Full wwPDB EM Validation Report

Aug 17, 2024 – 12:31 pm BST

PDB ID	:	8QBE
EMDB ID	:	EMD-18311
Title	:	Compact state - Pil1 in native eisosome lattice bound to plasma membrane microdomain
Authors	:	Kefauver, J.M.; Zou, L.; Desfosses, A.; Loewith, R.J.
Deposited on	:	2023-08-24
Resolution	:	3.67 Å(reported)
Based on initial model	:	.

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 (i) 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 (i)) were used in the production of this report:

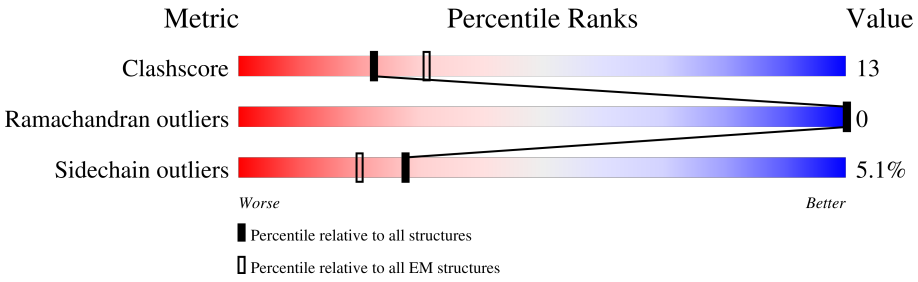
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.67 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	339	6% 54% 25% · 20%
1	B	339	6% 56% 22% · 20%
1	C	339	19% 55% 23% · 20%
1	D	339	42% 55% 24% · 20%
1	E	339	67% 56% 23% · 20%
1	F	339	24% 55% 24% · 20%
1	G	339	32% 56% 22% · 20%
1	H	339	51% 55% 24% · 20%

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Mol	Chain	Length	Quality of chain
1	I	339	26% 55% 24% 20%
1	J	339	33% 55% 23% 20%
1	K	339	56% 56% 22% 20%
1	L	339	17% 55% 24% 20%
1	M	339	47% 55% 24% 20%
1	N	339	69% 56% 23% 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 30058 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 Sphingolipid long chain base-responsive protein PIL1.

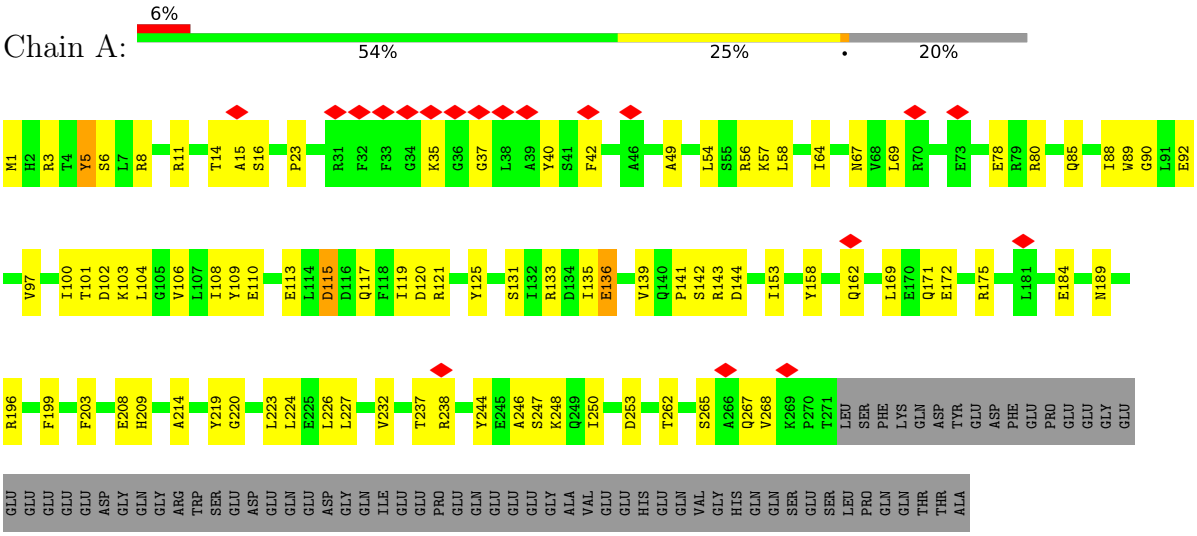
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	B	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	C	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	I	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	D	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	J	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	E	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	K	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	F	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	L	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	G	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	M	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	H	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		
1	N	271	Total	C	N	O	S	0	0
			2147	1346	374	425	2		

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.

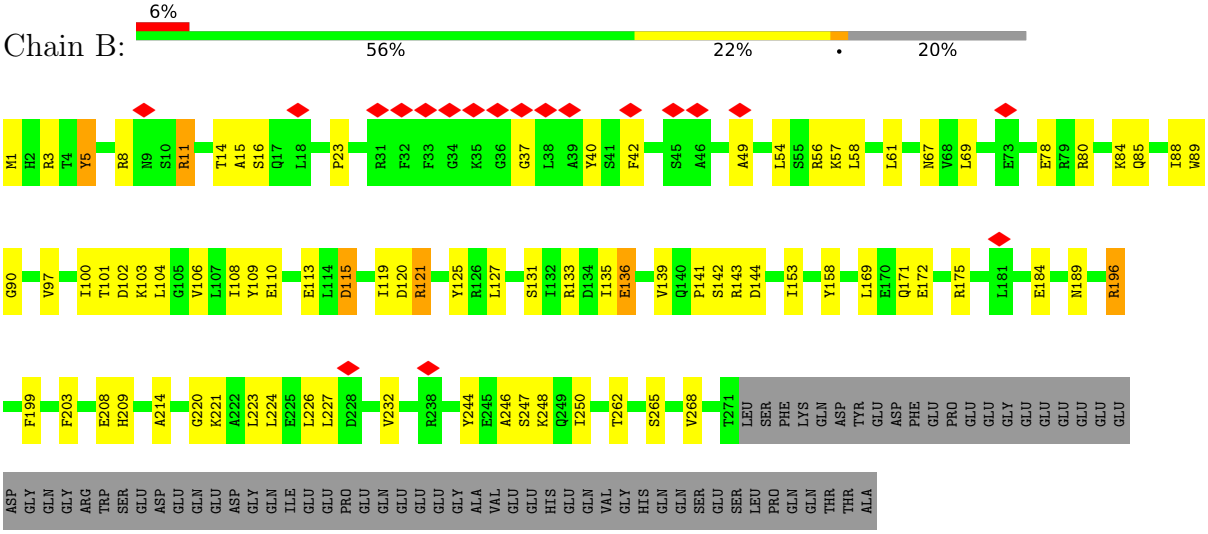
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain A:



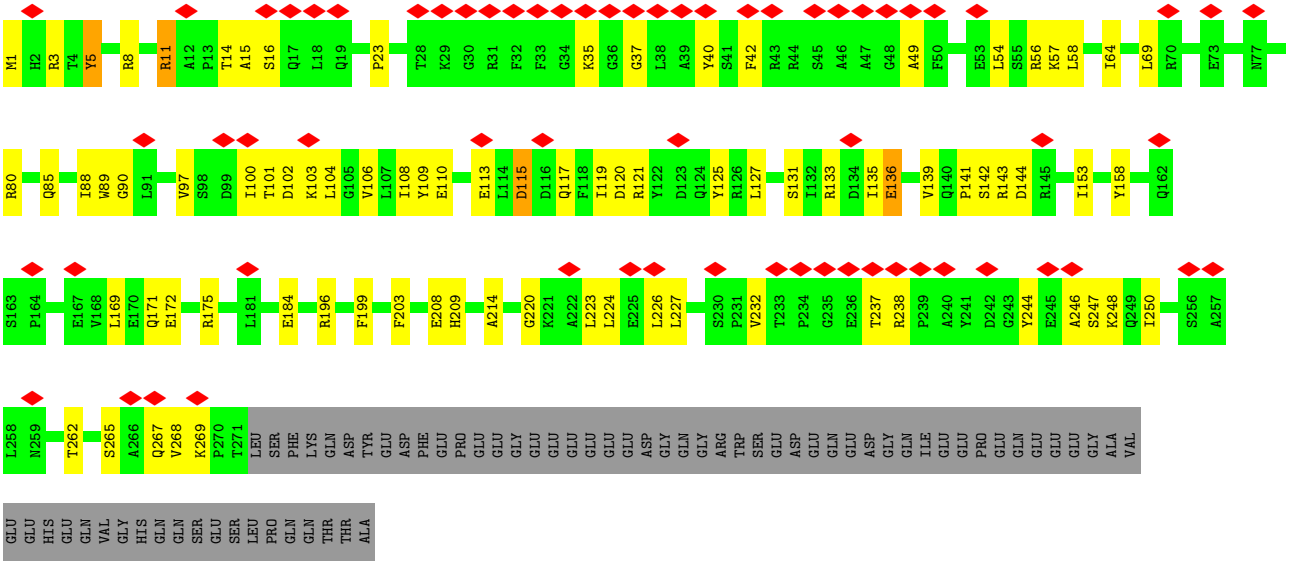
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain B:



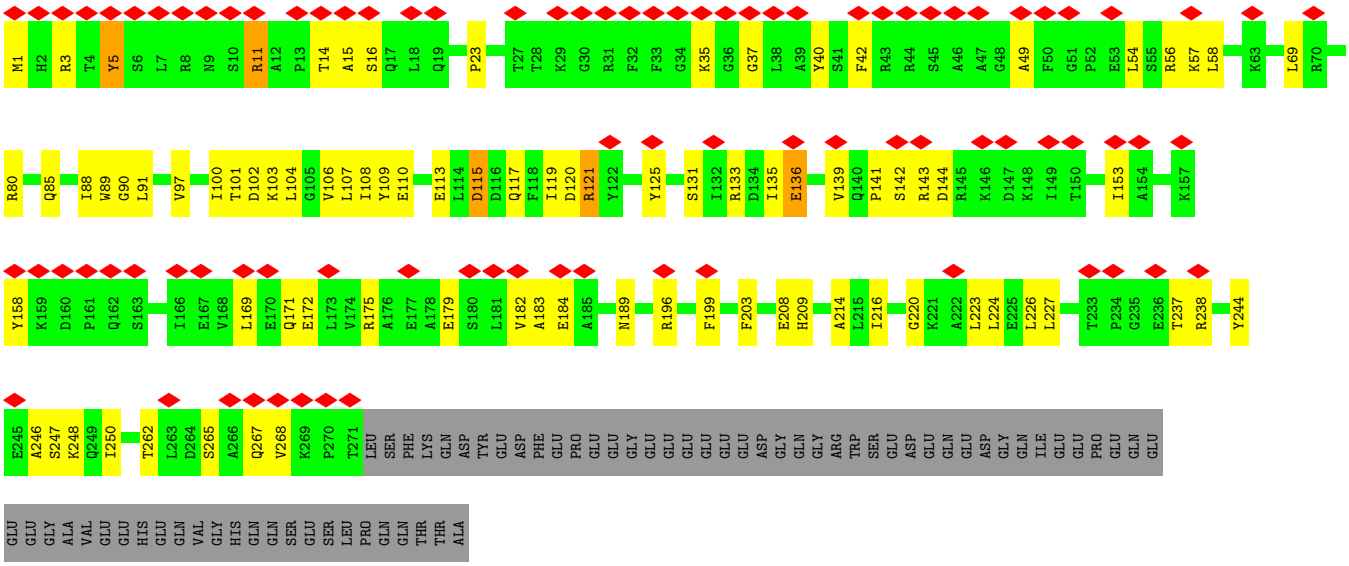
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain C:



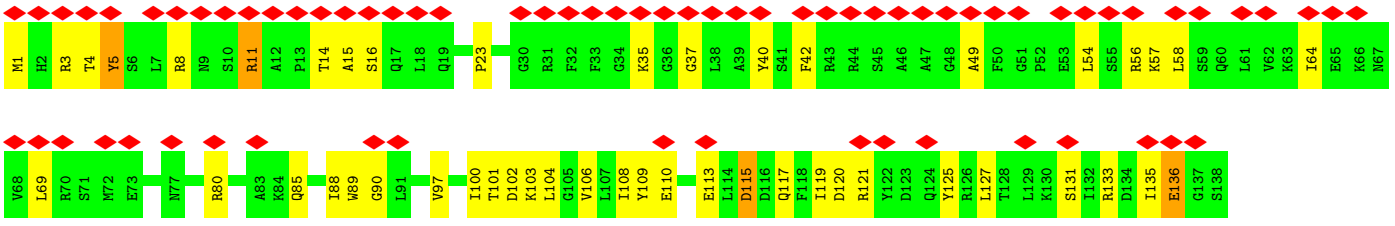
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

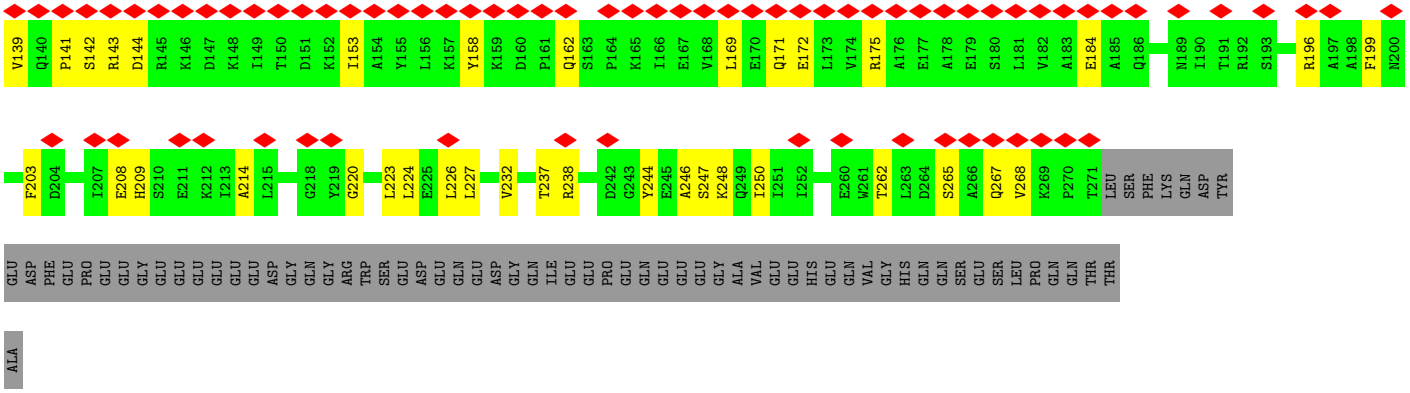
Chain I:



• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

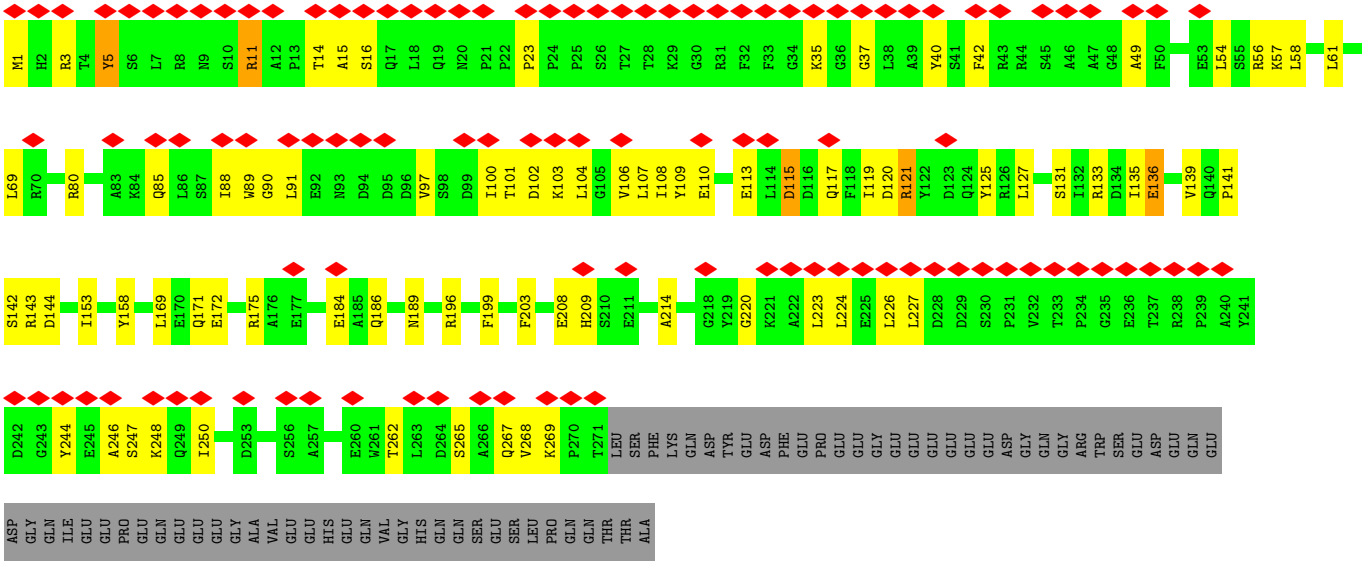
Chain D:





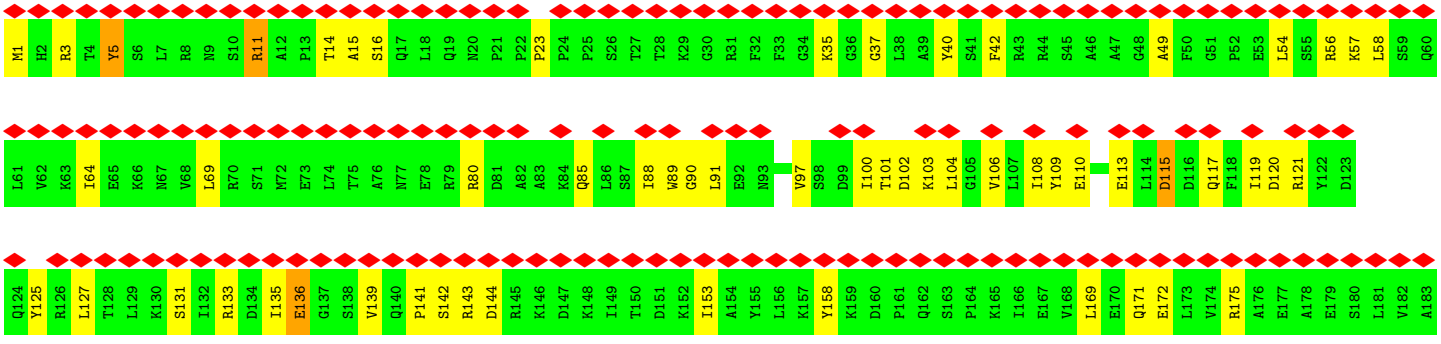
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

