE2	1.96	0.45
1:A:89:GLN:NE2	1:A:92:ASN:HB3	2.32	0.45
1:C:1121:SER:O	1:E:2149:ILE:CG2	2.60	0.45
1:C:1149:ILE:CD1	1:G:3122:GLU:HA	2.46	0.45
1:E:2182:LYS:O	1:G:3182:LYS:CG	2.51	0.45
1:G:3033:TYR:CZ	1:G:3090:ARG:NH1	2.74	0.45
1:C:1125:THR:HG21	1:E:2191:TYR:CD1	2.47	0.45
1:C:1182:LYS:CD	1:E:2185:TYR:CA	2.84	0.45
1:G:3089:GLN:NE2	1:G:3092:ASN:HB3	2.32	0.45
1:E:2089:GLN:NE2	1:E:2092:ASN:HB3	2.32	0.45
2:D:1197:THR:HG23	2:D:1214:LYS:HE3	1.99	0.45
2:H:3198:ILE:HG22	2:H:3215:ILE:HD11	1.98	0.45
1:C:1089:GLN:NE2	1:C:1092:ASN:HB3	2.32	0.44
1:E:2192:THR:HG23	1:E:2207:SER:HB2	1.99	0.44
2:H:3197:THR:HG23	2:H:3214:LYS:HE3	1.99	0.44
1:A:192:THR:HG23	1:A:207:SER:HB2	1.99	0.44
1:E:2124:LEU:HG	1:G:3187:ARG:CD	2.45	0.44
2:F:2197:THR:HG23	2:F:2214:LYS:HE3	1.99	0.44
2:H:3149:GLY:HA2	2:H:3179:LEU:HB3	2.00	0.44
1:C:1090:ARG:HB2	1:C:1091:THR:H	1.47	0.44
1:C:1192:THR:HG23	1:C:1207:SER:HB2	1.99	0.44
1:E:2154:ARG:NE	2:D:1127:TYR:OH	2.44	0.44
2:H:3076:SER:N	2:H:3077:SER:HB3	2.33	0.44
1:G:3011:MET:HE3	1:G:3021:MET:HG2	2.00	0.44
2:B:54:SER:HB2	2:B:55:ASP:CB	2.28	0.44
1:G:3090:ARG:HB2	1:G:3091:THR:H	1.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3192:THR:HG23	1:G:3207:SER:HB2	2.00	0.44
2:F:2034:MET:HB3	2:F:2034:MET:HE2	1.74	0.44
2:D:1149:GLY:HA2	2:D:1179:LEU:HB3	2.00	0.44
1:C:1128:GLY:C	1:E:2184:GLU:N	2.67	0.44
1:C:1184:GLU:N	1:G:3128:GLY:C	2.67	0.44
2:B:149:GLY:HA2	2:B:179:LEU:HB3	2.00	0.44
1:C:1124:LEU:CD2	1:E:2184:GLU:CA	2.88	0.43
2:H:3075:SER:N	2:H:3076:SER:C	2.66	0.43
2:D:1054:SER:HB2	2:D:1055:ASP:CB	2.28	0.43
2:F:2075:SER:N	2:F:2076:SER:C	2.66	0.43
2:D:1032:LYS:HD3	2:D:1100:VAL:HG22	2.01	0.43
1:C:1032:MET:HG3	1:C:1070:TYR:CG	2.54	0.43
1:E:2011:MET:HE3	1:E:2021:MET:HG2	2.01	0.43
2:B:197:THR:HG23	2:B:214:LYS:HE3	1.99	0.43
2:F:2076:SER:N	2:F:2077:SER:HB3	2.33	0.43
1:C:1184:GLU:HB3	1:G:3128:GLY:H	1.84	0.43
1:C:1184:GLU:HA	1:G:3124:LEU:N	2.26	0.43
1:E:2128:GLY:C	1:G:3184:GLU:N	2.67	0.43
1:G:3032:MET:HG3	1:G:3070:TYR:CG	2.54	0.43
1:E:2032:MET:HG3	1:E:2070:TYR:CG	2.54	0.43
1:E:2124:LEU:CB	1:G:3187:ARG:N	2.78	0.43
2:B:32:LYS:HD3	2:B:100:VAL:HG22	2.01	0.43
2:D:1102:ARG:HA	2:D:1103:GLY:HA2	1.68	0.43
2:F:2102:ARG:HA	2:F:2103:GLY:HA2	1.68	0.43
2:D:1204:HIS:HA	2:D:1205:PRO:HD3	1.88	0.43
1:A:32:MET:HG3	1:A:70:TYR:CG	2.54	0.43
1:C:1154:ARG:HH11	2:H:3127:TYR:HE1	1.67	0.43
1:C:1187:ARG:CD	1:G:3124:LEU:HG	2.45	0.43
2:B:50:ASN:HD21	2:B:59:HIS:CB	2.27	0.43
2:D:1076:SER:N	2:D:1077:SER:HB3	2.33	0.43
2:H:3065:LYS:HA	2:H:3066:ASP:HA	1.66	0.43
2:H:3102:ARG:HA	2:H:3103:GLY:HA2	1.68	0.43
2:F:2032:LYS:HD3	2:F:2100:VAL:HG22	2.01	0.43
2:F:2149:GLY:HA2	2:F:2179:LEU:HB3	2.00	0.43
1:C:1124:LEU:HG	1:E:2187:ARG:CD	2.45	0.42
1:C:1153:GLU:H	2:H:3213:LYS:NZ	2.04	0.42
1:C:1185:TYR:CA	1:G:3182:LYS:CD	2.84	0.42
1:C:1187:ARG:N	1:G:3124:LEU:CB	2.78	0.42
2:H:3050:ASN:HD22	2:H:3050:ASN:H	1.67	0.42
1:A:11:MET:HE3	1:A:21:MET:HG2	2.01	0.42
1:C:1125:THR:OG1	1:E:2149:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TYR:CZ	1:A:90:ARG:NH1	2.74	0.42
1:C:1149:ILE:HG23	1:G:3125:THR:OG1	2.19	0.42
1:C:1188:HIS:CE1	1:G:3120:SER:HB2	2.55	0.42
2:H:3032:LYS:HD3	2:H:3100:VAL:HG22	2.01	0.42
1:C:1011:MET:HE3	1:C:1021:MET:HG2	2.01	0.42
2:D:1075:SER:N	2:D:1076:SER:C	2.66	0.42
1:C:1120:SER:HB2	1:E:2188:HIS:CE1	2.55	0.42
