



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:09 AM UTC

PDB ID : 9KYY / pdb_00009kyx
EMDB ID : EMD-61456
Title : The scaffold tetramer of phage P22
Authors : Liu, H.R.; Xiao, H.
Deposited on : 2024-12-09
Resolution : 6.90 Å(reported)

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:

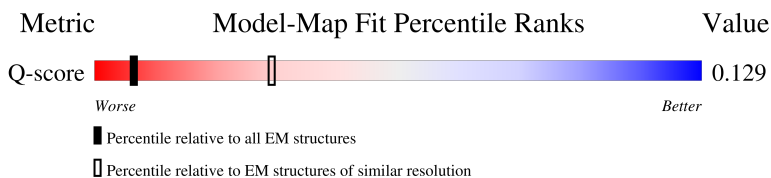
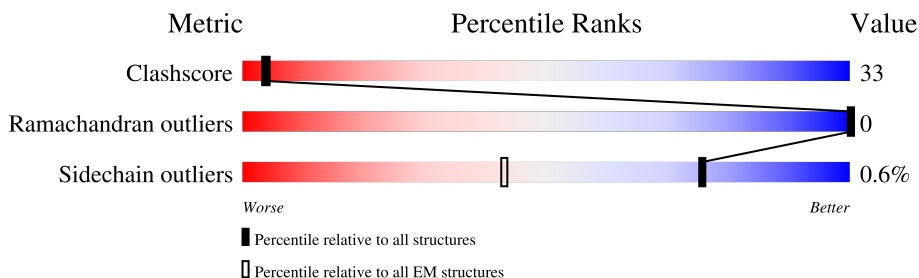
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 6.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	479 (6.40 - 7.40)

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 $\leq 5\%$. 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	303	21% 33% 23% 42%
1	B	303	14% 17% 18% 64%
1	C	303	21% 31% 25% 42%
1	D	303	25% 32% 25% 42%

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Mol	Chain	Length	Quality of chain
1	E	303	21% 31% 26% 42%
1	F	303	17% 17% 19% 64%
1	G	303	17% 17% 19% 64%
1	H	303	10% 17% 18% 64%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9112 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.

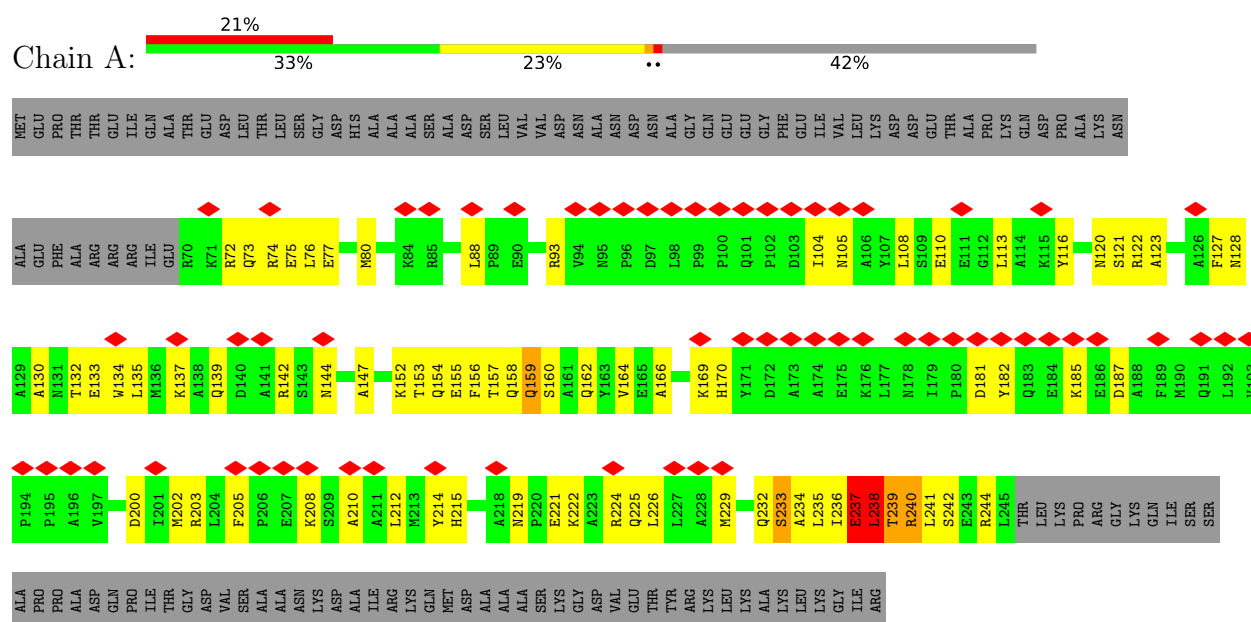
- Molecule 1 is a protein called Scaffolding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	B	109	Total	C	N	O	S	0	0
			877	548	159	165	5		
1	C	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	D	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	E	176	Total	C	N	O	S	0	0
			1401	870	252	273	6		
1	F	109	Total	C	N	O	S	0	0
			877	548	159	165	5		
1	G	109	Total	C	N	O	S	0	0
			877	548	159	165	5		
1	H	109	Total	C	N	O	S	0	0
			877	548	159	165	5		

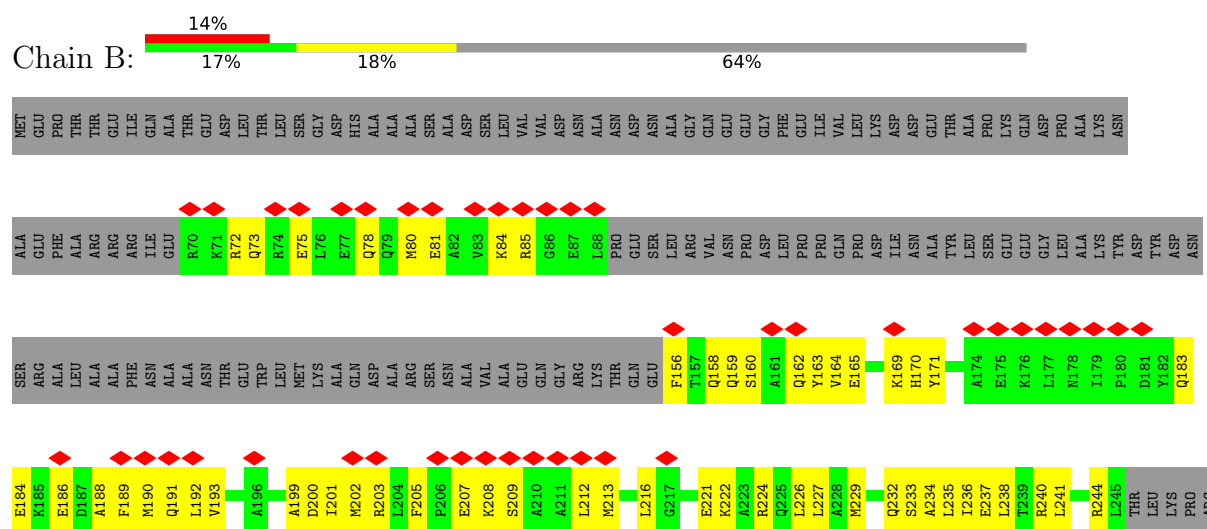
3 Residue-property plots

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: Scaffolding protein



• Molecule 1: Scaffolding protein



GLY
LYS
GLN
ILE
SER
SER
ALA
PRO
PRO
ALA
ASP
GLN
PRO
ILE
ILE
THR
GLY
ASP
VAL
SER
ALA
ALA
ASN
LYS
ASP
ALA
ILE
ARG
LYS
GLY
ASP
VAL
GLU
THR
TYR
ARG
LYS
LEU
LYS
ALA
LYS
LEU
LYS
GLY
ILE
ARG

• Molecule 1: Scaffolding protein

Chain C: 21% 31% 25% 42%

MET
GLU
PRO
THR
THR
GLU
GLN
THR
THR
ASP
GLU
LEU
THR
LEU
SER
GLY
ASP
HIS
ALA
ALA
SER
SER
ALA
ASP
SER
VAL
VAL
ASP
ASN
ALA
ASN
ASN
ASP
ALA
GLY
GLN
GLU
GLY
PHE
GLU
THR
TLE
VAL
LEU
LYS
ASP
ASP
GLU
THR
PRO
GLN
ASP
PRO
ALA
LYS
ASN

ALA
GLU
PHE
F127
ARG
ARG
ARG
ILE
GLU
R70
R71
R72
Q73
Q74
E75
L76
E77
M80
R85
G86
E87
L88
P89
E90
S91
E155
L92
R93
V94
N95
P96
D97
L98
P99
P100
Q101
P102
D103
I104
M105
A106
Y107
L108
S109
E110
E111
G112
L113
A114
K115
Y116
D117
Y118
D119
N120
S121
R122
A123
L124

A125
A126
F127
N128
A129
A130
N131
T132
E133
W134
L135
M136
K137
A138
Q139
D140
A141
R142
S143
N144
A147
K152
T153
E154
E155
F156
T157
Q158
Q159
S160
A161
Q162
V163
E165
A166
K169
H170
Y171
A174
E175
E176
L177
P180
D181
Y182
Q183
E184
K185
E186
D187
Q191
L192
V193

P194
P195
A196
V197
D200
L201
R202
L203
F205
P206
E207
K208
S209
A210
A211
L212
W213
Y214
H215
L216
G217
A218
A219
P220
E221
K222
A223
R224
Q225
L226
L227
A228
M229
D230
G231
Q232
S233
A234
L235
L236
E237
L238
T239
R240
L241
S242
E243
R244
L245
THR
LEU
LYS
PRO
ARG
GLY
LYS
ILE

SER
SER
ALA
PRO
PRO
ALA
ASP
GLN
THR
ILE
GLY
VAL
SER
ALA
ASN
LYS
ASP
ILE
ALA
GLN
MET
ASP
ALA
ALA
SER
LYS
GLY
ASP
VAL
GLU
THR
TYR
ARG
LYS
ILE
ARG

• Molecule 1: Scaffolding protein

Chain D: 25% 32% 25% 42%

MET
GLU
PRO
THR
THR
GLU
GLN
THR
THR
ASP
GLU
LEU
THR
LEU
SER
GLY
ASP
HIS
ALA
ALA
SER
SER
ALA
ASP
SER
VAL
VAL
ASP
ASN
ALA
ASN
ASP
ALA
ALA
GLY
GLN
GLU
GLY
PHE
GLU
THR
TLE
VAL
LEU
LYS
ASP
ASP
GLU
THR
PRO
GLN
ASP
PRO
ALA
LYS
ASN

ALA
GLU
PHE
A125
ARG
ARG
ARG
ILE
GLU
R70
R71
R72
Q73
Q74
E75
L76
E77
Q78
Q79
M80
V83
K84
R85
G86
E87
L88
P89
E90
S91
F156
L92
R93
V94
N95
P96
D97
L98
P99
P100
Q101
P102
D103
I104
M105
A106
Y107
L108
S109
E110
E111
G112
L113
A114
K115
Y116
D117
Y118
D119
N120
S121

R122
A123
L124
A125
A126
F127
N128
A129
A130
N131
T132
E133
W134
L135
M136
K137
A138
Q139
D140
A141
R142
S143
N144
A147
K152
T153
E154
E155
F156
T157
Q158
Q159
S160
A161
Q162
V163
E165
A166
K169
H170
Y171
D172
A173
A174
E175
K176
L177
N178
I179
P180
D181
Y182
Q183
E184
K185

E186
D187
F188
F189
M190
L192
P194
V197
A196
V197
G198
A199
D200
L201
R202
L203
L204
P206
E207
K208
S209
A210
A211
L212
W213
Y214
H215
V219
P220
E221
K222
A223
R224
Q225
L226
L227
A228
M229
D230
G231
Q232
S233
A234
L235
L236
E237
L238
T239
R240
L241
S242
E243
R244
L245
LEU

LYS
PRO
ARG
GLY
LYS
GLN
ILE
SER
SER
ALA
PRO
PRO
ALA
ASP
GLN
GLN
PRO
PRO
ILE
THR
GLY
ASP
VAL
SER
SER
ALA
ASN
LYS
ASP
ALA
ILE
ARG
LYS
GLN
MET
ASP
ASN
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ALA
SER
LYS
GLY
GLU
PHE
GLU
THR
TYR
ARG
LEU
LEU
LYS
LYS
LYS
LEU
LYS
GLY
ILE
ARG

• Molecule 1: Scaffolding protein

Chain E: 21% 31% 26% 42%

MET
GLU
PRO
THR
THR
GLU
GLN
THR
THR
ASP
GLU
LEU
THR
LEU
SER
GLY
ASP
HIS
ALA
ALA
SER
SER
ALA
ASP
SER
VAL
VAL
ASP
ASN
ALA
ASN
ASP
ALA
ALA
GLY
GLN
GLU
GLY
PHE
GLU
THR
TLE
VAL
LEU
LYS
LYS
ASP
ASP
GLU
THR
ALA
PRO
LYS
GLN
ASP
PRO
ALA
LYS
ASN

GLY	LYS	GLN	ILE	SER	ALA	PRO	PRO	ALA	ASP	GLN	PRO	ILE	THR	GLY	ASP	VAL	SER	ALA	ALA	LYS	ASP	ALA	ILE	ARG	GLN	MET	ASP	ALA	ALA	ALA	SER	LYS	GLY	ASP	VAL	GLU	THR	TYR	ARG	LYS	LEU	LYS	ALA	LYS	LYS	LEU	GLY	ILE	ARG
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● Molecule 1: Scaffolding protein



