



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:54 AM UTC

PDB ID : 5VVS / pdb_00005vvs
EMDB ID : EMD-8737
Title : RNA pol II elongation complex
Authors : Lahiri, I.; Leschziner, A.E.
Deposited on : 2017-05-20
Resolution : 6.40 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:

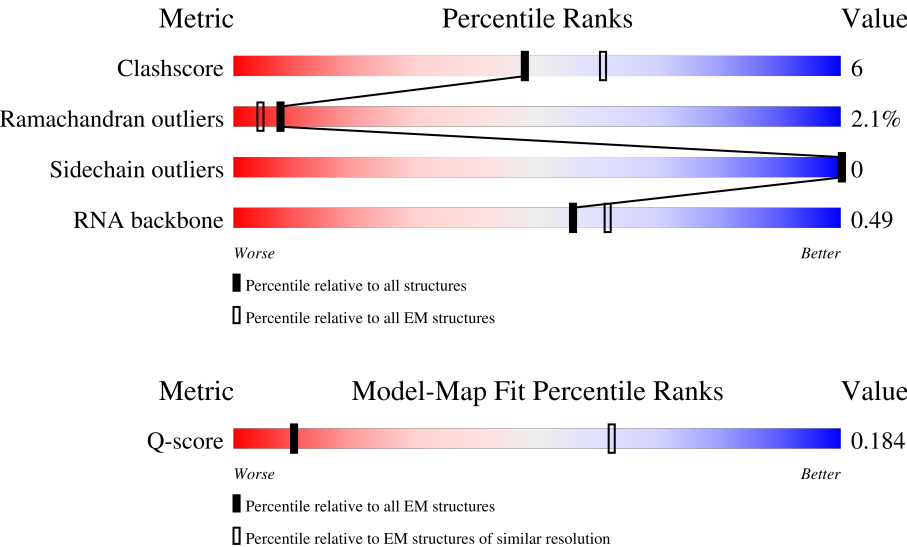
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.40 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	544 (5.90 - 6.90)

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	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	10	
14	N	47	
15	T	47	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33790 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1455	Total	C	N	O	S	0	0
			11444	7205	1997	2180	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1207	Total	C	N	O	S	0	0
			9608	6062	1678	1812	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1409	870	251	286	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	81	Total	C	N	O	S	0	0
			657	419	111	124	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			997	613	182	191	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 14 is a DNA chain called DNA (NTS).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	22	Total	C	N	O	P	0	0
			460	216	96	126	22		

- Molecule 15 is a DNA chain called DNA (TS).

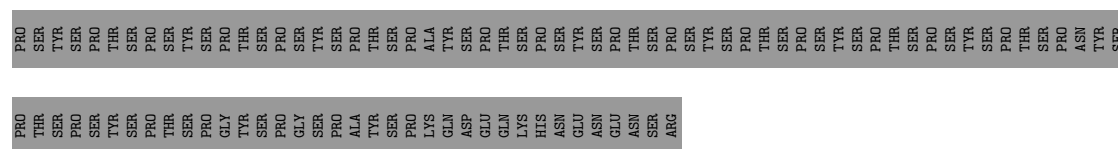
Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	38	Total	C	N	O	P	0	0
			763	365	124	236	38		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

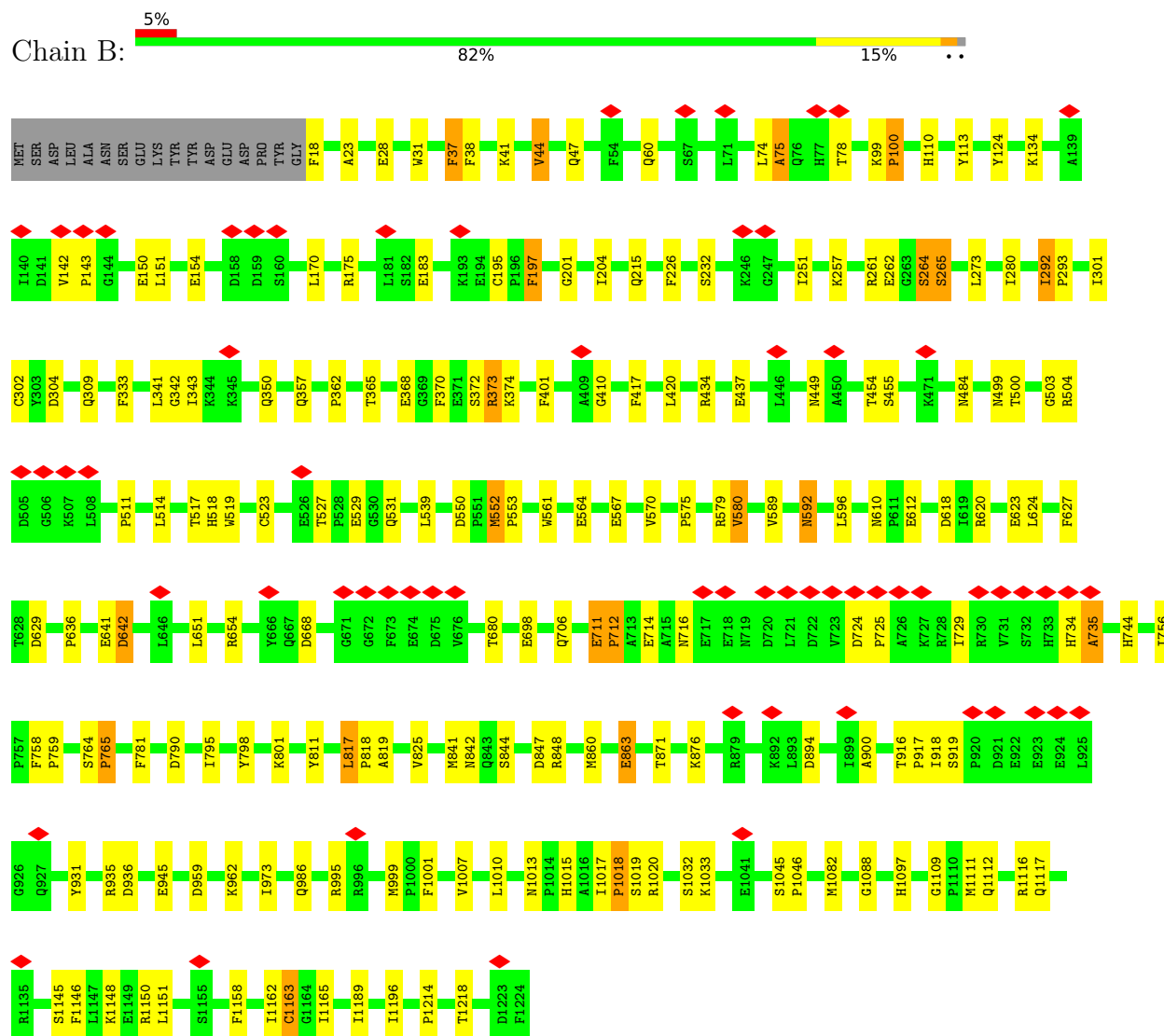
Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	C	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

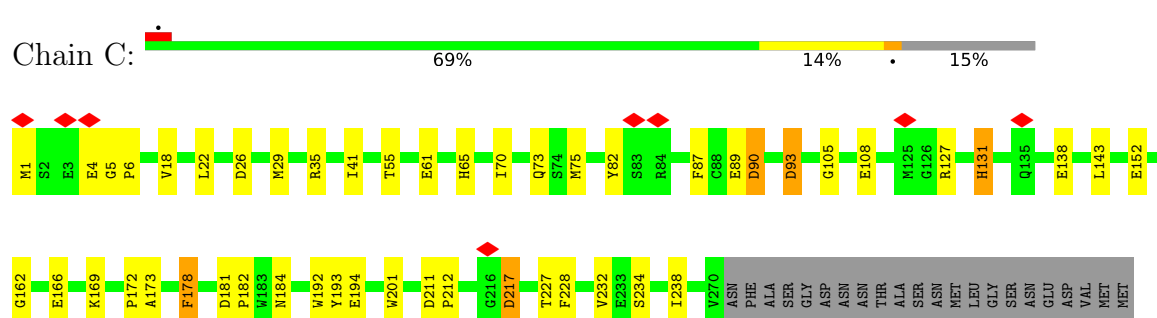
Mol	Chain	Residues	Atoms		AltConf
17	R	1	Total	Mg	0
			1	1	



• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



THR
GLY
ALA
GLU
GLN
ASP
PRO
TYR
SER
ASN
ALA
SER
GLN
MET
GLY
THR
GLY
SER
GLY
GLY
TYR
ASP
ASN
ALA
TRP

- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 

MET
ASN
VAL
S4
T5
S6
T7
F8
R11
R12
V18
E19
E20
E21
E22
N23
A24
N39
L52
R72
S73
GLN
LYS
LYS
HIS
LYS
LYS
HIS
LEU
LYS
HIS
GLU
ASN
ALA
ASN
ASP
GLU
THR
ALA
VAL
GLU
ASP
GLU
ASP
ASP
LEU
ASP
GLU
ASP
VAL
ASN

ALA
ASP
ASP
ASP
PHE
MET
HIS
SER
E117
E122
S125
I126
L129
L130
T134
G135
L141
K168
H173
A184
I195
E206
K212
T219
L220
Y221

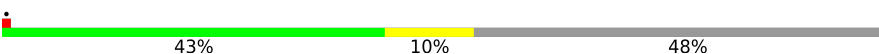
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 

M1
W13
K24
F29
I30
E33
P38
K45
S49
M50
G51
R52
R55
M68
N63
E66
I69
F72
P73
D74
L78
F82
P86
F110
V111
T117
V124
I127
P128
F135
M143
H146
P151
I154

E172
S173
Q174
L175
D182
E203
Y208
M215

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 

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

HIS
GLU
GLN
ILE
ARG
LYS
THR
LEU
LYS
GLU
LYS
ALA
ILE
P75
K76
D77
R97
M103
N104
A105
L111
D116
R119
T130
P131
L132
R135
L138
F143
E144
D145
E149
L155

- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 

M1
D6
H14
P15
P20
R21
M22
L30
V34
I54
D55
I56
Q57
L62
E69
K80
K83
G84
E85
V86
V87
D88
G89
T90
V91
H97
V101
G104
K107
L114
M115
P116
Q117
G124
S125
N126
P127
P128
S129
Y130
Q131
E134
D135

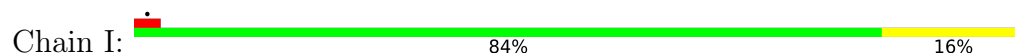
V136
I137
R142
I143
V154
I157
S162
I163
K164
I171