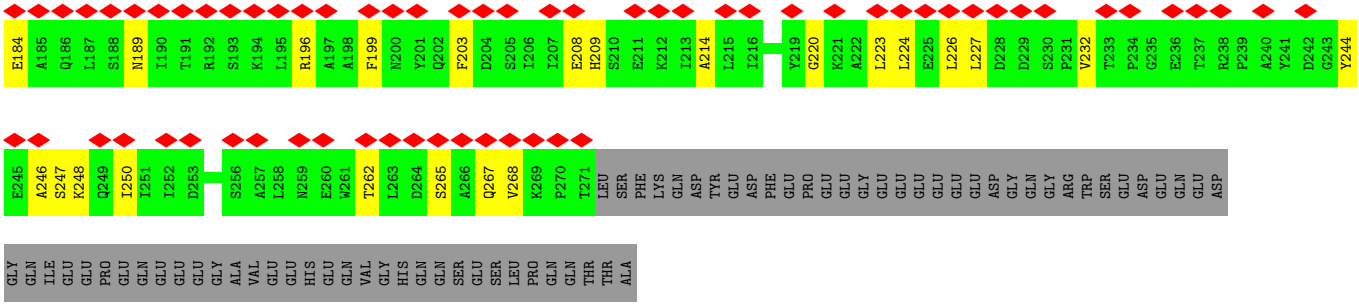
Chain J:



• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain E:



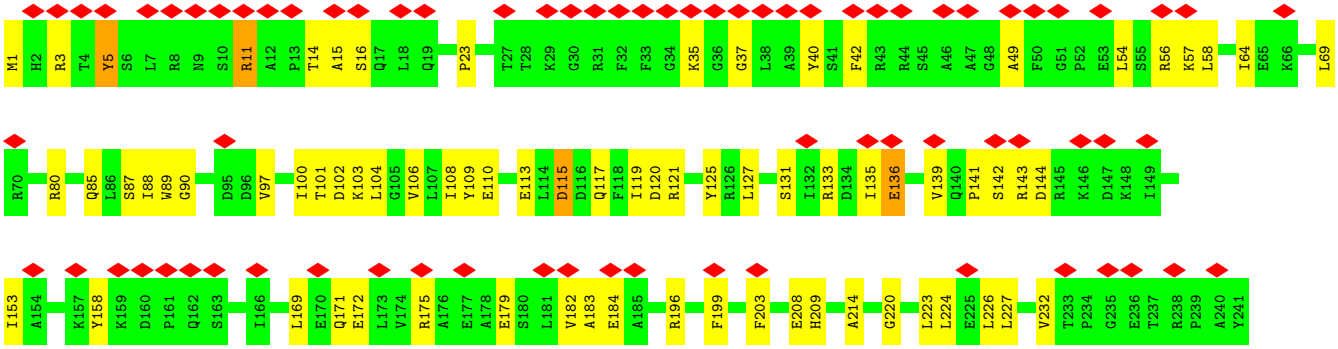


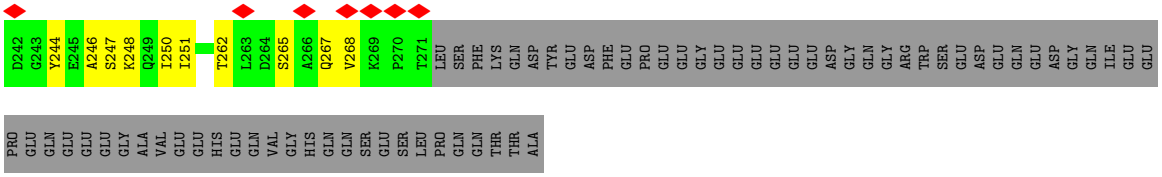
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain K:

• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

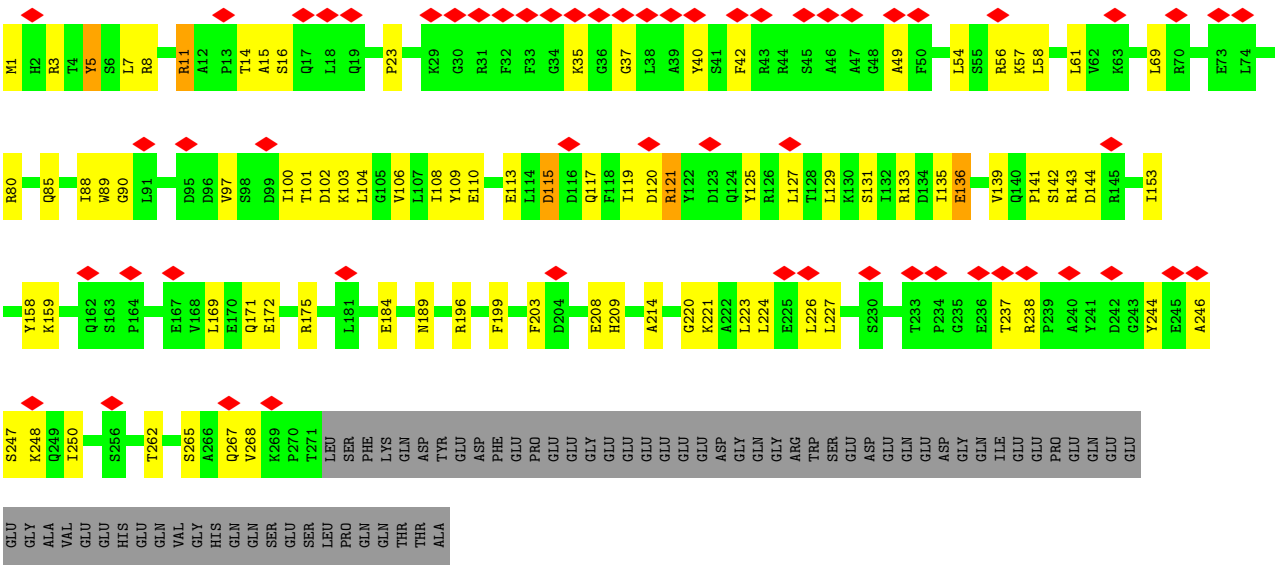
Chain F:





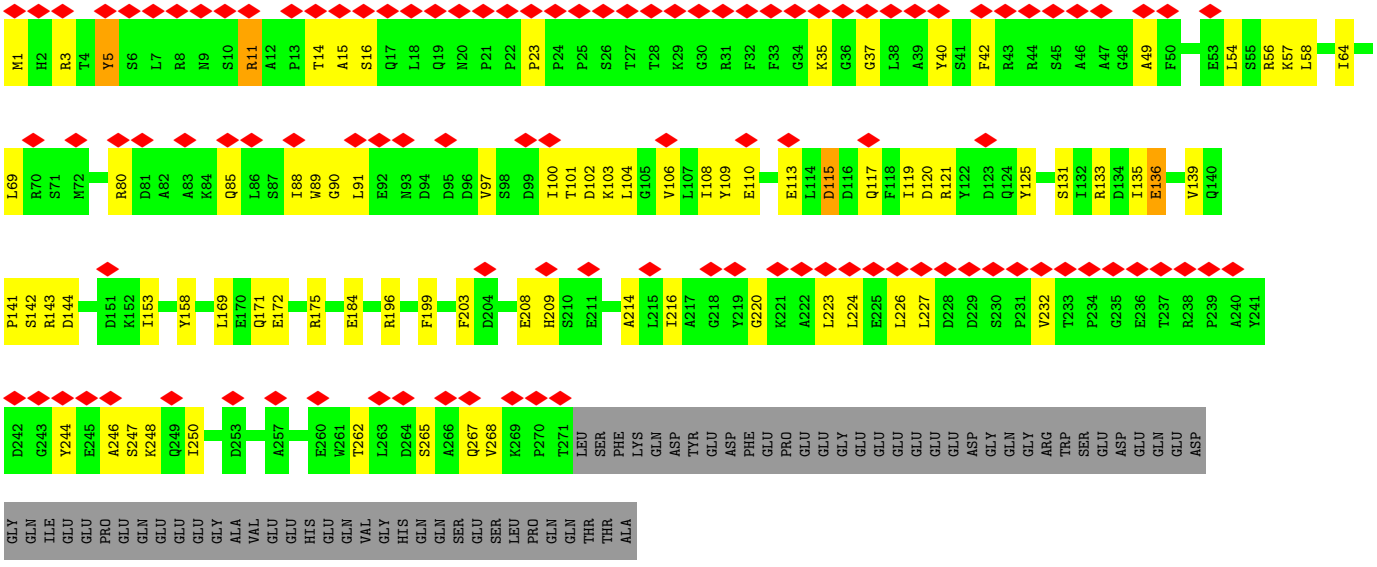
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain L:



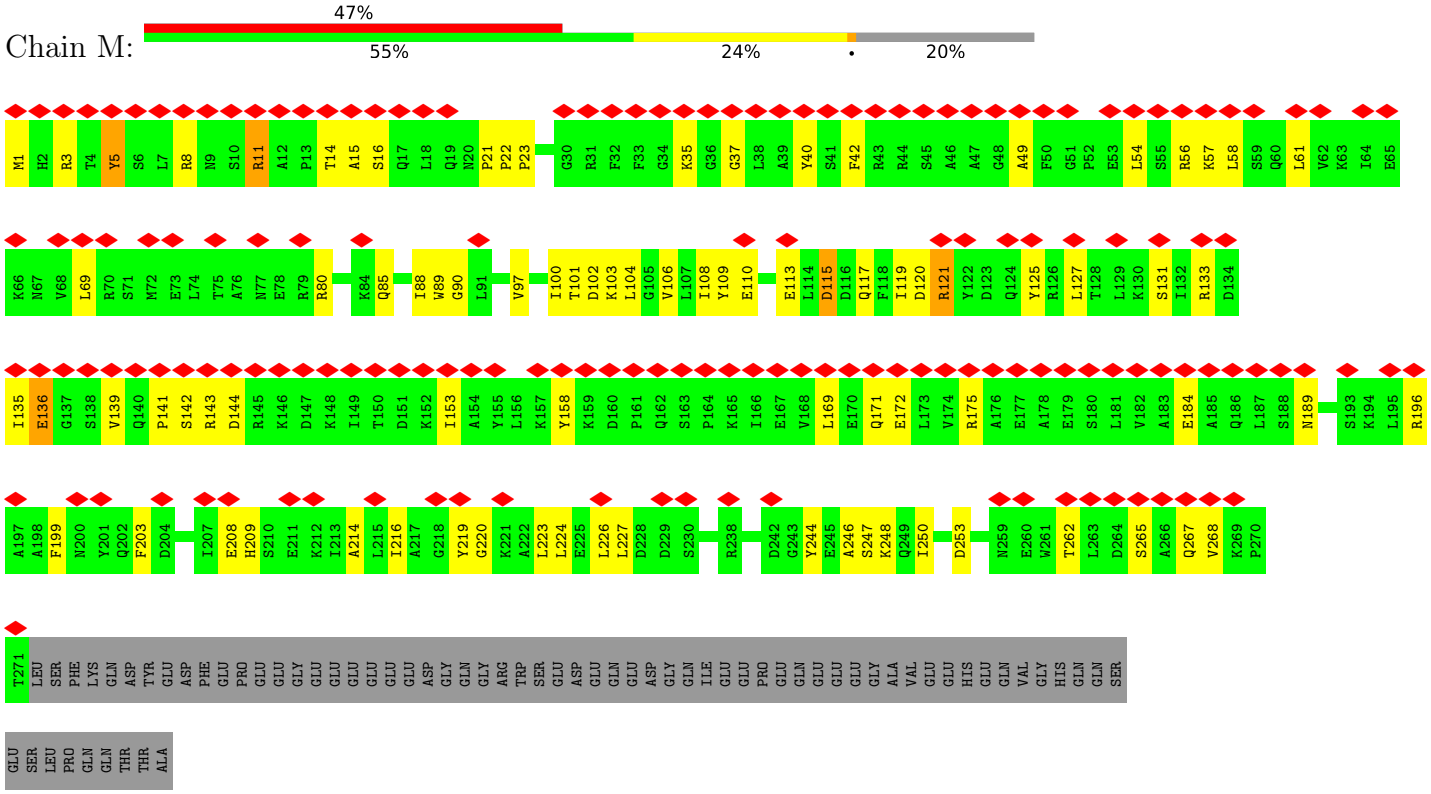
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain G:



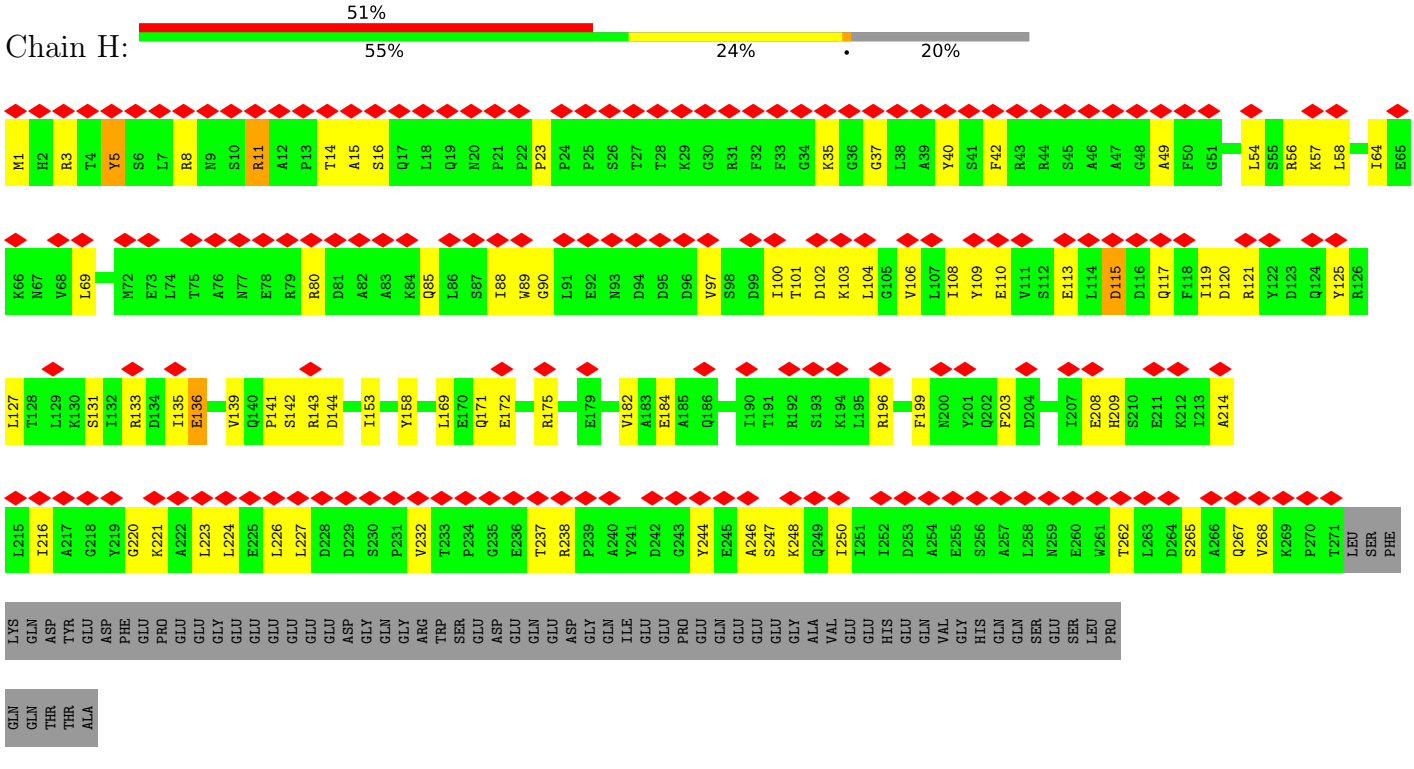
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain M:



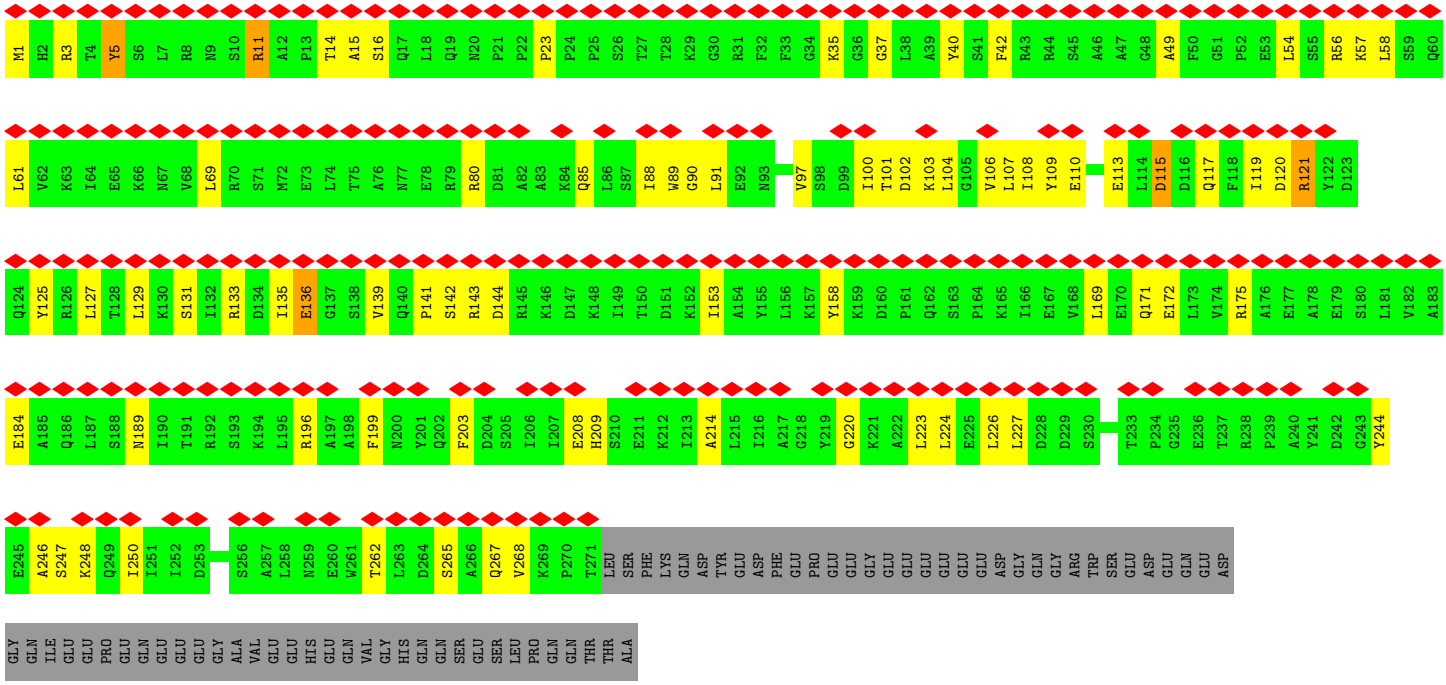
• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain H:



• Molecule 1: Sphingolipid long chain base-responsive protein PIL1

Chain N:


M1 H2 R3 T4 Y5 S6 L7 R8 N9 S10 R11 A12 P13 T14 A15 S16 Q17 L18 Q19 N20 P21 P22 P23 P24 P25 S26 T27 T28 K29 G30 R31 F32 F33 G34 K35 G36 G37 L38 A39 Y40 S41 F42 R43 R44 S45 A46 A47 G48 A49 F50 G51 P52 E53 L54 S55 R56 K57 L58 S59 Q60
L61 V62 K63 I64 E65 K66 N67 V68 L69 R70 S71 M72 E73 L74 T75 A76 N77 E78 R79 R80 D81 A82 A83 K84 Q85 L86 S87 I88 W89 G90 L91 E92 N93 V97 S98 D99 I100 T101 D102 K103 L104 G105 V106 L107 I108 Y109 E110 E113 L114 D115 D116 Q117 F118 I119 D120 R121 Y122 D123
Q124 Y125 R126 L127 T128 L129 K130 S131 I132 R133 D134 I135 E136 G137 S138 V139 Q140 P141 S142 R143 D144 R145 K146 D147 K148 I149 T150 D151 K152 I153 A154 Y155 L156 K157 Y158 K159 D160 P161 Q162 S163 P164 K165 I166 E167 V168 L169 E170 Q171 E172 L173 V174 R175 A176 E177 A178 E179 S180 L181 V182 A183
E184 A185 Q186 L187 S188 N189 I190 T191 R192 S193 K194 L195 R196 A197 A198 F199 N200 Y201 Q202 F203 D204 S205 I206 I207 E208 H209 S210 E211 K212 I213 A214 L215 I216 A217 G218 Y219 G220 K221 A222 L223 L224 E225 L226 L227 D228 D229 S230 T233 P234 G235 E236 T237 R238 P239 A240 Y241 D242 G243 Y244
E245 A246 S247 K248 Q249 I250 I251 I252 D253 S256 A257 L258 N259 E260 W261 T262 L263 D264 S265 A266 Q267 V268 K269 P270 T271 LEU SER PHE LYS GLN ASP TYR GLU ASP PHE GLU PRO GLU GLU GLY GLU GLU GLU GLU GLU GLU ASP GLY GLN GLY ARG TRP SER GLU ASP GLU GLN GLU ASP
GLY GLN ILE GLU GLU PRO GLU GLN GLU GLU GLU GLY ALA VAL GLU GLU HIS GLU GLN VAL GLY HIS GLN GLN SER GLU SER LEU PRO GLN GLN THR THR ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63118	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.476	Depositor
Minimum map value	-2.576	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	339.712, 339.712, 339.712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.327, 1.327, 1.327	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	0.27	0/2184	0.52	0/2952
1	B	0.27	0/2184	0.52	0/2952
1	C	0.27	0/2184	0.52	0/2952
1	D	0.27	0/2184	0.52	0/2952
1	E	0.27	0/2184	0.52	0/2952
1	F	0.27	0/2184	0.52	0/2952
1	G	0.27	0/2184	0.52	0/2952
1	H	0.27	0/2184	0.52	0/2952
1	I	0.27	0/2184	0.52	0/2952
1	J	0.27	0/2184	0.52	0/2952
1	K	0.27	0/2184	0.52	0/2952
1	L	0.27	0/2184	0.52	0/2952
1	M	0.27	0/2184	0.52	0/2952
1	N	0.27	0/2184	0.52	0/2952
All	All	0.27	0/30576	0.52	0/41328

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	2147	0	2150	79	0
1	B	2147	0	2150	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2147	0	2150	63	0
1	D	2147	0	2150	63	0
1	E	2147	0	2150	60	0
1	F	2147	0	2150	73	0
1	G	2147	0	2150	60	0
1	H	2147	0	2150	79	0
1	I	2147	0	2150	79	0
1	J	2147	0	2150	68	0
1	K	2147	0	2150	77	0
1	L	2147	0	2150	71	0
1	M	2147	0	2150	65	0
1	N	2147	0	2150	65	0
All	All	30058	0	30100	763	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 13.