1:E:2120:SER:CB	1:G:3188:HIS:CE1	3.02	0.42
1:E:2154:ARG:HH11	2:D:1127:TYR:HE1	1.67	0.42
2:F:2065:LYS:HA	2:F:2066:ASP:HA	1.66	0.42
2:H:3050:ASN:HD21	2:H:3059:HIS:CB	2.27	0.42
1:E:2122:GLU:HA	1:G:3149:ILE:HD13	2.02	0.42
2:B:34:MET:HE2	2:B:34:MET:HB3	1.81	0.42
1:E:2057:VAL:HA	1:E:2058:PRO:HD3	1.94	0.42
2:B:76:SER:N	2:B:77:SER:HB3	2.33	0.42
2:B:151:PHE:HA	2:B:152:PRO:HA	1.89	0.42
2:H:3012:VAL:HG21	2:H:3018:VAL:HG22	2.02	0.42
1:C:1033:TYR:CZ	1:C:1090:ARG:NH1	2.73	0.42
1:C:1120:SER:CB	1:E:2188:HIS:CE1	3.02	0.42
1:G:3154:ARG:HH11	2:F:2127:TYR:HE1	1.67	0.42
1:E:2125:THR:OG1	1:G:3149:ILE:HG23	2.20	0.41
2:D:1050:ASN:HD21	2:D:1059:HIS:CB	2.27	0.41
2:H:3039:GLN:HB2	2:H:3045:LEU:HD23	2.03	0.41
1:E:2120:SER:HB2	1:G:3188:HIS:CE1	2.55	0.41
1:E:2019:VAL:HB	1:E:2074:ILE:HB	2.02	0.41
2:B:50:ASN:ND2	2:B:50:ASN:N	2.67	0.41
1:C:1202:SER:HA	1:C:1203:PRO:HD3	1.88	0.41
2:B:50:ASN:HD22	2:B:50:ASN:H	1.67	0.41
2:D:1039:GLN:HB2	2:D:1045:LEU:HD23	2.03	0.41
2:F:2050:ASN:ND2	2:F:2050:ASN:N	2.67	0.41
1:A:117:PHE:HA	1:A:118:PRO:HD3	1.93	0.41
2:B:34:MET:HE1	2:B:96:CYS:SG	2.60	0.41
1:C:1119:PRO:O	1:E:2187:ARG:HB3	2.20	0.41
1:E:2156:ASN:CB	2:D:1125:SER:OG	2.63	0.41
2:D:1012:VAL:HG21	2:D:1018:VAL:HG22	2.02	0.41
1:C:1187:ARG:HB3	1:G:3119:PRO:O	2.20	0.41
1:E:2124:LEU:CG	1:G:3187:ARG:HD3	2.49	0.41
2:B:12:VAL:HG21	2:B:18:VAL:HG22	2.02	0.41
2:F:2023:LYS:HA	2:F:2078:THR:HG22	2.03	0.41
2:F:2039:GLN:HB2	2:F:2045:LEU:HD23	2.03	0.41
1:C:1188:HIS:CE1	1:G:3120:SER:CB	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2125:THR:HG21	1:G:3191:TYR:HD1	1.85	0.41
2:F:2050:ASN:HD21	2:F:2059:HIS:CB	2.27	0.41
2:F:2171:PHE:HA	2:F:2172:PRO:HD3	1.94	0.41
1:E:2033:TYR:CZ	1:E:2090:ARG:NH1	2.74	0.41
1:E:2119:PRO:O	1:G:3187:ARG:HB3	2.20	0.41
2:D:1023:LYS:HA	2:D:1078:THR:HG22	2.03	0.41
1:A:19:VAL:HB	1:A:74:ILE:HB	2.02	0.40
1:A:194:GLU:HG2	1:A:205:VAL:HG22	2.04	0.40
1:C:1191:TYR:CD1	1:G:3125:THR:HG21	2.47	0.40
2:D:1100:VAL:O	2:D:1101:THR:HG22	2.21	0.40
2:H:3023:LYS:HA	2:H:3078:THR:HG22	2.03	0.40
2:H:3100:VAL:O	2:H:3101:THR:HG22	2.21	0.40
1:C:1191:TYR:OH	1:G:3125:THR:HA	2.21	0.40
2:B:100:VAL:O	2:B:101:THR:HG22	2.21	0.40
2:F:2012:VAL:HG21	2:F:2018:VAL:HG22	2.02	0.40
1:C:1194:GLU:HG2	1:C:1205:VAL:HG22	2.04	0.40
1:G:3156:ASN:CB	2:F:2125:SER:OG	2.63	0.40
2:B:74:LYS:HE3	2:B:74:LYS:H	1.86	0.40
2:F:2010:GLU:HG2	2:F:2018:VAL:HG13	2.03	0.40
2:F:2100:VAL:O	2:F:2101:THR:HG22	2.21	0.40
1:C:1019:VAL:HB	1:C:1074:ILE:HB	2.02	0.40
1:G:3194:GLU:HG2	1:G:3205:VAL:HG22	2.04	0.40
2:B:10:GLU:HG2	2:B:18:VAL:HG13	2.03	0.40
2:D:1010:GLU:HG2	2:D:1018:VAL:HG13	2.03	0.40
1:C:1149:ILE:HD13	1:G:3122:GLU:HA	2.02	0.40
1:C:1154:ARG:HD3	2:H:3127:TYR:HE1	1.87	0.40
2:H:3010:GLU:HG2	2:H:3018:VAL:HG13	2.03	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%)	11	46
1	C	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	11	46
1	E	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	11	46
1	G	210/212 (99%)	195 (93%)	12 (6%)	3 (1%)	11	46
2	B	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	5	30
2	D	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	5	30
2	F	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	5	30
2	H	216/218 (99%)	188 (87%)	22 (10%)	6 (3%)	5	30
All	All	1704/1720 (99%)	1532 (90%)	136 (8%)	36 (2%)	10	36