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

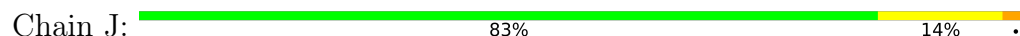
Chain H: 



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

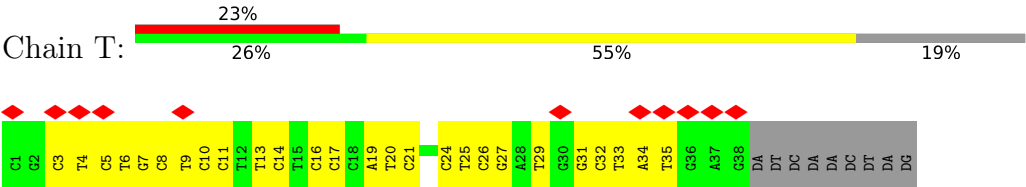


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19331	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	7.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0256	Depositor
Map size (Å)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.90	0/11651	1.25	137/15761 (0.9%)
2	B	0.90	0/9799	1.23	99/13221 (0.7%)
3	C	0.91	0/2163	1.22	26/2930 (0.9%)
4	D	0.83	0/1419	1.02	4/1903 (0.2%)
5	E	0.89	0/1796	1.26	18/2416 (0.7%)
6	F	0.94	0/669	1.26	9/903 (1.0%)
7	G	0.84	0/1368	1.27	16/1844 (0.9%)
8	H	0.87	0/1181	1.22	12/1602 (0.7%)
9	I	0.89	0/1016	1.26	13/1365 (1.0%)
10	J	0.87	0/587	1.13	4/786 (0.5%)
11	K	0.92	1/913 (0.1%)	1.29	13/1232 (1.1%)
12	L	0.83	0/366	1.19	1/485 (0.2%)
13	R	0.62	2/247 (0.8%)	0.52	0/384
14	N	0.25	0/518	0.43	0/796
15	T	0.28	0/849	0.54	0/1305
All	All	0.87	3/34542 (0.0%)	1.20	352/46933 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	6	G	C1'-N9	-6.67	1.38	1.48
13	R	10	A	C1'-N9	-5.29	1.40	1.48
11	K	60	ALA	CA-CB	-5.01	1.45	1.53