All (763) 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:B:88:ILE:HA	1:L:8:ARG:HH12	1.21	1.04
1:J:88:ILE:HA	1:K:8:ARG:HH12	1.36	0.89
1:M:8:ARG:NH1	1:N:91:LEU:HB2	1.91	0.85
1:I:183:ALA:HA	1:H:175:ARG:HH21	1.44	0.82
1:I:175:ARG:CZ	1:H:182:VAL:HG13	2.12	0.80
1:B:8:ARG:HH12	1:I:88:ILE:HA	1.46	0.80
1:A:88:ILE:HA	1:C:8:ARG:HH12	1.47	0.78
1:K:90:GLY:HA3	1:K:101:THR:HG21	1.67	0.77
1:L:90:GLY:HA3	1:L:101:THR:HG21	1.67	0.77
1:A:90:GLY:HA3	1:A:101:THR:HG21	1.67	0.77
1:I:90:GLY:HA3	1:I:101:THR:HG21	1.67	0.77
1:F:90:GLY:HA3	1:F:101:THR:HG21	1.67	0.77
1:M:90:GLY:HA3	1:M:101:THR:HG21	1.67	0.76
1:J:90:GLY:HA3	1:J:101:THR:HG21	1.67	0.76
1:N:90:GLY:HA3	1:N:101:THR:HG21	1.67	0.76
1:C:90:GLY:HA3	1:C:101:THR:HG21	1.67	0.76
1:D:90:GLY:HA3	1:D:101:THR:HG21	1.67	0.76
1:G:90:GLY:HA3	1:G:101:THR:HG21	1.67	0.76
1:B:90:GLY:HA3	1:B:101:THR:HG21	1.67	0.75
1:E:90:GLY:HA3	1:E:101:THR:HG21	1.67	0.75
1:H:90:GLY:HA3	1:H:101:THR:HG21	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:ILE:HD13	1:K:8:ARG:NH1	2.02	0.74
1:I:179:GLU:OE1	1:H:175:ARG:HB3	1.87	0.73
1:K:175:ARG:HH21	1:F:183:ALA:HA	1.55	0.72
1:G:88:ILE:HA	1:H:8:ARG:HH12	1.54	0.71
1:I:183:ALA:HA	1:H:175:ARG:NH2	2.06	0.70
1:M:5:TYR:CE1	1:N:248:LYS:NZ	2.60	0.69
1:K:182:VAL:HG13	1:F:175:ARG:CZ	2.24	0.68
1:E:57:LYS:HE2	1:K:89:TRP:HA	1.77	0.67
1:D:57:LYS:HE2	1:J:89:TRP:HA	1.77	0.67
1:K:175:ARG:HB3	1:F:179:GLU:OE1	1.96	0.66
1:A:57:LYS:HE2	1:B:89:TRP:HA	1.76	0.66
1:I:175:ARG:NH2	1:H:182:VAL:HG13	2.10	0.66
1:C:57:LYS:HE2	1:I:89:TRP:HA	1.77	0.66
1:F:57:LYS:HE2	1:L:89:TRP:HA	1.77	0.65
1:H:57:LYS:HE2	1:N:89:TRP:HA	1.77	0.65
1:G:57:LYS:HE2	1:M:89:TRP:HA	1.77	0.65
1:K:175:ARG:NH2	1:F:183:ALA:HA	2.11	0.65
1:B:88:ILE:HD13	1:L:8:ARG:NH1	2.13	0.64
1:B:106:VAL:HG21	1:L:5:TYR:O	1.99	0.63
1:I:175:ARG:NH1	1:H:182:VAL:HG13	2.13	0.63
1:J:115:ASP:OD1	1:J:209:HIS:NE2	2.34	0.61
1:C:115:ASP:OD1	1:C:209:HIS:NE2	2.34	0.61
1:M:8:ARG:HH11	1:N:91:LEU:HD13	1.65	0.61
1:G:120:ASP:HB3	1:M:23:PRO:HG2	1.83	0.61
1:A:115:ASP:OD1	1:A:209:HIS:NE2	2.34	0.61
1:D:115:ASP:OD1	1:D:209:HIS:NE2	2.33	0.61
1:K:182:VAL:HG13	1:F:175:ARG:NH1	2.16	0.61
1:F:120:ASP:HB3	1:L:23:PRO:HG2	1.83	0.61
1:F:115:ASP:OD1	1:F:209:HIS:NE2	2.34	0.61
1:B:115:ASP:OD1	1:B:209:HIS:NE2	2.33	0.61
1:N:115:ASP:OD1	1:N:209:HIS:NE2	2.34	0.60
1:B:8:ARG:HH22	1:I:88:ILE:N	1.99	0.60
1:E:115:ASP:OD1	1:E:209:HIS:NE2	2.33	0.60
1:M:115:ASP:OD1	1:M:209:HIS:NE2	2.34	0.60
1:C:120:ASP:HB3	1:I:23:PRO:HG2	1.83	0.60
1:L:115:ASP:OD1	1:L:209:HIS:NE2	2.33	0.60
1:H:120:ASP:HB3	1:N:23:PRO:HG2	1.83	0.60
1:K:115:ASP:OD1	1:K:209:HIS:NE2	2.33	0.60
1:H:115:ASP:OD1	1:H:209:HIS:NE2	2.34	0.60
1:G:115:ASP:OD1	1:G:209:HIS:NE2	2.33	0.59
1:E:120:ASP:HB3	1:K:23:PRO:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:GLY:N	1:J:40:TYR:OH	2.27	0.59
1:D:120:ASP:HB3	1:J:23:PRO:HG2	1.83	0.59
1:H:141:PRO:HA	1:H:144:ASP:HB3	1.85	0.59
1:J:102:ASP:O	1:J:106:VAL:HG23	2.03	0.59
1:G:102:ASP:O	1:G:106:VAL:HG23	2.03	0.59
1:G:141:PRO:HA	1:G:144:ASP:HB3	1.85	0.59
1:B:3:ARG:HH12	1:B:5:TYR:HA	1.68	0.59
1:F:141:PRO:HA	1:F:144:ASP:HB3	1.85	0.59
1:A:1:MET:SD	1:L:5:TYR:HD2	2.26	0.59
1:L:141:PRO:HA	1:L:144:ASP:HB3	1.85	0.59
1:N:3:ARG:HH12	1:N:5:TYR:HA	1.68	0.59
1:C:102:ASP:O	1:C:106:VAL:HG23	2.03	0.58
1:K:102:ASP:O	1:K:106:VAL:HG23	2.03	0.58
1:L:3:ARG:HH12	1:L:5:TYR:HA	1.68	0.58
1:H:102:ASP:O	1:H:106:VAL:HG23	2.03	0.58
1:B:37:GLY:N	1:B:40:TYR:OH	2.27	0.58
1:N:141:PRO:HA	1:N:144:ASP:HB3	1.85	0.58
1:I:141:PRO:HA	1:I:144:ASP:HB3	1.85	0.58
1:J:141:PRO:HA	1:J:144:ASP:HB3	1.85	0.58
1:M:102:ASP:O	1:M:106:VAL:HG23	2.03	0.58
1:I:102:ASP:O	1:I:106:VAL:HG23	2.03	0.58
1:C:141:PRO:HA	1:C:144:ASP:HB3	1.85	0.58
1:E:102:ASP:O	1:E:106:VAL:HG23	2.03	0.58
1:A:102:ASP:O	1:A:106:VAL:HG23	2.03	0.58
1:K:3:ARG:HH12	1:K:5:TYR:HA	1.68	0.58
1:N:102:ASP:O	1:N:106:VAL:HG23	2.03	0.58
1:D:102:ASP:O	1:D:106:VAL:HG23	2.03	0.58
1:K:141:PRO:HA	1:K:144:ASP:HB3	1.85	0.58
1:I:3:ARG:HH12	1:I:5:TYR:HA	1.68	0.58
1:D:141:PRO:HA	1:D:144:ASP:HB3	1.85	0.58
1:M:3:ARG:HH12	1:M:5:TYR:HA	1.68	0.58
1:M:100:ILE:HG21	1:M:227:LEU:HD12	1.86	0.58
1:A:141:PRO:HA	1:A:144:ASP:HB3	1.85	0.58
1:I:115:ASP:OD1	1:I:209:HIS:NE2	2.34	0.58
1:H:100:ILE:HG21	1:H:227:LEU:HD12	1.86	0.58
1:I:100:ILE:HG21	1:I:227:LEU:HD12	1.86	0.58
1:J:88:ILE:HD13	1:K:8:ARG:CZ	2.34	0.58
1:L:102:ASP:O	1:L:106:VAL:HG23	2.03	0.58
1:M:141:PRO:HA	1:M:144:ASP:HB3	1.85	0.58
1:B:102:ASP:O	1:B:106:VAL:HG23	2.03	0.57
1:E:141:PRO:HA	1:E:144:ASP:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:5:TYR:HE1	1:N:248:LYS:NZ	2.00	0.57
1:A:92:GLU:OE2	1:B:57:LYS:NZ	2.22	0.57
1:F:102:ASP:O	1:F:106:VAL:HG23	2.03	0.57
1:B:141:PRO:HA	1:B:144:ASP:HB3	1.85	0.57
1:C:3:ARG:HH12	1:C:5:TYR:HA	1.68	0.57
1:F:3:ARG:HH12	1:F:5:TYR:HA	1.68	0.57
1:D:3:ARG:HH12	1:D:5:TYR:HA	1.68	0.57
1:J:3:ARG:HH12	1:J:5:TYR:HA	1.68	0.57
1:J:100:ILE:HG21	1:J:227:LEU:HD12	1.86	0.57
1:M:37:GLY:N	1:M:40:TYR:OH	2.27	0.57
1:A:3:ARG:HH12	1:A:5:TYR:HA	1.68	0.57
1:K:100:ILE:HG21	1:K:227:LEU:HD12	1.86	0.57
1:B:100:ILE:HG21	1:B:227:LEU:HD12	1.86	0.57
1:J:91:LEU:HD13	1:K:8:ARG:HD2	1.87	0.57
1:E:100:ILE:HG21	1:E:227:LEU:HD12	1.86	0.57
1:G:3:ARG:HH12	1:G:5:TYR:HA	1.68	0.57
1:D:8:ARG:HH11	1:E:91:LEU:HD13	1.69	0.57
1:F:100:ILE:HG21	1:F:227:LEU:HD12	1.86	0.57
1:G:91:LEU:HB2	1:H:8:ARG:NH1	2.20	0.57
1:H:3:ARG:HH12	1:H:5:TYR:HA	1.68	0.57
1:A:3:ARG:NH2	1:L:3:ARG:NH2	2.53	0.56
1:N:100:ILE:HG21	1:N:227:LEU:HD12	1.86	0.56
1:I:182:VAL:HG13	1:H:175:ARG:NH1	2.20	0.56
1:C:143:ARG:NH2	1:C:184:GLU:OE1	2.39	0.56
1:D:100:ILE:HG21	1:D:227:LEU:HD12	1.86	0.56
1:J:143:ARG:NH2	1:J:184:GLU:OE1	2.39	0.56
1:L:100:ILE:HG21	1:L:227:LEU:HD12	1.86	0.56
1:G:100:ILE:HG21	1:G:227:LEU:HD12	1.86	0.56
1:B:244:TYR:O	1:B:248:LYS:HB2	2.06	0.56
1:I:244:TYR:O	1:I:248:LYS:HB2	2.06	0.56
1:M:143:ARG:NH2	1:M:184:GLU:OE1	2.39	0.56
1:A:100:ILE:HG21	1:A:227:LEU:HD12	1.86	0.56
1:B:143:ARG:NH2	1:B:184:GLU:OE1	2.39	0.56
1:C:100:ILE:HG21	1:C:227:LEU:HD12	1.86	0.56
1:E:3:ARG:HH12	1:E:5:TYR:HA	1.68	0.56
1:L:244:TYR:O	1:L:248:LYS:HB2	2.06	0.56
1:J:244:TYR:O	1:J:248:LYS:HB2	2.06	0.56
1:D:143:ARG:NH2	1:D:184:GLU:OE1	2.39	0.56
1:E:244:TYR:O	1:E:248:LYS:HB2	2.06	0.56
1:F:143:ARG:NH2	1:F:184:GLU:OE1	2.39	0.56
1:N:244:TYR:O	1:N:248:LYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD11	1:A:224:LEU:HD21	1.88	0.56
1:C:244:TYR:O	1:C:248:LYS:HB2	2.06	0.56
1:J:104:LEU:HD11	1:J:224:LEU:HD21	1.88	0.56
1:E:143:ARG:NH2	1:E:184:GLU:OE1	2.39	0.56
1:K:143:ARG:NH2	1:K:184:GLU:OE1	2.39	0.56
1:F:23:PRO:HG2	1:L:120:ASP:HB3	1.88	0.56
1:M:244:TYR:O	1:M:248:LYS:HB2	2.06	0.56
1:N:104:LEU:HD11	1:N:224:LEU:HD21	1.88	0.56
1:A:143:ARG:NH2	1:A:184:GLU:OE1	2.39	0.56
1:A:244:TYR:O	1:A:248:LYS:HB2	2.06	0.56
1:G:23:PRO:HG2	1:M:120:ASP:HB3	1.88	0.56
1:H:23:PRO:HG2	1:N:120:ASP:HB3	1.88	0.56
1:H:104:LEU:HD11	1:H:224:LEU:HD21	1.88	0.56
1:N:143:ARG:NH2	1:N:184:GLU:OE1	2.39	0.56
1:B:88:ILE:N	1:L:8:ARG:HH22	2.04	0.55
1:F:104:LEU:HD11	1:F:224:LEU:HD21	1.88	0.55
1:F:244:TYR:O	1:F:248:LYS:HB2	2.06	0.55
1:G:104:LEU:HD11	1:G:224:LEU:HD21	1.88	0.55
1:A:120:ASP:HB3	1:B:23:PRO:HG2	1.88	0.55
1:I:143:ARG:NH2	1:I:184:GLU:OE1	2.39	0.55
1:E:23:PRO:HG2	1:K:120:ASP:HB3	1.88	0.55
1:K:104:LEU:HD11	1:K:224:LEU:HD21	1.88	0.55
1:M:104:LEU:HD11	1:M:224:LEU:HD21	1.88	0.55
1:G:143:ARG:NH2	1:G:184:GLU:OE1	2.39	0.55
1:C:37:GLY:N	1:C:40:TYR:OH	2.27	0.55
1:L:37:GLY:N	1:L:40:TYR:OH	2.27	0.55
1:L:143:ARG:NH2	1:L:184:GLU:OE1	2.39	0.55
1:H:143:ARG:NH2	1:H:184:GLU:OE1	2.39	0.55
1:H:244:TYR:O	1:H:248:LYS:HB2	2.06	0.55
1:K:244:TYR:O	1:K:248:LYS:HB2	2.06	0.55
1:L:104:LEU:HD11	1:L:224:LEU:HD21	1.88	0.55
1:D:37:GLY:N	1:D:40:TYR:OH	2.27	0.55
1:G:244:TYR:O	1:G:248:LYS:HB2	2.06	0.55
1:M:8:ARG:HH11	1:N:91:LEU:HB2	1.70	0.55
1:I:104:LEU:HD11	1:I:224:LEU:HD21	1.88	0.55
1:I:182:VAL:HG13	1:H:175:ARG:HH12	1.72	0.55
1:D:244:TYR:O	1:D:248:LYS:HB2	2.06	0.55
1:H:37:GLY:N	1:H:40:TYR:OH	2.27	0.55
1:C:23:PRO:HG2	1:I:120:ASP:HB3	1.88	0.54
1:C:104:LEU:HD11	1:C:224:LEU:HD21	1.88	0.54
1:B:104:LEU:HD11	1:B:224:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PHE:HB3	1:B:224:LEU:HD11	1.90	0.54
1:D:23:PRO:HG2	1:J:120:ASP:HB3	1.88	0.54
1:E:104:LEU:HD11	1:E:224:LEU:HD21	1.88	0.54
1:M:8:ARG:HH12	1:N:91:LEU:HB2	1.67	0.54
1:A:8:ARG:HH12	1:F:88:ILE:HA	1.73	0.54
1:G:199:PHE:HB3	1:M:224:LEU:HD11	1.90	0.54
1:E:214:ALA:HB1	1:K:268:VAL:HG21	1.90	0.53
1:H:214:ALA:HB1	1:N:268:VAL:HG21	1.90	0.53
1:D:104:LEU:HD11	1:D:224:LEU:HD21	1.88	0.53
1:E:199:PHE:HB3	1:K:224:LEU:HD11	1.90	0.53
1:E:37:GLY:N	1:E:40:TYR:OH	2.27	0.53
1:C:214:ALA:HB1	1:I:268:VAL:HG21	1.90	0.53
1:I:37:GLY:N	1:I:40:TYR:OH	2.27	0.53
1:K:182:VAL:O	1:F:175:ARG:NH2	2.42	0.53
1:F:199:PHE:HB3	1:L:224:LEU:HD11	1.90	0.53
1:D:199:PHE:HB3	1:J:224:LEU:HD11	1.90	0.53
1:A:8:ARG:NH2	1:F:87:SER:HB2	2.24	0.52
1:I:175:ARG:NH2	1:H:182:VAL:O	2.41	0.52
1:K:182:VAL:HG13	1:F:175:ARG:NH2	2.24	0.52
1:D:5:TYR:CE1	1:E:248:LYS:NZ	2.78	0.52
1:G:214:ALA:HB1	1:M:268:VAL:HG21	1.91	0.52
1:C:199:PHE:HB3	1:I:224:LEU:HD11	1.90	0.52
1:D:214:ALA:HB1	1:J:268:VAL:HG21	1.91	0.52
1:F:214:ALA:HB1	1:L:268:VAL:HG21	1.90	0.52
1:J:88:ILE:HD13	1:K:8:ARG:HH12	1.73	0.52
1:A:85:GLN:HE21	1:B:61:LEU:HA	1.74	0.52
1:B:88:ILE:HA	1:L:8:ARG:NH1	2.06	0.52
1:F:37:GLY:N	1:F:40:TYR:OH	2.27	0.52
1:I:175:ARG:NH1	1:H:182:VAL:CG1	2.73	0.52
1:K:37:GLY:N	1:K:40:TYR:OH	2.27	0.52
1:G:37:GLY:N	1:G:40:TYR:OH	2.27	0.52
1:H:199:PHE:HB3	1:N:224:LEU:HD11	1.90	0.52
1:A:23:PRO:HG2	1:B:120:ASP:HB3	1.91	0.51
1:A:232:VAL:HG12	1:B:189:ASN:OD1	2.10	0.51
1:J:88:ILE:HA	1:K:8:ARG:NH1	2.15	0.51
1:N:37:GLY:H	1:N:40:TYR:HH	1.52	0.51
1:E:89:TRP:HA	1:K:57:LYS:HE2	1.93	0.51
1:H:89:TRP:HA	1:N:57:LYS:HE2	1.93	0.51
1:G:89:TRP:HA	1:M:57:LYS:HE2	1.93	0.51
1:A:232:VAL:O	1:B:189:ASN:ND2	2.39	0.51
1:F:89:TRP:HA	1:L:57:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:GLY:N	1:N:40:TYR:OH	2.27	0.51
1:A:78:GLU:OE2	1:B:67:ASN:ND2	2.43	0.51
1:A:89:TRP:HA	1:B:57:LYS:HE2	1.93	0.51
1:A:203:PHE:CE2	1:B:220:GLY:HA3	2.46	0.51
1:A:220:GLY:HA3	1:B:203:PHE:CE2	2.46	0.51
1:D:89:TRP:HA	1:J:57:LYS:HE2	1.93	0.51
1:A:106:VAL:HG21	1:C:5:TYR:O	2.11	0.51
1:K:175:ARG:NH1	1:F:182:VAL:HG13	2.25	0.50
1:A:214:ALA:HB1	1:B:268:VAL:HG21	1.91	0.50
1:I:131:SER:O	1:I:135:ILE:HG22	2.12	0.50
1:D:131:SER:O	1:D:135:ILE:HG22	2.12	0.50
1:J:131:SER:O	1:J:135:ILE:HG22	2.12	0.50
1:E:131:SER:O	1:E:135:ILE:HG22	2.12	0.50
1:K:131:SER:O	1:K:135:ILE:HG22	2.12	0.50
1:F:131:SER:O	1:F:135:ILE:HG22	2.12	0.50
1:G:37:GLY:H	1:G:40:TYR:HH	1.57	0.50
1:G:131:SER:O	1:G:135:ILE:HG22	2.12	0.49
1:N:131:SER:O	1:N:135:ILE:HG22	2.12	0.49
1:L:131:SER:O	1:L:135:ILE:HG22	2.12	0.49
1:H:131:SER:O	1:H:135:ILE:HG22	2.12	0.49
1:A:203:PHE:HE2	1:B:220:GLY:HA3	1.77	0.49
1:C:131:SER:O	1:C:135:ILE:HG22	2.12	0.49
1:I:3:ARG:NH1	1:I:5:TYR:HA	2.28	0.49
1:E:49:ALA:O	1:E:56:ARG:NH2	2.46	0.49
1:F:49:ALA:O	1:F:56:ARG:NH2	2.46	0.49
1:H:3:ARG:NH1	1:H:5:TYR:HA	2.28	0.49
1:H:49:ALA:O	1:H:56:ARG:NH2	2.46	0.49
1:J:91:LEU:HB2	1:K:8:ARG:NH1	2.28	0.49
1:E:117:GLN:NE2	1:K:11:ARG:HH22	2.11	0.49
1:G:88:ILE:N	1:H:8:ARG:HH22	2.11	0.49
1:G:117:GLN:NE2	1:M:11:ARG:HH22	2.11	0.49
1:A:49:ALA:O	1:A:56:ARG:NH2	2.46	0.49
1:A:224:LEU:HD11	1:B:199:PHE:HB3	1.95	0.49
1:D:3:ARG:NH1	1:D:5:TYR:HA	2.28	0.49
1:D:117:GLN:NE2	1:J:11:ARG:HH22	2.11	0.49
1:J:1:MET:CE	1:J:3:ARG:HE	2.26	0.49
1:M:131:SER:O	1:M:135:ILE:HG22	2.12	0.49
1:H:1:MET:CE	1:H:3:ARG:HE	2.26	0.49
1:E:1:MET:CE	1:E:3:ARG:HE	2.26	0.49
1:K:3:ARG:NH1	1:K:5:TYR:HA	2.28	0.49
1:F:1:MET:CE	1:F:3:ARG:HE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:MET:CE	1:L:3:ARG:HE	2.26	0.49
1:L:3:ARG:NH1	1:L:5:TYR:HA	2.28	0.49
1:B:49:ALA:O	1:B:56:ARG:NH2	2.46	0.49
1:C:89:TRP:HA	1:I:57:LYS:HE2	1.93	0.49
1:D:49:ALA:O	1:D:56:ARG:NH2	2.46	0.49
1:F:117:GLN:NE2	1:L:11:ARG:HH22	2.11	0.49
1:B:131:SER:O	1:B:135:ILE:HG22	2.12	0.48
1:D:8:ARG:NH1	1:E:91:LEU:HB2	2.28	0.48
1:I:49:ALA:O	1:I:56:ARG:NH2	2.46	0.48
1:D:1:MET:CE	1:D:3:ARG:HE	2.26	0.48
1:J:49:ALA:O	1:J:56:ARG:NH2	2.46	0.48
1:L:49:ALA:O	1:L:56:ARG:NH2	2.46	0.48
1:M:49:ALA:O	1:M:56:ARG:NH2	2.46	0.48
1:M:262:THR:H	1:M:265:SER:HB2	1.79	0.48
1:A:3:ARG:NH1	1:A:5:TYR:HA	2.28	0.48
1:A:6:SER:HA	1:F:106:VAL:CG2	2.42	0.48
1:A:131:SER:O	1:A:135:ILE:HG22	2.12	0.48
1:K:80:ARG:HD3	1:K:109:TYR:HE1	1.79	0.48
1:F:3:ARG:NH1	1:F:5:TYR:HA	2.28	0.48
1:N:1:MET:CE	1:N:3:ARG:HE	2.26	0.48
1:A:1:MET:CE	1:A:3:ARG:HE	2.26	0.48
1:A:262:THR:H	1:A:265:SER:HB2	1.79	0.48
1:B:3:ARG:NH1	1:B:5:TYR:HA	2.28	0.48
1:I:1:MET:CE	1:I:3:ARG:HE	2.26	0.48
1:G:80:ARG:HD3	1:G:109:TYR:HE1	1.79	0.48
1:N:3:ARG:NH1	1:N:5:TYR:HA	2.28	0.48
1:A:80:ARG:HD3	1:A:109:TYR:HE1	1.79	0.48
1:A:223:LEU:HB2	1:A:250:ILE:HG21	1.96	0.48
1:C:80:ARG:HD3	1:C:109:TYR:HE1	1.79	0.48
1:I:223:LEU:HB2	1:I:250:ILE:HG21	1.96	0.48
1:D:203:PHE:CE2	1:J:220:GLY:HA3	2.49	0.48
1:J:262:THR:H	1:J:265:SER:HB2	1.79	0.48
1:H:80:ARG:HD3	1:H:109:TYR:HE1	1.79	0.48
1:H:117:GLN:NE2	1:N:11:ARG:HH22	2.11	0.48
1:N:49:ALA:O	1:N:56:ARG:NH2	2.46	0.48
1:C:1:MET:CE	1:C:3:ARG:HE	2.26	0.48
1:C:49:ALA:O	1:C:56:ARG:NH2	2.46	0.48
1:C:262:THR:H	1:C:265:SER:HB2	1.79	0.48
1:J:80:ARG:HD3	1:J:109:TYR:HE1	1.79	0.48
1:E:223:LEU:HB2	1:E:250:ILE:HG21	1.96	0.48
1:K:49:ALA:O	1:K:56:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:ALA:O	1:G:56:ARG:NH2	2.46	0.48
1:H:203:PHE:CE2	1:N:220:GLY:HA3	2.49	0.48
1:B:1:MET:CE	1:B:3:ARG:HE	2.26	0.48
1:C:117:GLN:NE2	1:I:11:ARG:HH22	2.11	0.48
1:K:1:MET:CE	1:K:3:ARG:HE	2.26	0.48
1:K:262:THR:H	1:K:265:SER:HB2	1.79	0.48
1:D:23:PRO:HG3	1:J:121:ARG:HD3	1.96	0.48
1:J:3:ARG:NH1	1:J:5:TYR:HA	2.28	0.48
1:E:203:PHE:CE2	1:K:220:GLY:HA3	2.49	0.48
1:F:80:ARG:HD3	1:F:109:TYR:HE1	1.79	0.48
1:G:3:ARG:NH1	1:G:5:TYR:HA	2.28	0.48
1:G:223:LEU:HB2	1:G:250:ILE:HG21	1.96	0.48
1:B:5:TYR:O	1:I:106:VAL:HG21	2.13	0.48
1:I:262:THR:H	1:I:265:SER:HB2	1.79	0.48
1:E:3:ARG:NH1	1:E:5:TYR:HA	2.28	0.48
1:K:175:ARG:HH12	1:F:182:VAL:HG13	1.79	0.48
1:F:203:PHE:CE2	1:L:220:GLY:HA3	2.49	0.48
1:M:80:ARG:HD3	1:M:109:TYR:HE1	1.79	0.48
1:H:223:LEU:HB2	1:H:250:ILE:HG21	1.96	0.48
1:N:80:ARG:HD3	1:N:109:TYR:HE1	1.79	0.48
1:A:89:TRP:NE1	1:B:58:LEU:HD22	2.29	0.48
1:A:136:GLU:O	1:A:139:VAL:HG12	2.14	0.48
1:B:80:ARG:HD3	1:B:109:TYR:HE1	1.79	0.48
1:E:262:THR:H	1:E:265:SER:HB2	1.79	0.48
1:K:223:LEU:HB2	1:K:250:ILE:HG21	1.96	0.48
1:L:136:GLU:O	1:L:139:VAL:HG12	2.14	0.48
1:L:262:THR:H	1:L:265:SER:HB2	1.79	0.48
1:G:262:THR:H	1:G:265:SER:HB2	1.79	0.48
1:M:1:MET:CE	1:M:3:ARG:HE	2.26	0.48
1:H:23:PRO:HG3	1:N:121:ARG:HD3	1.96	0.48
1:N:223:LEU:HB2	1:N:250:ILE:HG21	1.96	0.48
1:C:203:PHE:CE2	1:I:220:GLY:HA3	2.49	0.47
1:D:136:GLU:O	1:D:139:VAL:HG12	2.14	0.47
1:E:23:PRO:HG3	1:K:121:ARG:HD3	1.96	0.47
1:E:80:ARG:HD3	1:E:109:TYR:HE1	1.79	0.47
1:M:3:ARG:NH1	1:M:5:TYR:HA	2.28	0.47
1:A:64:ILE:HD12	1:B:85:GLN:NE2	2.28	0.47
1:D:80:ARG:HD3	1:D:109:TYR:HE1	1.79	0.47
1:F:136:GLU:O	1:F:139:VAL:HG12	2.14	0.47
1:F:262:THR:H	1:F:265:SER:HB2	1.79	0.47
1:G:1:MET:CE	1:G:3:ARG:HE	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:GLU:O	1:C:139:VAL:HG12	2.14	0.47
1:M:223:LEU:HB2	1:M:250:ILE:HG21	1.96	0.47
1:H:136:GLU:O	1:H:139:VAL:HG12	2.14	0.47
1:A:23:PRO:HG3	1:B:121:ARG:HD3	1.96	0.47
1:B:223:LEU:HB2	1:B:250:ILE:HG21	1.96	0.47
1:B:262:THR:H	1:B:265:SER:HB2	1.79	0.47
1:I:136:GLU:O	1:I:139:VAL:HG12	2.14	0.47
1:D:262:THR:H	1:D:265:SER:HB2	1.79	0.47
1:E:58:LEU:HB3	1:E:133:ARG:HG2	1.97	0.47
1:L:80:ARG:HD3	1:L:109:TYR:HE1	1.78	0.47
1:M:136:GLU:O	1:M:139:VAL:HG12	2.14	0.47
1:C:223:LEU:HB2	1:C:250:ILE:HG21	1.96	0.47
1:J:267:GLN:OE1	1:J:267:GLN:N	2.45	0.47
1:E:136:GLU:O	1:E:139:VAL:HG12	2.14	0.47
1:H:58:LEU:HB3	1:H:133:ARG:HG2	1.97	0.47
1:H:262:THR:H	1:H:265:SER:HB2	1.79	0.47
1:A:8:ARG:NH2	1:F:87:SER:CB	2.77	0.47
1:B:136:GLU:O	1:B:139:VAL:HG12	2.14	0.47
1:I:182:VAL:HG13	1:H:175:ARG:NH2	2.29	0.47
1:J:88:ILE:N	1:K:8:ARG:HH22	2.12	0.47
1:F:58:LEU:HB3	1:F:133:ARG:HG2	1.97	0.47
1:F:223:LEU:HB2	1:F:250:ILE:HG21	1.96	0.47
1:A:67:ASN:ND2	1:B:78:GLU:OE2	2.48	0.47
1:C:3:ARG:NH1	1:C:5:TYR:HA	2.28	0.47
1:C:23:PRO:HG3	1:I:121:ARG:HD3	1.96	0.47
1:I:80:ARG:HD3	1:I:109:TYR:HE1	1.79	0.47
1:D:11:ARG:HH22	1:J:117:GLN:NE2	2.13	0.47
1:D:223:LEU:HB2	1:D:250:ILE:HG21	1.96	0.47
1:J:223:LEU:HB2	1:J:250:ILE:HG21	1.96	0.47
1:E:11:ARG:HH22	1:K:117:GLN:NE2	2.13	0.47
1:B:37:GLY:H	1:B:40:TYR:HH	1.57	0.47
1:C:11:ARG:HH22	1:I:117:GLN:NE2	2.13	0.47
1:I:58:LEU:HB3	1:I:133:ARG:HG2	1.97	0.47
1:J:58:LEU:HB3	1:J:133:ARG:HG2	1.97	0.47
1:F:23:PRO:HG3	1:L:121:ARG:HD3	1.96	0.47
1:G:203:PHE:HE2	1:M:220:GLY:HA3	1.80	0.47
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.79	0.47
1:H:11:ARG:HH22	1:N:117:GLN:NE2	2.13	0.47
1:A:58:LEU:HB3	1:A:133:ARG:HG2	1.97	0.46
1:K:58:LEU:HB3	1:K:133:ARG:HG2	1.97	0.46
1:L:14:THR:OG1	1:L:15:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:223:LEU:HB2	1:L:250:ILE:HG21	1.96	0.46
1:G:203:PHE:CE2	1:M:220:GLY:HA3	2.49	0.46
1:N:262:THR:H	1:N:265:SER:HB2	1.79	0.46
1:C:203:PHE:HE2	1:I:220:GLY:HA3	1.80	0.46
1:D:58:LEU:HB3	1:D:133:ARG:HG2	1.97	0.46
1:K:136:GLU:O	1:K:139:VAL:HG12	2.14	0.46
1:B:14:THR:OG1	1:B:15:ALA:N	2.49	0.46
1:J:153:ILE:HD11	1:J:169:LEU:O	2.16	0.46
1:F:11:ARG:HH22	1:L:117:GLN:NE2	2.13	0.46
1:G:136:GLU:O	1:G:139:VAL:HG12	2.14	0.46
1:B:8:ARG:NH1	1:I:91:LEU:HB2	2.30	0.46