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
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

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Mol	Chain	Res	Type
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%)	25 51
1	C	187/187 (100%)	178 (95%)	9 (5%)	25 51
1	E	187/187 (100%)	178 (95%)	9 (5%)	25 51
1	G	187/187 (100%)	178 (95%)	9 (5%)	25 51
2	B	189/189 (100%)	182 (96%)	7 (4%)	34 58
2	D	189/189 (100%)	182 (96%)	7 (4%)	34 58
2	F	189/189 (100%)	182 (96%)	7 (4%)	34 58
2	H	189/189 (100%)	182 (96%)	7 (4%)	34 58
All	All	1504/1504 (100%)	1440 (96%)	64 (4%)	33 53

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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
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

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Mol	Chain	Res	Type
2	H	3050	ASN
2	H	3061	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

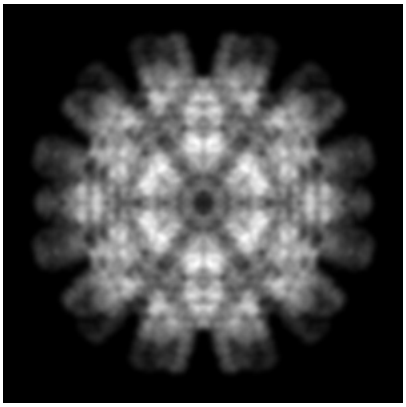
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5579. These allow visual inspection of the internal detail of the map and identification of artifacts.

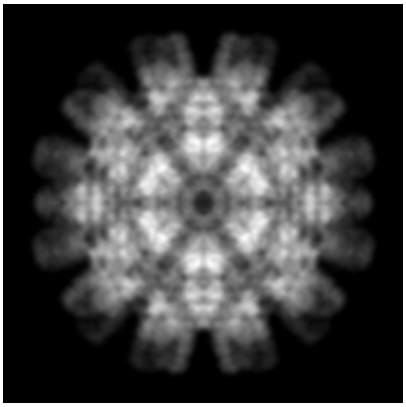
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

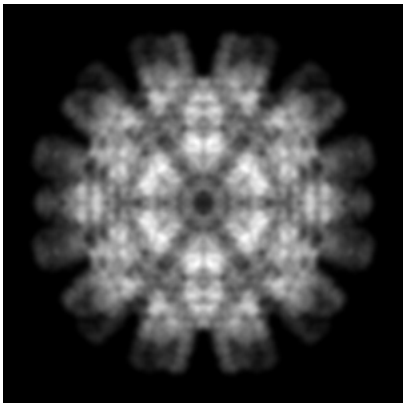
6.1.1 Primary map



X



Y

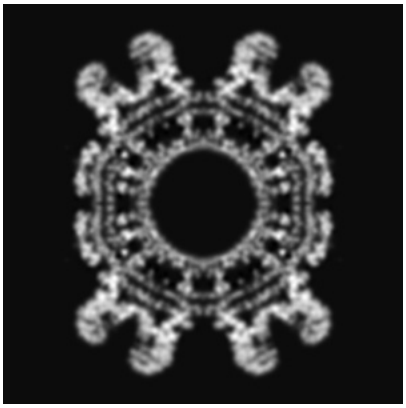


Z

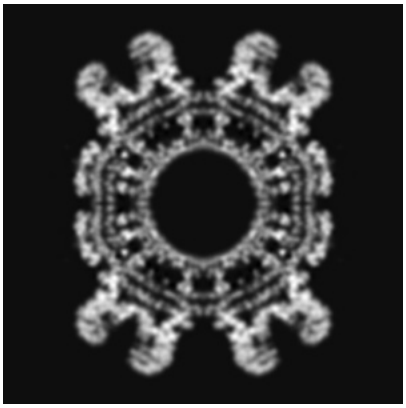
The images above show the map projected in three orthogonal directions.