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	GLY	CA-C-N	9.80	129.46	119.56
1	A	638	GLY	C-N-CA	9.80	129.46	119.56
5	E	63	ASN	CA-C-N	9.79	129.88	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	63	ASN	C-N-CA	9.79	129.88	119.89
2	B	1109	GLY	CA-C-N	9.63	129.72	119.90
2	B	1109	GLY	C-N-CA	9.63	129.72	119.90
7	G	62	LEU	CA-C-N	9.62	129.25	119.82
7	G	62	LEU	C-N-CA	9.62	129.25	119.82
2	B	1088	GLY	CA-C-N	9.38	129.44	119.78
2	B	1088	GLY	C-N-CA	9.38	129.44	119.78
1	A	1301	GLU	CA-C-N	9.38	129.14	119.76
1	A	1301	GLU	C-N-CA	9.38	129.14	119.76
1	A	1137	ALA	CA-C-N	-9.36	110.78	122.48
1	A	1137	ALA	C-N-CA	-9.36	110.78	122.48
1	A	513	SER	CA-C-N	9.18	131.32	119.84
1	A	513	SER	C-N-CA	9.18	131.32	119.84
1	A	909	ASP	CA-C-N	9.14	128.89	119.56
1	A	909	ASP	C-N-CA	9.14	128.89	119.56
1	A	1163	ILE	CA-C-N	9.07	129.66	119.32
1	A	1163	ILE	C-N-CA	9.07	129.66	119.32
2	B	38	PHE	CA-CB-CG	-9.02	104.78	113.80
1	A	157	ASP	CA-C-N	8.87	130.92	119.84
1	A	157	ASP	C-N-CA	8.87	130.92	119.84
9	I	68	LEU	CA-C-N	8.79	128.84	119.78
9	I	68	LEU	C-N-CA	8.79	128.84	119.78
1	A	239	LEU	CA-C-N	8.60	128.53	119.85
1	A	239	LEU	C-N-CA	8.60	128.53	119.85
1	A	171	GLN	CA-C-N	8.56	128.50	119.85
1	A	171	GLN	C-N-CA	8.56	128.50	119.85
1	A	356	ASP	CA-C-N	8.55	128.20	119.82
1	A	356	ASP	C-N-CA	8.55	128.20	119.82
1	A	1332	PHE	CA-CB-CG	-8.55	105.25	113.80
2	B	500	THR	CA-C-N	8.54	128.41	120.21
2	B	500	THR	C-N-CA	8.54	128.41	120.21
3	C	217	ASP	CA-C-N	8.53	128.74	119.87
3	C	217	ASP	C-N-CA	8.53	128.74	119.87
2	B	1045	SER	CA-C-N	8.51	128.46	120.03
2	B	1045	SER	C-N-CA	8.51	128.46	120.03
1	A	1138	ILE	N-CA-C	8.45	120.08	107.15
2	B	570	VAL	CA-C-N	8.44	129.26	119.47
2	B	570	VAL	C-N-CA	8.44	129.26	119.47
1	A	599	SER	CA-C-N	8.41	128.14	119.56
1	A	599	SER	C-N-CA	8.41	128.14	119.56
2	B	592	ASN	CA-C-N	8.39	128.03	119.56
2	B	592	ASN	C-N-CA	8.39	128.03	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	706	GLN	CA-C-N	8.34	127.98	119.56
2	B	706	GLN	C-N-CA	8.34	127.98	119.56
4	D	195	ILE	CA-C-N	8.25	129.04	119.47
4	D	195	ILE	C-N-CA	8.25	129.04	119.47
1	A	491	VAL	CA-C-N	8.25	128.26	119.76
1	A	491	VAL	C-N-CA	8.25	128.26	119.76
1	A	1244	ARG	CA-C-N	8.25	130.15	119.84
1	A	1244	ARG	C-N-CA	8.25	130.15	119.84
2	B	23	ALA	CA-C-N	8.22	129.78	120.98
2	B	23	ALA	C-N-CA	8.22	129.78	120.98
5	E	58	MET	N-CA-C	-8.18	102.33	111.82
1	A	553	VAL	CA-C-N	8.15	127.80	119.56
1	A	553	VAL	C-N-CA	8.15	127.80	119.56
1	A	463	ILE	CA-C-N	8.13	128.57	120.52
1	A	463	ILE	C-N-CA	8.13	128.57	120.52
8	H	80	ARG	CA-C-N	8.13	128.76	120.38
8	H	80	ARG	C-N-CA	8.13	128.76	120.38
1	A	977	LYS	CA-C-N	8.13	128.14	119.76
1	A	977	LYS	C-N-CA	8.13	128.14	119.76
1	A	1155	ASP	CA-C-N	8.13	128.59	119.32
1	A	1155	ASP	C-N-CA	8.13	128.59	119.32
1	A	1319	VAL	CA-C-N	8.11	128.25	120.31
1	A	1319	VAL	C-N-CA	8.11	128.25	120.31
11	K	82	ASP	CA-C-N	8.09	128.54	119.32
11	K	82	ASP	C-N-CA	8.09	128.54	119.32
11	K	27	ALA	CA-C-N	8.05	127.98	119.85
11	K	27	ALA	C-N-CA	8.05	127.98	119.85
1	A	1121	GLU	CA-C-N	8.03	128.78	119.47
1	A	1121	GLU	C-N-CA	8.03	128.78	119.47
5	E	175	LEU	CA-C-N	8.02	128.04	119.78
5	E	175	LEU	C-N-CA	8.02	128.04	119.78
2	B	523	CYS	CA-C-N	8.00	127.64	119.56
2	B	523	CYS	C-N-CA	8.00	127.64	119.56
7	G	115	MET	CA-C-N	8.00	128.06	119.90
7	G	115	MET	C-N-CA	8.00	128.06	119.90
2	B	999	MET	CA-C-N	7.95	128.43	119.92
2	B	999	MET	C-N-CA	7.95	128.43	119.92
11	K	3	ALA	CA-C-N	7.93	129.47	120.98
11	K	3	ALA	C-N-CA	7.93	129.47	120.98
2	B	410	GLY	CA-C-N	7.88	127.80	119.05
2	B	410	GLY	C-N-CA	7.88	127.80	119.05
2	B	1013	ASN	CA-C-N	7.87	127.59	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1013	ASN	C-N-CA	7.87	127.59	119.56
2	B	417	PHE	CA-CB-CG	-7.84	105.96	113.80
1	A	518	LYS	CA-C-N	7.81	127.80	119.76
1	A	518	LYS	C-N-CA	7.81	127.80	119.76
2	B	610	ASN	CA-C-N	7.77	128.49	119.47
2	B	610	ASN	C-N-CA	7.77	128.49	119.47
2	B	801	LYS	CA-C-N	7.74	127.67	119.85
2	B	801	LYS	C-N-CA	7.74	127.67	119.85
8	H	16	ASP	CA-C-N	7.73	128.13	119.32
8	H	16	ASP	C-N-CA	7.73	128.13	119.32
2	B	232	SER	CA-C-N	7.72	127.36	119.56
2	B	232	SER	C-N-CA	7.72	127.36	119.56
2	B	758	PHE	CA-C-N	7.68	127.40	119.56
2	B	758	PHE	C-N-CA	7.68	127.40	119.56
1	A	560	ILE	CA-C-N	7.61	127.77	120.31
1	A	560	ILE	C-N-CA	7.61	127.77	120.31
1	A	395	GLY	CA-C-N	7.54	128.52	120.83
1	A	395	GLY	C-N-CA	7.54	128.52	120.83
2	B	1007	VAL	CA-C-N	7.54	127.54	119.78
2	B	1007	VAL	C-N-CA	7.54	127.54	119.78
5	E	127	ILE	N-CA-C	7.50	116.17	107.77
1	A	1157	ASP	CA-C-N	7.48	128.42	120.12
1	A	1157	ASP	C-N-CA	7.48	128.42	120.12
11	K	65	HIS	CA-C-N	7.48	128.14	119.47
11	K	65	HIS	C-N-CA	7.48	128.14	119.47
10	J	3	VAL	CA-C-N	7.47	127.52	119.90
10	J	3	VAL	C-N-CA	7.47	127.52	119.90
6	F	138	LEU	CA-C-N	7.46	127.17	119.56
6	F	138	LEU	C-N-CA	7.46	127.17	119.56
6	F	105	ALA	CA-C-N	7.44	127.44	119.78
6	F	105	ALA	C-N-CA	7.44	127.44	119.78
6	F	116	ASP	CA-C-N	7.42	128.07	119.47
6	F	116	ASP	C-N-CA	7.42	128.07	119.47
3	C	211	ASP	CA-C-N	7.37	127.97	120.38
3	C	211	ASP	C-N-CA	7.37	127.97	120.38
1	A	1323	ASP	CA-C-N	7.32	127.48	119.87
1	A	1323	ASP	C-N-CA	7.32	127.48	119.87
3	C	41	ILE	CA-C-N	7.20	127.18	119.76
3	C	41	ILE	C-N-CA	7.20	127.18	119.76
11	K	22	ASP	CA-C-N	7.17	127.60	119.93
11	K	22	ASP	C-N-CA	7.17	127.60	119.93
9	I	40	SER	CA-C-N	7.15	126.78	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	40	SER	C-N-CA	7.15	126.78	119.56
11	K	40	HIS	CA-CB-CG	-7.12	106.68	113.80
2	B	795	ILE	N-CA-C	7.10	118.12	107.75
2	B	527	THR	CA-C-N	7.09	127.02	120.21
2	B	527	THR	C-N-CA	7.09	127.02	120.21
5	E	117	THR	CA-C-N	7.08	127.69	119.47
5	E	117	THR	C-N-CA	7.08	127.69	119.47
1	A	376	TYR	CA-C-N	7.06	128.67	119.84
1	A	376	TYR	C-N-CA	7.06	128.67	119.84
9	I	65	ASP	CA-C-N	7.06	126.76	119.56
9	I	65	ASP	C-N-CA	7.06	126.76	119.56
2	B	817	LEU	CA-C-N	7.04	128.64	119.84
2	B	817	LEU	C-N-CA	7.04	128.64	119.84
2	B	197	PHE	CA-CB-CG	-7.03	106.77	113.80
2	B	1117	GLN	CA-C-N	7.02	126.99	119.76
2	B	1117	GLN	C-N-CA	7.02	126.99	119.76
9	I	15	TYR	CA-C-N	7.02	126.99	119.76
9	I	15	TYR	C-N-CA	7.02	126.99	119.76
4	D	173	HIS	CA-C-N	7.00	127.30	119.32
4	D	173	HIS	C-N-CA	7.00	127.30	119.32
2	B	195	CYS	CA-C-N	6.94	126.92	119.28
2	B	195	CYS	C-N-CA	6.94	126.92	119.28
7	G	87	VAL	N-CA-C	6.94	118.11	108.12
1	A	241	VAL	CA-C-N	6.94	127.52	120.38
1	A	241	VAL	C-N-CA	6.94	127.52	120.38
5	E	72	PHE	CA-C-N	6.93	128.50	119.84
5	E	72	PHE	C-N-CA	6.93	128.50	119.84
1	A	243	PRO	CA-C-N	6.90	127.49	120.38
1	A	243	PRO	C-N-CA	6.90	127.49	120.38
1	A	247	ARG	CA-C-N	6.88	128.44	119.84
1	A	247	ARG	C-N-CA	6.88	128.44	119.84
1	A	582	ILE	CA-C-N	6.87	126.83	120.03
1	A	582	ILE	C-N-CA	6.87	126.83	120.03
1	A	152	VAL	CA-C-N	6.83	128.37	119.84
1	A	152	VAL	C-N-CA	6.83	128.37	119.84
2	B	273	LEU	CA-C-N	6.80	128.34	119.84
2	B	273	LEU	C-N-CA	6.80	128.34	119.84
1	A	440	ASP	CA-C-N	6.77	128.30	119.84
1	A	440	ASP	C-N-CA	6.77	128.30	119.84
2	B	292	ILE	CA-C-N	6.76	126.72	119.76
2	B	292	ILE	C-N-CA	6.76	126.72	119.76
7	G	127	PRO	CA-C-N	6.74	128.27	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	127	PRO	C-N-CA	6.74	128.27	119.84
8	H	81	PRO	CA-C-N	6.72	128.25	119.84
8	H	81	PRO	C-N-CA	6.72	128.25	119.84
1	A	1293	SER	CA-C-N	6.70	127.56	120.12
1	A	1293	SER	C-N-CA	6.70	127.56	120.12
2	B	564	GLU	CA-C-N	6.69	126.65	119.76
2	B	564	GLU	C-N-CA	6.69	126.65	119.76
2	B	900	ALA	CA-C-N	6.69	126.65	119.76
2	B	900	ALA	C-N-CA	6.69	126.65	119.76
3	C	5	GLY	CA-C-N	6.63	128.12	119.84
3	C	5	GLY	C-N-CA	6.63	128.12	119.84
1	A	1113	THR	CA-C-N	6.62	128.12	119.84
1	A	1113	THR	C-N-CA	6.62	128.12	119.84
2	B	113	TYR	CA-C-N	6.62	128.12	119.84
2	B	113	TYR	C-N-CA	6.62	128.12	119.84
3	C	232	VAL	N-CA-C	6.60	117.35	108.11
5	E	52	ARG	CA-C-N	6.54	128.02	119.84
5	E	52	ARG	C-N-CA	6.54	128.02	119.84
9	I	13	MET	N-CA-C	6.54	119.77	109.96
1	A	562	THR	CA-C-N	6.49	126.41	119.85
1	A	562	THR	C-N-CA	6.49	126.41	119.85
9	I	75	CYS	CA-C-N	6.41	126.91	119.47
9	I	75	CYS	C-N-CA	6.41	126.91	119.47
7	G	104	GLY	CA-C-N	6.41	128.79	121.04
7	G	104	GLY	C-N-CA	6.41	128.79	121.04
3	C	192	TRP	CB-CA-C	-6.39	108.54	117.23
6	F	130	ILE	CA-C-N	6.38	127.81	119.84
6	F	130	ILE	C-N-CA	6.38	127.81	119.84
2	B	142	VAL	CA-C-N	6.37	127.80	119.84
2	B	142	VAL	C-N-CA	6.37	127.80	119.84
1	A	88	LYS	CA-C-N	6.31	126.81	119.99
1	A	88	LYS	C-N-CA	6.31	126.81	119.99
3	C	70	ILE	CA-C-N	6.31	126.83	120.14
3	C	70	ILE	C-N-CA	6.31	126.83	120.14
2	B	550	ASP	CA-C-N	6.30	127.44	120.45
2	B	550	ASP	C-N-CA	6.30	127.44	120.45
3	C	212	PRO	CA-C-N	6.28	127.69	119.84
3	C	212	PRO	C-N-CA	6.28	127.69	119.84
1	A	809	THR	CA-C-N	6.26	126.46	119.32
1	A	809	THR	C-N-CA	6.26	126.46	119.32
2	B	434	ARG	N-CA-C	6.24	117.74	111.07
2	B	744	HIS	CA-C-N	6.23	127.63	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	744	HIS	C-N-CA	6.23	127.63	119.84
2	B	863	GLU	N-CA-C	6.22	117.94	111.03
12	L	29	TYR	N-CA-C	6.22	118.00	108.42
8	H	7	ASP	N-CA-C	6.19	117.28	108.74
1	A	381	THR	CA-C-N	6.18	126.08	119.28
1	A	381	THR	C-N-CA	6.18	126.08	119.28
1	A	784	LEU	CA-C-N	6.16	126.96	120.12
1	A	784	LEU	C-N-CA	6.16	126.96	120.12
1	A	793	SER	CA-C-N	6.14	125.70	119.19
1	A	793	SER	C-N-CA	6.14	125.70	119.19
2	B	876	LYS	CA-C-N	6.13	128.23	120.51
2	B	876	LYS	C-N-CA	6.13	128.23	120.51
3	C	201	TRP	CA-C-N	6.12	126.48	119.93
3	C	201	TRP	C-N-CA	6.12	126.48	119.93
2	B	373	ARG	N-CA-C	6.12	117.62	111.07
7	G	69	GLU	N-CA-C	6.07	118.41	108.52
2	B	1189	ILE	N-CA-C	6.04	117.16	111.48
3	C	18	VAL	N-CA-C	6.03	116.30	107.37
1	A	218	ASP	CA-CB-CG	-6.02	106.58	112.60
1	A	956	LEU	CA-C-N	6.02	125.64	119.56
1	A	956	LEU	C-N-CA	6.02	125.64	119.56
2	B	589	VAL	N-CA-C	6.01	117.25	108.53
7	G	80	LYS	CA-C-N	6.00	128.08	120.51
7	G	80	LYS	C-N-CA	6.00	128.08	120.51
1	A	1137	ALA	N-CA-C	-5.97	101.20	110.10
5	E	110	PHE	CA-CB-CG	-5.93	107.87	113.80
1	A	284	ALA	CA-C-N	5.93	125.87	119.76
1	A	284	ALA	C-N-CA	5.93	125.87	119.76
2	B	919	SER	CA-C-N	5.92	128.06	120.89
2	B	919	SER	C-N-CA	5.92	128.06	120.89
1	A	1140	HIS	N-CA-C	5.91	117.51	108.52
2	B	257	LYS	N-CA-C	5.91	118.58	109.07
5	E	124	VAL	CA-C-N	5.91	126.01	119.87
5	E	124	VAL	C-N-CA	5.91	126.01	119.87
2	B	280	ILE	CA-C-N	5.88	126.22	119.93
2	B	280	ILE	C-N-CA	5.88	126.22	119.93
1	A	507	VAL	CA-C-N	5.86	126.26	119.47
1	A	507	VAL	C-N-CA	5.86	126.26	119.47
2	B	798	TYR	CA-C-N	5.83	125.59	119.76
2	B	798	TYR	C-N-CA	5.83	125.59	119.76
1	A	954	TRP	CA-C-N	5.80	127.10	119.84
1	A	954	TRP	C-N-CA	5.80	127.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ASP	N-CA-C	5.80	117.05	107.20
5	E	182	ASP	CA-C-N	5.79	127.07	119.84
5	E	182	ASP	C-N-CA	5.79	127.07	119.84
7	G	14	HIS	CA-C-N	5.78	125.45	119.56
7	G	14	HIS	C-N-CA	5.78	125.45	119.56
3	C	181	ASP	CA-C-N	5.76	127.03	119.84
3	C	181	ASP	C-N-CA	5.76	127.03	119.84
2	B	449	ASN	CA-CB-CG	-5.75	106.85	112.60
8	H	75	ALA	N-CA-C	-5.75	100.40	108.96
2	B	552	MET	CA-C-N	5.71	125.83	119.32
2	B	552	MET	C-N-CA	5.71	125.83	119.32
2	B	781	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	9	ALA	CA-C-N	5.63	125.39	119.76
1	A	9	ALA	C-N-CA	5.63	125.39	119.76
1	A	463	ILE	CB-CA-C	-5.63	102.97	110.97
1	A	242	PRO	CA-C-N	5.63	126.18	120.38
1	A	242	PRO	C-N-CA	5.63	126.18	120.38
1	A	366	VAL	N-CA-C	5.62	113.44	107.76
1	A	476	SER	CA-C-N	5.60	125.12	119.19
1	A	476	SER	C-N-CA	5.60	125.12	119.19
3	C	178	PHE	CA-CB-CG	-5.56	108.24	113.80
2	B	668	ASP	CA-C-N	-5.55	115.83	122.22
2	B	668	ASP	C-N-CA	-5.55	115.83	122.22
1	A	1189	SER	CA-C-N	5.55	126.03	120.04
1	A	1189	SER	C-N-CA	5.55	126.03	120.04
1	A	77	CYS	CA-C-N	5.51	125.98	120.14
1	A	77	CYS	C-N-CA	5.51	125.98	120.14
1	A	1319	VAL	N-CA-C	5.49	113.35	108.63
1	A	1058	VAL	N-CA-C	5.49	116.66	109.58
2	B	973	ILE	CA-C-N	5.48	126.69	119.84
2	B	973	ILE	C-N-CA	5.48	126.69	119.84
2	B	37	PHE	CA-CB-CG	-5.47	108.33	113.80
2	B	333	PHE	CA-CB-CG	-5.45	108.35	113.80
10	J	64	ASN	CA-C-N	5.45	126.65	119.84
10	J	64	ASN	C-N-CA	5.45	126.65	119.84
8	H	118	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	366	VAL	CA-C-N	5.43	126.62	119.84
1	A	366	VAL	C-N-CA	5.43	126.62	119.84
1	A	1183	GLN	N-CA-C	5.41	119.37	112.34
1	A	835	GLY	N-CA-C	-5.39	106.24	112.50
1	A	1454	MET	CA-C-N	5.35	126.53	119.84
1	A	1454	MET	C-N-CA	5.35	126.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1163	CYS	CA-C-N	5.34	126.03	119.99
2	B	1163	CYS	C-N-CA	5.34	126.03	119.99
3	C	65	HIS	CA-CB-CG	5.34	119.14	113.80
9	I	6	PHE	N-CA-C	5.34	118.03	110.50
1	A	174	ILE	N-CA-C	5.33	116.15	108.48
2	B	265	SER	N-CA-C	5.32	119.03	112.54
2	B	110	HIS	N-CA-C	5.32	116.60	108.52
1	A	673	GLY	CA-C-N	5.31	125.13	119.28
1	A	673	GLY	C-N-CA	5.31	125.13	119.28
3	C	131	HIS	CA-C-N	5.31	125.25	119.78
3	C	131	HIS	C-N-CA	5.31	125.25	119.78
5	E	154	ILE	N-CA-C	5.31	115.50	107.80
1	A	463	ILE	N-CA-C	5.30	114.81	108.45
1	A	813	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	244	PRO	CA-C-N	5.30	125.36	119.32
1	A	244	PRO	C-N-CA	5.30	125.36	119.32
3	C	238	ILE	CA-C-N	5.26	125.56	119.93
3	C	238	ILE	C-N-CA	5.26	125.56	119.93
1	A	659	HIS	CA-CB-CG	-5.25	108.55	113.80
6	F	132	LEU	N-CA-C	5.24	117.04	108.55
1	A	567	LYS	CA-C-N	5.23	126.38	119.84
1	A	567	LYS	C-N-CA	5.23	126.38	119.84
2	B	756	ILE	CA-C-N	5.23	125.14	119.76
2	B	756	ILE	C-N-CA	5.23	125.14	119.76
8	H	68	THR	CA-C-N	5.22	125.22	119.90
8	H	68	THR	C-N-CA	5.22	125.22	119.90
11	K	61	TYR	N-CA-C	5.21	116.90	109.14
1	A	23	SER	CA-C-N	5.21	126.35	119.84
1	A	23	SER	C-N-CA	5.21	126.35	119.84
1	A	600	PRO	CA-C-N	5.20	127.24	120.28
1	A	600	PRO	C-N-CA	5.20	127.24	120.28
1	A	91	PHE	CA-CB-CG	5.18	118.98	113.80
2	B	680	THR	N-CA-C	5.17	117.73	110.23
1	A	37	PHE	CA-C-N	5.16	129.75	120.88
1	A	37	PHE	C-N-CA	5.16	129.75	120.88
9	I	83	ASN	CA-CB-CG	-5.15	107.45	112.60
11	K	109	TRP	N-CA-C	5.14	117.67	111.40
2	B	226	PHE	N-CA-C	5.14	116.88	108.55
2	B	18	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	213	HIS	CA-CB-CG	5.12	118.92	113.80
1	A	263	THR	N-CA-C	-5.11	105.79	111.36
1	A	1278	ASN	CA-C-N	-5.11	116.34	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1278	ASN	C-N-CA	-5.11	116.34	122.22
8	H	74	SER	N-CA-C	-5.11	108.79	114.62
1	A	1143	LEU	N-CA-C	5.11	117.24	111.11
7	G	34	VAL	N-CA-C	5.11	115.77	110.82
7	G	91	VAL	N-CA-C	5.09	115.61	108.89
1	A	1030	ARG	N-CA-C	-5.09	105.81	111.36
1	A	308	ILE	N-CA-C	5.08	114.61	106.88
2	B	945	GLU	N-CA-C	5.08	115.76	108.74
2	B	170	LEU	CA-C-N	5.06	125.29	119.83
2	B	170	LEU	C-N-CA	5.06	125.29	119.83
1	A	95	PHE	CA-CB-CG	-5.04	108.76	113.80
3	C	87	PHE	CA-CB-CG	-5.04	108.76	113.80
2	B	627	PHE	CA-CB-CG	-5.03	108.77	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11444	0	11502	105	0
2	B	9608	0	9578	124	0
3	C	2125	0	2094	28	0
4	D	1409	0	1423	10	0
5	E	1760	0	1788	20	0
6	F	657	0	673	10	0
7	G	1340	0	1357	9	0
8	H	1161	0	1124	14	0
9	I	997	0	959	8	0
10	J	578	0	590	5	0
11	K	895	0	903	12	0
12	L	364	0	389	1	0
13	R	220	0	110	13	0
14	N	460	0	246	14	0
15	T	763	0	431	35	0
16	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	R	1	0	0	0	0
All	All	33790	0	33167	395	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 6.