MET	GLU	PRO	THR	THR	GLU	ILE	GLN	ALA	THR	GLU	ASP	LEU	THR	SER	GLY	ASP	HIS	ALA	ALA	ALA	SER	LYS	ASP	ALA	ILE	ARG	VAL	VAL	ASP	ASN	ALA	ASN	ASN	ALA	ALA	GLY	GLN	GLU	GLU	GLY	PHE	GLU	ILE	VAL	LEU	LYS	ASP	GLU	THR	ALA	ALA	LYS	GLN	ASP	PRO	ALA	LYS	ASN
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ALA	GLU	PHE	ALA	ARG	ARG	ILE	GLU	R70	R71	R72	Q73	R74	E75	Q78	Q79	M80	E81	R84	R85	G86	E87	I88	PRO	GLU	SER	SER	LEU	VAL	VAL	ASP	ASN	ALA	ASN	ASN	VAL	ASN	PRO	ASP	ASP	LEU	PRO	PRO	GLN	PRO	GLN	PRO	ASP	TYR	LEU	SER	GLY	GLU	GLU	PRO	ALA	LYS	TYR	ASP	ASP	ASN	SER	ARG
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ALA	LEU	ALA	ALA	PHE	ASN	ALA	ALA	ASN	THR	THR	TRP	LEU	MET	LYS	ALA	ALA	GLN	ASP	ASP	ALA	ARG	SER	ASN	ALA	VAL	ALA	GLU	GLN	GLY	ARG	LYS	THR	GLU	F156	T157	Q158	Q159	S160	A161	Q162	Y163	V164	E165	K169	H170	Y171	K176	Q183	E184	K185	E186	D187	A188	F189	M190	Q191	L192
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V193	P194	P195	A196	A199	D200	I201	M202	R203	L204	F205	P206	E207	K208	S209	A210	A211	L212	M213	L216	E221	K222	A223	R224	Q225	L226	L227	A228	M229	Q232	S233	A234	L235	I236	E237	L238	T239	R240	L241	R244	L245	THR	LEU	LYS	PRO	ARG	GLY	LYS	GLN	ILE	SER	SER	ALA	PRO	PRO
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	ASP	GLN	PRO	ILE	THR	GLY	ASP	VAL	SER	ALA	ASN	ALA	ALA	GLY	ILE	LYS	GLN	MET	ASP	ALA	ALA	ALA	SER	LYS	GLY	ASP	VAL	GLU	THR	TYR	ARG	LYS	LYS	LYS	ALA	LYS	LEU	LEU	LEU	LYS	LYS	GLY	ILE	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.942	Depositor
Minimum map value	-6.079	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.767	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.12, 2.12, 2.12	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	0.45	0/1425	0.68	5/1923 (0.3%)
1	B	0.19	0/889	0.50	0/1191
1	C	0.43	3/1425 (0.2%)	0.74	4/1923 (0.2%)
1	D	0.38	1/1425 (0.1%)	0.66	3/1923 (0.2%)
1	E	0.34	1/1425 (0.1%)	0.65	2/1923 (0.1%)
1	F	0.19	0/889	0.50	0/1191
1	G	0.19	0/889	0.50	0/1191
1	H	0.19	0/889	0.50	0/1191
All	All	0.34	5/9256 (0.1%)	0.62	14/12456 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	ILE	CA-C	-7.27	1.44	1.52
1	D	236	ILE	CA-C	-6.26	1.45	1.52
1	C	237	GLU	N-CA	-5.58	1.39	1.46
1	E	236	ILE	CA-C	-5.33	1.46	1.52
1	C	232	GLN	N-CA	-5.09	1.40	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	232	GLN	N-CA-C	-10.33	100.01	111.07
1	A	239	THR	N-CA-C	-9.44	99.90	111.33
1	C	236	ILE	N-CA-C	-9.12	100.75	110.23
1	D	236	ILE	N-CA-C	-8.54	102.22	110.42
1	A	238	LEU	N-CA-C	-6.95	102.28	111.24
1	E	234	ALA	N-CA-C	-6.61	103.33	111.33
1	E	159	GLN	N-CA-C	-6.37	104.27	111.14
1	C	236	ILE	CB-CA-C	-6.31	103.62	111.70
1	D	236	ILE	CB-CA-C	-5.95	104.35	111.97
1	C	159	GLN	N-CA-C	-5.67	105.01	111.07
1	A	237	GLU	N-CA-C	-5.49	99.11	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	GLU	N-CA-C	-5.21	102.83	111.37
1	A	159	GLN	N-CA-C	-5.11	105.61	111.07
1	A	233	SER	N-CA-C	-5.01	105.50	110.97

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	1401	0	1376	111	0
1	B	877	0	880	55	0
1	C	1401	0	1376	107	0
1	D	1401	0	1376	105	0
1	E	1401	0	1376	98	0
1	F	877	0	880	55	0
1	G	877	0	880	57	0
1	H	877	0	880	54	0
All	All	9112	0	9024	607	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 33.