6.2 Central slices

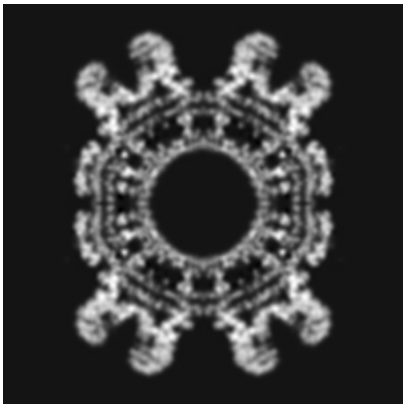
6.2.1 Primary map



X Index: 200



Y Index: 200

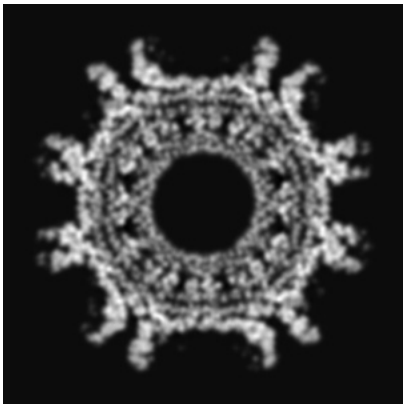


Z Index: 200

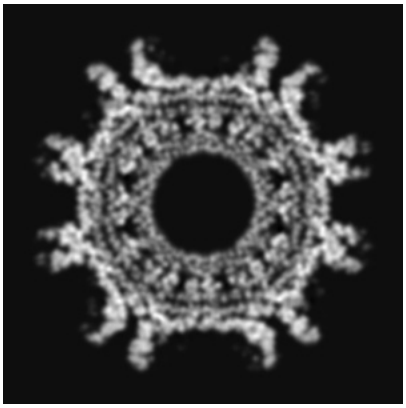
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

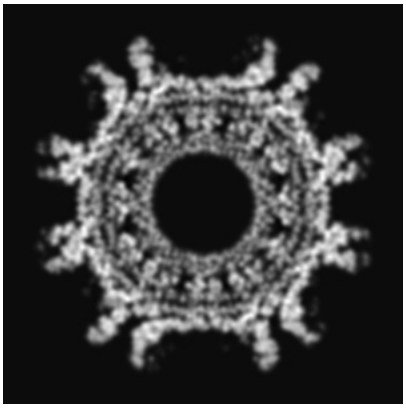
6.3.1 Primary map



X Index: 186



Y Index: 186

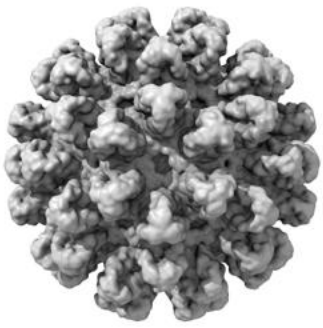


Z Index: 214

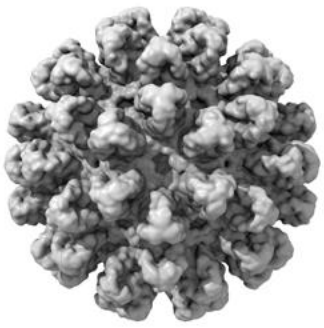
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

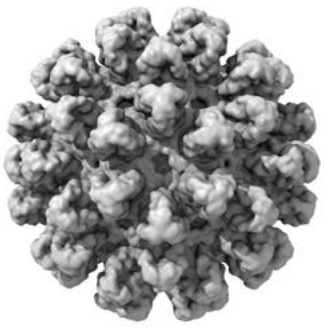
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