All (395) 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)
15:T:3:DC:H2''	15:T:4:DT:H72	1.50	0.94
2:B:343:ILE:HG22	2:B:343:ILE:O	1.74	0.88
15:T:19:DA:C8	15:T:20:DT:H72	2.11	0.85
5:E:208:TYR:CD2	5:E:208:TYR:O	2.32	0.83
2:B:580:VAL:HG12	2:B:580:VAL:O	1.77	0.82
2:B:251:ILE:HG22	2:B:251:ILE:O	1.81	0.80
10:J:70:ASP:OXT	10:J:70:ASP:OD1	2.05	0.74
2:B:519:TRP:O	2:B:519:TRP:CE3	2.42	0.73
7:G:131:GLN:OE1	7:G:131:GLN:O	2.07	0.73
1:A:69:THR:O	1:A:69:THR:HG22	1.86	0.73
2:B:44:VAL:HG12	2:B:44:VAL:O	1.88	0.73
14:N:34:DG:H2'	14:N:35:DA:C8	2.24	0.72
15:T:9:DT:H2''	15:T:10:DC:C5	2.25	0.71
1:A:1363:VAL:HG12	1:A:1363:VAL:O	1.91	0.70
1:A:1191:TRP:HA	1:A:1191:TRP:CE3	2.24	0.70
1:A:868:TYR:C	1:A:868:TYR:CD2	2.70	0.70
1:A:145:LYS:O	1:A:145:LYS:HG2	1.91	0.69
2:B:518:HIS:C	2:B:518:HIS:CD2	2.69	0.68
2:B:539:LEU:HD12	2:B:539:LEU:O	1.95	0.67
15:T:3:DC:H2''	15:T:4:DT:C7	2.24	0.67
3:C:108:GLU:OE1	3:C:108:GLU:N	2.26	0.67
2:B:60:GLN:N	2:B:60:GLN:OE1	2.28	0.67
15:T:10:DC:H2'	15:T:11:DC:C6	2.28	0.67
2:B:518:HIS:HD2	2:B:518:HIS:O	1.79	0.66
13:R:5:A:O5'	13:R:5:A:H8	1.79	0.66
15:T:5:DC:C5	15:T:6:DT:H73	2.30	0.66
6:F:149:GLU:OE1	6:F:149:GLU:N	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:TYR:C	1:A:551:TYR:CD2	2.74	0.65
2:B:1015:HIS:ND1	2:B:1015:HIS:C	2.54	0.65
15:T:16:DC:N3	15:T:17:DC:N4	2.45	0.65
2:B:175:ARG:O	2:B:175:ARG:HG2	1.96	0.64
13:R:4:G:O5'	13:R:4:G:H8	1.80	0.64
14:N:42:DA:C2	15:T:7:DG:C2	2.86	0.64
1:A:1191:TRP:HA	1:A:1191:TRP:HE3	1.62	0.64
15:T:3:DC:C2'	15:T:4:DT:H72	2.25	0.64
1:A:247:ARG:O	1:A:247:ARG:HG3	1.96	0.64
2:B:341:LEU:O	2:B:341:LEU:HD23	1.98	0.64
1:A:226:GLU:N	1:A:226:GLU:OE1	2.32	0.63
15:T:26:DC:H2''	15:T:27:DG:H5'	1.80	0.63
2:B:37:PHE:O	2:B:37:PHE:CD1	2.52	0.63
2:B:261:ARG:N	2:B:261:ARG:HD2	2.15	0.62
1:A:1271:ILE:O	1:A:1271:ILE:HG22	1.98	0.62
14:N:40:DG:H2''	14:N:41:DC:C6	2.35	0.61
14:N:34:DG:C6	14:N:35:DA:C6	2.90	0.60
1:A:453:MET:SD	1:A:453:MET:N	2.75	0.60
8:H:61:SER:OG	8:H:62:SER:N	2.35	0.60
11:K:29:ASN:ND2	11:K:77:THR:OG1	2.35	0.60
1:A:742:ASN:OD1	1:A:742:ASN:N	2.34	0.60
15:T:9:DT:H2''	15:T:10:DC:C6	2.37	0.59
1:A:549:MET:SD	1:A:549:MET:C	2.85	0.59
2:B:183:GLU:N	2:B:183:GLU:OE1	2.35	0.59
15:T:4:DT:H2''	15:T:5:DC:C6	2.38	0.59
1:A:461:LYS:HD3	1:A:461:LYS:C	2.27	0.59
2:B:343:ILE:O	2:B:343:ILE:CG2	2.47	0.59
2:B:529:GLU:N	2:B:529:GLU:OE1	2.36	0.59
2:B:624:LEU:C	2:B:624:LEU:HD23	2.27	0.59
15:T:5:DC:C6	15:T:6:DT:H71	2.38	0.58
15:T:34:DA:H2''	15:T:35:DT:C7	2.34	0.58
15:T:5:DC:C6	15:T:6:DT:C7	2.87	0.58
2:B:341:LEU:HD23	2:B:341:LEU:C	2.29	0.58
2:B:518:HIS:CD2	2:B:518:HIS:O	2.58	0.57
2:B:714:GLU:OE1	2:B:714:GLU:N	2.35	0.57
1:A:1086:PHE:O	1:A:1086:PHE:CD1	2.57	0.57
13:R:1:A:C2'	13:R:2:U:H5'	2.33	0.57
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.30	0.57
2:B:871:THR:HG23	2:B:871:THR:O	2.05	0.57
1:A:551:TYR:CD2	1:A:551:TYR:O	2.58	0.56
3:C:169:LYS:HD2	3:C:169:LYS:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:HG22	1:A:191:THR:O	2.05	0.56
3:C:227:THR:HG22	3:C:227:THR:O	2.06	0.56
2:B:251:ILE:O	2:B:251:ILE:CG2	2.52	0.56
2:B:518:HIS:C	2:B:518:HIS:HD2	2.13	0.56
3:C:127:ARG:O	3:C:127:ARG:HG2	2.06	0.56
3:C:55:THR:OG1	3:C:152:GLU:N	2.39	0.56
13:R:1:A:H3'	13:R:2:U:C6	2.40	0.56
6:F:145:ASP:OD1	6:F:145:ASP:C	2.49	0.55
2:B:44:VAL:O	2:B:44:VAL:CG1	2.54	0.55
9:I:26:LEU:C	9:I:26:LEU:HD12	2.31	0.55
9:I:54:GLU:N	9:I:54:GLU:OE1	2.39	0.55
1:A:68:GLN:O	1:A:68:GLN:HG2	2.07	0.55
1:A:496:GLU:CD	1:A:496:GLU:H	2.15	0.55
1:A:1024:SER:OG	1:A:1025:ARG:N	2.39	0.55
1:A:1421:CYS:O	1:A:1421:CYS:SG	2.65	0.55
1:A:959:ASN:C	1:A:959:ASN:OD1	2.50	0.54
14:N:13:DA:H1'	14:N:14:DT:H5'	1.88	0.54
1:A:463:ILE:O	1:A:463:ILE:HG13	2.07	0.54
15:T:25:DT:H2''	15:T:26:DC:C6	2.42	0.54
13:R:1:A:OP2	13:R:1:A:H8	1.90	0.54
2:B:651:LEU:O	2:B:654:ARG:NH1	2.41	0.54
3:C:166:GLU:HA	3:C:166:GLU:OE1	2.07	0.54
2:B:592:ASN:OD1	2:B:592:ASN:C	2.50	0.54
1:A:868:TYR:CD2	1:A:868:TYR:O	2.61	0.54
1:A:431:LYS:HD2	1:A:431:LYS:N	2.23	0.54
8:H:89:LEU:C	8:H:89:LEU:HD12	2.33	0.54
14:N:40:DG:H2''	14:N:41:DC:H6	1.71	0.54
10:J:37:SER:OG	10:J:38:ARG:NH1	2.41	0.54
2:B:918:ILE:HG23	2:B:918:ILE:O	2.09	0.53
8:H:43:ASN:OD1	8:H:43:ASN:C	2.50	0.53
2:B:372:SER:OG	2:B:373:ARG:N	2.41	0.53
2:B:894:ASP:OD1	2:B:894:ASP:C	2.49	0.53
15:T:34:DA:H2''	15:T:35:DT:H71	1.90	0.53
1:A:525:GLN:OE1	1:A:525:GLN:N	2.39	0.53
2:B:78:THR:O	2:B:78:THR:HG22	2.08	0.53
1:A:1215:ARG:NH1	1:A:1219:THR:OG1	2.42	0.53
15:T:19:DA:N9	15:T:20:DT:H72	2.23	0.53
2:B:529:GLU:CD	2:B:529:GLU:H	2.17	0.52
2:B:357:GLN:O	2:B:365:THR:OG1	2.28	0.52
6:F:111:LEU:HD23	6:F:111:LEU:O	2.08	0.52
2:B:531:GLN:OE1	2:B:531:GLN:N	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:42:DA:H2''	14:N:43:DG:O5'	2.08	0.52
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.52
3:C:22:LEU:HB2	3:C:228:PHE:HB2	1.91	0.52
1:A:320:ARG:O	1:A:321:PRO:C	2.52	0.52
6:F:119:ARG:HA	6:F:119:ARG:NE	2.25	0.52
2:B:561:TRP:HA	2:B:561:TRP:CE3	2.45	0.52
2:B:1150:ARG:HA	2:B:1150:ARG:NE	2.25	0.52
2:B:514:LEU:C	2:B:514:LEU:HD23	2.35	0.51
9:I:60:GLN:OE1	9:I:60:GLN:N	2.36	0.51
2:B:580:VAL:O	2:B:580:VAL:CG1	2.50	0.51
1:A:53:LEU:O	1:A:54:ASN:HB2	2.10	0.51
2:B:567:GLU:H	2:B:567:GLU:CD	2.16	0.51
3:C:194:GLU:OE1	3:C:194:GLU:HA	2.10	0.51
13:R:1:A:H3'	13:R:2:U:C5	2.46	0.51
2:B:629:ASP:C	2:B:629:ASP:OD1	2.50	0.51
2:B:341:LEU:O	2:B:341:LEU:CD2	2.58	0.51
2:B:484:ASN:OD1	2:B:484:ASN:C	2.54	0.51
1:A:376:TYR:C	1:A:376:TYR:CD2	2.89	0.50
1:A:461:LYS:HD3	1:A:461:LYS:O	2.11	0.50
3:C:29:MET:SD	3:C:29:MET:C	2.94	0.50
2:B:261:ARG:HD2	2:B:261:ARG:H	1.76	0.50
2:B:1019:SER:OG	2:B:1020:ARG:NH2	2.44	0.50
14:N:36:DA:C2	14:N:37:DG:C4	2.99	0.50
14:N:45:DG:H2''	14:N:46:DC:C5	2.47	0.50
1:A:205:GLU:CD	1:A:205:GLU:H	2.19	0.50
2:B:711:GLU:HB3	2:B:712:PRO:HD2	1.94	0.50
11:K:101:LEU:C	11:K:101:LEU:HD23	2.36	0.50
15:T:20:DT:H2'	15:T:21:DC:C6	2.46	0.50
1:A:569:LYS:HE2	1:A:569:LYS:HA	1.93	0.50
1:A:1386:ARG:HA	1:A:1390:ASN:HB3	1.94	0.50
2:B:28:GLU:OE1	2:B:28:GLU:N	2.37	0.50
2:B:519:TRP:O	2:B:519:TRP:CD2	2.64	0.50
1:A:567:LYS:O	1:A:569:LYS:N	2.45	0.49
5:E:172:GLU:C	5:E:172:GLU:OE1	2.55	0.49
2:B:596:LEU:HD23	2:B:596:LEU:C	2.37	0.49
7:G:126:ASN:HA	7:G:127:PRO:C	2.37	0.49
15:T:7:DG:H2'	15:T:8:DC:C6	2.47	0.49
2:B:368:GLU:OE1	2:B:368:GLU:N	2.35	0.49
3:C:143:LEU:HD23	3:C:143:LEU:C	2.37	0.49
14:N:38:DG:H2''	14:N:39:DA:C8	2.47	0.49
2:B:539:LEU:HD12	2:B:539:LEU:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:ASP:C	1:A:1198:ASP:OD1	2.56	0.49
9:I:98:VAL:O	9:I:98:VAL:HG13	2.12	0.49
8:H:43:ASN:OD1	8:H:43:ASN:O	2.30	0.49
11:K:79:GLU:H	11:K:79:GLU:CD	2.20	0.49
2:B:197:PHE:C	2:B:197:PHE:CD2	2.91	0.49
2:B:698:GLU:CD	2:B:698:GLU:C	2.80	0.49
1:A:1335:ILE:O	1:A:1339:LEU:N	2.46	0.49
1:A:196:GLU:O	1:A:197:PRO:C	2.56	0.48
1:A:551:TYR:C	1:A:551:TYR:HD2	2.19	0.48
2:B:215:GLN:HG2	2:B:499:ASN:HB2	1.95	0.48
2:B:1111:MET:SD	2:B:1111:MET:C	2.95	0.48
1:A:423:ASP:C	1:A:423:ASP:OD1	2.55	0.48
1:A:1221:LYS:N	1:A:1221:LYS:HD2	2.28	0.48
2:B:454:THR:OG1	2:B:455:SER:N	2.47	0.48
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.89	0.48
2:B:1112:GLN:O	2:B:1116:ARG:N	2.46	0.48
15:T:19:DA:H2''	15:T:20:DT:H73	1.95	0.48
1:A:69:THR:O	1:A:69:THR:CG2	2.59	0.48
2:B:37:PHE:CD1	2:B:37:PHE:C	2.82	0.48
7:G:127:PRO:O	7:G:129:SER:N	2.46	0.48
13:R:5:A:O2'	13:R:6:G:H5'	2.13	0.48
2:B:1162:ILE:HG23	2:B:1162:ILE:O	2.13	0.48
4:D:39:ASN:OD1	4:D:39:ASN:C	2.56	0.48
1:A:849:MET:SD	1:A:849:MET:C	2.97	0.48
1:A:1176:LEU:O	1:A:1177:LEU:CB	2.61	0.48
5:E:13:TRP:O	5:E:13:TRP:HD1	1.97	0.48
2:B:74:LEU:O	2:B:75:ALA:C	2.57	0.48
2:B:309:GLN:OE1	2:B:309:GLN:N	2.40	0.48
1:A:1405:THR:OG1	1:A:1406:VAL:N	2.47	0.48
2:B:31:TRP:O	2:B:811:TYR:OH	2.31	0.47
2:B:99:LYS:O	2:B:100:PRO:C	2.56	0.47
5:E:33:GLU:OE1	5:E:33:GLU:N	2.33	0.47
2:B:1163:CYS:SG	2:B:1165:ILE:HG22	2.53	0.47
3:C:193:TYR:CD1	3:C:193:TYR:C	2.92	0.47
9:I:101:PHE:HB2	9:I:110:PHE:HB2	1.95	0.47
2:B:618:ASP:OD1	2:B:618:ASP:C	2.58	0.47
2:B:1001:PHE:HD1	2:B:1001:PHE:O	1.97	0.47
1:A:552:TRP:HA	11:K:62:LYS:HD2	1.96	0.47
3:C:93:ASP:OD1	3:C:93:ASP:N	2.48	0.47
1:A:453:MET:O	1:A:454:SER:CB	2.63	0.47
11:K:39:ASP:OD1	11:K:39:ASP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:OE1	1:A:259:GLU:N	2.40	0.46
2:B:620:ARG:HB3	2:B:620:ARG:CZ	2.45	0.46
15:T:5:DC:C5	15:T:6:DT:C7	2.97	0.46
1:A:1329:THR:OG1	1:A:1330:ASN:N	2.48	0.46
3:C:217:ASP:OD1	3:C:217:ASP:C	2.55	0.46
13:R:4:G:H2'	13:R:5:A:C8	2.49	0.46
3:C:35:ARG:NH1	11:K:40:HIS:NE2	2.62	0.46
2:B:641:GLU:O	2:B:642:ASP:CB	2.64	0.46
5:E:78:LEU:C	5:E:78:LEU:HD23	2.40	0.46
5:E:208:TYR:O	5:E:208:TYR:HD2	1.93	0.46
1:A:1323:ASP:OD1	1:A:1323:ASP:C	2.59	0.46
2:B:1001:PHE:CD1	2:B:1001:PHE:O	2.69	0.46
15:T:31:DG:H2''	15:T:32:DC:OP2	2.14	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.97	0.46