All (607) 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:139:GLN:HG3	1:D:139:GLN:HE22	1.17	1.08
1:A:108:LEU:HD22	1:C:125:ALA:HB2	1.35	1.07
1:D:236:ILE:HG23	1:G:239:THR:HG23	1.36	1.04
1:D:108:LEU:HD23	1:E:121:SER:HB2	1.50	0.91
1:A:240:ARG:HG2	1:A:240:ARG:HH11	1.38	0.89
1:E:224:ARG:NH1	1:E:225:GLN:OE1	2.06	0.89
1:E:234:ALA:O	1:E:237:GLU:HB3	1.74	0.88
1:C:224:ARG:NH1	1:C:225:GLN:OE1	2.06	0.88
1:A:224:ARG:NH1	1:A:225:GLN:OE1	2.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ARG:NH1	1:D:225:GLN:OE1	2.06	0.86
1:A:182:TYR:HA	1:A:185:LYS:HE3	1.57	0.86
1:E:182:TYR:HA	1:E:185:LYS:HE3	1.57	0.86
1:A:236:ILE:HD12	1:A:239:THR:HB	1.58	0.84
1:D:182:TYR:HA	1:D:185:LYS:HE3	1.57	0.84
1:C:229:MET:HE1	1:C:233:SER:C	2.03	0.83
1:C:234:ALA:O	1:C:237:GLU:HB3	1.78	0.83
1:C:135:LEU:HD21	1:D:132:THR:HA	1.60	0.83
1:C:182:TYR:HA	1:C:185:LYS:HE3	1.57	0.83
1:E:229:MET:HE1	1:E:234:ALA:N	1.94	0.83
1:A:236:ILE:C	1:A:238:LEU:H	1.87	0.83
1:C:142:ARG:HH21	1:D:139:GLN:HE21	1.24	0.82
1:B:209:SER:HA	1:B:212:LEU:HD12	1.63	0.81
1:D:234:ALA:O	1:D:237:GLU:HB3	1.79	0.80
1:G:209:SER:HA	1:G:212:LEU:HD12	1.63	0.80
1:F:209:SER:HA	1:F:212:LEU:HD12	1.63	0.80
1:C:139:GLN:CG	1:D:139:GLN:HE22	1.94	0.80
1:H:209:SER:HA	1:H:212:LEU:HD12	1.63	0.79
1:A:229:MET:HE1	1:A:233:SER:HB3	1.65	0.78
1:A:155:GLU:O	1:A:159:GLN:HG2	1.83	0.78
1:E:108:LEU:HG	1:E:123:ALA:HB1	1.67	0.77
1:A:237:GLU:CA	1:A:240:ARG:HB3	2.15	0.77
1:C:201:ILE:HG12	1:C:238:LEU:HD22	1.66	0.77
1:E:155:GLU:O	1:E:159:GLN:HG2	1.83	0.77
1:A:135:LEU:HD22	1:C:136:MET:HE3	1.65	0.77
1:A:232:GLN:O	1:A:235:LEU:HB3	1.85	0.77
1:C:236:ILE:HG22	1:C:240:ARG:HD2	1.67	0.76
1:A:108:LEU:HG	1:A:123:ALA:HB1	1.67	0.76
1:E:201:ILE:HG12	1:E:238:LEU:HD22	1.66	0.76
1:D:201:ILE:HG12	1:D:238:LEU:HD22	1.66	0.75
1:C:108:LEU:HG	1:C:123:ALA:HB1	1.67	0.75
1:C:229:MET:HE1	1:C:234:ALA:N	2.01	0.75
1:E:226:LEU:HD21	1:E:237:GLU:HG2	1.69	0.75
1:C:139:GLN:HG3	1:D:139:GLN:NE2	1.98	0.75
1:D:108:LEU:HG	1:D:123:ALA:HB1	1.67	0.75
1:D:235:LEU:O	1:D:238:LEU:HB3	1.87	0.73
1:C:142:ARG:NH2	1:D:139:GLN:HE21	1.87	0.72
1:C:237:GLU:OE2	1:C:241:LEU:HB2	1.89	0.71
1:D:235:LEU:HG	1:D:236:ILE:HD13	1.71	0.71
1:B:207:GLU:HG2	1:B:208:LYS:HG3	1.73	0.70
1:C:155:GLU:O	1:C:159:GLN:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:MET:HE1	1:E:233:SER:C	2.17	0.70
1:H:213:MET:HA	1:H:216:LEU:HG	1.73	0.70
1:F:207:GLU:HG2	1:F:208:LYS:HG3	1.73	0.70
1:A:236:ILE:C	1:A:238:LEU:N	2.48	0.69
1:C:226:LEU:HD12	1:C:234:ALA:HB1	1.74	0.69
1:H:207:GLU:HG2	1:H:208:LYS:HG3	1.73	0.69
1:D:108:LEU:CD2	1:E:121:SER:HB2	2.21	0.69
1:D:212:LEU:HD13	1:D:238:LEU:HD11	1.74	0.69
1:C:212:LEU:HD13	1:C:238:LEU:HD11	1.74	0.69
1:E:212:LEU:HD13	1:E:238:LEU:HD11	1.74	0.69
1:A:237:GLU:HA	1:A:240:ARG:CZ	2.22	0.69
1:D:229:MET:HE1	1:D:234:ALA:N	2.08	0.69
1:G:201:ILE:HD11	1:G:212:LEU:HD13	1.75	0.69
1:H:201:ILE:HD11	1:H:212:LEU:HD13	1.75	0.69
1:B:213:MET:HA	1:B:216:LEU:HG	1.73	0.69
1:G:207:GLU:HG2	1:G:208:LYS:HG3	1.73	0.69
1:A:240:ARG:HH11	1:A:240:ARG:CG	2.05	0.68
1:F:201:ILE:HD11	1:F:212:LEU:HD13	1.75	0.68
1:F:213:MET:HA	1:F:216:LEU:HG	1.73	0.68
1:B:201:ILE:HD13	1:B:238:LEU:HD13	1.76	0.68
1:F:226:LEU:HD13	1:F:229:MET:HB3	1.75	0.68
1:G:201:ILE:HD13	1:G:238:LEU:HD13	1.75	0.68
1:G:213:MET:HA	1:G:216:LEU:HG	1.73	0.68
1:B:226:LEU:HD13	1:B:229:MET:HB3	1.75	0.68
1:B:201:ILE:HD11	1:B:212:LEU:HD13	1.75	0.67
1:A:169:LYS:HE2	1:A:202:MET:HB2	1.77	0.67
1:A:237:GLU:HA	1:A:240:ARG:HB3	1.76	0.67
1:A:236:ILE:CD1	1:A:239:THR:HB	2.25	0.67
1:C:116:TYR:O	1:C:122:ARG:NH2	2.26	0.67
1:F:201:ILE:HD13	1:F:238:LEU:HD13	1.75	0.67
1:D:169:LYS:HE2	1:D:202:MET:HB2	1.77	0.67
1:E:237:GLU:OE2	1:E:240:ARG:NH1	2.28	0.67
1:G:226:LEU:HD13	1:G:229:MET:HB3	1.75	0.66
1:H:226:LEU:HD13	1:H:229:MET:HB3	1.75	0.66
1:H:201:ILE:HD13	1:H:238:LEU:HD13	1.76	0.66
1:C:169:LYS:HE2	1:C:202:MET:HB2	1.76	0.66
1:C:229:MET:CE	1:C:233:SER:HB3	2.25	0.66
1:E:169:LYS:HE2	1:E:202:MET:HB2	1.77	0.65
1:C:135:LEU:HD22	1:D:136:MET:HE2	1.76	0.65
1:A:234:ALA:O	1:A:238:LEU:HB3	1.95	0.65
1:E:116:TYR:O	1:E:122:ARG:NH2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:OG	1:A:122:ARG:NH1	2.30	0.65
1:E:235:LEU:O	1:E:236:ILE:C	2.36	0.65
1:F:158:GLN:O	1:F:162:GLN:NE2	2.31	0.64
1:C:225:GLN:O	1:C:229:MET:HG3	1.98	0.64
1:B:192:LEU:HD12	1:B:193:VAL:HG13	1.80	0.64
1:C:236:ILE:O	1:C:237:GLU:C	2.39	0.64
1:G:192:LEU:HD12	1:G:193:VAL:HG13	1.80	0.64
1:A:225:GLN:O	1:A:229:MET:HG3	1.98	0.64
1:H:158:GLN:O	1:H:162:GLN:NE2	2.31	0.64
1:E:225:GLN:O	1:E:229:MET:HG3	1.98	0.64
1:D:121:SER:OG	1:D:122:ARG:NH1	2.30	0.63
1:F:170:HIS:HD2	1:F:202:MET:HG2	1.64	0.63
1:F:192:LEU:HD12	1:F:193:VAL:HG13	1.80	0.63
1:H:170:HIS:HD2	1:H:202:MET:HG2	1.64	0.63
1:A:116:TYR:O	1:A:122:ARG:NH2	2.26	0.63
1:C:121:SER:OG	1:C:122:ARG:NH1	2.30	0.63
1:E:121:SER:OG	1:E:122:ARG:NH1	2.30	0.63
1:G:170:HIS:HD2	1:G:202:MET:HG2	1.64	0.63
1:H:192:LEU:HD12	1:H:193:VAL:HG13	1.80	0.63
1:B:158:GLN:O	1:B:162:GLN:NE2	2.31	0.63
1:B:170:HIS:HD2	1:B:202:MET:HG2	1.64	0.63
1:G:158:GLN:O	1:G:162:GLN:NE2	2.31	0.63
1:D:116:TYR:O	1:D:122:ARG:NH2	2.26	0.63
1:A:240:ARG:HD2	1:A:244:ARG:NH2	2.13	0.62
1:E:235:LEU:O	1:E:238:LEU:N	2.32	0.62
1:H:156:PHE:O	1:H:159:GLN:NE2	2.27	0.62
1:C:219:ASN:HB3	1:C:222:LYS:HE2	1.82	0.62
1:D:134:TRP:HA	1:D:137:LYS:HG2	1.82	0.62
1:E:236:ILE:O	1:E:237:GLU:C	2.41	0.62
1:A:205:PHE:HZ	1:A:239:THR:HG23	1.65	0.62
1:D:225:GLN:O	1:D:229:MET:HG3	1.98	0.62
1:E:219:ASN:HB3	1:E:222:LYS:HE2	1.82	0.62
1:A:229:MET:CE	1:A:233:SER:HB3	2.30	0.62
1:A:237:GLU:C	1:A:240:ARG:HB3	2.25	0.62
1:D:219:ASN:HB3	1:D:222:LYS:HE2	1.82	0.61
1:C:104:ILE:HB	1:D:125:ALA:HB1	1.83	0.61
1:A:219:ASN:HB3	1:A:222:LYS:HE2	1.82	0.61
1:H:81:GLU:HA	1:H:84:LYS:HG2	1.82	0.61
1:D:236:ILE:HG22	1:D:240:ARG:HD2	1.82	0.61
1:A:134:TRP:HA	1:A:137:LYS:HG2	1.82	0.61
1:A:238:LEU:HG	1:A:239:THR:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:GLU:HA	1:F:84:LYS:HG2	1.82	0.61
1:F:156:PHE:O	1:F:159:GLN:NE2	2.27	0.61
1:C:142:ARG:HH21	1:D:139:GLN:NE2	1.96	0.61
1:C:226:LEU:HD21	1:C:237:GLU:HG2	1.82	0.60
1:D:226:LEU:HD12	1:D:234:ALA:HB1	1.84	0.60
1:E:134:TRP:HA	1:E:137:LYS:HG2	1.82	0.60
1:G:81:GLU:HA	1:G:84:LYS:HG2	1.82	0.60
1:D:72:ARG:HH12	1:D:187:ASP:HA	1.67	0.60
1:C:134:TRP:HA	1:C:137:LYS:HG2	1.82	0.60
1:E:229:MET:SD	1:E:234:ALA:HA	2.41	0.60
1:C:72:ARG:HH12	1:C:187:ASP:HA	1.67	0.60
1:C:235:LEU:O	1:C:236:ILE:C	2.41	0.60
1:D:236:ILE:O	1:D:237:GLU:C	2.40	0.60
1:E:72:ARG:HH12	1:E:187:ASP:HA	1.67	0.60
1:D:229:MET:HE1	1:D:233:SER:HB3	1.83	0.59
1:E:235:LEU:O	1:E:238:LEU:HB3	2.01	0.59
1:A:237:GLU:HA	1:A:240:ARG:NE	2.16	0.59
1:C:229:MET:HE2	1:C:233:SER:HB3	1.83	0.59
1:C:232:GLN:CD	1:C:232:GLN:H	2.10	0.59
1:C:221:GLU:O	1:C:225:GLN:NE2	2.35	0.59
1:A:72:ARG:HH12	1:A:187:ASP:HA	1.67	0.59
1:A:221:GLU:O	1:A:225:GLN:NE2	2.35	0.59
1:B:81:GLU:HA	1:B:84:LYS:HG2	1.82	0.59
1:D:229:MET:CE	1:D:233:SER:HB3	2.33	0.59
1:E:221:GLU:O	1:E:225:GLN:NE2	2.35	0.59
1:A:238:LEU:O	1:A:239:THR:C	2.45	0.59
1:D:221:GLU:O	1:D:225:GLN:NE2	2.35	0.59
1:E:226:LEU:HD12	1:E:234:ALA:HB1	1.83	0.59
1:H:240:ARG:HB3	1:H:244:ARG:NH1	2.18	0.59
1:G:240:ARG:HB3	1:G:244:ARG:NH1	2.18	0.59
1:F:80:MET:HG3	1:F:164:VAL:HG22	1.85	0.58
1:H:80:MET:HG3	1:H:164:VAL:HG22	1.85	0.58
1:A:185:LYS:NZ	1:A:210:ALA:O	2.34	0.58
1:D:185:LYS:NZ	1:D:210:ALA:O	2.34	0.58
1:B:156:PHE:O	1:B:159:GLN:NE2	2.27	0.58
1:B:80:MET:HG3	1:B:164:VAL:HG22	1.85	0.58
1:A:233:SER:O	1:A:234:ALA:C	2.44	0.58
1:A:235:LEU:O	1:A:238:LEU:HB3	2.03	0.58
1:B:240:ARG:HB3	1:B:244:ARG:NH1	2.18	0.58
1:C:104:ILE:HG13	1:C:105:ASN:H	1.69	0.58
1:E:104:ILE:HG13	1:E:105:ASN:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:ARG:HB3	1:F:244:ARG:NH1	2.18	0.58
1:D:104:ILE:HG13	1:D:105:ASN:N	2.19	0.58
1:F:159:GLN:O	1:F:163:TYR:HD2	1.87	0.58
1:D:109:SER:HA	1:E:122:ARG:NH1	2.19	0.58
1:C:104:ILE:HG13	1:C:105:ASN:N	2.19	0.57
1:C:230:ASP:O	1:C:234:ALA:N	2.36	0.57
1:E:185:LYS:NZ	1:E:210:ALA:O	2.34	0.57
1:C:237:GLU:O	1:C:238:LEU:C	2.43	0.57
1:E:233:SER:HA	1:E:236:ILE:HG12	1.86	0.57
1:G:170:HIS:CD2	1:G:202:MET:HG2	2.39	0.57
1:E:104:ILE:HG13	1:E:105:ASN:H	1.69	0.57
1:H:170:HIS:CD2	1:H:202:MET:HG2	2.39	0.57
1:B:170:HIS:CD2	1:B:202:MET:HG2	2.39	0.57
1:C:135:LEU:HD21	1:D:132:THR:CA	2.34	0.57
1:C:235:LEU:O	1:C:238:LEU:N	2.37	0.57
1:G:159:GLN:O	1:G:163:TYR:HD2	1.87	0.57
1:B:159:GLN:O	1:B:163:TYR:HD2	1.87	0.57
1:D:109:SER:HA	1:E:122:ARG:HH11	1.69	0.57
1:G:80:MET:HG3	1:G:164:VAL:HG22	1.85	0.57
1:A:104:ILE:HG13	1:A:105:ASN:H	1.69	0.57
1:D:104:ILE:HG13	1:D:105:ASN:H	1.69	0.57
1:B:81:GLU:OE1	1:B:85:ARG:NH2	2.38	0.57
1:G:81:GLU:OE1	1:G:85:ARG:NH2	2.38	0.57
1:H:81:GLU:OE1	1:H:85:ARG:NH2	2.38	0.57
1:C:104:ILE:HG22	1:C:127:PHE:CZ	2.40	0.56
1:E:104:ILE:HG22	1:E:127:PHE:CZ	2.40	0.56
1:G:156:PHE:O	1:G:159:GLN:NE2	2.27	0.56
1:D:104:ILE:HG22	1:D:127:PHE:CZ	2.40	0.56
1:F:170:HIS:CD2	1:F:202:MET:HG2	2.39	0.56
1:A:104:ILE:HG13	1:A:105:ASN:N	2.19	0.56
1:F:81:GLU:OE1	1:F:85:ARG:NH2	2.38	0.56
1:A:236:ILE:HG13	1:A:237:GLU:H	1.71	0.56
1:F:240:ARG:HB3	1:F:244:ARG:HH12	1.71	0.56
1:H:240:ARG:HB3	1:H:244:ARG:HH12	1.71	0.56
1:G:240:ARG:HB3	1:G:244:ARG:HH12	1.71	0.55
1:A:104:ILE:HG22	1:A:127:PHE:CZ	2.40	0.55
1:G:212:LEU:HA	1:G:241:LEU:HD13	1.88	0.55
1:H:159:GLN:O	1:H:163:TYR:HD2	1.87	0.55
1:A:166:ALA:O	1:A:169:LYS:HG3	2.07	0.55
1:A:144:ASN:O	1:A:147:ALA:N	2.40	0.55
1:C:144:ASN:O	1:C:147:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLU:O	1:D:238:LEU:C	2.50	0.55
1:A:80:MET:HE1	1:A:160:SER:HA	1.88	0.55
1:A:240:ARG:CZ	1:A:244:ARG:NH1	2.70	0.55
1:A:132:THR:CG2	1:E:135:LEU:HD21	2.37	0.55
1:E:166:ALA:O	1:E:169:LYS:HG3	2.07	0.55
1:A:237:GLU:HB3	1:A:240:ARG:NH2	2.22	0.55
1:B:212:LEU:HA	1:B:241:LEU:HD13	1.88	0.55
1:B:240:ARG:HB3	1:B:244:ARG:HH12	1.71	0.55
1:C:80:MET:HE1	1:C:160:SER:HA	1.88	0.55
1:E:80:MET:HE1	1:E:160:SER:HA	1.88	0.55
1:F:212:LEU:HA	1:F:241:LEU:HD13	1.88	0.55
1:B:237:GLU:HG3	1:B:240:ARG:NH2	2.22	0.55
1:C:166:ALA:O	1:C:169:LYS:HG3	2.07	0.55
1:E:144:ASN:O	1:E:147:ALA:N	2.40	0.55
1:H:237:GLU:HG3	1:H:240:ARG:NH2	2.22	0.54
1:A:215:HIS:CE1	1:A:241:LEU:HD11	2.43	0.54
1:D:166:ALA:O	1:D:169:LYS:HG3	2.07	0.54
1:C:215:HIS:CE1	1:C:241:LEU:HD11	2.42	0.54
1:C:235:LEU:O	1:C:238:LEU:HB3	2.07	0.54
1:D:215:HIS:CE1	1:D:241:LEU:HD11	2.43	0.54
1:A:237:GLU:O	1:A:240:ARG:NH1	2.41	0.54
1:G:237:GLU:HG3	1:G:240:ARG:NH2	2.22	0.54
1:D:80:MET:HE1	1:D:160:SER:HA	1.88	0.54
1:E:215:HIS:CE1	1:E:241:LEU:HD11	2.42	0.54
1:F:237:GLU:HG3	1:F:240:ARG:NH2	2.22	0.54
1:C:160:SER:O	1:C:164:VAL:HG23	2.07	0.54
1:C:235:LEU:O	1:C:239:THR:N	2.36	0.54
1:H:212:LEU:HA	1:H:241:LEU:HD13	1.88	0.54
1:A:132:THR:HG22	1:E:135:LEU:HD21	1.90	0.54
1:D:160:SER:O	1:D:164:VAL:HG23	2.07	0.54
1:D:144:ASN:O	1:D:147:ALA:N	2.40	0.54
1:E:160:SER:O	1:E:164:VAL:HG23	2.07	0.54
1:C:135:LEU:CD2	1:D:136:MET:HE2	2.38	0.53
1:A:160:SER:O	1:A:164:VAL:HG23	2.08	0.53
1:D:236:ILE:O	1:D:239:THR:N	2.41	0.53
1:D:235:LEU:O	1:D:239:THR:N	2.41	0.53
1:G:189:PHE:O	1:G:193:VAL:HG22	2.09	0.53
1:F:232:GLN:O	1:F:236:ILE:HG12	2.09	0.53
1:H:189:PHE:O	1:H:193:VAL:HG22	2.09	0.53
1:C:222:LYS:O	1:C:226:LEU:HD23	2.09	0.53
1:F:189:PHE:O	1:F:193:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLN:O	1:B:236:ILE:HG12	2.09	0.53
1:E:222:LYS:O	1:E:226:LEU:HD23	2.09	0.53
1:D:222:LYS:O	1:D:226:LEU:HD23	2.09	0.53
1:H:232:GLN:O	1:H:236:ILE:HG12	2.09	0.53
1:A:222:LYS:O	1:A:226:LEU:HD23	2.09	0.53
1:B:189:PHE:O	1:B:193:VAL:HG22	2.09	0.53
1:G:232:GLN:O	1:G:236:ILE:HG12	2.09	0.52
1:A:236:ILE:O	1:A:237:GLU:HB2	2.10	0.52
1:A:104:ILE:HD12	1:C:126:ALA:HB2	1.92	0.51
1:A:73:GLN:NE2	1:A:170:HIS:HB3	2.26	0.51
1:C:221:GLU:CD	1:C:225:GLN:HE22	2.18	0.51
1:C:208:LYS:HG2	1:C:212:LEU:HG	1.93	0.51
1:D:208:LYS:HG2	1:D:212:LEU:HG	1.93	0.51
1:C:212:LEU:HD22	1:C:238:LEU:HD12	1.93	0.51
1:A:236:ILE:HG13	1:A:237:GLU:N	2.25	0.51
1:D:73:GLN:NE2	1:D:170:HIS:HB3	2.26	0.51
1:E:212:LEU:HD22	1:E:238:LEU:HD12	1.93	0.51
1:D:221:GLU:CD	1:D:225:GLN:HE22	2.18	0.51
1:E:221:GLU:CD	1:E:225:GLN:HE22	2.18	0.51
1:A:208:LYS:HG2	1:A:212:LEU:HG	1.93	0.50
1:F:226:LEU:HD11	1:F:233:SER:OG	2.11	0.50
1:H:226:LEU:HD11	1:H:233:SER:OG	2.11	0.50
1:A:152:LYS:O	1:A:155:GLU:HG3	2.11	0.50
1:B:226:LEU:HD11	1:B:233:SER:OG	2.11	0.50
1:C:239:THR:HG22	1:F:243:GLU:OE2	2.11	0.50
1:E:73:GLN:NE2	1:E:170:HIS:HB3	2.26	0.50
1:E:152:LYS:O	1:E:155:GLU:HG3	2.11	0.50
1:D:212:LEU:HD22	1:D:238:LEU:HD12	1.93	0.50
1:G:186:GLU:O	1:G:190:MET:HG3	2.12	0.50
1:A:221:GLU:CD	1:A:225:GLN:HE22	2.18	0.50
1:A:240:ARG:NH1	1:A:244:ARG:NH1	2.60	0.50
1:B:186:GLU:O	1:B:190:MET:HG3	2.12	0.50
1:C:113:LEU:HD22	1:C:120:ASN:HA	1.94	0.50
1:D:113:LEU:HD22	1:D:120:ASN:HA	1.94	0.50
1:E:113:LEU:HD22	1:E:120:ASN:HA	1.94	0.50
1:B:165:GLU:HB3	1:B:169:LYS:NZ	2.27	0.50
1:C:73:GLN:NE2	1:C:170:HIS:HB3	2.26	0.50
1:F:186:GLU:O	1:F:190:MET:HG3	2.12	0.50
1:H:186:GLU:O	1:H:190:MET:HG3	2.12	0.50
1:E:229:MET:CE	1:E:233:SER:HB3	2.42	0.50
1:G:226:LEU:HD11	1:G:233:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD22	1:A:120:ASN:HA	1.94	0.49
1:C:108:LEU:HD23	1:C:108:LEU:O	2.12	0.49
1:C:152:LYS:O	1:C:155:GLU:HG3	2.11	0.49
1:G:165:GLU:HB3	1:G:169:LYS:NZ	2.27	0.49
1:B:165:GLU:HB3	1:B:169:LYS:HZ3	1.76	0.49
1:E:208:LYS:HG2	1:E:212:LEU:HG	1.93	0.49
1:C:154:GLN:O	1:C:157:THR:OG1	2.24	0.49
1:D:108:LEU:HD23	1:D:108:LEU:O	2.12	0.49
1:D:152:LYS:O	1:D:155:GLU:HG3	2.11	0.49
1:C:222:LYS:HA	1:C:225:GLN:HE21	1.78	0.49
1:H:165:GLU:HB3	1:H:169:LYS:NZ	2.27	0.49
1:A:108:LEU:O	1:A:108:LEU:HD23	2.12	0.49
1:D:222:LYS:HA	1:D:225:GLN:HE21	1.78	0.49
1:E:236:ILE:HG22	1:E:240:ARG:HD2	1.94	0.49
1:F:165:GLU:HB3	1:F:169:LYS:HZ3	1.76	0.49
1:B:163:TYR:CD1	1:B:202:MET:HE3	2.48	0.49
1:H:163:TYR:CD1	1:H:202:MET:HE3	2.48	0.49