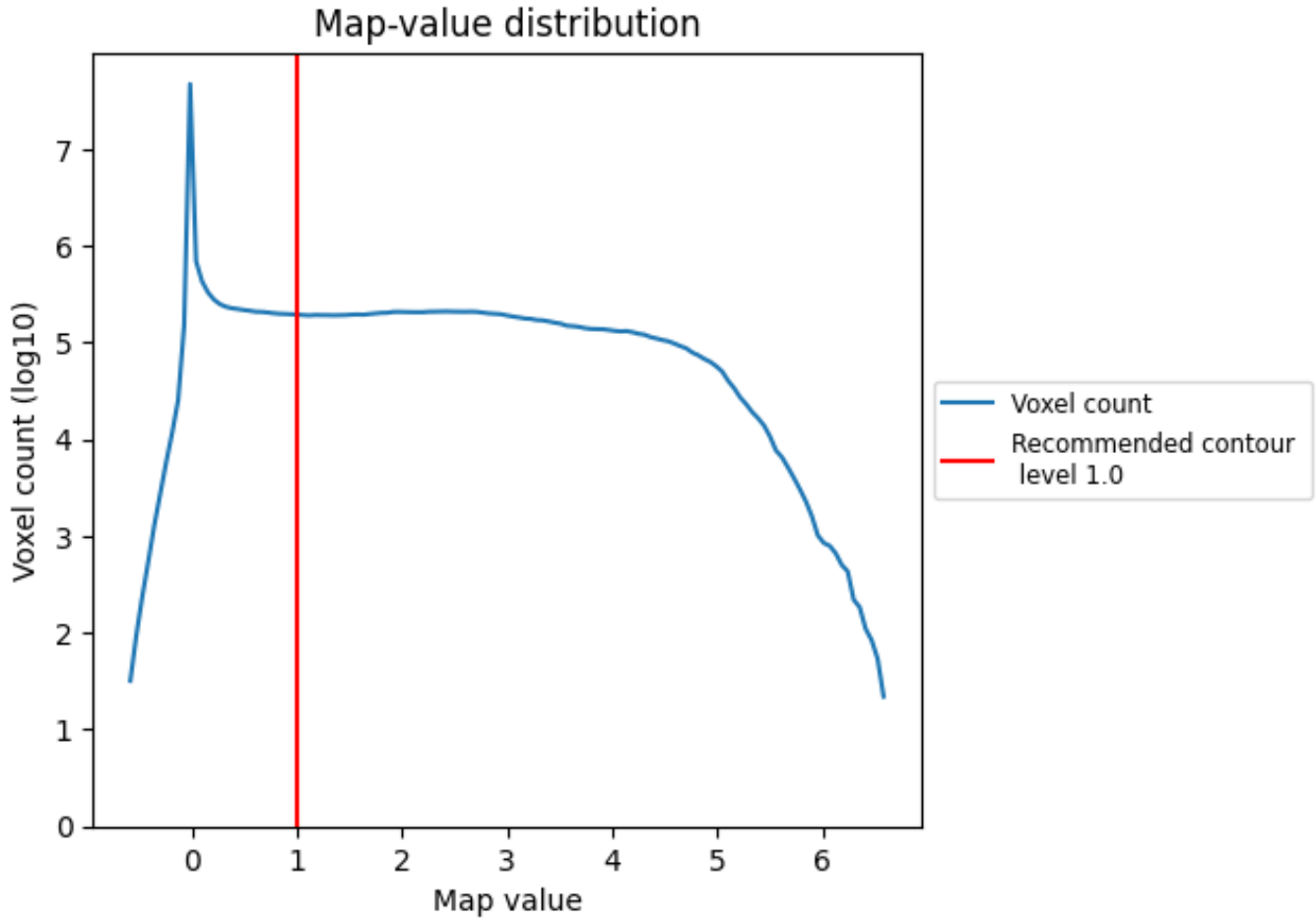
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

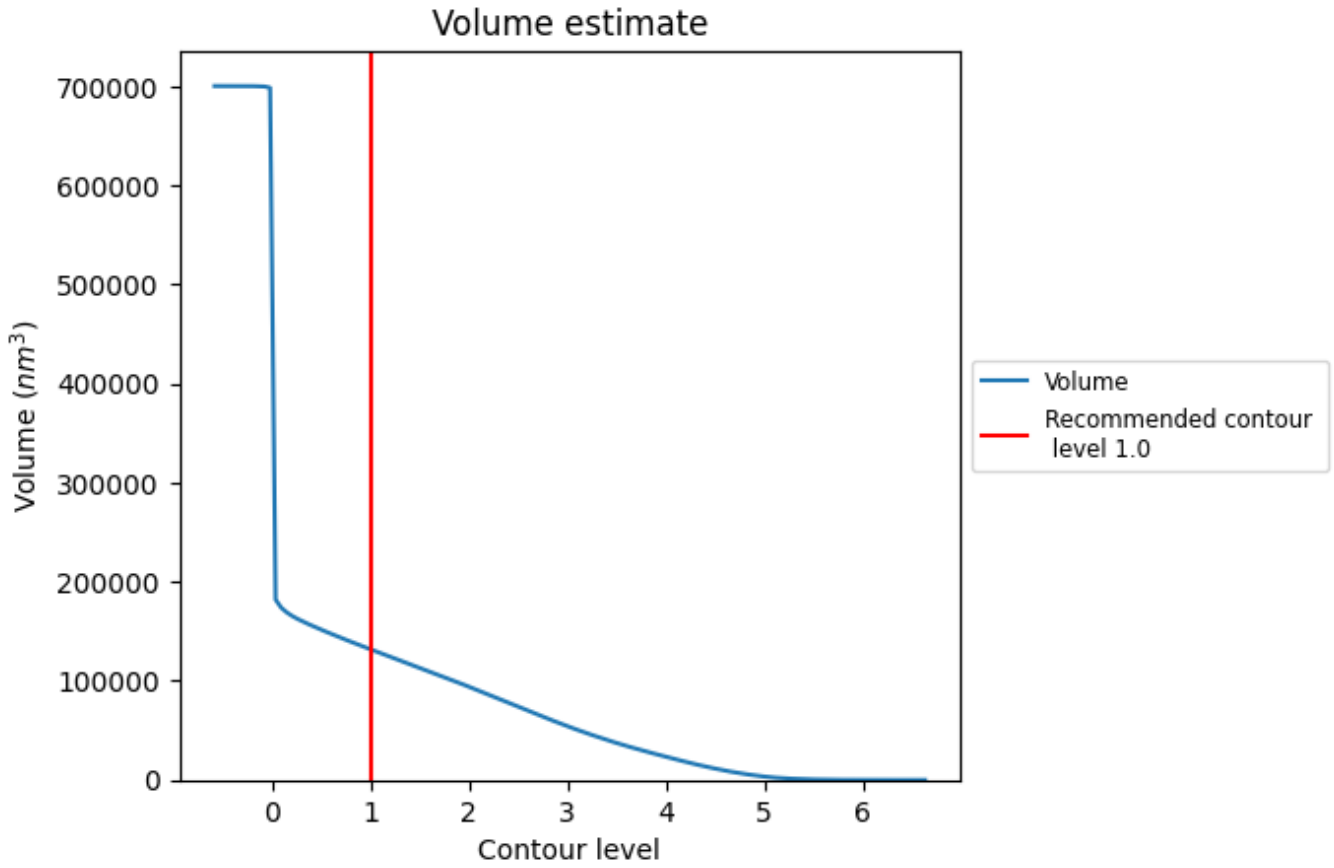
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