1:A:496:GLU:CD	1:A:496:GLU:N	2.74	0.46
1:A:1155:ASP:OD1	1:A:1155:ASP:C	2.55	0.46
5:E:13:TRP:O	5:E:13:TRP:CD1	2.68	0.46
8:H:59:ILE:O	8:H:60:ALA:C	2.59	0.46
6:F:111:LEU:HD23	6:F:111:LEU:C	2.41	0.45
8:H:38:LEU:C	8:H:38:LEU:HD23	2.41	0.45
1:A:344:ARG:HD3	1:A:344:ARG:N	2.30	0.45
2:B:1017:ILE:N	2:B:1018:PRO:CD	2.79	0.45
8:H:39:THR:O	8:H:123:MET:HG3	2.16	0.45
2:B:580:VAL:HA	2:B:624:LEU:HB3	1.99	0.45
2:B:592:ASN:OD1	2:B:592:ASN:O	2.34	0.45
3:C:89:GLU:O	3:C:90:ASP:CB	2.64	0.45
4:D:220:LEU:O	4:D:221:TYR:C	2.59	0.45
15:T:5:DC:C2	15:T:6:DT:C5	3.05	0.45
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.98	0.45
5:E:69:ILE:HB	5:E:73:PRO:HA	1.98	0.45
9:I:17:ARG:HG3	9:I:28:GLU:HB3	1.98	0.45
15:T:24:DC:H5''	15:T:24:DC:H6	1.82	0.45
15:T:29:DT:OP2	15:T:29:DT:H3'	2.16	0.45
1:A:107:CYS:SG	1:A:148:CYS:SG	3.11	0.45
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.99	0.45
2:B:1032:SER:OG	2:B:1033:LYS:N	2.50	0.45
3:C:61:GLU:OE1	3:C:61:GLU:N	2.35	0.45
3:C:73:GLN:N	3:C:131:HIS:O	2.44	0.45
1:A:311:GLN:HB3	1:A:312:PRO:HD3	1.97	0.45
1:A:635:ARG:NH1	1:A:877:HIS:ND1	2.63	0.45
1:A:1119:TYR:CD1	1:A:1119:TYR:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:GLU:OE1	2:B:150:GLU:N	2.36	0.45
5:E:13:TRP:CD1	5:E:13:TRP:C	2.94	0.45
6:F:77:ASP:C	6:F:77:ASP:OD1	2.60	0.45
1:A:453:MET:O	1:A:454:SER:HB3	2.16	0.45
3:C:178:PHE:CD1	3:C:178:PHE:C	2.95	0.45
7:G:131:GLN:O	7:G:131:GLN:CD	2.58	0.45
15:T:13:DT:H2''	15:T:14:DC:H6	1.81	0.45
2:B:302:CYS:O	2:B:302:CYS:SG	2.75	0.45
2:B:734:HIS:O	2:B:735:ALA:C	2.60	0.45
8:H:55:LEU:C	8:H:55:LEU:HD12	2.41	0.45
1:A:230:ARG:HB3	1:A:231:PRO:HD2	1.99	0.44
2:B:936:ASP:OD1	2:B:936:ASP:C	2.58	0.44
3:C:4:GLU:HA	11:K:97:LYS:HG3	1.99	0.44
3:C:169:LYS:N	3:C:169:LYS:CD	2.80	0.44
2:B:552:MET:HB3	2:B:553:PRO:HD3	1.99	0.44
4:D:206:GLU:OE1	4:D:206:GLU:HA	2.17	0.44
3:C:22:LEU:N	3:C:22:LEU:HD12	2.32	0.44
5:E:29:PHE:CD2	5:E:29:PHE:O	2.70	0.44
1:A:67:CYS:SG	1:A:67:CYS:O	2.74	0.44
2:B:1082:MET:SD	2:B:1082:MET:C	3.01	0.44
1:A:1263:ILE:O	1:A:1267:MET:N	2.49	0.44
2:B:264:SER:OG	2:B:265:SER:N	2.50	0.44
4:D:52:LEU:HD23	4:D:52:LEU:C	2.42	0.44
15:T:19:DA:C2'	15:T:20:DT:C7	2.95	0.44
1:A:109:HIS:H	1:A:213:HIS:HE2	1.65	0.44
1:A:483:ASP:C	1:A:483:ASP:OD1	2.59	0.44
1:A:1391:ARG:O	1:A:1391:ARG:HG2	2.17	0.44
13:R:1:A:H2'	13:R:2:U:H5'	1.99	0.44
7:G:30:LEU:C	7:G:30:LEU:HD23	2.42	0.44
1:A:451:HIS:N	1:A:451:HIS:CD2	2.84	0.44
8:H:93:TYR:CD1	8:H:93:TYR:C	2.95	0.44
10:J:5:VAL:O	10:J:6:ARG:HB2	2.18	0.44
13:R:2:U:C5	13:R:2:U:OP2	2.71	0.43
15:T:16:DC:C4	15:T:17:DC:N4	2.85	0.43
15:T:34:DA:H2''	15:T:35:DT:C5	2.52	0.43
1:A:34:LYS:O	1:A:36:ARG:NH1	2.52	0.43
1:A:1189:SER:HB2	1:A:1190:PRO:HD2	1.99	0.43
2:B:134:LYS:N	2:B:134:LYS:HD3	2.32	0.43
4:D:19:GLU:O	4:D:20:GLU:HB2	2.18	0.43
2:B:292:ILE:HB	2:B:293:PRO:HD3	2.01	0.43
5:E:24:LYS:HB3	5:E:30:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:959:ASP:OD1	2:B:959:ASP:C	2.56	0.43
5:E:143:ASN:O	5:E:146:HIS:ND1	2.51	0.43
13:R:6:G:H2'	13:R:7:A:C8	2.53	0.43
15:T:16:DC:C2	15:T:17:DC:C4	3.07	0.43
1:A:105:CYS:HB3	1:A:142:CYS:SG	2.58	0.43
1:A:399:HIS:N	1:A:400:PRO:HD2	2.33	0.43
2:B:567:GLU:OE1	2:B:567:GLU:N	2.46	0.43
2:B:1145:SER:OG	2:B:1146:PHE:N	2.51	0.43
8:H:146:ARG:OXT	8:H:146:ARG:HG3	2.18	0.43
1:A:65:LEU:O	1:A:66:LYS:C	2.61	0.43
2:B:124:TYR:HB2	2:B:204:ILE:HB	2.01	0.43
2:B:729:ILE:O	2:B:729:ILE:HG23	2.17	0.43
2:B:764:SER:O	2:B:765:PRO:C	2.61	0.43
2:B:1111:MET:SD	2:B:1116:ARG:HA	2.59	0.43
3:C:82:TYR:CE1	3:C:162:GLY:HA2	2.53	0.43
5:E:55:ARG:HD3	5:E:82:PHE:CE2	2.54	0.43
8:H:115:TYR:N	8:H:115:TYR:CD1	2.86	0.43
13:R:1:A:OP2	13:R:1:A:C8	2.71	0.43
2:B:47:GLN:CD	2:B:47:GLN:N	2.77	0.43
2:B:420:LEU:HD23	2:B:420:LEU:C	2.42	0.43
2:B:995:ARG:HD3	2:B:995:ARG:HA	1.86	0.43
5:E:33:GLU:H	5:E:33:GLU:CD	2.22	0.43
5:E:111:VAL:HA	5:E:135:PHE:O	2.18	0.43
1:A:868:TYR:O	1:A:868:TYR:HD2	2.01	0.42
2:B:37:PHE:O	2:B:41:LYS:N	2.51	0.42
2:B:519:TRP:CD2	2:B:519:TRP:C	2.94	0.42
2:B:1158:PHE:N	2:B:1196:ILE:O	2.51	0.42
3:C:1:MET:SD	11:K:48:ALA:O	2.77	0.42
7:G:143:ILE:HG23	7:G:143:ILE:O	2.19	0.42
8:H:82:PRO:O	8:H:83:GLN:C	2.62	0.42
2:B:844:SER:O	2:B:848:ARG:HG2	2.19	0.42
2:B:863:GLU:HB2	2:B:962:LYS:HB3	2.01	0.42
3:C:173:ALA:HA	3:C:234:SER:HA	2.01	0.42
1:A:23:SER:O	1:A:26:GLU:N	2.52	0.42
1:A:1285:MET:O	1:A:1285:MET:SD	2.77	0.42
15:T:13:DT:H2''	15:T:14:DC:C6	2.54	0.42
1:A:50:ILE:HB	1:A:53:LEU:O	2.18	0.42
1:A:632:VAL:O	1:A:635:ARG:HB3	2.18	0.42
1:A:862:ASN:HA	5:E:174:GLN:HA	2.01	0.42
9:I:118:ARG:HA	9:I:118:ARG:NE	2.34	0.42
10:J:2:ILE:O	10:J:3:VAL:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:CYS:SG	12:L:51:CYS:SG	3.17	0.42
1:A:1086:PHE:O	1:A:1086:PHE:HD1	2.02	0.42
1:A:1245:PRO:HA	1:A:1249:ASP:HB3	2.01	0.42
2:B:841:MET:SD	2:B:1010:LEU:HD13	2.59	0.42
3:C:26:ASP:C	3:C:26:ASP:OD1	2.62	0.42
5:E:203:GLU:OE1	5:E:203:GLU:HA	2.19	0.42
1:A:55:ASP:OD1	1:A:55:ASP:C	2.62	0.42
1:A:25:GLU:CD	1:A:25:GLU:H	2.26	0.42
2:B:790:ASP:C	2:B:790:ASP:OD1	2.60	0.42
2:B:842:ASN:OD1	2:B:842:ASN:C	2.62	0.42
15:T:16:DC:C2	15:T:17:DC:N4	2.87	0.42
1:A:567:LYS:HB2	1:A:567:LYS:HE2	1.84	0.42
2:B:503:GLY:O	2:B:504:ARG:HB2	2.20	0.42
2:B:847:ASP:O	3:C:169:LYS:NZ	2.53	0.42
2:B:1017:ILE:O	2:B:1018:PRO:C	2.63	0.42
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.83	0.42
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.20	0.42
2:B:817:LEU:N	2:B:818:PRO:HD3	2.35	0.42
4:D:24:ALA:HA	7:G:83:LYS:HB3	2.02	0.42
2:B:552:MET:SD	2:B:552:MET:C	3.03	0.42
4:D:212:LYS:HA	4:D:212:LYS:HD3	1.78	0.42
14:N:44:DA:H2''	14:N:45:DG:C8	2.55	0.42
1:A:1171:GLN:C	1:A:1171:GLN:CD	2.88	0.41
2:B:262:GLU:OE1	2:B:262:GLU:N	2.44	0.41
2:B:579:ARG:N	2:B:579:ARG:HD2	2.35	0.41
4:D:39:ASN:HB2	7:G:6:ASP:HB3	2.02	0.41
8:H:1:MET:HB3	8:H:62:SER:O	2.19	0.41
9:I:101:PHE:CD1	9:I:101:PHE:N	2.88	0.41
1:A:507:VAL:HB	1:A:508:PRO:HD3	2.01	0.41
1:A:1281:ARG:CZ	1:A:1281:ARG:HB2	2.50	0.41
2:B:860:MET:SD	2:B:860:MET:N	2.93	0.41
2:B:917:PRO:O	2:B:918:ILE:C	2.61	0.41
4:D:72:ARG:HA	4:D:72:ARG:NE	2.35	0.41
11:K:5:ASP:C	11:K:5:ASP:OD1	2.62	0.41
14:N:32:DG:H2''	14:N:33:DA:OP2	2.19	0.41
1:A:858:ASN:OD1	1:A:858:ASN:C	2.59	0.41
1:A:974:ASP:OD1	1:A:974:ASP:C	2.63	0.41
10:J:6:ARG:HA	10:J:12:LYS:O	2.20	0.41
2:B:825:VAL:HG12	2:B:1010:LEU:HB3	2.02	0.41
3:C:75:MET:SD	3:C:75:MET:N	2.87	0.41
6:F:103:MET:SD	7:G:15:PRO:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:39:DA:H2''	14:N:40:DG:H8	1.85	0.41
1:A:791:ASP:C	1:A:791:ASP:OD1	2.63	0.41
3:C:127:ARG:O	3:C:127:ARG:CG	2.69	0.41
15:T:19:DA:C2'	15:T:20:DT:H72	2.51	0.41
2:B:304:ASP:OD1	2:B:304:ASP:C	2.64	0.41
13:R:6:G:H2'	13:R:7:A:H8	1.85	0.41
1:A:179:LEU:HD13	1:A:179:LEU:HA	1.91	0.41
2:B:370:PHE:HA	2:B:374:LYS:HB2	2.02	0.41
2:B:401:PHE:HB3	2:B:517:THR:HB	2.03	0.41
2:B:716:ASN:OD1	2:B:716:ASN:C	2.64	0.41
2:B:916:THR:O	2:B:935:ARG:N	2.54	0.41
14:N:15:DA:H61	15:T:33:DT:H3	1.69	0.41
1:A:14:VAL:HA	2:B:1218:THR:HA	2.03	0.41
1:A:709:THR:O	1:A:710:LEU:C	2.62	0.41
1:A:1453:TYR:CE1	6:F:131:PRO:HA	2.56	0.41
2:B:342:GLY:O	2:B:343:ILE:C	2.64	0.41
2:B:918:ILE:O	2:B:918:ILE:CG2	2.68	0.41
5:E:208:TYR:O	5:E:208:TYR:CG	2.69	0.41
6:F:135:ARG:HG3	6:F:143:PHE:HB2	2.01	0.41
1:A:1185:PHE:O	1:A:1186:ASP:C	2.64	0.41
2:B:350:GLN:CD	2:B:350:GLN:C	2.89	0.41
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	2.03	0.41
2:B:931:TYR:O	2:B:931:TYR:CD1	2.74	0.41
5:E:143:ASN:C	5:E:143:ASN:OD1	2.63	0.40
11:K:46:ILE:O	11:K:49:GLU:HG2	2.22	0.40
11:K:82:ASP:HA	11:K:83:PRO:HD3	1.93	0.40
1:A:174:ILE:HG23	1:A:181:LEU:HB3	2.03	0.40
1:A:414:ASP:C	1:A:414:ASP:OD1	2.63	0.40
1:A:476:SER:HB3	1:A:477:PRO:CD	2.51	0.40
1:A:784:LEU:HB3	1:A:785:PRO:HD2	2.02	0.40
1:A:813:PHE:CD2	1:A:813:PHE:C	2.99	0.40
2:B:151:LEU:O	2:B:154:GLU:HB3	2.21	0.40
11:K:94:ILE:O	11:K:97:LYS:HB3	2.21	0.40
2:B:618:ASP:HB3	2:B:623:GLU:HB2	2.04	0.40
5:E:66:GLU:C	5:E:66:GLU:CD	2.89	0.40
1:A:1208:THR:O	1:A:1208:THR:HG23	2.21	0.40
2:B:1148:LYS:HA	2:B:1151:LEU:HB3	2.04	0.40
8:H:143:LEU:HD23	8:H:143:LEU:C	2.46	0.40
1:A:186:LYS:O	1:A:187:LYS:C	2.64	0.40
4:D:5:THR:OG1	4:D:6:SER:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1453/1733 (84%)	1292 (89%)	137 (9%)	24 (2%)	7	36
2	B	1205/1224 (98%)	1089 (90%)	90 (8%)	26 (2%)	5	29
3	C	268/318 (84%)	232 (87%)	28 (10%)	8 (3%)	3	22
4	D	171/221 (77%)	157 (92%)	12 (7%)	2 (1%)	10	43
5	E	213/215 (99%)	190 (89%)	15 (7%)	8 (4%)	2	19
6	F	79/155 (51%)	73 (92%)	6 (8%)	0	100	100
7	G	169/171 (99%)	153 (90%)	12 (7%)	4 (2%)	4	27
8	H	144/146 (99%)	118 (82%)	23 (16%)	3 (2%)	5	30
9	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	7	36
10	J	68/70 (97%)	59 (87%)	5 (7%)	4 (6%)	1	13
11	K	109/120 (91%)	103 (94%)	4 (4%)	2 (2%)	6	34
12	L	44/70 (63%)	35 (80%)	7 (16%)	2 (4%)	2	16
All	All	4043/4565 (89%)	3603 (89%)	355 (9%)	85 (2%)	8	30