1:D:201:ILE:HG23	1:D:238:LEU:HD21	1.95	0.49
1:E:108:LEU:HD23	1:E:108:LEU:O	2.12	0.49
1:F:165:GLU:HB3	1:F:169:LYS:NZ	2.27	0.49
1:B:226:LEU:HA	1:B:229:MET:HB3	1.94	0.49
1:C:237:GLU:OE2	1:C:240:ARG:NH1	2.46	0.49
1:D:104:ILE:CD1	1:E:126:ALA:HB2	2.43	0.49
1:E:110:GLU:HA	1:E:113:LEU:HG	1.95	0.49
1:F:163:TYR:CD1	1:F:202:MET:HE3	2.48	0.49
1:A:108:LEU:CD2	1:C:125:ALA:HB2	2.25	0.48
1:C:110:GLU:HA	1:C:113:LEU:HG	1.95	0.48
1:E:222:LYS:HA	1:E:225:GLN:HE21	1.78	0.48
1:F:226:LEU:HA	1:F:229:MET:HB3	1.94	0.48
1:G:163:TYR:CD1	1:G:202:MET:HE3	2.48	0.48
1:A:154:GLN:O	1:A:157:THR:OG1	2.24	0.48
1:E:154:GLN:O	1:E:157:THR:OG1	2.24	0.48
1:A:132:THR:HB	1:E:135:LEU:HD21	1.95	0.48
1:A:219:ASN:HB3	1:A:222:LYS:HB2	1.95	0.48
1:C:159:GLN:O	1:C:162:GLN:HG3	2.14	0.48
1:C:229:MET:HE1	1:C:233:SER:HB3	1.93	0.48
1:D:235:LEU:HG	1:D:236:ILE:N	2.28	0.48
1:H:226:LEU:HA	1:H:229:MET:HB3	1.94	0.48
1:C:77:GLU:O	1:C:80:MET:HB2	2.14	0.48
1:C:219:ASN:HB3	1:C:222:LYS:HB2	1.95	0.48
1:D:72:ARG:NH1	1:D:187:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:MET:SD	1:E:234:ALA:CA	3.02	0.48
1:A:229:MET:HE1	1:A:233:SER:CB	2.41	0.48
1:A:236:ILE:O	1:A:237:GLU:CB	2.60	0.48
1:C:185:LYS:NZ	1:C:210:ALA:O	2.34	0.48
1:E:159:GLN:O	1:E:162:GLN:HG3	2.14	0.48
1:E:219:ASN:HB3	1:E:222:LYS:HB2	1.95	0.48
1:E:72:ARG:NH1	1:E:187:ASP:OD1	2.47	0.48
1:F:226:LEU:HG	1:F:234:ALA:HB2	1.96	0.48
1:G:226:LEU:HA	1:G:229:MET:HB3	1.94	0.48
1:D:219:ASN:HB3	1:D:222:LYS:HB2	1.95	0.48
1:E:107:TYR:HE1	1:E:116:TYR:HH	1.61	0.48
1:C:208:LYS:HZ1	1:C:245:LEU:HD12	1.79	0.48
1:A:222:LYS:HA	1:A:225:GLN:HE21	1.78	0.48
1:E:128:ASN:O	1:E:132:THR:HG23	2.14	0.48
1:H:73:GLN:HG2	1:H:171:TYR:HE2	1.79	0.48
1:H:160:SER:O	1:H:164:VAL:HG23	2.14	0.48
1:D:128:ASN:O	1:D:132:THR:HG23	2.14	0.47
1:D:236:ILE:HG23	1:G:239:THR:CG2	2.25	0.47
1:B:226:LEU:HG	1:B:234:ALA:HB2	1.96	0.47
1:G:226:LEU:HG	1:G:234:ALA:HB2	1.96	0.47
1:C:72:ARG:NH1	1:C:187:ASP:OD1	2.47	0.47
1:C:72:ARG:O	1:C:75:GLU:HG3	2.15	0.47
1:C:128:ASN:O	1:C:132:THR:HG23	2.14	0.47
1:C:229:MET:CE	1:C:233:SER:CB	2.90	0.47
1:D:110:GLU:HA	1:D:113:LEU:HG	1.95	0.47
1:E:77:GLU:O	1:E:80:MET:HB2	2.14	0.47
1:F:73:GLN:HG2	1:F:171:TYR:HE2	1.79	0.47
1:C:201:ILE:HG23	1:C:238:LEU:HD21	1.95	0.47
1:D:77:GLU:O	1:D:80:MET:HB2	2.14	0.47
1:A:72:ARG:NH1	1:A:187:ASP:OD1	2.47	0.47
1:A:240:ARG:O	1:A:241:LEU:C	2.57	0.47
1:D:104:ILE:HG22	1:D:127:PHE:HZ	1.80	0.47
1:H:226:LEU:HG	1:H:234:ALA:HB2	1.96	0.47
1:A:77:GLU:O	1:A:80:MET:HB2	2.14	0.47
1:B:73:GLN:HG2	1:B:171:TYR:HE2	1.79	0.47
1:B:160:SER:O	1:B:164:VAL:HG23	2.14	0.47
1:E:201:ILE:HG23	1:E:238:LEU:HD21	1.95	0.47
1:F:160:SER:O	1:F:164:VAL:HG23	2.14	0.47
1:A:104:ILE:HG22	1:A:127:PHE:HZ	1.80	0.47
1:A:110:GLU:HA	1:A:113:LEU:HG	1.95	0.47
1:A:234:ALA:O	1:A:235:LEU:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ARG:O	1:E:75:GLU:HG3	2.15	0.47
1:G:73:GLN:HG2	1:G:171:TYR:HE2	1.79	0.47
1:C:127:PHE:HE2	1:D:128:ASN:HB2	1.80	0.47
1:E:229:MET:HE1	1:E:233:SER:CB	2.44	0.47
1:A:128:ASN:O	1:A:132:THR:HG23	2.14	0.46
1:A:233:SER:O	1:A:235:LEU:N	2.48	0.46
1:F:158:GLN:HG2	1:F:159:GLN:N	2.31	0.46
1:E:134:TRP:CD1	1:E:137:LYS:HZ3	2.34	0.46
1:E:208:LYS:HZ1	1:E:242:SER:HA	1.80	0.46
1:E:229:MET:HE1	1:E:233:SER:HB3	1.95	0.46
1:A:139:GLN:O	1:A:142:ARG:HG3	2.16	0.46
1:D:72:ARG:O	1:D:75:GLU:HG3	2.15	0.46
1:D:139:GLN:O	1:D:142:ARG:HG3	2.16	0.46
1:A:155:GLU:HA	1:A:158:GLN:HG3	1.98	0.46
1:D:208:LYS:HZ1	1:D:242:SER:HA	1.81	0.46
1:D:229:MET:HE1	1:D:233:SER:CB	2.45	0.46
1:G:160:SER:O	1:G:164:VAL:HG23	2.14	0.46
1:A:208:LYS:HZ1	1:A:242:SER:HA	1.81	0.46
1:A:233:SER:C	1:A:235:LEU:N	2.70	0.46
1:B:221:GLU:HG2	1:B:222:LYS:N	2.31	0.46
1:A:72:ARG:O	1:A:75:GLU:HG3	2.15	0.46
1:C:155:GLU:HA	1:C:158:GLN:HG3	1.98	0.46
1:H:221:GLU:HG2	1:H:222:LYS:N	2.31	0.46
1:A:134:TRP:CD1	1:A:137:LYS:HZ3	2.34	0.46
1:E:74:ARG:O	1:E:77:GLU:HG3	2.16	0.46
1:E:155:GLU:HA	1:E:158:GLN:HG3	1.98	0.46
1:C:139:GLN:O	1:C:142:ARG:HG3	2.16	0.46
1:E:139:GLN:O	1:E:142:ARG:HG3	2.16	0.46
1:A:110:GLU:CD	1:C:122:ARG:HH12	2.24	0.46
1:D:236:ILE:HD12	1:G:239:THR:OG1	2.16	0.46
1:C:229:MET:HE1	1:C:233:SER:CB	2.45	0.45
1:D:74:ARG:O	1:D:77:GLU:HG3	2.16	0.45
1:F:239:THR:O	1:F:242:SER:OG	2.23	0.45
1:A:74:ARG:O	1:A:77:GLU:HG3	2.16	0.45
1:D:154:GLN:O	1:D:157:THR:OG1	2.24	0.45
1:B:73:GLN:HG2	1:B:171:TYR:CE2	2.52	0.45
1:A:237:GLU:HA	1:A:240:ARG:CB	2.46	0.45
1:B:158:GLN:HG2	1:B:159:GLN:N	2.31	0.45
1:C:226:LEU:CD1	1:C:234:ALA:HB1	2.45	0.45
1:E:235:LEU:HD12	1:E:238:LEU:HB3	1.99	0.45
1:F:221:GLU:HA	1:F:224:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:GLN:HG2	1:H:159:GLN:N	2.31	0.45
1:H:163:TYR:HD1	1:H:202:MET:HE3	1.82	0.45
1:C:74:ARG:O	1:C:77:GLU:HG3	2.16	0.45
1:F:241:LEU:HD23	1:F:244:ARG:HH21	1.82	0.45
1:G:221:GLU:HG2	1:G:222:LYS:N	2.31	0.45
1:G:241:LEU:HD23	1:G:244:ARG:HH21	1.82	0.45
1:A:132:THR:HA	1:A:135:LEU:HD12	1.99	0.45
1:B:241:LEU:HD23	1:B:244:ARG:HH21	1.82	0.45
1:D:134:TRP:CD1	1:D:137:LYS:HZ3	2.35	0.45
1:F:73:GLN:HG2	1:F:171:TYR:CE2	2.52	0.45
1:B:221:GLU:HA	1:B:224:ARG:CZ	2.47	0.45
1:D:236:ILE:O	1:D:240:ARG:N	2.38	0.45
1:E:221:GLU:O	1:E:224:ARG:HD3	2.17	0.45
1:F:221:GLU:HG2	1:F:222:LYS:N	2.31	0.45
1:H:73:GLN:HG2	1:H:171:TYR:CE2	2.52	0.45
1:C:221:GLU:O	1:C:224:ARG:HD3	2.17	0.45
1:E:233:SER:O	1:E:234:ALA:C	2.57	0.45
1:G:158:GLN:HG2	1:G:159:GLN:N	2.31	0.45
1:G:221:GLU:HA	1:G:224:ARG:CZ	2.47	0.45
1:C:134:TRP:CD1	1:C:137:LYS:HZ3	2.35	0.44
1:E:104:ILE:HG22	1:E:127:PHE:HZ	1.80	0.44
1:D:155:GLU:HA	1:D:158:GLN:HG3	1.98	0.44
1:D:221:GLU:O	1:D:224:ARG:HD3	2.17	0.44
1:E:132:THR:HA	1:E:135:LEU:HD12	1.99	0.44
1:F:189:PHE:CD1	1:F:216:LEU:HD11	2.53	0.44
1:G:189:PHE:CD1	1:G:216:LEU:HD11	2.53	0.44
1:H:221:GLU:HA	1:H:224:ARG:CZ	2.47	0.44
1:G:163:TYR:HD1	1:G:202:MET:HE3	1.82	0.44
1:A:232:GLN:O	1:A:233:SER:C	2.61	0.44
1:B:163:TYR:HD1	1:B:202:MET:HE3	1.82	0.44
1:G:73:GLN:HG2	1:G:171:TYR:CE2	2.52	0.44
1:A:208:LYS:NZ	1:A:242:SER:HA	2.33	0.44
1:B:224:ARG:HA	1:B:227:LEU:HD12	2.00	0.44
1:D:208:LYS:NZ	1:D:242:SER:HA	2.33	0.44
1:B:233:SER:HA	1:B:236:ILE:HG12	1.99	0.44
1:C:132:THR:HA	1:C:135:LEU:HD12	1.99	0.44
1:F:163:TYR:HD1	1:F:202:MET:HE3	1.82	0.44
1:G:233:SER:HA	1:G:236:ILE:HG12	1.99	0.44
1:H:189:PHE:CD1	1:H:216:LEU:HD11	2.53	0.44
1:H:224:ARG:HA	1:H:227:LEU:HD12	2.00	0.44
1:A:232:GLN:H	1:A:232:GLN:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:CA	1:A:240:ARG:CB	2.93	0.44
1:D:185:LYS:HD2	1:D:214:TYR:HA	2.00	0.44
1:E:159:GLN:O	1:E:160:SER:C	2.60	0.44
1:B:183:GLN:O	1:B:186:GLU:HG3	2.18	0.43
1:E:208:LYS:NZ	1:E:242:SER:HA	2.33	0.43
1:F:224:ARG:HA	1:F:227:LEU:HD12	2.00	0.43
1:F:233:SER:HA	1:F:236:ILE:HG12	2.00	0.43
1:A:221:GLU:O	1:A:224:ARG:HD3	2.17	0.43
1:C:185:LYS:HD2	1:C:214:TYR:HA	2.00	0.43
1:G:224:ARG:HA	1:G:227:LEU:HD12	2.00	0.43
1:A:153:THR:O	1:A:157:THR:HG23	2.18	0.43
1:C:208:LYS:NZ	1:C:242:SER:HA	2.33	0.43
1:D:132:THR:HA	1:D:135:LEU:HD12	1.99	0.43
1:E:230:ASP:OD1	1:E:231:GLY:N	2.50	0.43
1:G:183:GLN:O	1:G:186:GLU:HG3	2.18	0.43
1:G:212:LEU:HD22	1:G:238:LEU:HD22	2.01	0.43
1:D:237:GLU:HA	1:D:240:ARG:CD	2.48	0.43
1:H:232:GLN:O	1:H:235:LEU:HB3	2.19	0.43
1:H:241:LEU:HD23	1:H:244:ARG:HH21	1.82	0.43
1:A:236:ILE:O	1:A:238:LEU:N	2.48	0.43
1:G:186:GLU:OE1	1:G:190:MET:HE2	2.19	0.43
1:H:163:TYR:CE1	1:H:199:ALA:HB1	2.54	0.43
1:B:186:GLU:OE1	1:B:190:MET:HE2	2.19	0.43
1:B:189:PHE:CD1	1:B:216:LEU:HD11	2.53	0.43
1:F:232:GLN:O	1:F:235:LEU:HB3	2.19	0.43
1:A:159:GLN:O	1:A:162:GLN:HG3	2.18	0.43
1:A:237:GLU:O	1:A:241:LEU:N	2.33	0.43
1:B:212:LEU:HD22	1:B:238:LEU:HD22	2.01	0.43
1:D:235:LEU:O	1:D:236:ILE:C	2.58	0.43
1:E:159:GLN:OE1	1:E:159:GLN:HA	2.19	0.43
1:E:236:ILE:HD11	1:H:235:LEU:HG	2.00	0.43
1:F:212:LEU:HD22	1:F:238:LEU:HD22	2.01	0.43
1:H:212:LEU:HD22	1:H:238:LEU:HD22	2.01	0.43
1:H:233:SER:HA	1:H:236:ILE:HG12	2.00	0.43
1:A:238:LEU:C	1:A:240:ARG:N	2.70	0.43
1:B:232:GLN:O	1:B:235:LEU:HB3	2.19	0.43
1:D:159:GLN:O	1:D:162:GLN:HG3	2.19	0.43
1:F:186:GLU:OE1	1:F:190:MET:HE2	2.19	0.43
1:H:183:GLN:O	1:H:186:GLU:HG3	2.18	0.43
1:B:200:ASP:O	1:B:203:ARG:HG3	2.19	0.43
1:C:104:ILE:HG22	1:C:127:PHE:HZ	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:THR:O	1:C:157:THR:HG23	2.19	0.43
1:D:153:THR:O	1:D:157:THR:HG23	2.19	0.43
1:H:186:GLU:OE1	1:H:190:MET:HE2	2.19	0.43
1:E:205:PHE:HZ	1:E:239:THR:HG23	1.84	0.42
1:G:232:GLN:O	1:G:235:LEU:HB3	2.19	0.42
1:E:134:TRP:HD1	1:E:137:LYS:HZ3	1.66	0.42
1:A:76:LEU:O	1:A:80:MET:HG2	2.19	0.42
1:A:134:TRP:HD1	1:A:137:LYS:HZ3	1.67	0.42
1:A:200:ASP:OD1	1:A:203:ARG:NH2	2.53	0.42
1:B:163:TYR:CE1	1:B:199:ALA:HB1	2.54	0.42
1:C:108:LEU:HD12	1:C:127:PHE:HB2	2.02	0.42
1:G:163:TYR:CE1	1:G:199:ALA:HB1	2.54	0.42
1:A:132:THR:CB	1:E:135:LEU:HD21	2.49	0.42
1:A:237:GLU:CA	1:A:240:ARG:CZ	2.95	0.42
1:C:205:PHE:HZ	1:C:239:THR:HG23	1.84	0.42
1:D:76:LEU:O	1:D:80:MET:HG2	2.19	0.42
1:H:165:GLU:HB3	1:H:169:LYS:HZ1	1.83	0.42
1:H:200:ASP:O	1:H:203:ARG:HG3	2.19	0.42
1:C:76:LEU:O	1:C:80:MET:HG2	2.19	0.42
1:D:108:LEU:HD12	1:D:127:PHE:HB2	2.01	0.42
1:D:159:GLN:OE1	1:D:162:GLN:NE2	2.53	0.42
1:G:80:MET:SD	1:G:160:SER:HB2	2.60	0.42
1:A:185:LYS:HD2	1:A:214:TYR:HA	2.00	0.42
1:E:185:LYS:HD2	1:E:214:TYR:HA	2.00	0.42
1:H:188:ALA:O	1:H:191:GLN:HG3	2.19	0.42
1:B:80:MET:SD	1:B:160:SER:HB2	2.60	0.42
1:C:142:ARG:HE	1:D:139:GLN:NE2	2.17	0.42
1:C:159:GLN:OE1	1:C:162:GLN:NE2	2.52	0.42
1:C:200:ASP:OD1	1:C:203:ARG:NH2	2.53	0.42
1:E:153:THR:O	1:E:157:THR:HG23	2.19	0.42
1:F:80:MET:SD	1:F:160:SER:HB2	2.60	0.42
1:F:183:GLN:O	1:F:186:GLU:HG3	2.18	0.42
1:F:200:ASP:O	1:F:203:ARG:HG3	2.19	0.42
1:A:169:LYS:CE	1:A:202:MET:HB2	2.48	0.42
1:C:230:ASP:OD1	1:C:231:GLY:N	2.51	0.42
1:D:200:ASP:OD1	1:D:203:ARG:NH2	2.53	0.42
1:F:163:TYR:CE1	1:F:199:ALA:HB1	2.54	0.42
1:B:183:GLN:HG2	1:B:184:GLU:N	2.35	0.42
1:D:237:GLU:OE2	1:D:240:ARG:NH1	2.53	0.42
1:F:188:ALA:O	1:F:191:GLN:HG3	2.19	0.42
1:G:188:ALA:O	1:G:191:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:ASP:O	1:G:203:ARG:HG3	2.19	0.42
1:D:104:ILE:HD12	1:E:126:ALA:HB2	2.02	0.41
1:H:222:LYS:HG3	1:H:226:LEU:HD23	2.02	0.41
1:C:104:ILE:HG13	1:C:105:ASN:OD1	2.21	0.41
1:E:200:ASP:OD1	1:E:203:ARG:NH2	2.53	0.41
1:H:72:ARG:O	1:H:75:GLU:HG3	2.21	0.41
1:A:108:LEU:HD12	1:A:127:PHE:HB2	2.01	0.41
1:E:76:LEU:O	1:E:80:MET:HG2	2.19	0.41
1:E:153:THR:HA	1:E:156:PHE:CD2	2.55	0.41
1:B:188:ALA:O	1:B:191:GLN:HG3	2.19	0.41
1:C:88:LEU:HD22	1:C:93:ARG:HD2	2.02	0.41
1:D:88:LEU:HD22	1:D:93:ARG:HD2	2.02	0.41
1:D:240:ARG:HB2	1:G:243:GLU:HG2	2.03	0.41
1:E:88:LEU:HD22	1:E:93:ARG:HD2	2.02	0.41
1:G:72:ARG:O	1:G:75:GLU:HG3	2.20	0.41
1:H:80:MET:SD	1:H:160:SER:HB2	2.59	0.41
1:D:134:TRP:HD1	1:D:137:LYS:HZ3	1.67	0.41
1:D:205:PHE:HZ	1:D:239:THR:HG23	1.84	0.41
1:D:230:ASP:OD1	1:D:231:GLY:N	2.50	0.41
1:F:222:LYS:HE3	1:F:226:LEU:HD21	2.03	0.41
1:G:183:GLN:HG2	1:G:184:GLU:N	2.35	0.41
1:A:153:THR:HA	1:A:156:PHE:CD2	2.55	0.41
1:A:235:LEU:CD2	1:B:235:LEU:HD22	2.50	0.41
1:B:205:PHE:HD2	1:B:212:LEU:HD11	1.86	0.41
1:C:153:THR:HA	1:C:156:PHE:CD2	2.55	0.41
1:C:237:GLU:CD	1:C:240:ARG:NH1	2.79	0.41
1:D:153:THR:HA	1:D:156:PHE:CD2	2.55	0.41
1:A:104:ILE:HG13	1:A:105:ASN:OD1	2.20	0.41
1:B:222:LYS:HG3	1:B:226:LEU:HD23	2.02	0.41
1:C:229:MET:SD	1:C:234:ALA:HA	2.61	0.41
1:E:104:ILE:HG13	1:E:105:ASN:OD1	2.21	0.41
1:G:205:PHE:HD2	1:G:212:LEU:HD11	1.86	0.41
1:C:113:LEU:O	1:C:118:TYR:N	2.51	0.41
1:C:169:LYS:CE	1:C:202:MET:HB2	2.48	0.41
1:F:222:LYS:HG3	1:F:226:LEU:HD23	2.03	0.41
1:A:234:ALA:O	1:A:236:ILE:O	2.39	0.41
1:D:144:ASN:O	1:D:145:ALA:C	2.64	0.41
1:D:235:LEU:HD12	1:D:239:THR:OG1	2.21	0.41
1:E:108:LEU:HD12	1:E:127:PHE:HB2	2.01	0.41
1:E:232:GLN:O	1:E:235:LEU:HB3	2.21	0.41
1:F:205:PHE:HD2	1:F:212:LEU:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ALA:HA	1:G:191:GLN:HG3	2.03	0.41
1:H:183:GLN:HG2	1:H:184:GLU:N	2.35	0.41
1:H:205:PHE:HD2	1:H:212:LEU:HD11	1.86	0.41
1:A:88:LEU:HD22	1:A:93:ARG:HD2	2.02	0.41
1:B:72:ARG:O	1:B:75:GLU:HG3	2.20	0.41
1:C:181:ASP:OD1	1:C:181:ASP:N	2.54	0.41
1:D:233:SER:O	1:D:234:ALA:C	2.63	0.41
1:F:183:GLN:HG2	1:F:184:GLU:N	2.35	0.41
1:E:169:LYS:CE	1:E:202:MET:HB2	2.48	0.40
1:F:72:ARG:O	1:F:75:GLU:HG3	2.21	0.40
1:B:78:GLN:O	1:B:81:GLU:HG3	2.22	0.40
1:D:104:ILE:HG13	1:D:105:ASN:OD1	2.21	0.40
1:A:130:ALA:HA	1:A:133:GLU:HG3	2.03	0.40
1:B:188:ALA:HA	1:B:191:GLN:HG3	2.03	0.40
1:E:130:ALA:HA	1:E:133:GLU:HG3	2.03	0.40
1:G:222:LYS:HE3	1:G:226:LEU:HD21	2.03	0.40
1:G:222:LYS:HG3	1:G:226:LEU:HD23	2.03	0.40
1:F:188:ALA:HA	1:F:191:GLN:HG3	2.03	0.40
1:G:78:GLN:O	1:G:81:GLU:HG3	2.22	0.40
1:H:78:GLN:O	1:H:81:GLU:HG3	2.22	0.40
1:H:188:ALA:HA	1:H:191:GLN:HG3	2.03	0.40
1:A:181:ASP:OD1	1:A:181:ASP:N	2.54	0.40
1:B:226:LEU:CG	1:B:234:ALA:HB2	2.52	0.40
1:E:173:ALA:HA	1:E:177:LEU:HD23	2.04	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	174/303 (57%)	158 (91%)	16 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
1	C	174/303 (57%)	163 (94%)	11 (6%)	0	100	100
1	D	174/303 (57%)	161 (92%)	13 (8%)	0	100	100
1	E	174/303 (57%)	161 (92%)	13 (8%)	0	100	100
1	F	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
1	G	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
1	H	105/303 (35%)	104 (99%)	1 (1%)	0	100	100
All	All	1116/2424 (46%)	1059 (95%)	57 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	144/244 (59%)	141 (98%)	3 (2%)	47	65
1	B	90/244 (37%)	90 (100%)	0	100	100
1	C	144/244 (59%)	143 (99%)	1 (1%)	76	81
1	D	144/244 (59%)	143 (99%)	1 (1%)	76	81
1	E	144/244 (59%)	143 (99%)	1 (1%)	76	81
1	F	90/244 (37%)	90 (100%)	0	100	100
1	G	90/244 (37%)	90 (100%)	0	100	100
1	H	90/244 (37%)	90 (100%)	0	100	100
All	All	936/1952 (48%)	930 (99%)	6 (1%)	76	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	GLU
1	A	238	LEU