1:K:14:THR:OG1	1:K:15:ALA:N	2.49	0.46
1:F:14:THR:OG1	1:F:15:ALA:N	2.49	0.46
1:L:172:GLU:OE1	1:L:172:GLU:HA	2.16	0.46
1:G:267:GLN:OE1	1:G:267:GLN:N	2.45	0.46
1:M:58:LEU:HB3	1:M:133:ARG:HG2	1.97	0.46
1:N:153:ILE:HD11	1:N:169:LEU:O	2.16	0.46
1:J:127:LEU:HA	1:J:127:LEU:HD23	1.79	0.46
1:G:58:LEU:HB3	1:G:133:ARG:HG2	1.97	0.46
1:N:136:GLU:O	1:N:139:VAL:HG12	2.14	0.46
1:B:58:LEU:HB3	1:B:133:ARG:HG2	1.97	0.46
1:C:58:LEU:HB3	1:C:133:ARG:HG2	1.97	0.46
1:I:267:GLN:OE1	1:I:267:GLN:N	2.45	0.46
1:D:14:THR:OG1	1:D:15:ALA:N	2.49	0.46
1:D:203:PHE:HE2	1:J:220:GLY:HA3	1.80	0.46
1:D:267:GLN:OE1	1:D:267:GLN:N	2.45	0.46
1:G:11:ARG:HH22	1:M:117:GLN:NE2	2.13	0.46
1:G:23:PRO:HG3	1:M:121:ARG:HD3	1.96	0.46
1:A:153:ILE:HD11	1:A:169:LEU:O	2.16	0.46
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.16	0.46
1:M:153:ILE:HD11	1:M:169:LEU:O	2.16	0.46
1:A:3:ARG:NH2	1:L:3:ARG:HH21	2.14	0.46
1:I:153:ILE:HD11	1:I:169:LEU:O	2.16	0.46
1:J:136:GLU:O	1:J:139:VAL:HG12	2.14	0.46
1:F:127:LEU:HD23	1:F:127:LEU:HA	1.79	0.46
1:F:153:ILE:HD11	1:F:169:LEU:O	2.16	0.46
1:A:6:SER:HA	1:F:106:VAL:HG22	1.98	0.46
1:B:153:ILE:HD11	1:B:169:LEU:O	2.16	0.46
1:J:14:THR:OG1	1:J:15:ALA:N	2.49	0.46
1:E:14:THR:OG1	1:E:15:ALA:N	2.49	0.46
1:K:172:GLU:OE1	1:K:172:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:LEU:HB2	1:H:8:ARG:HH11	1.79	0.46
1:H:14:THR:OG1	1:H:15:ALA:N	2.49	0.46
1:A:220:GLY:HA3	1:B:203:PHE:HE2	1.81	0.46
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.16	0.46
1:J:172:GLU:HA	1:J:172:GLU:OE1	2.16	0.46
1:L:58:LEU:HB3	1:L:133:ARG:HG2	1.97	0.46
1:H:172:GLU:HA	1:H:172:GLU:OE1	2.16	0.46
1:B:172:GLU:OE1	1:B:172:GLU:HA	2.16	0.45
1:C:14:THR:OG1	1:C:15:ALA:N	2.49	0.45
1:C:172:GLU:HA	1:C:172:GLU:OE1	2.16	0.45
1:C:267:GLN:OE1	1:C:267:GLN:N	2.45	0.45
1:D:4:THR:OG1	1:E:248:LYS:HE2	2.15	0.45
1:L:153:ILE:HD11	1:L:169:LEU:O	2.16	0.45
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.79	0.45
1:I:172:GLU:OE1	1:I:172:GLU:HA	2.16	0.45
1:K:153:ILE:HD11	1:K:169:LEU:O	2.16	0.45
1:H:153:ILE:HD11	1:H:169:LEU:O	2.16	0.45
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.79	0.45
1:M:219:TYR:OH	1:M:253:ASP:OD1	2.26	0.45
1:N:14:THR:OG1	1:N:15:ALA:N	2.49	0.45
1:N:58:LEU:HB3	1:N:133:ARG:HG2	1.97	0.45
1:A:37:GLY:N	1:A:40:TYR:OH	2.27	0.45
1:C:153:ILE:HD11	1:C:169:LEU:O	2.16	0.45
1:E:172:GLU:HA	1:E:172:GLU:OE1	2.16	0.45
1:M:14:THR:OG1	1:M:15:ALA:N	2.49	0.45
1:M:172:GLU:HA	1:M:172:GLU:OE1	2.16	0.45
1:N:172:GLU:OE1	1:N:172:GLU:HA	2.16	0.45
1:C:58:LEU:HD12	1:C:58:LEU:HA	1.83	0.45
1:I:14:THR:OG1	1:I:15:ALA:N	2.49	0.45
1:D:224:LEU:HD11	1:J:199:PHE:HB3	1.99	0.45
1:F:37:GLY:H	1:F:40:TYR:HH	1.57	0.45
1:H:224:LEU:HD11	1:N:199:PHE:HB3	1.99	0.45
1:A:14:THR:OG1	1:A:15:ALA:N	2.49	0.45
1:F:203:PHE:HE2	1:L:220:GLY:HA3	1.80	0.45
1:G:14:THR:OG1	1:G:15:ALA:N	2.49	0.45
1:F:172:GLU:HA	1:F:172:GLU:OE1	2.16	0.45
1:G:172:GLU:OE1	1:G:172:GLU:HA	2.16	0.45
1:H:203:PHE:HE2	1:N:220:GLY:HA3	1.80	0.45
1:C:224:LEU:HD11	1:I:199:PHE:HB3	1.99	0.45
1:D:153:ILE:HD11	1:D:169:LEU:O	2.16	0.45
1:N:127:LEU:HD23	1:N:127:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ILE:HD11	1:E:169:LEU:O	2.16	0.45
1:A:175:ARG:NH2	1:J:186:GLN:HB2	2.32	0.44
1:L:127:LEU:HD23	1:L:127:LEU:HA	1.79	0.44
1:M:37:GLY:H	1:M:40:TYR:HH	1.56	0.44
1:I:226:LEU:HD21	1:I:246:ALA:HB3	2.00	0.44
1:N:226:LEU:HD21	1:N:246:ALA:HB3	2.00	0.44
1:A:104:LEU:HD13	1:B:199:PHE:CD1	2.52	0.44
1:B:226:LEU:HD21	1:B:246:ALA:HB3	2.00	0.44
1:C:110:GLU:O	1:C:113:GLU:HG2	2.18	0.44
1:K:226:LEU:HD21	1:K:246:ALA:HB3	2.00	0.44
1:G:153:ILE:HD11	1:G:169:LEU:O	2.16	0.44
1:A:3:ARG:HH21	1:L:3:ARG:NH2	2.15	0.44
1:D:103:LYS:HG3	1:D:247:SER:OG	2.18	0.44
1:D:110:GLU:O	1:D:113:GLU:HG2	2.18	0.44
1:E:226:LEU:HD21	1:E:246:ALA:HB3	2.00	0.44
1:F:232:VAL:O	1:L:189:ASN:ND2	2.46	0.44
1:L:267:GLN:OE1	1:L:267:GLN:N	2.45	0.44
1:A:110:GLU:O	1:A:113:GLU:HG2	2.18	0.44
1:D:58:LEU:HD12	1:D:58:LEU:HA	1.83	0.44
1:E:203:PHE:HE2	1:K:220:GLY:HA3	1.80	0.44
1:C:220:GLY:HA3	1:I:203:PHE:CE2	2.53	0.44
1:I:110:GLU:O	1:I:113:GLU:HG2	2.18	0.44
1:K:110:GLU:O	1:K:113:GLU:HG2	2.18	0.44
1:L:226:LEU:HD21	1:L:246:ALA:HB3	2.00	0.44
1:G:220:GLY:HA3	1:M:203:PHE:CE2	2.53	0.44
1:M:226:LEU:HD21	1:M:246:ALA:HB3	2.00	0.44
1:I:103:LYS:HG3	1:I:247:SER:OG	2.18	0.44
1:D:226:LEU:HD21	1:D:246:ALA:HB3	2.00	0.44
1:E:220:GLY:HA3	1:K:203:PHE:CE2	2.53	0.44
1:K:1:MET:HE3	1:K:3:ARG:HE	1.83	0.44
1:F:267:GLN:OE1	1:F:267:GLN:N	2.45	0.44
1:M:267:GLN:OE1	1:M:267:GLN:N	2.45	0.44
1:H:220:GLY:HA3	1:N:203:PHE:CE2	2.53	0.44
1:A:227:LEU:HD22	1:B:196:ARG:HD3	1.99	0.44
1:C:103:LYS:HG3	1:C:247:SER:OG	2.18	0.44
1:I:182:VAL:HG13	1:H:175:ARG:CZ	2.48	0.44
1:E:58:LEU:HD12	1:E:58:LEU:HA	1.83	0.44
1:G:226:LEU:HD21	1:G:246:ALA:HB3	2.00	0.44
1:H:267:GLN:HE21	1:N:268:VAL:HA	1.83	0.44
1:N:103:LYS:HG3	1:N:247:SER:OG	2.18	0.44
1:A:226:LEU:HD21	1:A:246:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ARG:HH11	1:I:91:LEU:HB2	1.83	0.43
1:K:182:VAL:CG1	1:F:175:ARG:NH1	2.81	0.43
1:F:103:LYS:HG3	1:F:247:SER:OG	2.18	0.43
1:F:220:GLY:HA3	1:L:203:PHE:CE2	2.53	0.43
1:L:103:LYS:HG3	1:L:247:SER:OG	2.18	0.43
1:G:110:GLU:O	1:G:113:GLU:HG2	2.18	0.43
1:G:224:LEU:HD11	1:M:199:PHE:HB3	1.99	0.43
1:H:232:VAL:O	1:N:189:ASN:ND2	2.46	0.43
1:J:226:LEU:HD21	1:J:246:ALA:HB3	2.00	0.43
1:K:103:LYS:HG3	1:K:247:SER:OG	2.18	0.43
1:G:103:LYS:HG3	1:G:247:SER:OG	2.18	0.43
1:M:103:LYS:HG3	1:M:247:SER:OG	2.18	0.43
1:N:1:MET:HE3	1:N:3:ARG:HE	1.83	0.43
1:A:117:GLN:NE2	1:B:11:ARG:HH22	2.17	0.43
1:B:54:LEU:HD23	1:B:54:LEU:O	2.19	0.43
1:E:103:LYS:HG3	1:E:247:SER:OG	2.18	0.43
1:A:54:LEU:O	1:A:54:LEU:HD23	2.19	0.43
1:A:175:ARG:HH21	1:J:186:GLN:CB	2.32	0.43
1:C:267:GLN:HE21	1:I:268:VAL:HA	1.83	0.43
1:L:54:LEU:HD23	1:L:54:LEU:O	2.19	0.43
1:L:110:GLU:O	1:L:113:GLU:HG2	2.18	0.43
1:H:103:LYS:HG3	1:H:247:SER:OG	2.18	0.43
1:H:226:LEU:HD21	1:H:246:ALA:HB3	2.00	0.43
1:B:103:LYS:HG3	1:B:247:SER:OG	2.18	0.43
1:B:110:GLU:O	1:B:113:GLU:HG2	2.18	0.43
1:I:54:LEU:HD23	1:I:54:LEU:O	2.19	0.43
1:D:220:GLY:HA3	1:J:203:PHE:CE2	2.53	0.43
1:J:110:GLU:O	1:J:113:GLU:HG2	2.18	0.43
1:E:224:LEU:HD11	1:K:199:PHE:HB3	1.99	0.43
1:F:224:LEU:HD11	1:L:199:PHE:HB3	1.99	0.43
1:G:64:ILE:HD12	1:M:85:GLN:NE2	2.34	0.43
1:A:103:LYS:HG3	1:A:247:SER:OG	2.18	0.43
1:K:37:GLY:H	1:K:40:TYR:HH	1.60	0.43
1:K:171:GLN:HE22	1:K:175:ARG:HE	1.67	0.43
1:H:110:GLU:O	1:H:113:GLU:HG2	2.18	0.43
1:B:97:VAL:HA	1:B:100:ILE:HG22	2.01	0.43
1:C:97:VAL:HA	1:C:100:ILE:HG22	2.01	0.43
1:I:182:VAL:CG1	1:H:175:ARG:HH12	2.32	0.43
1:D:64:ILE:HD12	1:J:85:GLN:NE2	2.34	0.43
1:K:85:GLN:HA	1:K:88:ILE:HB	2.01	0.43
1:F:226:LEU:HD21	1:F:246:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:GLY:H	1:H:40:TYR:HH	1.55	0.43
1:H:64:ILE:HD12	1:N:85:GLN:NE2	2.34	0.43
1:H:267:GLN:OE1	1:H:267:GLN:N	2.45	0.43
1:N:85:GLN:HA	1:N:88:ILE:HB	2.01	0.43
1:N:97:VAL:HA	1:N:100:ILE:HG22	2.01	0.43
1:B:58:LEU:HD12	1:B:58:LEU:HA	1.83	0.43
1:I:183:ALA:CA	1:H:175:ARG:NH2	2.79	0.43
1:J:103:LYS:HG3	1:J:247:SER:OG	2.18	0.43
1:J:171:GLN:HE22	1:J:175:ARG:HE	1.67	0.43
1:K:54:LEU:O	1:K:54:LEU:HD23	2.19	0.43
1:G:85:GLN:HA	1:G:88:ILE:HB	2.01	0.43
1:N:110:GLU:O	1:N:113:GLU:HG2	2.18	0.43
1:C:54:LEU:O	1:C:54:LEU:HD23	2.19	0.43
1:I:97:VAL:HA	1:I:100:ILE:HG22	2.01	0.43
1:I:171:GLN:HE22	1:I:175:ARG:HE	1.67	0.43
1:D:97:VAL:HA	1:D:100:ILE:HG22	2.01	0.43
1:J:97:VAL:HA	1:J:100:ILE:HG22	2.01	0.43
1:E:110:GLU:O	1:E:113:GLU:HG2	2.18	0.43
1:E:267:GLN:HE21	1:K:268:VAL:HA	1.83	0.43
1:F:110:GLU:O	1:F:113:GLU:HG2	2.18	0.43
1:G:54:LEU:HD23	1:G:54:LEU:O	2.19	0.43
1:G:171:GLN:HE22	1:G:175:ARG:HE	1.67	0.43
1:G:267:GLN:HE21	1:M:268:VAL:HA	1.83	0.43
1:M:110:GLU:O	1:M:113:GLU:HG2	2.18	0.43
1:H:58:LEU:HD12	1:H:58:LEU:HA	1.82	0.43
1:N:54:LEU:HD23	1:N:54:LEU:O	2.19	0.43
1:A:162:GLN:H	1:A:162:GLN:HG3	1.73	0.43
1:C:64:ILE:HD12	1:I:85:GLN:NE2	2.34	0.43
1:J:37:GLY:H	1:J:40:TYR:HH	1.58	0.43
1:L:58:LEU:HD12	1:L:58:LEU:HA	1.83	0.43
1:H:69:LEU:HD11	1:H:119:ILE:HG23	2.01	0.43
1:A:88:ILE:HD13	1:C:8:ARG:NH1	2.34	0.42
1:A:97:VAL:HA	1:A:100:ILE:HG22	2.01	0.42
1:C:85:GLN:HA	1:C:88:ILE:HB	2.01	0.42
1:I:107:LEU:HD23	1:I:107:LEU:HA	1.87	0.42
1:D:54:LEU:HD23	1:D:54:LEU:O	2.19	0.42
1:E:64:ILE:HD12	1:K:85:GLN:NE2	2.34	0.42
1:F:97:VAL:HA	1:F:100:ILE:HG22	2.01	0.42
1:F:267:GLN:HE21	1:L:268:VAL:HA	1.83	0.42
1:L:171:GLN:HE22	1:L:175:ARG:HE	1.67	0.42
1:M:97:VAL:HA	1:M:100:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:LEU:O	1:H:54:LEU:HD23	2.19	0.42
1:D:171:GLN:HE22	1:D:175:ARG:HE	1.67	0.42
1:L:97:VAL:HA	1:L:100:ILE:HG22	2.01	0.42
1:M:69:LEU:HD11	1:M:119:ILE:HG23	2.01	0.42
1:H:171:GLN:HE22	1:H:175:ARG:HE	1.67	0.42
1:N:69:LEU:HD11	1:N:119:ILE:HG23	2.02	0.42
1:J:85:GLN:HA	1:J:88:ILE:HB	2.01	0.42
1:E:127:LEU:HD23	1:E:127:LEU:HA	1.79	0.42
1:E:189:ASN:ND2	1:K:232:VAL:O	2.47	0.42
1:K:97:VAL:HA	1:K:100:ILE:HG22	2.01	0.42
1:F:54:LEU:O	1:F:54:LEU:HD23	2.19	0.42
1:G:97:VAL:HA	1:G:100:ILE:HG22	2.01	0.42
1:M:85:GLN:HA	1:M:88:ILE:HB	2.01	0.42
1:H:216:ILE:HD13	1:H:216:ILE:HA	1.89	0.42
1:B:171:GLN:HE22	1:B:175:ARG:HE	1.67	0.42
1:I:35:LYS:HD3	1:I:40:TYR:HE1	1.85	0.42
1:I:216:ILE:HD13	1:I:216:ILE:HA	1.89	0.42
1:D:267:GLN:HE21	1:J:268:VAL:HA	1.83	0.42
1:D:268:VAL:HG21	1:J:214:ALA:HB1	2.02	0.42
1:E:97:VAL:HA	1:E:100:ILE:HG22	2.01	0.42
1:E:268:VAL:HG21	1:K:214:ALA:HB1	2.02	0.42
1:A:35:LYS:HD3	1:A:40:TYR:HE1	1.85	0.42
1:A:85:GLN:HA	1:A:88:ILE:HB	2.01	0.42
1:A:189:ASN:ND2	1:B:232:VAL:O	2.45	0.42
1:A:219:TYR:OH	1:A:253:ASP:OD1	2.26	0.42
1:B:84:LYS:HG3	1:L:7:LEU:HG	2.01	0.42
1:E:54:LEU:HD23	1:E:54:LEU:O	2.19	0.42
1:G:69:LEU:HD11	1:G:119:ILE:HG23	2.01	0.42
1:H:85:GLN:HA	1:H:88:ILE:HB	2.01	0.42
1:N:171:GLN:HE22	1:N:175:ARG:HE	1.67	0.42
1:I:85:GLN:HA	1:I:88:ILE:HB	2.01	0.42
1:K:58:LEU:HD23	1:K:133:ARG:HA	2.02	0.42
1:A:268:VAL:HG21	1:B:214:ALA:HB1	2.00	0.42
1:C:226:LEU:HD21	1:C:246:ALA:HB3	2.00	0.42
1:E:69:LEU:HD11	1:E:119:ILE:HG23	2.02	0.42
1:E:267:GLN:OE1	1:E:267:GLN:N	2.45	0.42
1:F:64:ILE:HD12	1:L:85:GLN:NE2	2.34	0.42
1:M:58:LEU:HD23	1:M:133:ARG:HA	2.02	0.42
1:H:35:LYS:HD3	1:H:40:TYR:HE1	1.85	0.42
1:A:171:GLN:HE22	1:A:175:ARG:HE	1.67	0.42
1:I:69:LEU:HD11	1:I:119:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:LYS:HD3	1:J:40:TYR:HE1	1.85	0.42
1:J:54:LEU:HD23	1:J:54:LEU:O	2.19	0.42
1:F:1:MET:H2	1:L:110:GLU:CD	2.23	0.42
1:L:85:GLN:HA	1:L:88:ILE:HB	2.01	0.42
1:G:268:VAL:HG21	1:M:214:ALA:HB1	2.02	0.42
1:H:268:VAL:HG21	1:N:214:ALA:HB1	2.02	0.42
1:D:69:LEU:HD11	1:D:119:ILE:HG23	2.01	0.42
1:M:127:LEU:HD23	1:M:127:LEU:HA	1.79	0.42
1:B:69:LEU:HD11	1:B:119:ILE:HG23	2.02	0.42
1:C:69:LEU:HD11	1:C:119:ILE:HG23	2.01	0.42
1:C:232:VAL:HG12	1:I:189:ASN:OD1	2.20	0.42
1:E:85:GLN:HA	1:E:88:ILE:HB	2.01	0.42
1:F:58:LEU:HD23	1:F:133:ARG:HA	2.02	0.42
1:F:171:GLN:HE22	1:F:175:ARG:HE	1.67	0.42
1:L:35:LYS:HD3	1:L:40:TYR:HE1	1.85	0.42
1:M:54:LEU:O	1:M:54:LEU:HD23	2.19	0.42
1:A:89:TRP:CG	1:B:58:LEU:HD13	2.55	0.41
1:C:268:VAL:HG21	1:I:214:ALA:HB1	2.02	0.41
1:J:107:LEU:HD23	1:J:107:LEU:HA	1.87	0.41
1:E:35:LYS:HD3	1:E:40:TYR:HE1	1.85	0.41
1:E:232:VAL:HG12	1:K:189:ASN:OD1	2.20	0.41
1:K:69:LEU:HD11	1:K:119:ILE:HG23	2.02	0.41
1:L:58:LEU:HD23	1:L:133:ARG:HA	2.02	0.41
1:G:104:LEU:O	1:G:108:ILE:HG13	2.20	0.41
1:G:216:ILE:HD13	1:G:216:ILE:HA	1.90	0.41
1:G:232:VAL:HG12	1:M:189:ASN:OD1	2.20	0.41
1:H:104:LEU:O	1:H:108:ILE:HG13	2.20	0.41
1:H:127:LEU:HD23	1:H:127:LEU:HA	1.79	0.41
1:N:267:GLN:OE1	1:N:267:GLN:N	2.45	0.41
1:A:153:ILE:HD11	1:A:169:LEU:C	2.41	0.41
1:B:3:ARG:NH2	1:C:3:ARG:NH2	2.68	0.41
1:C:104:LEU:O	1:C:108:ILE:HG13	2.20	0.41
1:D:85:GLN:HA	1:D:88:ILE:HB	2.01	0.41
1:D:104:LEU:O	1:D:108:ILE:HG13	2.20	0.41
1:D:153:ILE:HD11	1:D:169:LEU:C	2.41	0.41
1:E:104:LEU:O	1:E:108:ILE:HG13	2.20	0.41
1:G:35:LYS:HD3	1:G:40:TYR:HE1	1.85	0.41
1:M:21:PRO:HA	1:M:22:PRO:HD3	1.97	0.41
1:H:232:VAL:HG12	1:N:189:ASN:OD1	2.20	0.41
1:N:35:LYS:HD3	1:N:40:TYR:HE1	1.85	0.41
1:B:58:LEU:HD23	1:B:133:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLN:HE22	1:C:175:ARG:HE	1.67	0.41
1:I:182:VAL:HG13	1:H:175:ARG:HH22	1.83	0.41
1:D:232:VAL:HG12	1:J:189:ASN:OD1	2.20	0.41
1:G:153:ILE:HD11	1:G:169:LEU:C	2.41	0.41
1:M:58:LEU:HD12	1:M:58:LEU:HA	1.83	0.41
1:A:69:LEU:HD11	1:A:119:ILE:HG23	2.01	0.41
1:E:171:GLN:HE22	1:E:175:ARG:HE	1.67	0.41
1:F:153:ILE:HD11	1:F:169:LEU:C	2.41	0.41
1:L:221:LYS:HB2	1:L:221:LYS:HE3	1.92	0.41
1:G:58:LEU:HD23	1:G:133:ARG:HA	2.02	0.41
1:B:221:LYS:HB2	1:B:221:LYS:HE3	1.92	0.41
1:I:58:LEU:HD23	1:I:133:ARG:HA	2.02	0.41
1:F:35:LYS:HD3	1:F:40:TYR:HE1	1.85	0.41
1:M:171:GLN:HE22	1:M:175:ARG:HE	1.67	0.41
1:N:129:LEU:HD23	1:N:129:LEU:HA	1.91	0.41
1:A:58:LEU:HD23	1:A:133:ARG:HA	2.02	0.41
1:A:104:LEU:O	1:A:108:ILE:HG13	2.20	0.41
1:A:267:GLN:OE1	1:A:267:GLN:N	2.45	0.41
1:B:85:GLN:HA	1:B:88:ILE:HB	2.01	0.41
1:I:104:LEU:O	1:I:108:ILE:HG13	2.20	0.41
1:J:69:LEU:HD11	1:J:119:ILE:HG23	2.01	0.41
1:F:58:LEU:HD12	1:F:58:LEU:HA	1.83	0.41
1:F:85:GLN:HA	1:F:88:ILE:HB	2.01	0.41
1:L:1:MET:HE3	1:L:3:ARG:HE	1.84	0.41
1:H:97:VAL:HA	1:H:100:ILE:HG22	2.01	0.41
1:D:58:LEU:HD23	1:D:133:ARG:HA	2.02	0.41
1:E:153:ILE:HD11	1:E:169:LEU:C	2.41	0.41
1:F:104:LEU:O	1:F:108:ILE:HG13	2.21	0.41
1:L:69:LEU:HD11	1:L:119:ILE:HG23	2.01	0.41
1:M:35:LYS:HD3	1:M:40:TYR:HE1	1.85	0.41
1:H:58:LEU:HD23	1:H:133:ARG:HA	2.02	0.41
1:H:153:ILE:HD11	1:H:169:LEU:C	2.41	0.41
1:N:104:LEU:O	1:N:108:ILE:HG13	2.20	0.41
1:K:58:LEU:HD12	1:K:58:LEU:HA	1.83	0.41
1:L:129:LEU:HD23	1:L:129:LEU:HA	1.91	0.41
1:C:35:LYS:HD3	1:C:40:TYR:HE1	1.85	0.41
1:C:58:LEU:HD23	1:C:133:ARG:HA	2.02	0.41
1:C:153:ILE:HD11	1:C:169:LEU:C	2.41	0.41
1:C:232:VAL:O	1:I:189:ASN:ND2	2.46	0.41
1:I:88:ILE:HA	1:I:88:ILE:HD13	1.94	0.41
1:I:153:ILE:HD11	1:I:169:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LYS:HD3	1:D:40:TYR:HE1	1.85	0.41
1:D:85:GLN:HE21	1:J:61:LEU:HA	1.86	0.41
1:D:162:GLN:H	1:D:162:GLN:HG3	1.72	0.41
1:J:58:LEU:HD23	1:J:133:ARG:HA	2.02	0.41
1:E:1:MET:H2	1:K:110:GLU:CD	2.24	0.41
1:K:153:ILE:HD11	1:K:169:LEU:C	2.41	0.41
1:F:69:LEU:HD11	1:F:119:ILE:HG23	2.02	0.41
1:F:85:GLN:HE21	1:L:61:LEU:HA	1.86	0.41
1:F:268:VAL:HG21	1:L:214:ALA:HB1	2.02	0.41
1:G:85:GLN:HE21	1:M:61:LEU:HA	1.86	0.41
1:M:216:ILE:HD13	1:M:216:ILE:HA	1.90	0.41
1:D:169:LEU:HD13	1:D:169:LEU:HA	1.97	0.41
1:J:269:LYS:HD3	1:J:269:LYS:HA	1.96	0.41
1:G:58:LEU:HA	1:G:58:LEU:HD12	1.83	0.41
1:N:58:LEU:HD23	1:N:133:ARG:HA	2.02	0.41
1:N:107:LEU:HD23	1:N:107:LEU:HA	1.87	0.41
1:C:1:MET:H2	1:I:110:GLU:CD	2.25	0.40
1:I:1:MET:HE3	1:I:3:ARG:HE	1.86	0.40
1:K:129:LEU:HD23	1:K:129:LEU:HA	1.91	0.40
1:H:85:GLN:HE21	1:N:61:LEU:HA	1.86	0.40
1:N:153:ILE:HD11	1:N:169:LEU:C	2.41	0.40
1:A:237:THR:OG1	1:A:238:ARG:N	2.55	0.40
1:C:88:ILE:HD13	1:C:88:ILE:HA	1.94	0.40
1:K:35:LYS:HD3	1:K:40:TYR:HE1	1.85	0.40
1:F:251:ILE:HD12	1:F:251:ILE:HA	1.93	0.40
1:M:104:LEU:O	1:M:108:ILE:HG13	2.20	0.40
1:H:221:LYS:HB2	1:H:221:LYS:HE3	1.92	0.40
1:C:237:THR:OG1	1:C:238:ARG:N	2.55	0.40
1:I:237:THR:OG1	1:I:238:ARG:N	2.55	0.40
1:J:88:ILE:CA	1:K:8:ARG:HH22	2.33	0.40
1:J:104:LEU:O	1:J:108:ILE:HG13	2.20	0.40
1:E:58:LEU:HD23	1:E:133:ARG:HA	2.02	0.40
1:L:237:THR:OG1	1:L:238:ARG:N	2.55	0.40
1:A:37:GLY:H	1:A:40:TYR:HH	1.60	0.40
1:D:1:MET:H2	1:J:110:GLU:CD	2.25	0.40
1:D:237:THR:OG1	1:D:238:ARG:N	2.55	0.40
1:K:88:ILE:HD13	1:K:88:ILE:HA	1.94	0.40
1:L:159:LYS:HA	1:L:159:LYS:HD3	1.93	0.40
1:M:153:ILE:HD11	1:M:169:LEU:C	2.41	0.40
1:B:88:ILE:HD13	1:L:8:ARG:HH12	1.83	0.40
1:B:104:LEU:O	1:B:108:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LYS:HD3	1:C:269:LYS:HA	1.96	0.40
1:K:267:GLN:OE1	1:K:267:GLN:N	2.45	0.40
1:L:104:LEU:O	1:L:108:ILE:HG13	2.20	0.40
1:H:237:THR:OG1	1:H:238:ARG:N	2.55	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	269/339 (79%)	263 (98%)	6 (2%)	0	100	100
1	B	269/339 (79%)	263 (98%)	6 (2%)	0	100	100
1	C	269/339 (79%)	263 (98%)	6 (2%)	0	100	100
1	D	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
1	E	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
1	F	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
1	G	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
1	H	269/339 (79%)	263 (98%)	6 (2%)	0	100	100
1	I	269/339 (79%)	263 (98%)	6 (2%)	0	100	100
1	J	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
1	K	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
1	L	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
1	M	269/339 (79%)	263 (98%)	6 (2%)	0	100	100
1	N	269/339 (79%)	264 (98%)	5 (2%)	0	100	100
All	All	3766/4746 (79%)	3690 (98%)	76 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	B	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	C	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	D	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	E	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	F	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	G	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	H	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	I	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	J	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	K	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	L	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	M	234/294 (80%)	222 (95%)	12 (5%)	24	55
1	N	234/294 (80%)	222 (95%)	12 (5%)	24	55
All	All	3276/4116 (80%)	3108 (95%)	168 (5%)	27	55