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	66	LYS
1	A	119	ASN
1	A	186	LYS
1	A	250	ILE
1	A	321	PRO
1	A	568	PRO
1	A	593	GLU
1	A	1177	LEU
2	B	100	PRO
2	B	642	ASP
2	B	711	GLU

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Mol	Chain	Res	Type
2	B	725	PRO
2	B	1018	PRO
2	B	1214	PRO
3	C	90	ASP
3	C	172	PRO
5	E	128	PRO
7	G	22	MET
9	I	62	ILE
11	K	41	THR
1	A	164	ARG
1	A	317	LYS
1	A	408	ASP
1	A	454	SER
1	A	871	ASP
2	B	44	VAL
2	B	75	ALA
2	B	201	GLY
2	B	712	PRO
2	B	735	ALA
3	C	105	GLY
3	C	184	ASN
7	G	128	PRO
8	H	67	ASP
8	H	83	GLN
9	I	93	LYS
10	J	65	PRO
1	A	197	PRO
1	A	224	PHE
1	A	833	GLU
2	B	575	PRO
2	B	986	GLN
3	C	93	ASP
4	D	8	PHE
5	E	29	PHE
5	E	45	LYS
7	G	20	PRO
7	G	57	GLN
8	H	61	SER
10	J	26	GLN
11	K	3	ALA
1	A	1087	ALA
2	B	143	PRO