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Mol	Chain	Res	Type
1	A	240	ARG
1	C	235	LEU
1	D	235	LEU
1	E	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	95	ASN
1	A	128	ASN
1	A	149	GLN
1	A	162	GLN
1	B	162	GLN
1	C	78	GLN
1	C	95	ASN
1	C	149	GLN
1	C	162	GLN
1	D	73	GLN
1	D	78	GLN
1	D	95	ASN
1	D	139	GLN
1	D	149	GLN
1	D	162	GLN
1	D	232	GLN
1	E	78	GLN
1	E	95	ASN
1	E	128	ASN
1	E	149	GLN
1	E	162	GLN
1	F	162	GLN
1	G	162	GLN
1	H	162	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

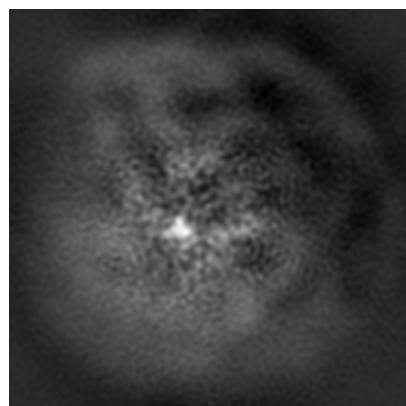
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61456. These allow visual inspection of the internal detail of the map and identification of artifacts.