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	11	ARG
1	A	16	SER
1	A	42	PHE
1	A	115	ASP
1	A	121	ARG
1	A	125	TYR
1	A	136	GLU
1	A	142	SER
1	A	158	TYR
1	A	196	ARG

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Mol	Chain	Res	Type
1	A	208	GLU
1	B	5	TYR
1	B	11	ARG
1	B	16	SER
1	B	42	PHE
1	B	115	ASP
1	B	121	ARG
1	B	125	TYR
1	B	136	GLU
1	B	142	SER
1	B	158	TYR
1	B	196	ARG
1	B	208	GLU
1	C	5	TYR
1	C	11	ARG
1	C	16	SER
1	C	42	PHE
1	C	115	ASP
1	C	121	ARG
1	C	125	TYR
1	C	136	GLU
1	C	142	SER
1	C	158	TYR
1	C	196	ARG
1	C	208	GLU
1	I	5	TYR
1	I	11	ARG
1	I	16	SER
1	I	42	PHE
1	I	115	ASP
1	I	121	ARG
1	I	125	TYR
1	I	136	GLU
1	I	142	SER
1	I	158	TYR
1	I	196	ARG
1	I	208	GLU
1	D	5	TYR
1	D	11	ARG
1	D	16	SER
1	D	42	PHE
1	D	115	ASP

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Mol	Chain	Res	Type
1	D	121	ARG
1	D	125	TYR
1	D	136	GLU
1	D	142	SER
1	D	158	TYR
1	D	196	ARG
1	D	208	GLU
1	J	5	TYR
1	J	11	ARG
1	J	16	SER
1	J	42	PHE
1	J	115	ASP
1	J	121	ARG
1	J	125	TYR
1	J	136	GLU
1	J	142	SER
1	J	158	TYR
1	J	196	ARG
1	J	208	GLU
1	E	5	TYR
1	E	11	ARG
1	E	16	SER
1	E	42	PHE
1	E	115	ASP
1	E	121	ARG
1	E	125	TYR
1	E	136	GLU
1	E	142	SER
1	E	158	TYR
1	E	196	ARG
1	E	208	GLU
1	K	5	TYR
1	K	11	ARG
1	K	16	SER
1	K	42	PHE
1	K	115	ASP
1	K	121	ARG
1	K	125	TYR
1	K	136	GLU
1	K	142	SER
1	K	158	TYR
1	K	196	ARG

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Mol	Chain	Res	Type
1	K	208	GLU
1	F	5	TYR
1	F	11	ARG
1	F	16	SER
1	F	42	PHE
1	F	115	ASP
1	F	121	ARG
1	F	125	TYR
1	F	136	GLU
1	F	142	SER
1	F	158	TYR
1	F	196	ARG
1	F	208	GLU
1	L	5	TYR
1	L	11	ARG
1	L	16	SER
1	L	42	PHE
1	L	115	ASP
1	L	121	ARG
1	L	125	TYR
1	L	136	GLU
1	L	142	SER
1	L	158	TYR
1	L	196	ARG
1	L	208	GLU
1	G	5	TYR
1	G	11	ARG
1	G	16	SER
1	G	42	PHE
1	G	115	ASP
1	G	121	ARG
1	G	125	TYR
1	G	136	GLU
1	G	142	SER
1	G	158	TYR
1	G	196	ARG
1	G	208	GLU
1	M	5	TYR
1	M	11	ARG
1	M	16	SER
1	M	42	PHE
1	M	115	ASP

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Continued from previous page...

Mol	Chain	Res	Type
1	M	121	ARG
1	M	125	TYR
1	M	136	GLU
1	M	142	SER
1	M	158	TYR
1	M	196	ARG
1	M	208	GLU
1	H	5	TYR
1	H	11	ARG
1	H	16	SER
1	H	42	PHE
1	H	115	ASP
1	H	121	ARG
1	H	125	TYR
1	H	136	GLU
1	H	142	SER
1	H	158	TYR
1	H	196	ARG
1	H	208	GLU
1	N	5	TYR
1	N	11	ARG
1	N	16	SER
1	N	42	PHE
1	N	115	ASP
1	N	121	ARG
1	N	125	TYR
1	N	136	GLU
1	N	142	SER
1	N	158	TYR
1	N	196	ARG
1	N	208	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	67	ASN
1	A	85	GLN
1	A	117	GLN
1	A	171	GLN
1	B	60	GLN
1	B	67	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	B	85	GLN
1	B	117	GLN
1	C	60	GLN
1	C	67	ASN
1	C	85	GLN
1	C	117	GLN
1	I	60	GLN
1	I	67	ASN
1	I	85	GLN
1	I	117	GLN
1	I	171	GLN
1	D	60	GLN
1	D	67	ASN
1	D	85	GLN
1	D	117	GLN
1	J	60	GLN
1	J	67	ASN
1	J	85	GLN
1	J	117	GLN
1	J	171	GLN
1	E	60	GLN
1	E	67	ASN
1	E	85	GLN
1	E	117	GLN
1	K	60	GLN
1	K	67	ASN
1	K	85	GLN
1	K	117	GLN
1	F	60	GLN
1	F	67	ASN
1	F	85	GLN
1	F	117	GLN
1	L	60	GLN
1	L	67	ASN
1	L	85	GLN
1	L	117	GLN
1	G	60	GLN
1	G	67	ASN
1	G	85	GLN
1	G	117	GLN
1	G	171	GLN
1	M	60	GLN

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Mol	Chain	Res	Type
1	M	67	ASN
1	M	85	GLN
1	M	117	GLN
1	H	60	GLN
1	H	67	ASN
1	H	85	GLN
1	H	117	GLN
1	N	60	GLN
1	N	67	ASN
1	N	85	GLN
1	N	117	GLN

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.

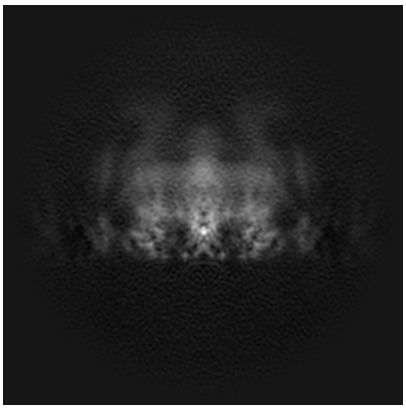
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18311. These allow visual inspection of the internal detail of the map and identification of artifacts.