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Mol	Chain	Res	Type
2	B	264	SER
2	B	362	PRO
2	B	511	PRO
2	B	636	PRO
2	B	819	ALA
5	E	38	PRO
5	E	151	PRO
12	L	59	ALA
1	A	35	ILE
1	A	248	PRO
1	A	1271	ILE
2	B	437	GLU
2	B	612	GLU
2	B	1097	HIS
3	C	138	GLU
4	D	20	GLU
5	E	74	ASP
5	E	86	PRO
10	J	2	ILE
12	L	56	LEU
2	B	580	VAL
2	B	724	ASP
2	B	301	ILE
10	J	15	GLY
1	A	55	ASP
1	A	158	PRO
1	A	780	VAL
2	B	765	PRO
3	C	6	PRO
3	C	182	PRO
5	E	73	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1271/1520 (84%)	1271 (100%)	0	100	100
2	B	1046/1061 (99%)	1046 (100%)	0	100	100
3	C	238/274 (87%)	238 (100%)	0	100	100
4	D	157/200 (78%)	157 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	72/137 (53%)	72 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	128/128 (100%)	128 (100%)	0	100	100
9	I	116/116 (100%)	116 (100%)	0	100	100
10	J	65/65 (100%)	65 (100%)	0	100	100
11	K	96/102 (94%)	96 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3578/4009 (89%)	3578 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	447	GLN
1	A	1052	GLN
1	A	1188	GLN
1	A	1367	HIS
2	B	83	ASN
2	B	325	GLN
2	B	518	HIS
2	B	1093	GLN
3	C	231	ASN
5	E	61	GLN
5	E	113	GLN
9	I	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U
13	R	3	C

There are no RNA pucker outliers to report.

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](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

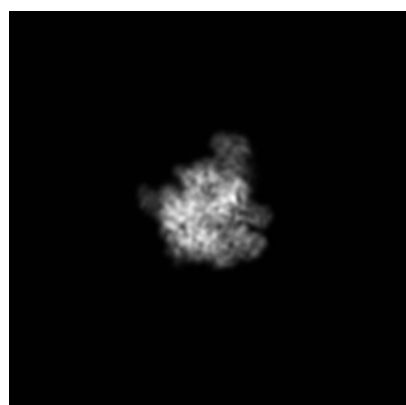
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8737. These allow visual inspection of the internal detail of the map and identification of artifacts.