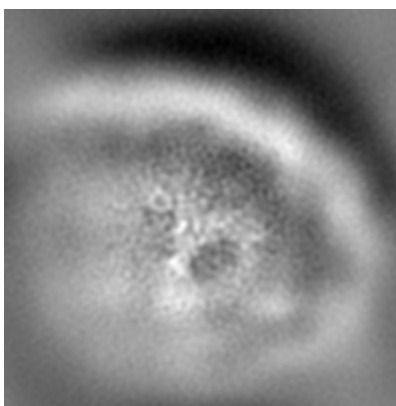
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

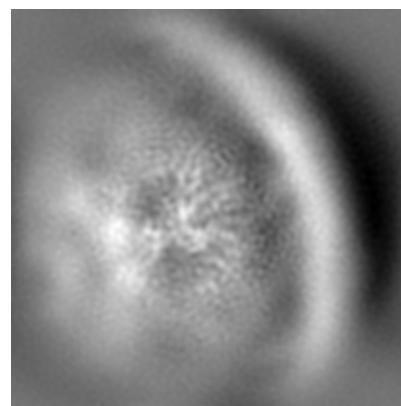
6.1.1 Primary map



X

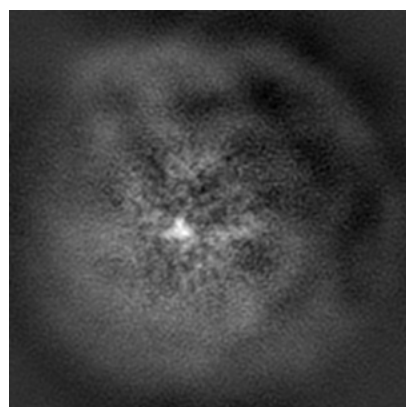


Y

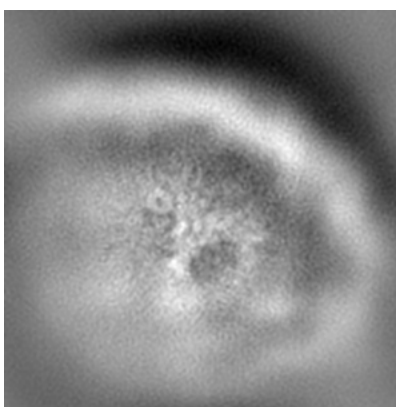


Z

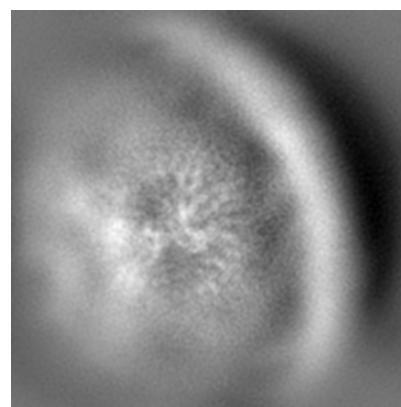
6.1.2 Raw map



X



Y

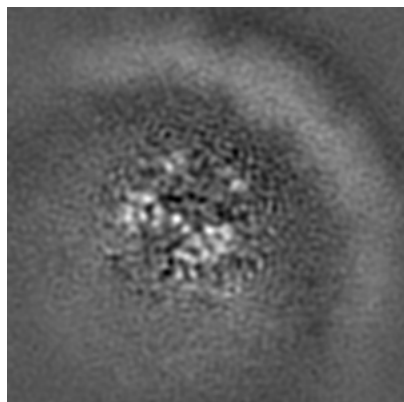


Z

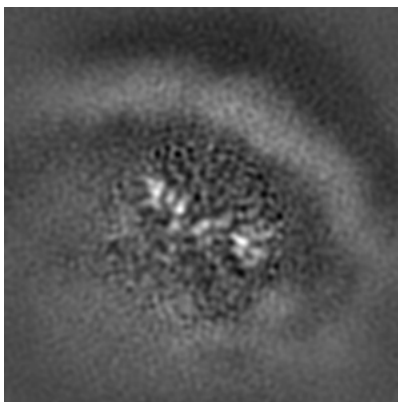
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

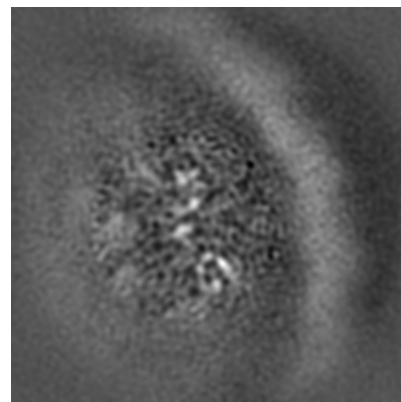
6.2.1 Primary map



X Index: 80

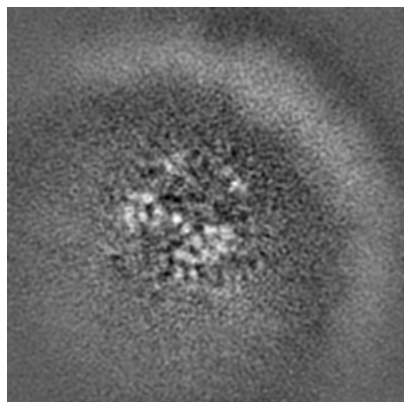


Y Index: 80

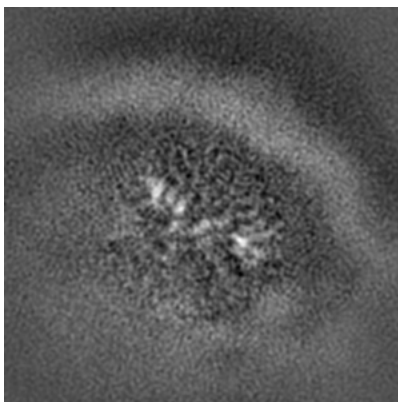


Z Index: 80

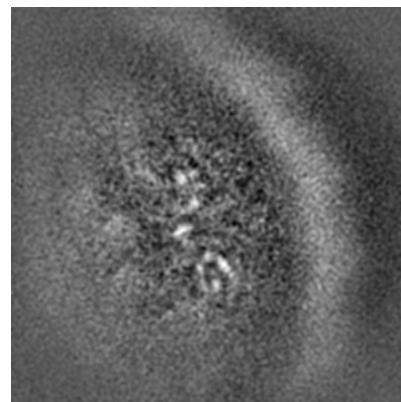
6.2.2 Raw map



X Index: 80



Y Index: 80

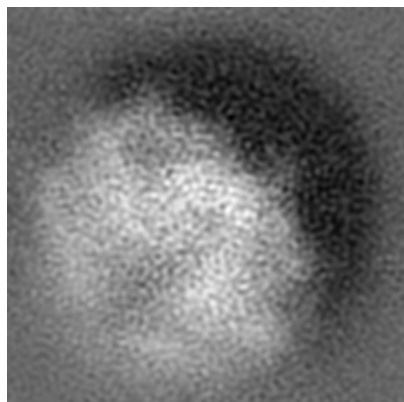


Z Index: 80

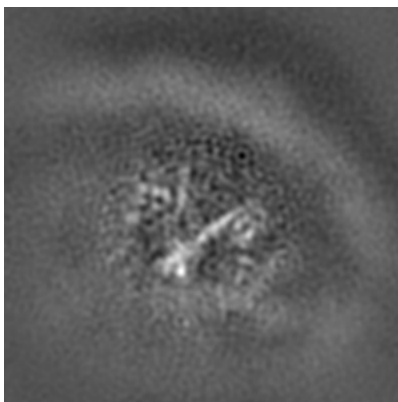
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

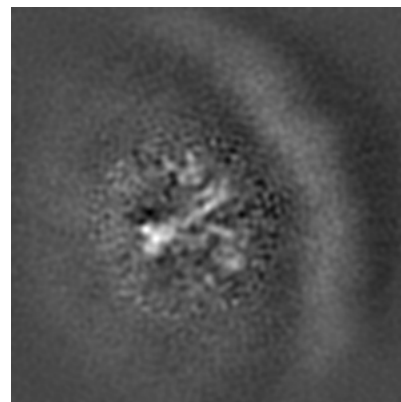
6.3.1 Primary map



X Index: 123

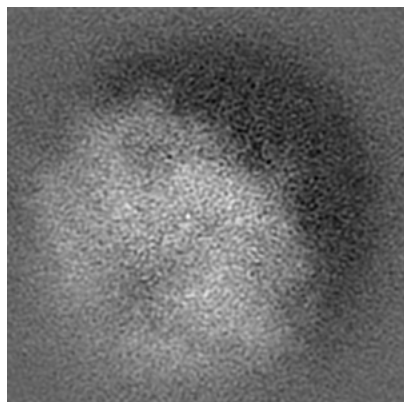


Y Index: 70

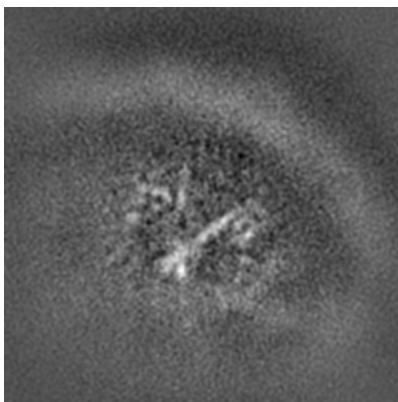


Z Index: 70

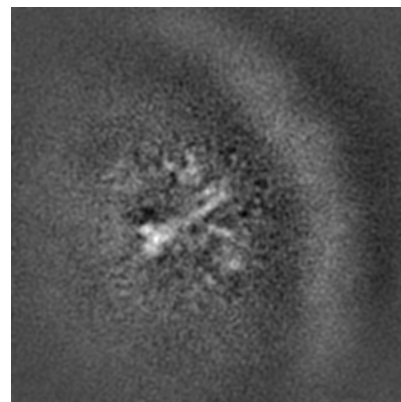
6.3.2 Raw map



X Index: 123



Y Index: 70

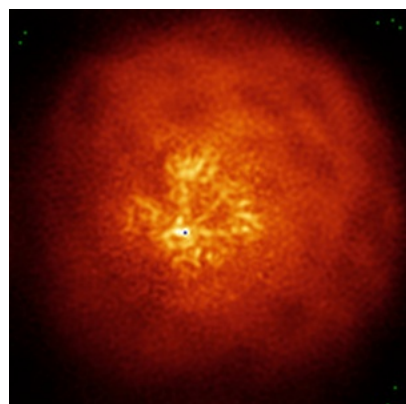


Z Index: 70

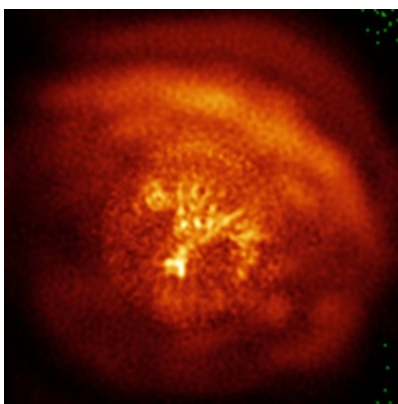
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