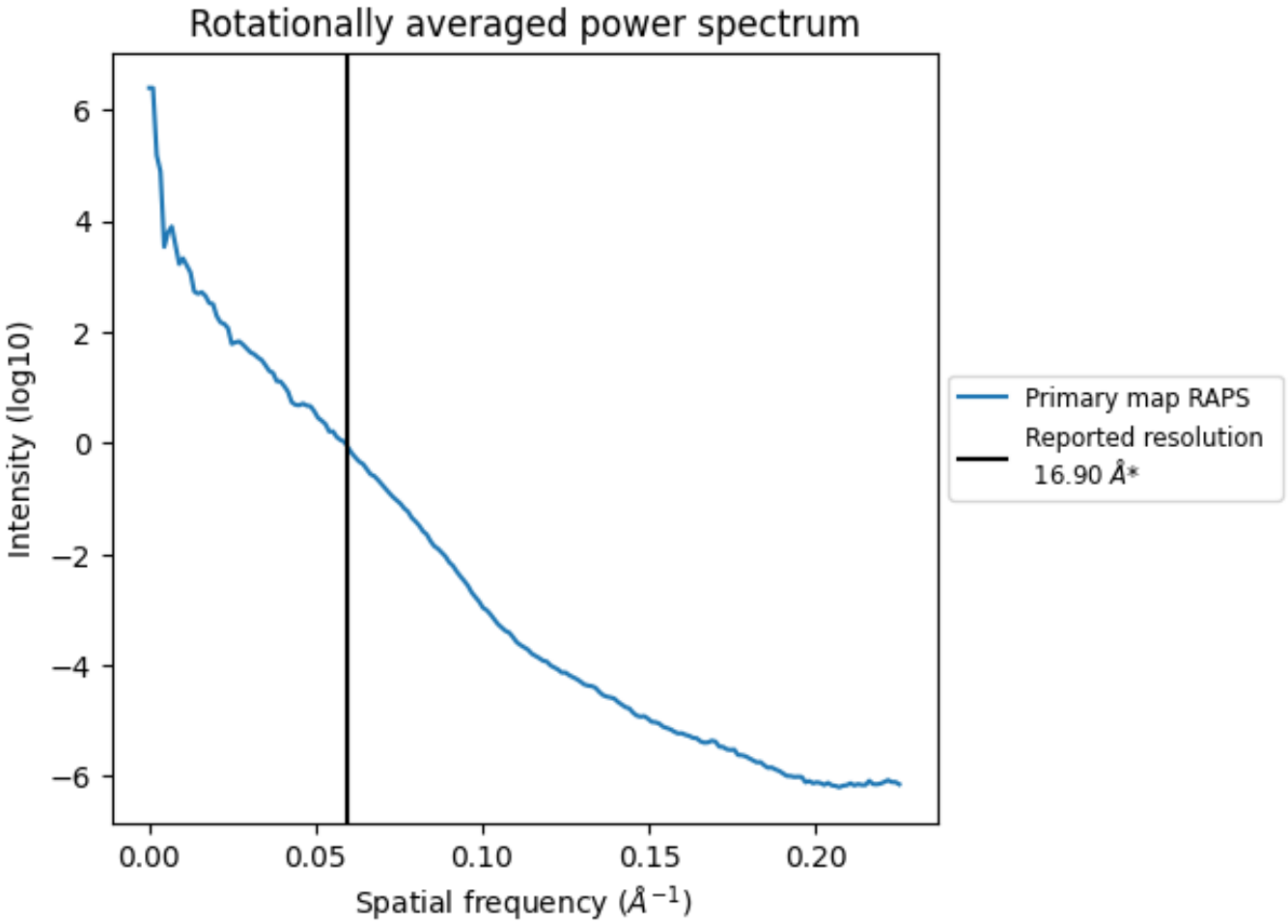
7.2 Volume estimate



The volume at the recommended contour level is 131853 nm^3; this corresponds to an approximate mass of 119106 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.059 Å^{-1}

8 Fourier-Shell correlation

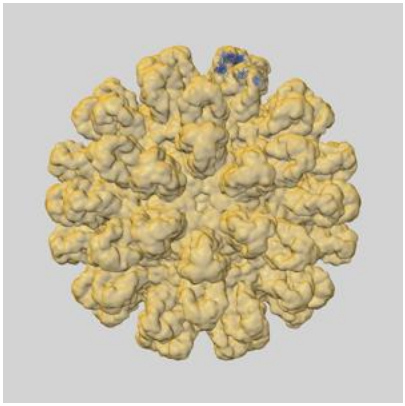
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