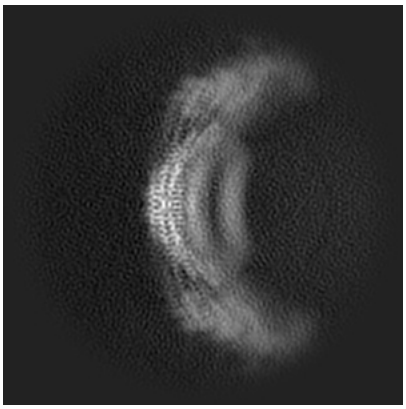
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

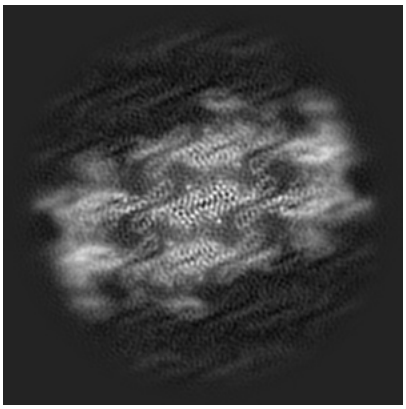
6.1.1 Primary map



X

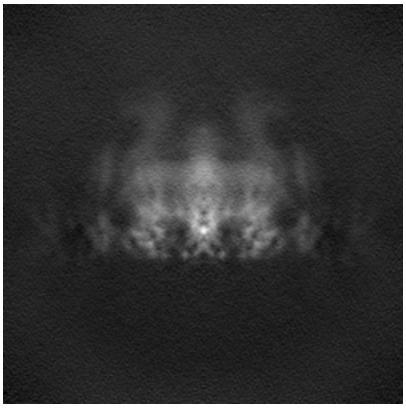


Y

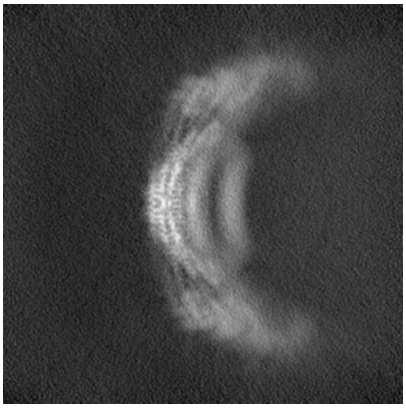


Z

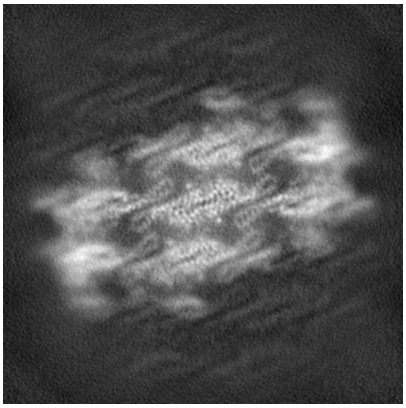
6.1.2 Raw map



X



Y

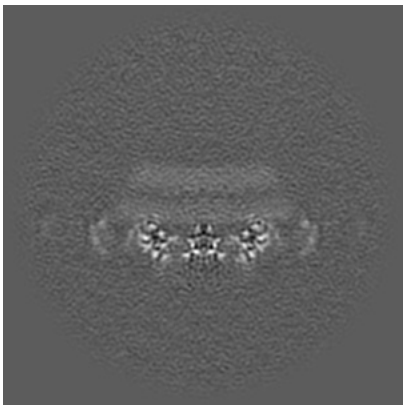


Z

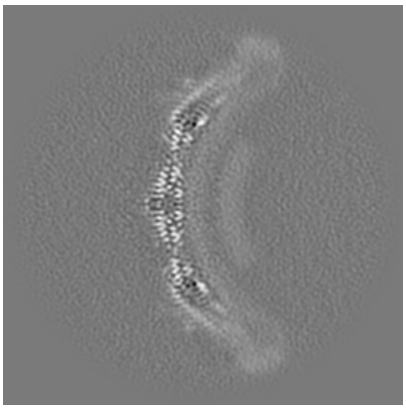
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

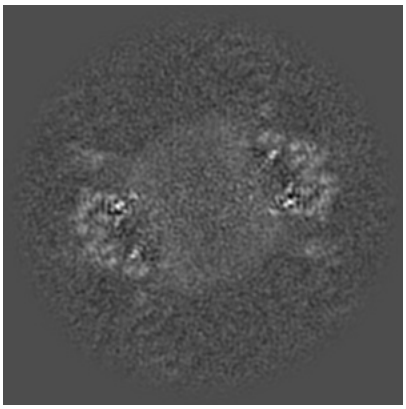
6.2.1 Primary map



X Index: 128

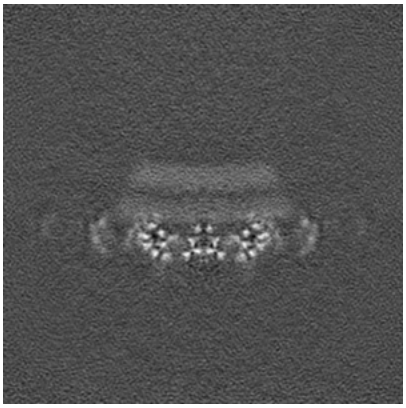


Y Index: 128

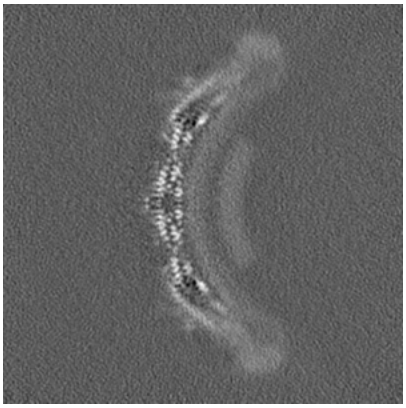


Z Index: 128

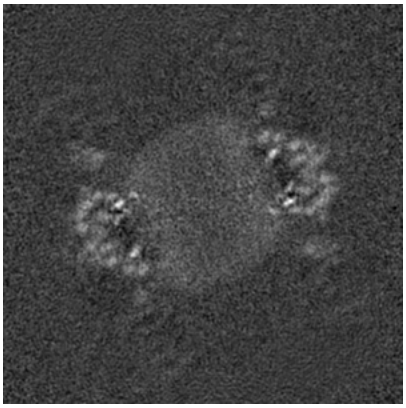
6.2.2 Raw map



X Index: 128



Y Index: 128

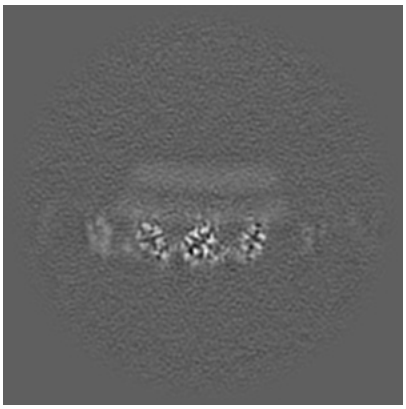


Z Index: 128

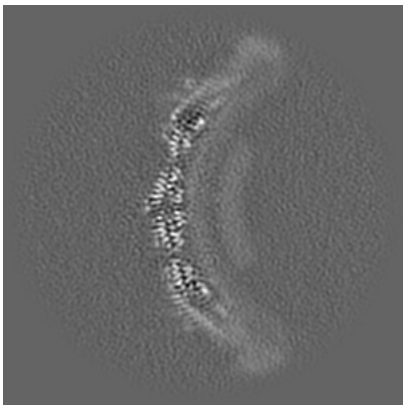
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

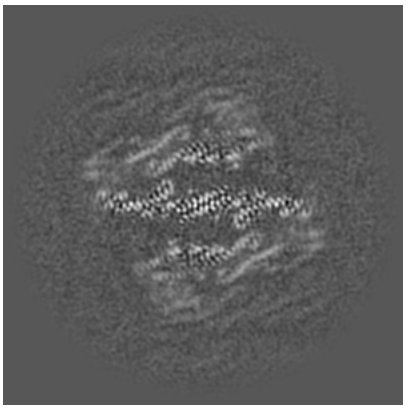
6.3.1 Primary map



X Index: 123

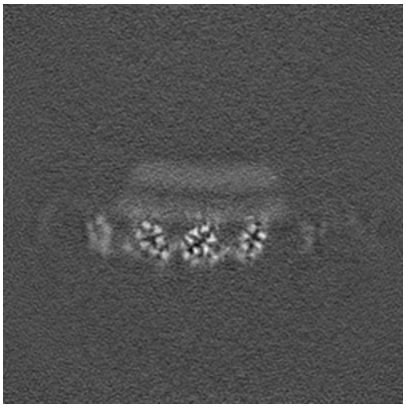


Y Index: 127

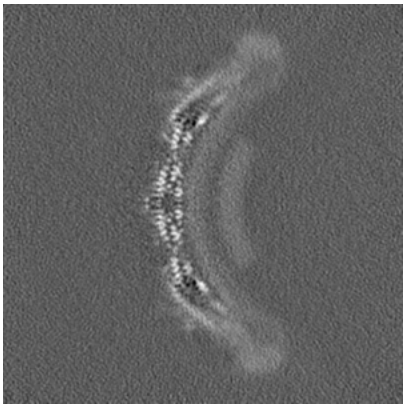


Z Index: 111

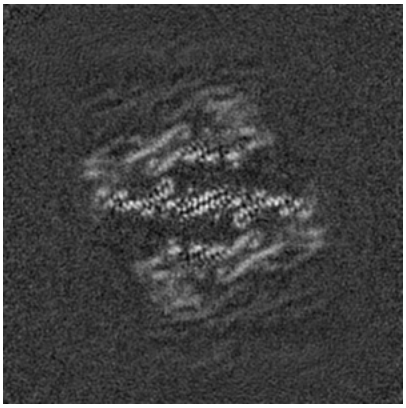
6.3.2 Raw map



X Index: 123



Y Index: 128

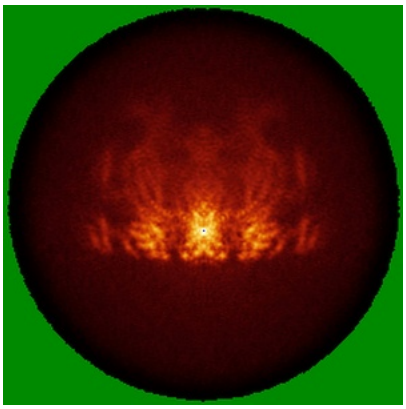


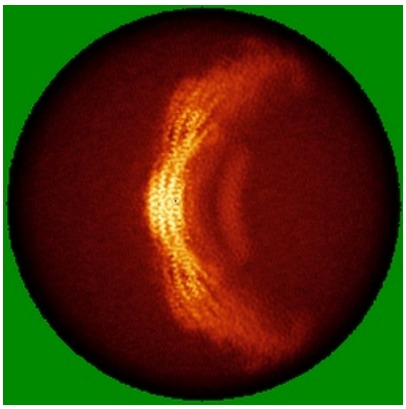
Z Index: 111

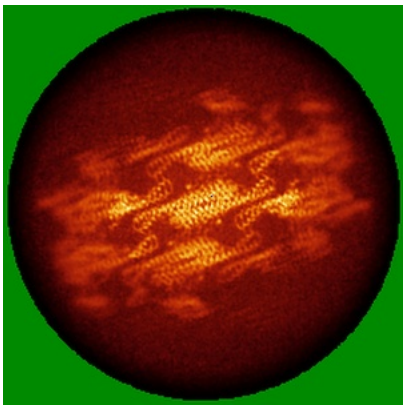
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

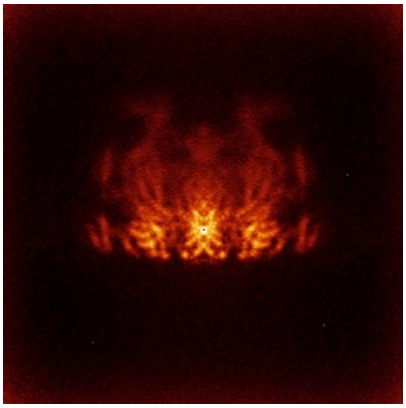
6.4.1 Primary map

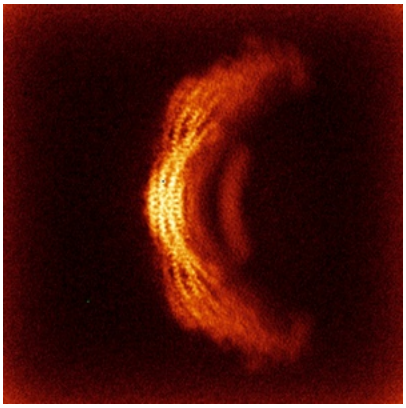

X

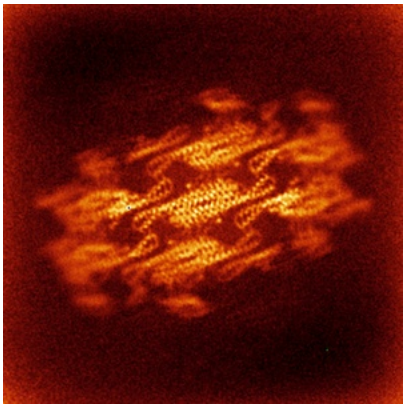

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

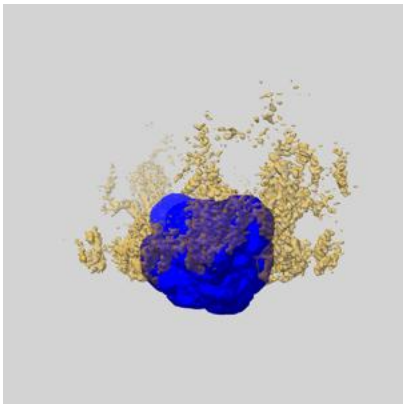
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

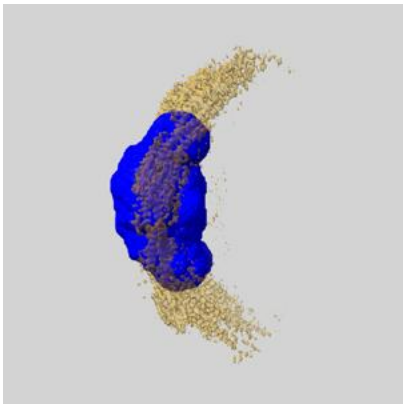
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

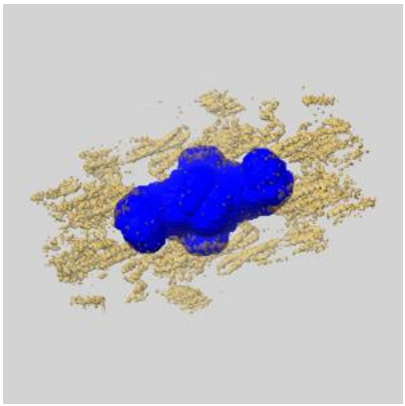
6.6.1 emd_18311_msk_1.map (i)