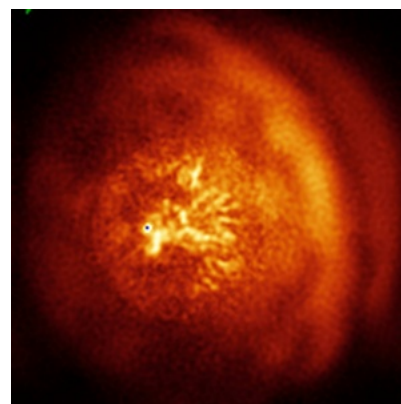
6.4.1 Primary map



X

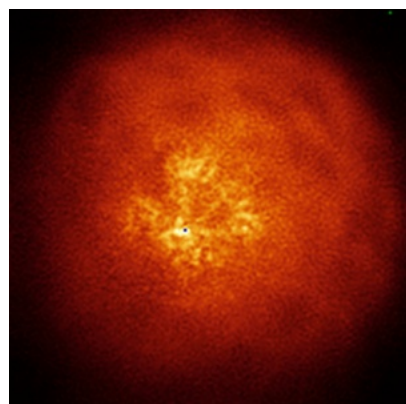


Y

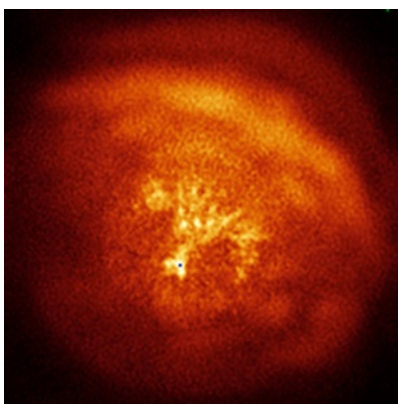


Z

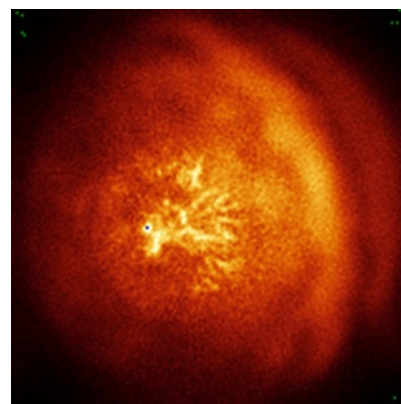
6.4.2 Raw map



X



Y

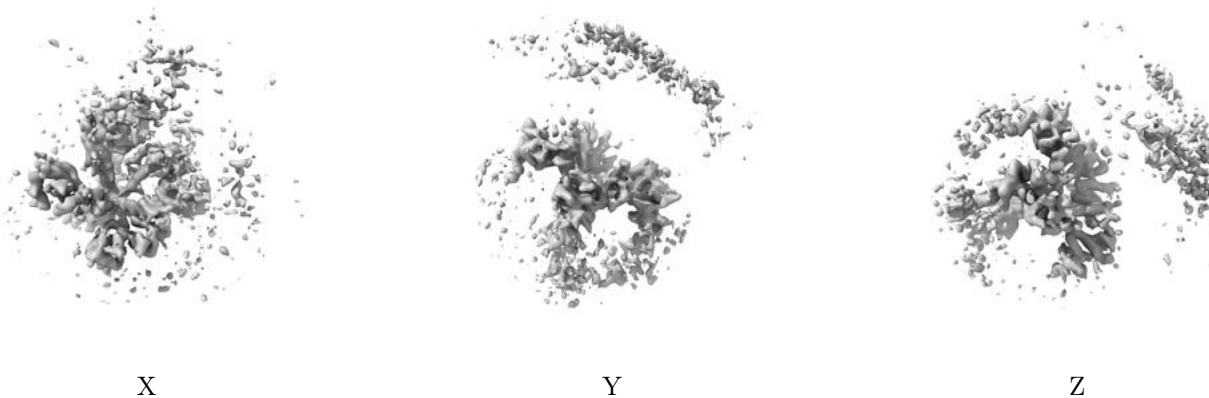


Z

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



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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



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.

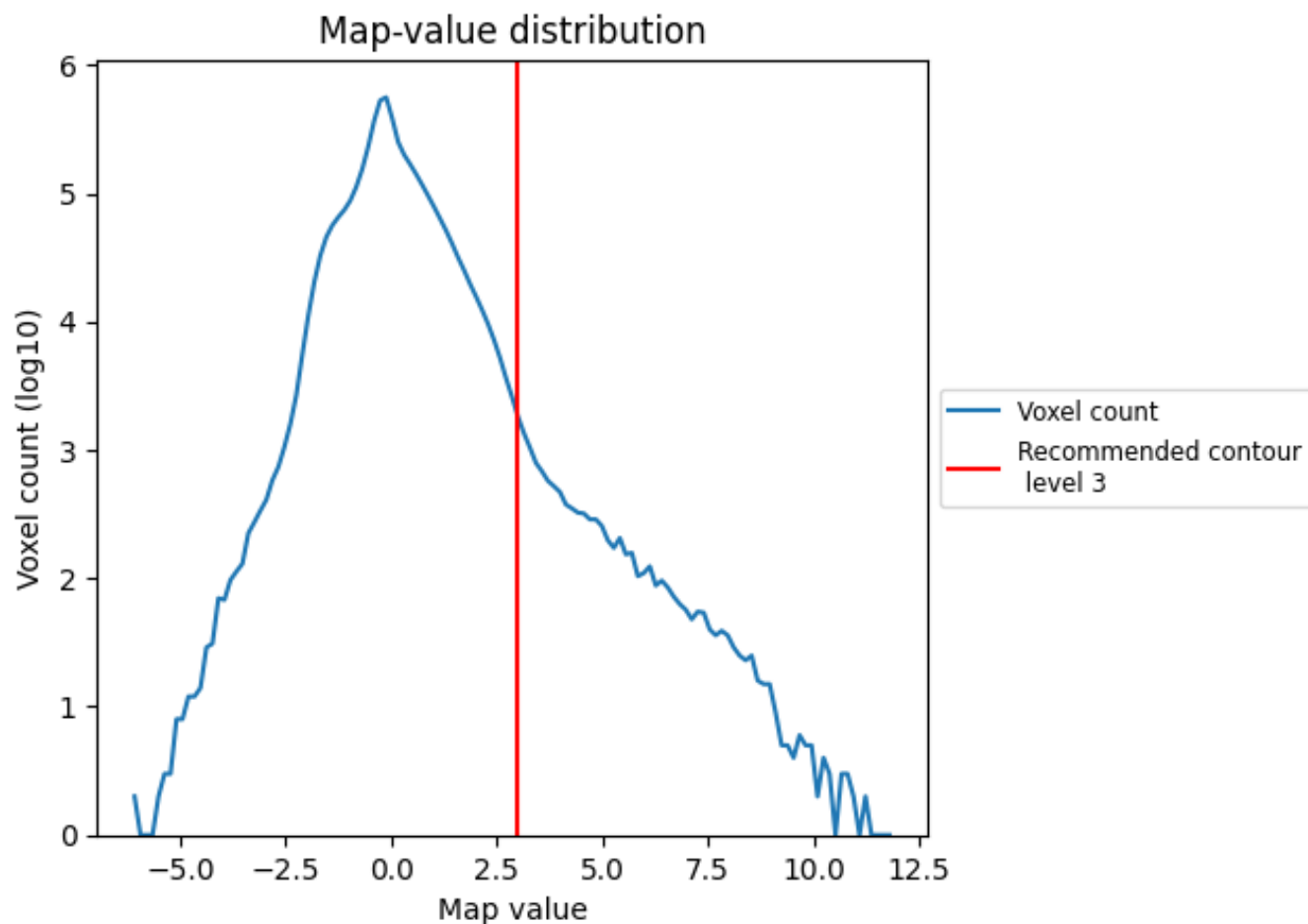
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

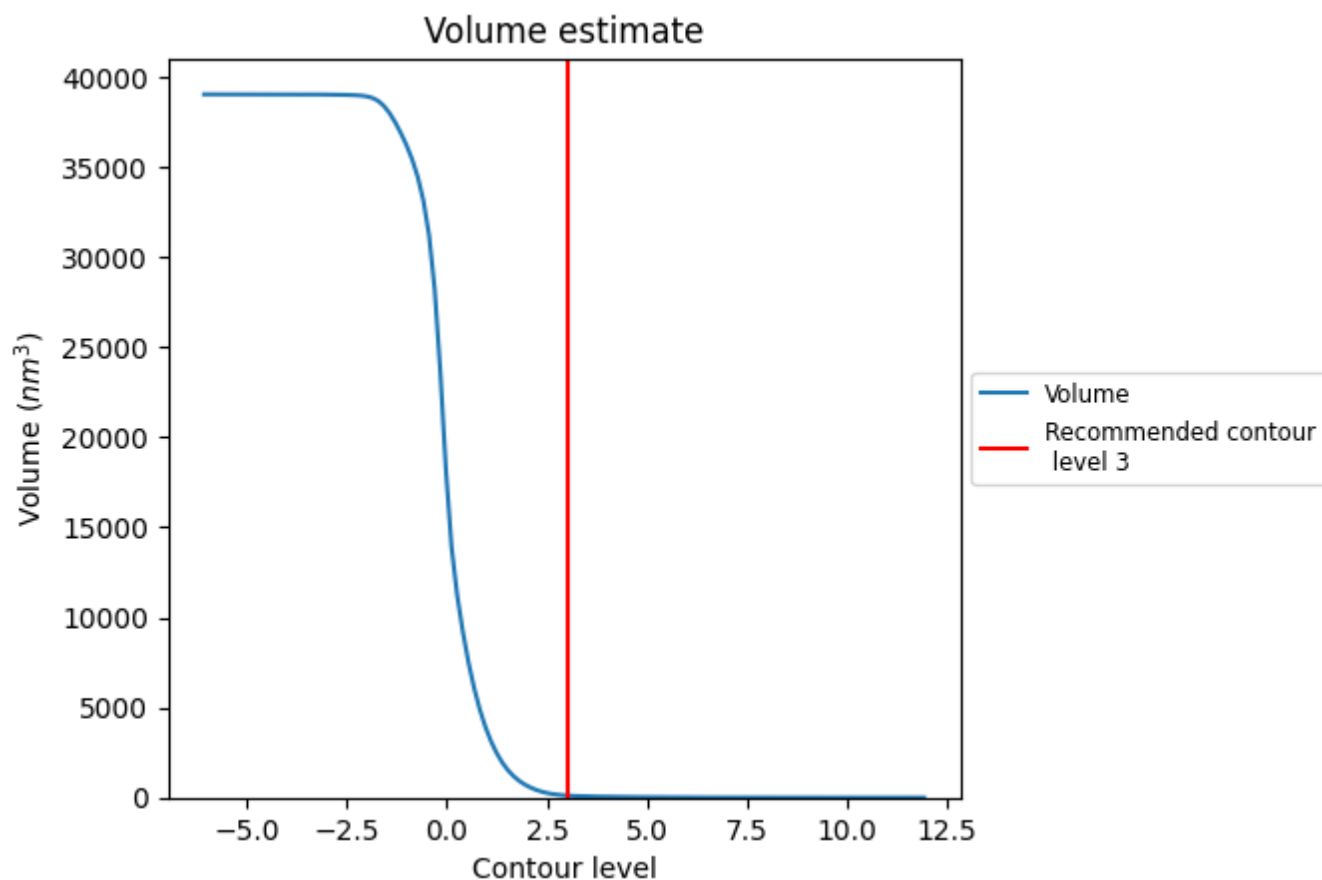
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

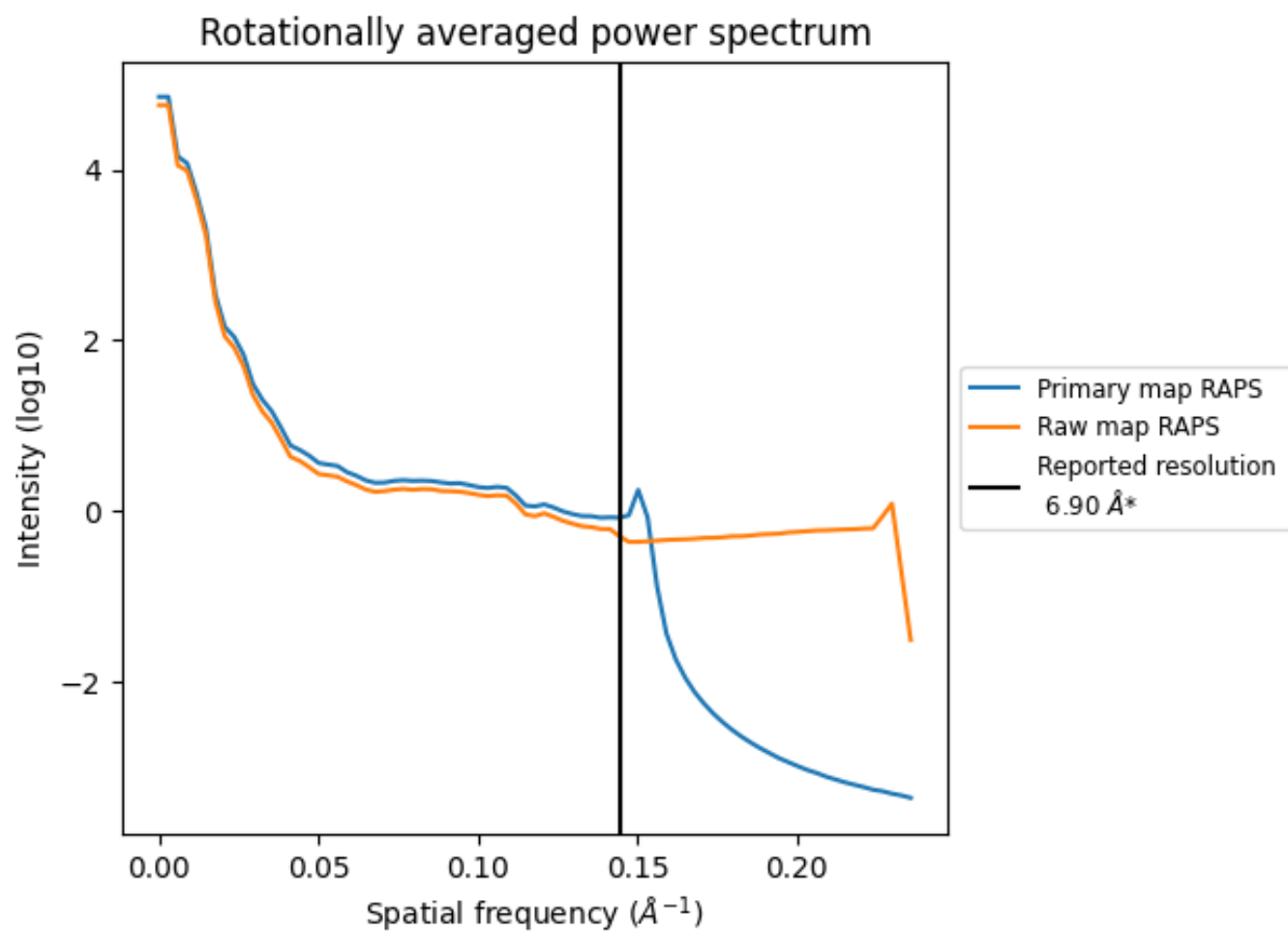
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