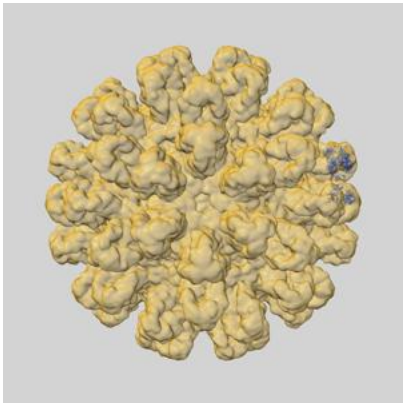
This section contains information regarding the fit between EMDB map EMD-5579 and PDB model 3J2Z. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

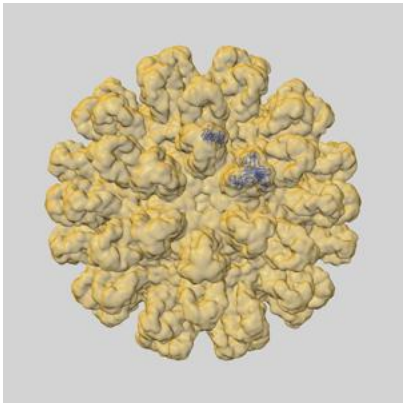
9.1.1 Map-model overlay



X

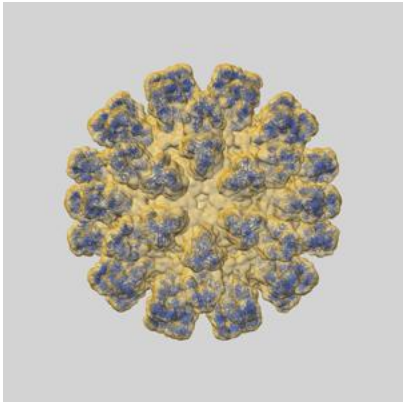


Y

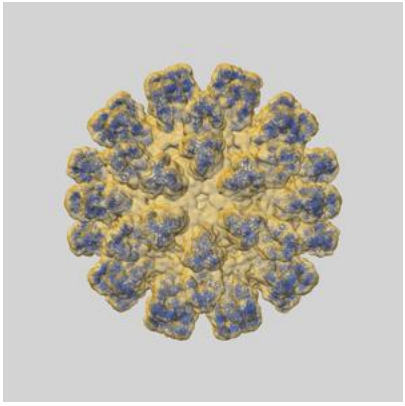


Z

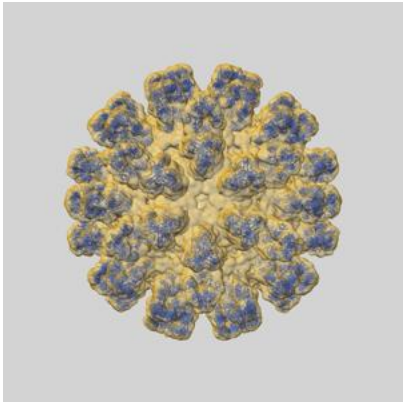
9.1.2 Map-model assembly overlay



X



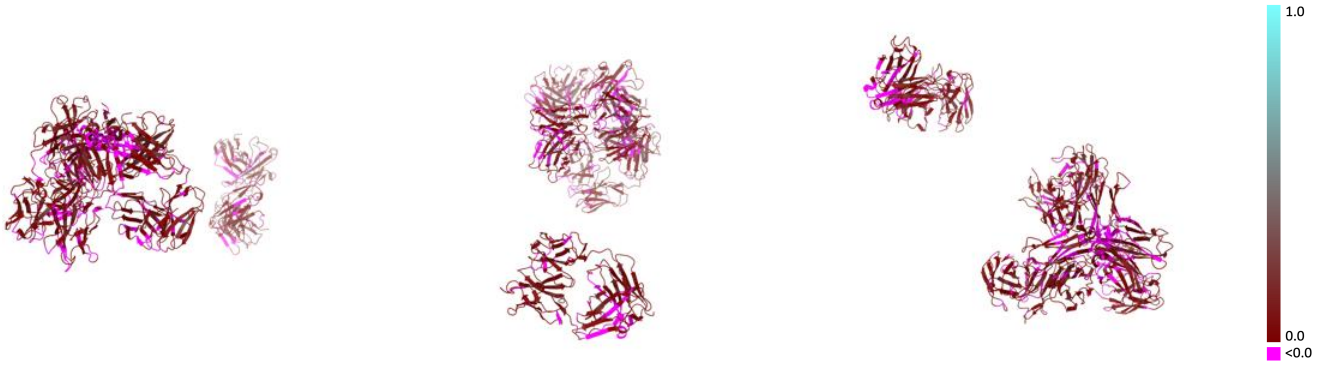
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