X



Y

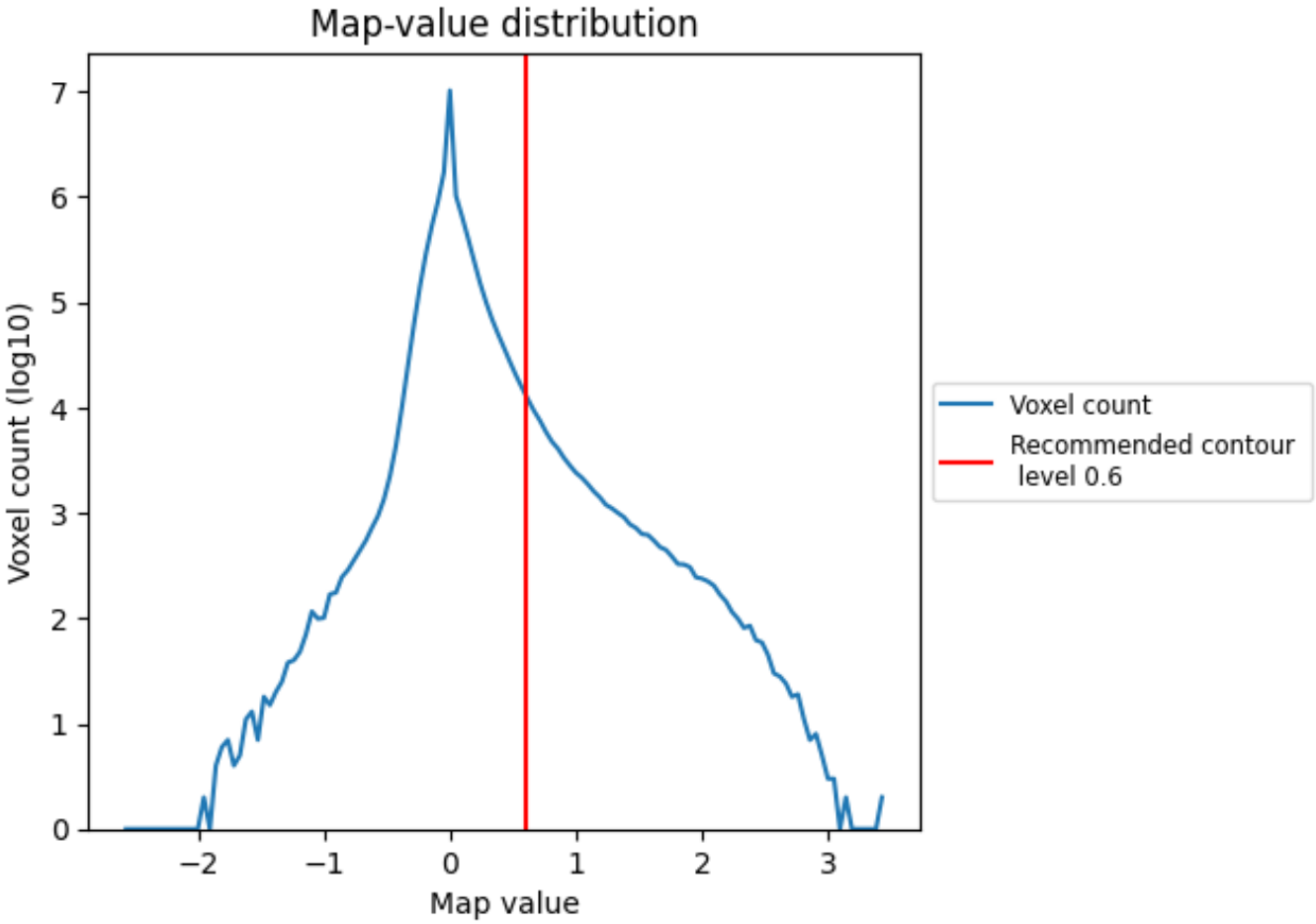


Z

7 Map analysis

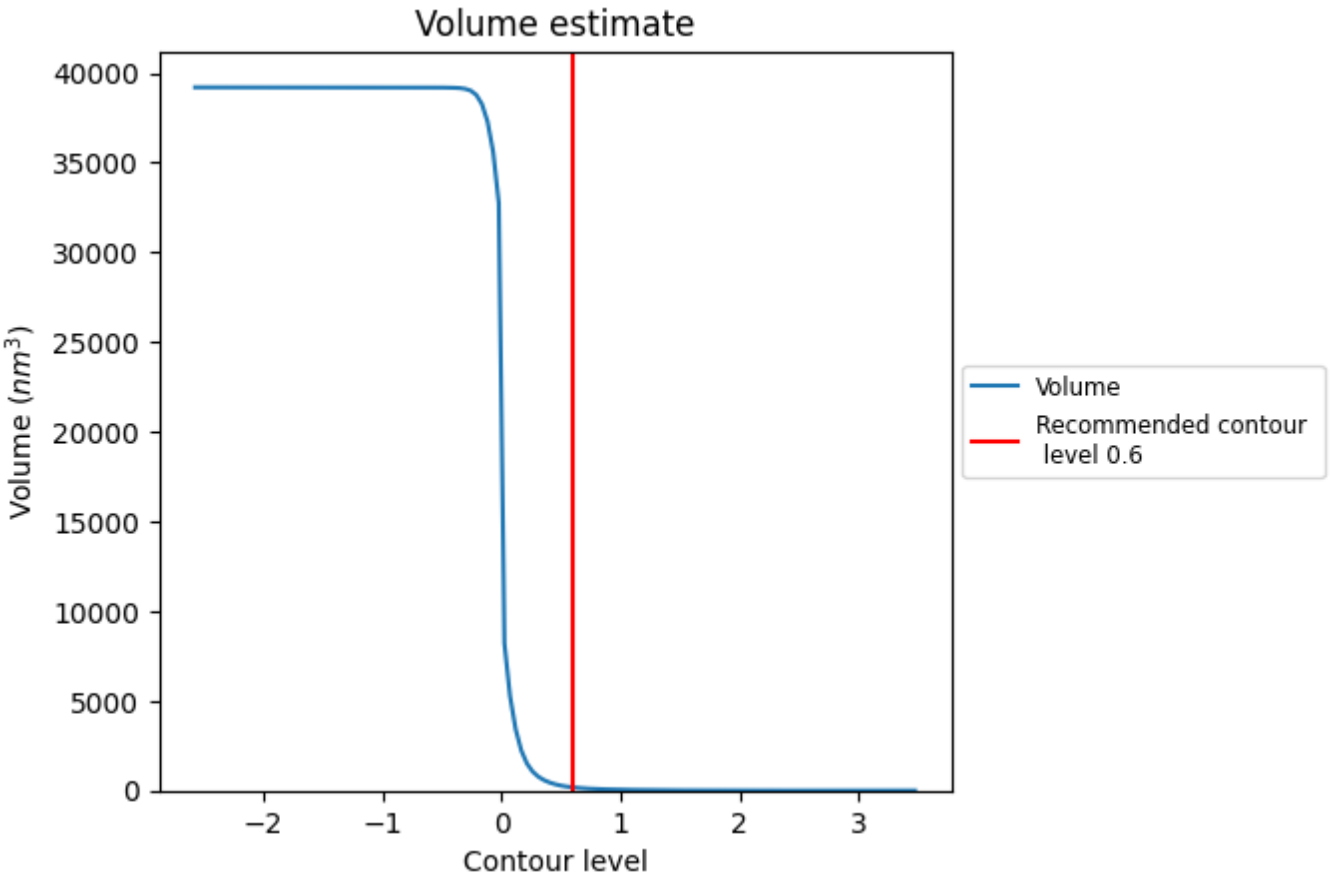
This section contains the results of statistical analysis of the map.

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.

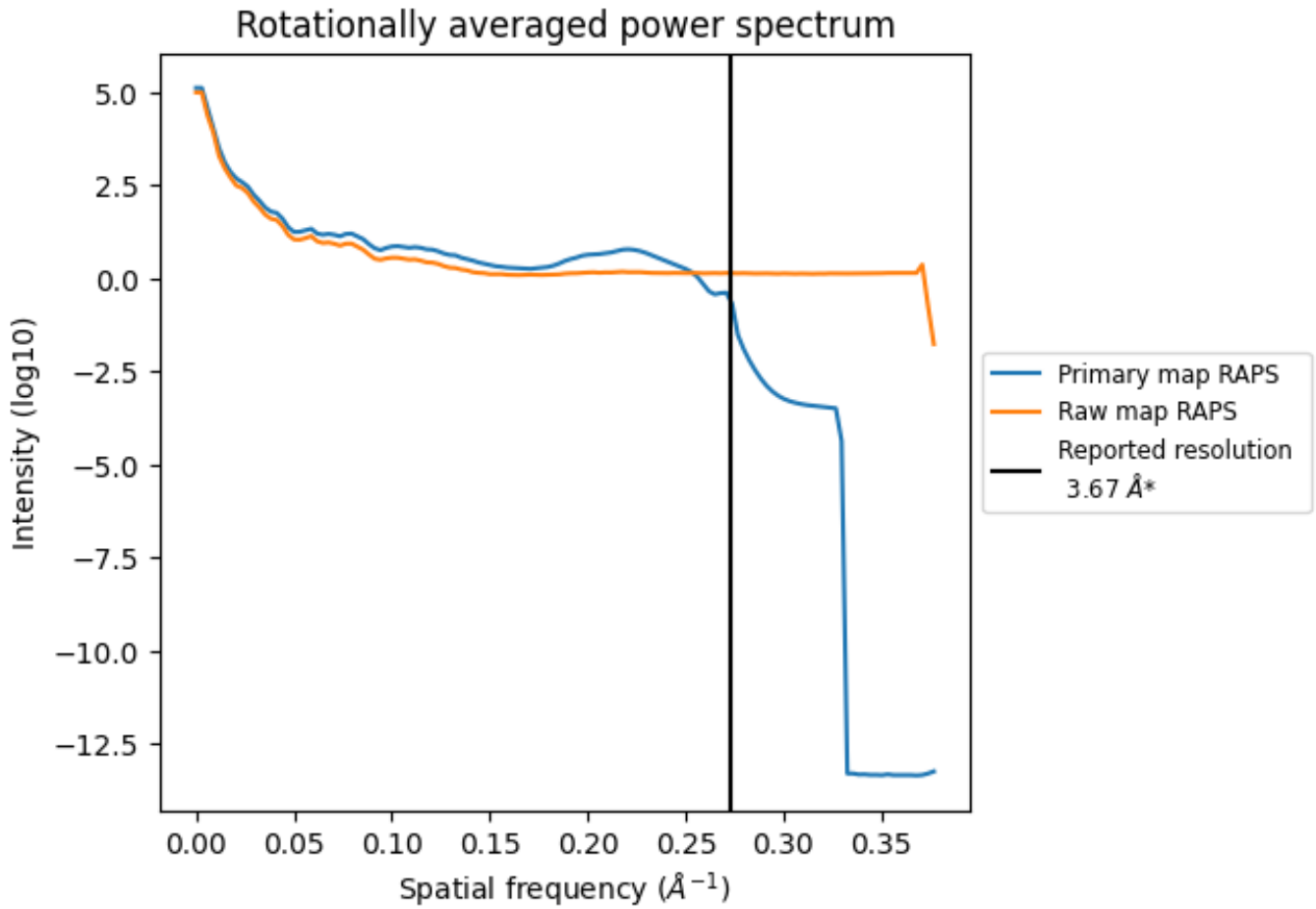
7.2 Volume estimate



The volume at the recommended contour level is 178 nm^3; this corresponds to an approximate mass of 161 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)

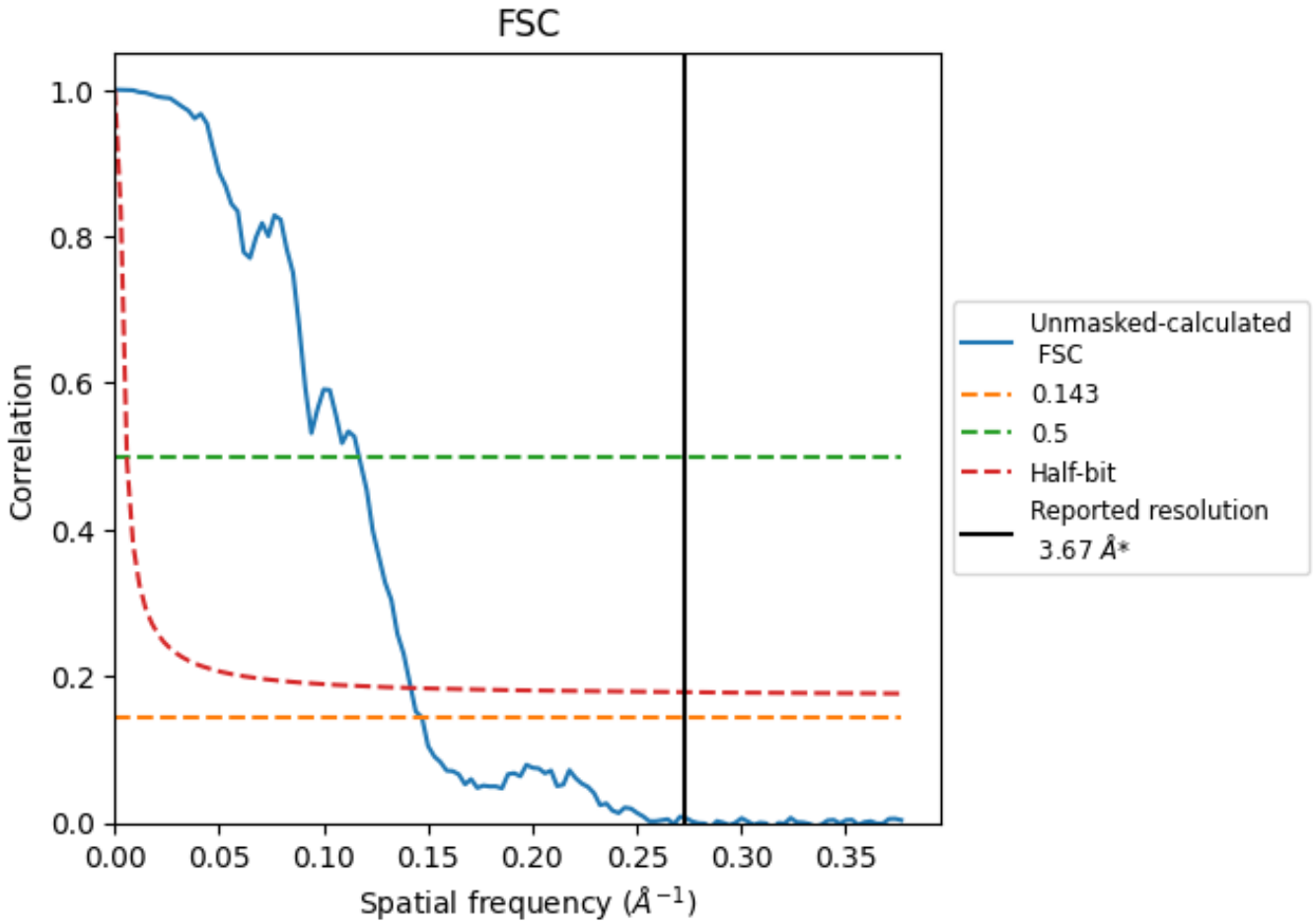


*Reported resolution corresponds to spatial frequency of 0.272 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.272 Å^{-1}

8.2 Resolution estimates (i)

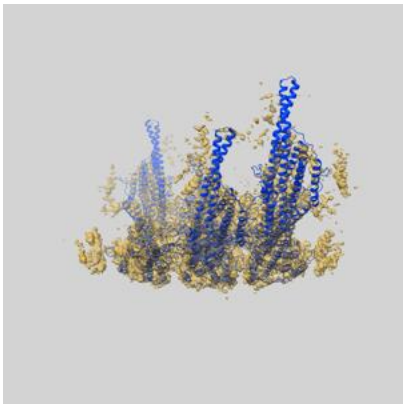
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.79	8.55	7.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.79 differs from the reported value 3.67 by more than 10 %

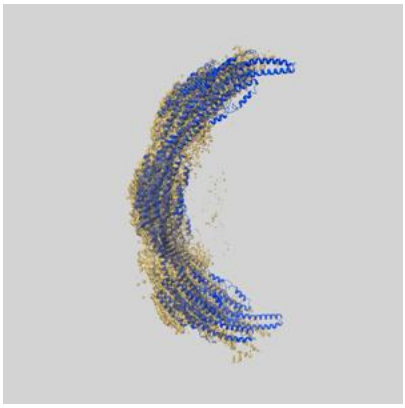
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18311 and PDB model 8QBE. Per-residue inclusion information can be found in section 3 on page 5.

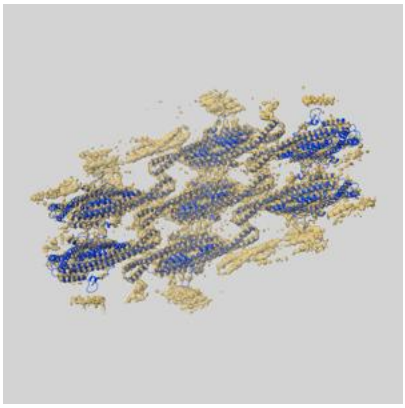
9.1 Map-model overlay



X



Y



Z

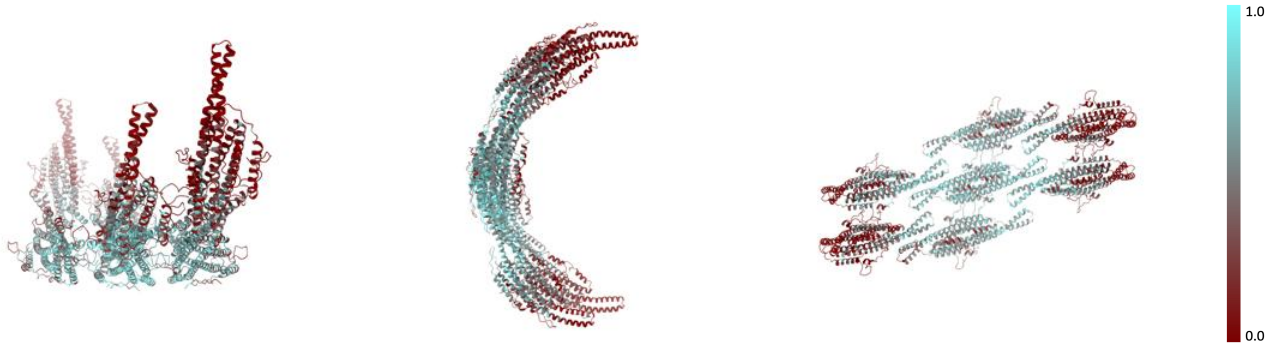
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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.

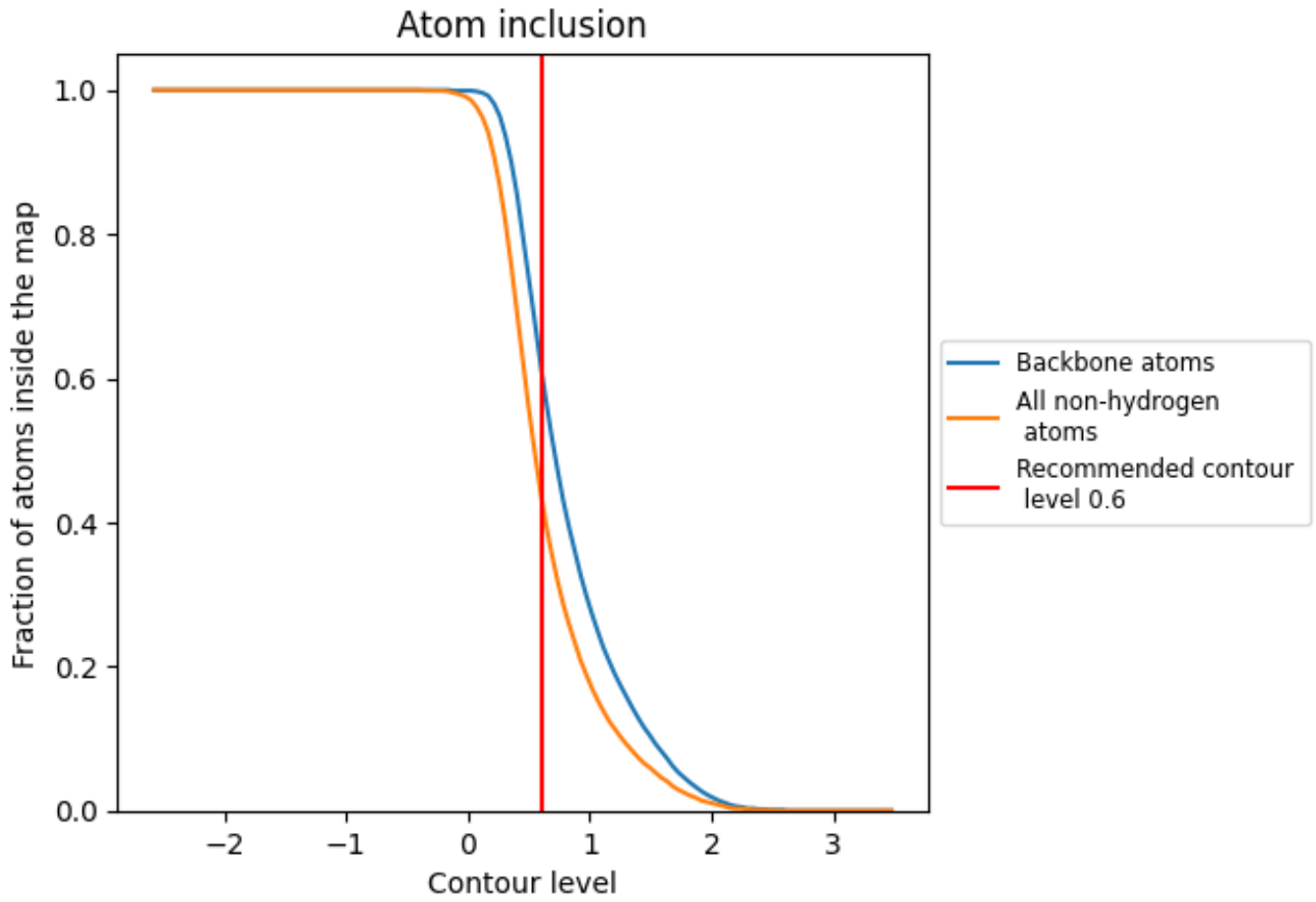
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 44% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4370	0.2280
A	0.7200	0.3950
B	0.7090	0.3800
C	0.5650	0.2870
D	0.3580	0.1970
E	0.1640	0.1070
F	0.5180	0.2690
G	0.4680	0.2340
H	0.2890	0.1340
I	0.5120	0.2550
J	0.4690	0.2320
K	0.2780	0.1460
L	0.5770	0.2890
M	0.3440	0.1700
N	0.1480	0.0980