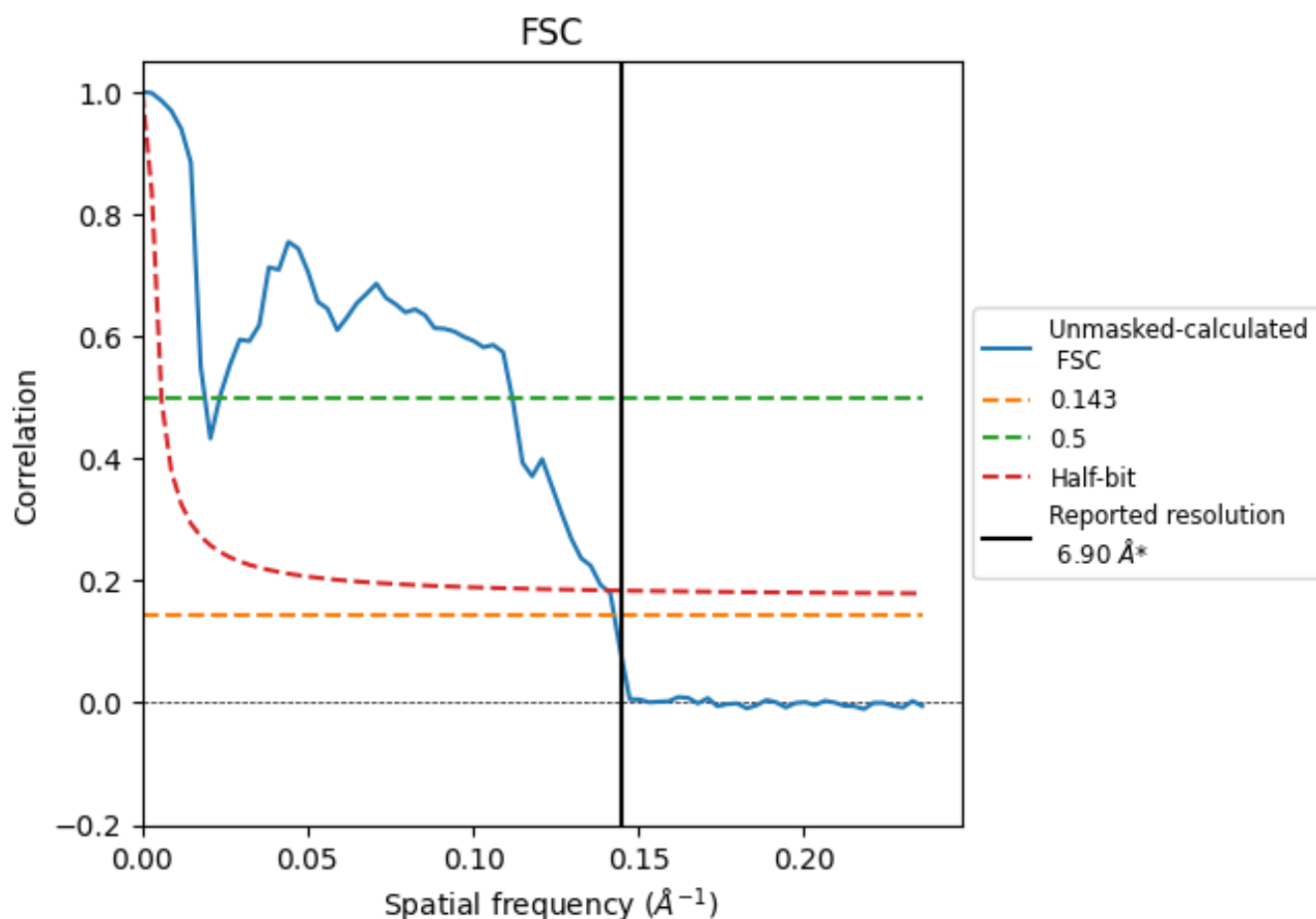


*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.145 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

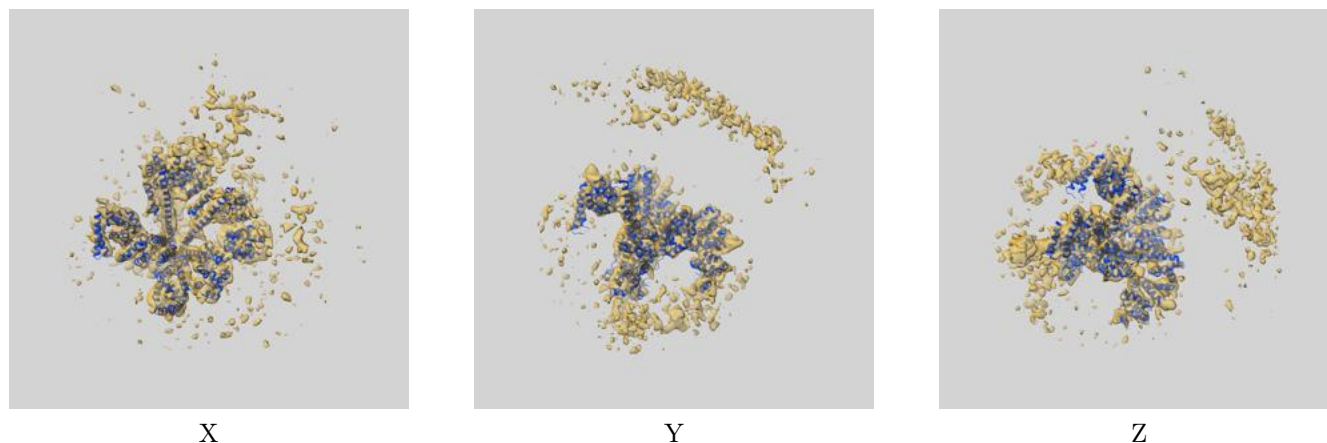
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.01	52.91	7.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

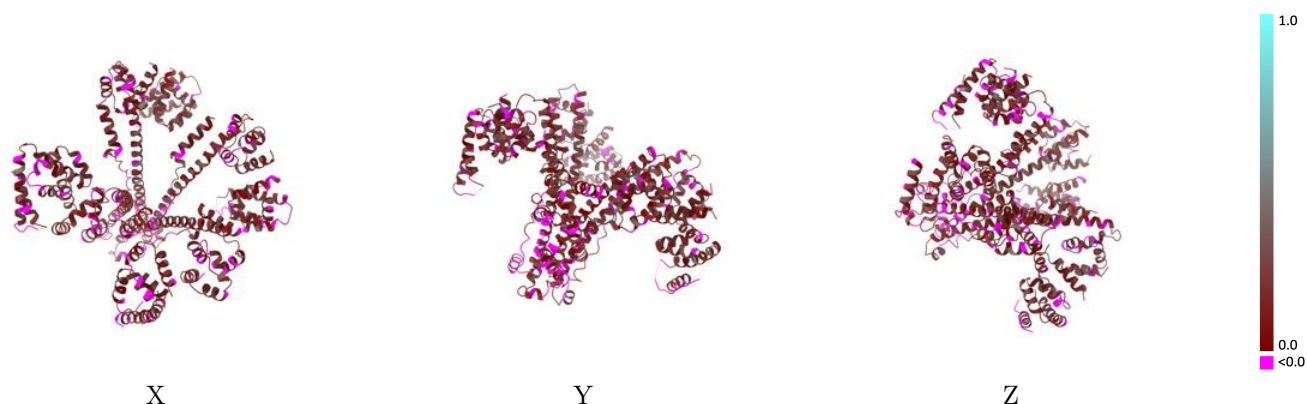
This section contains information regarding the fit between EMDB map EMD-61456 and PDB model 9KYX. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



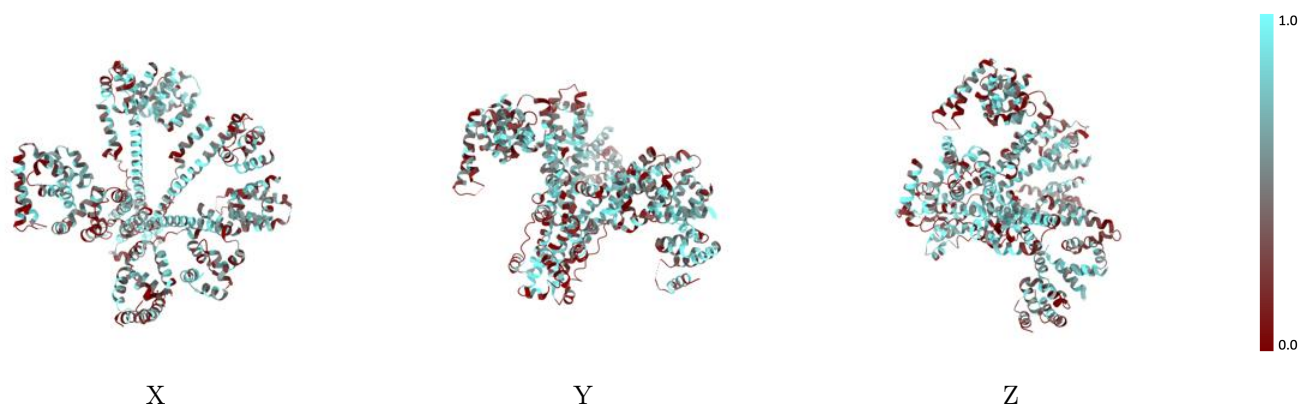
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



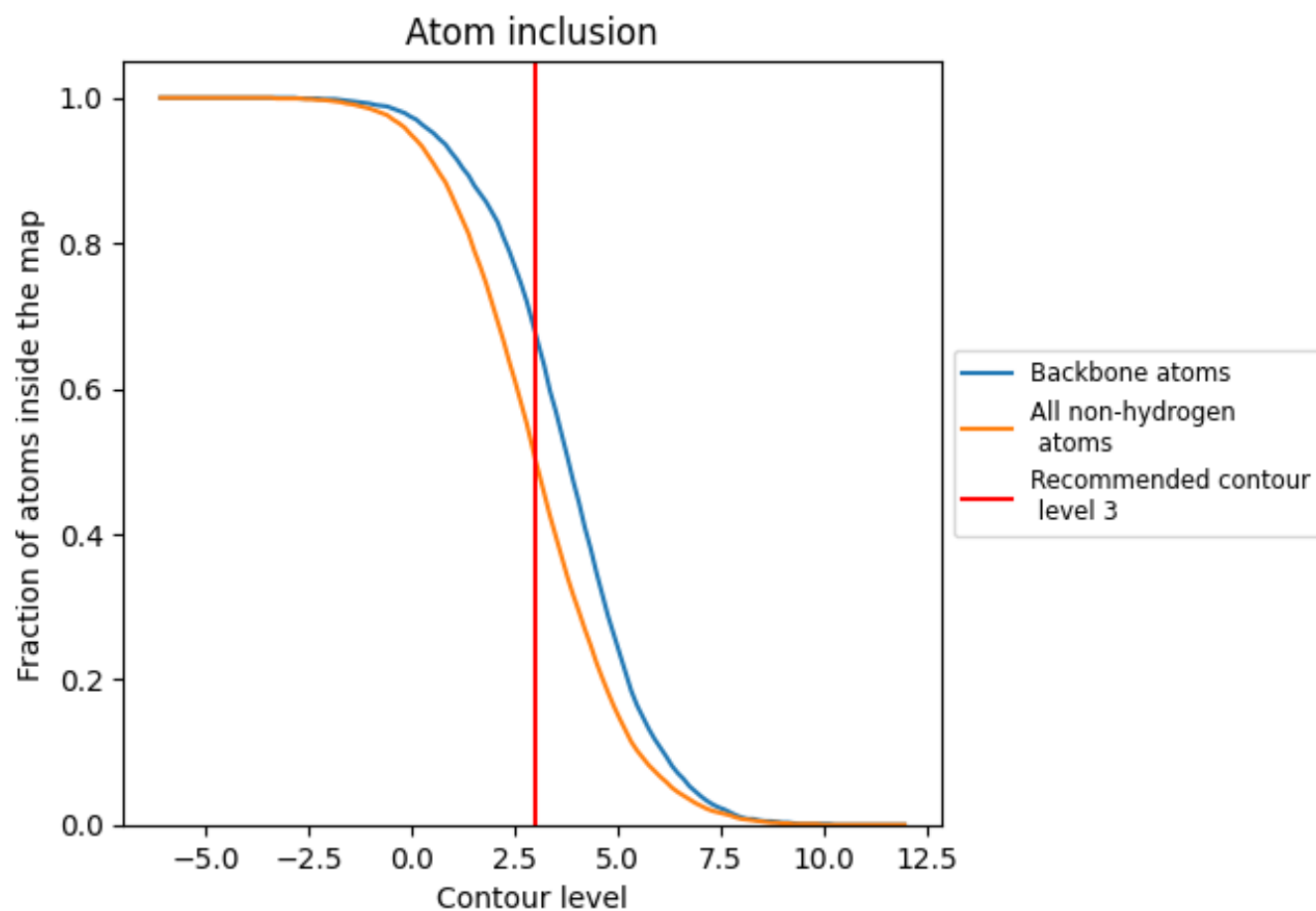
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 50% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5020	0.1290
A	0.5110	0.1470
B	0.4530	0.1430
C	0.5220	0.1150
D	0.4910	0.1240
E	0.5350	0.1300
F	0.4550	0.1240
G	0.4200	0.0890
H	0.6010	0.1560

1.0

0.0

<0.0