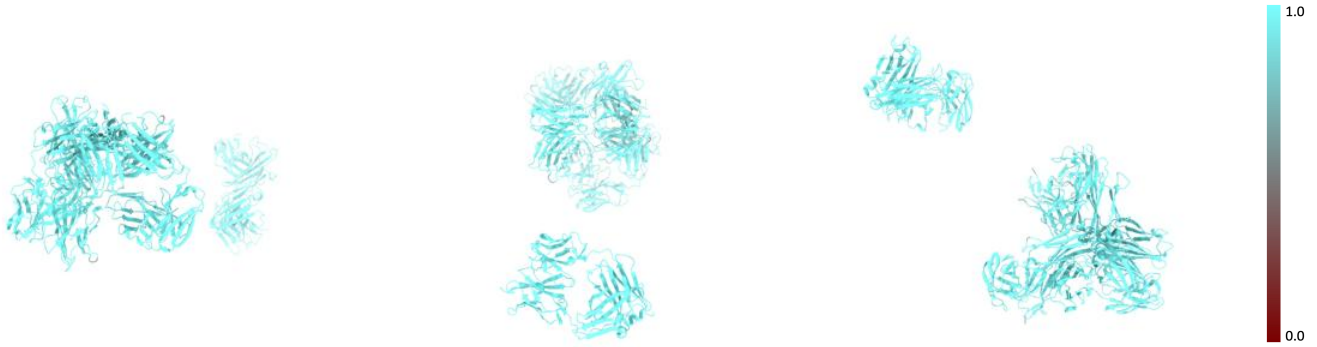
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

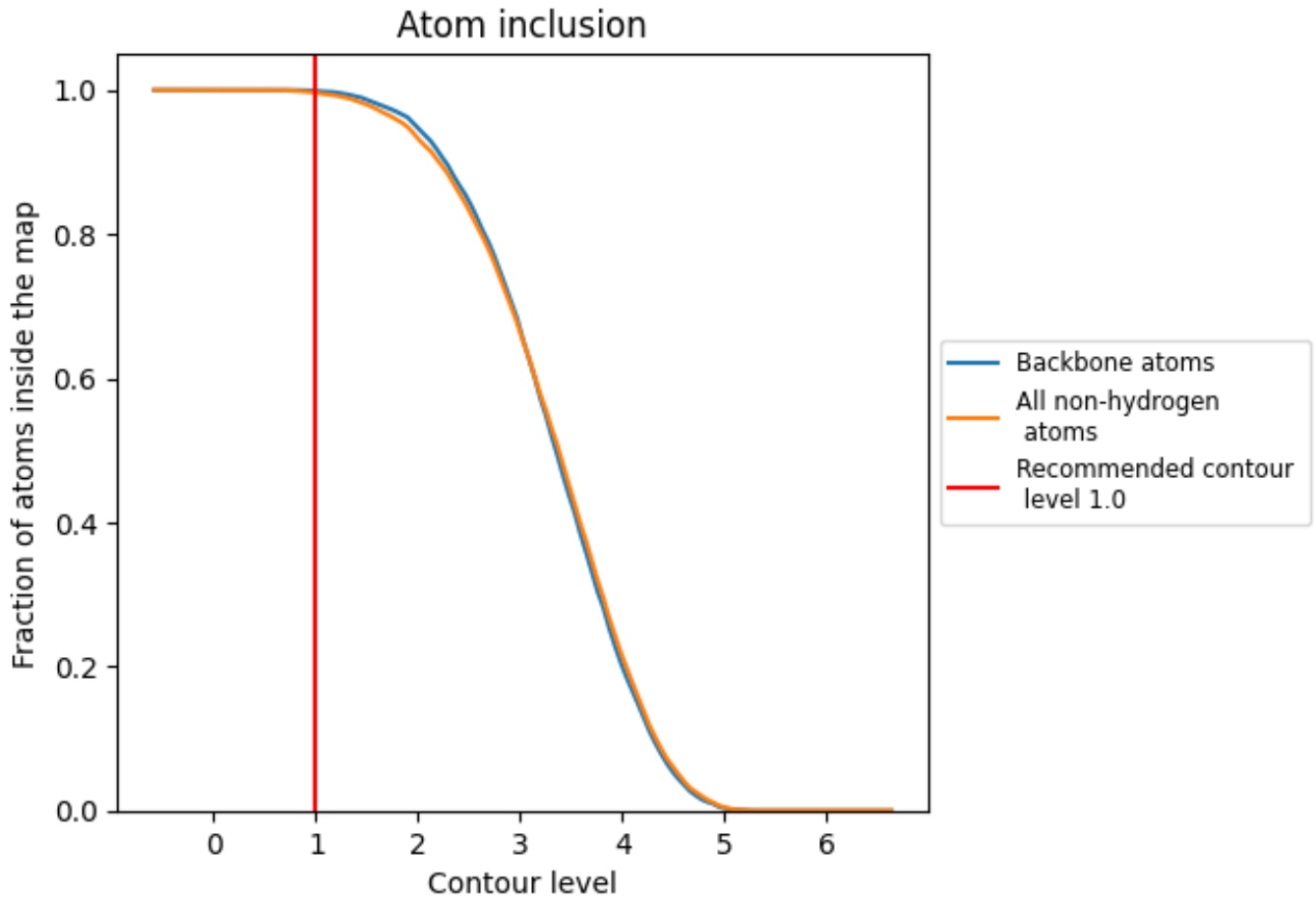
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9964	0.0550
A	1.0000	0.0580
B	0.9988	0.0680
C	0.9956	0.0520
D	0.9975	0.0610
E	0.9969	0.0450
F	0.9951	0.0500
G	1.0000	0.0460
H	0.9871	0.0640