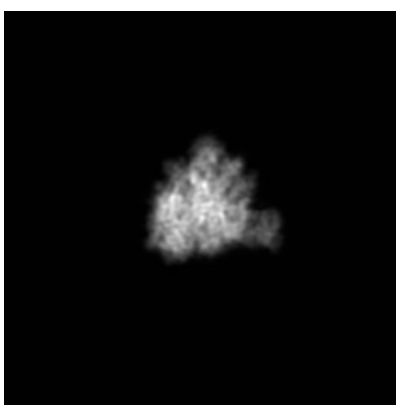
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

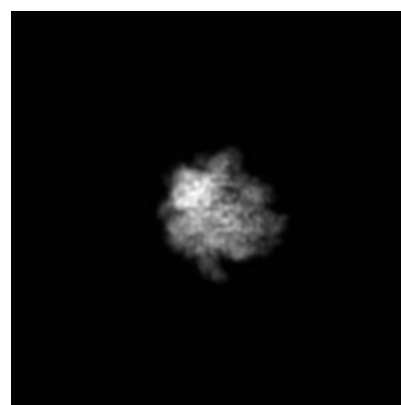
6.1.1 Primary map



X



Y

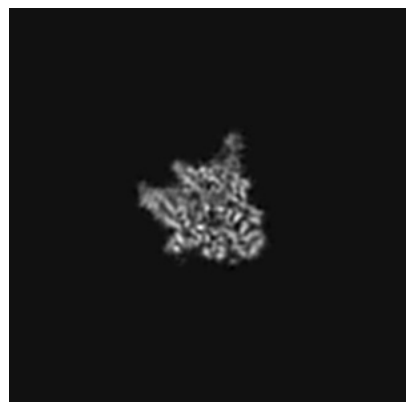


Z

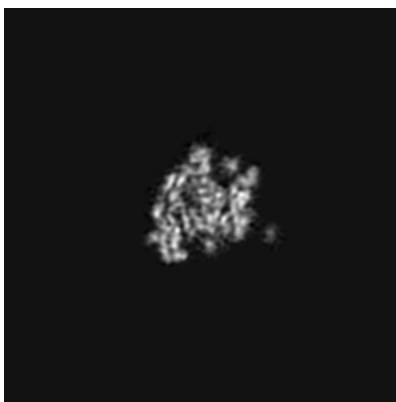
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

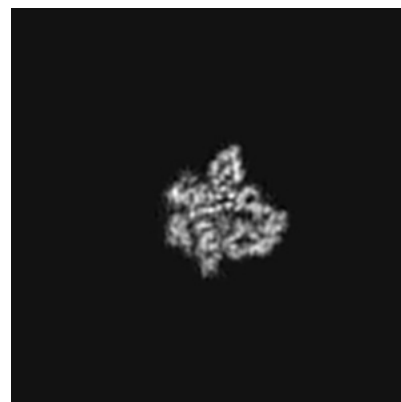
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

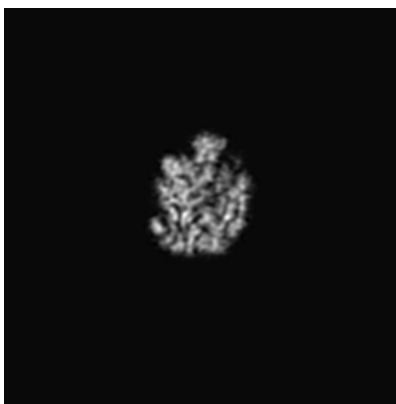
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

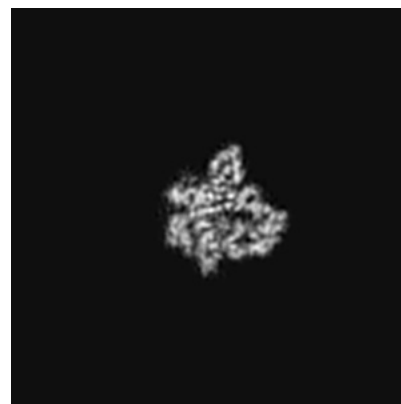
6.3.1 Primary map



X Index: 185



Y Index: 173

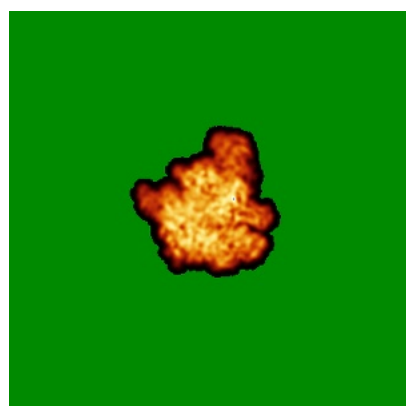


Z Index: 191

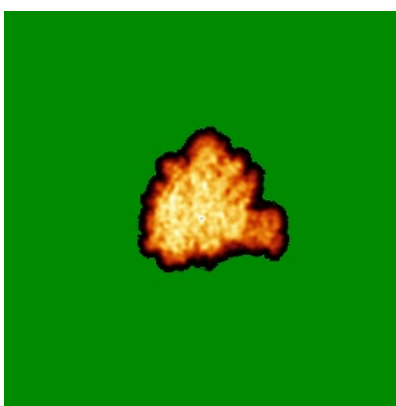
The images above show the largest variance slices of the map in three orthogonal directions.

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

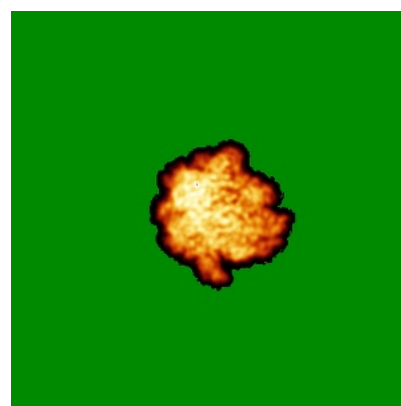
6.4.1 Primary map



X



Y

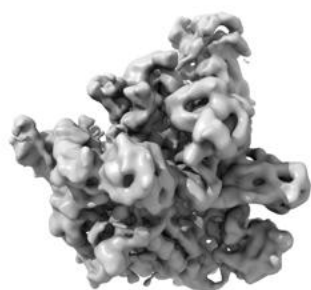


Z

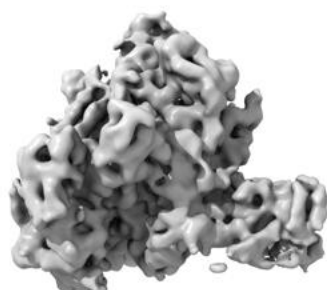
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

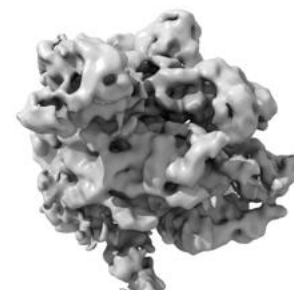
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

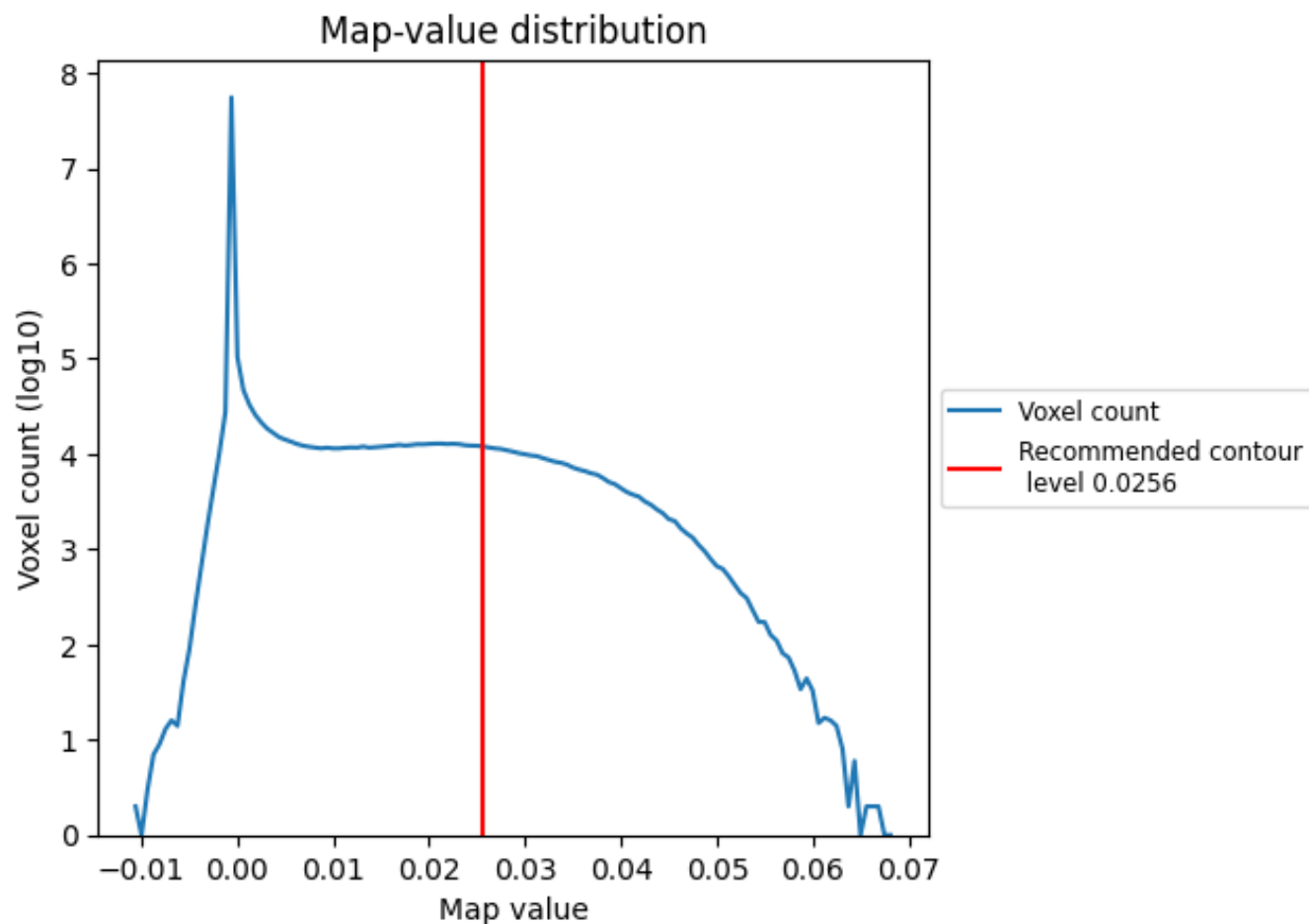
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

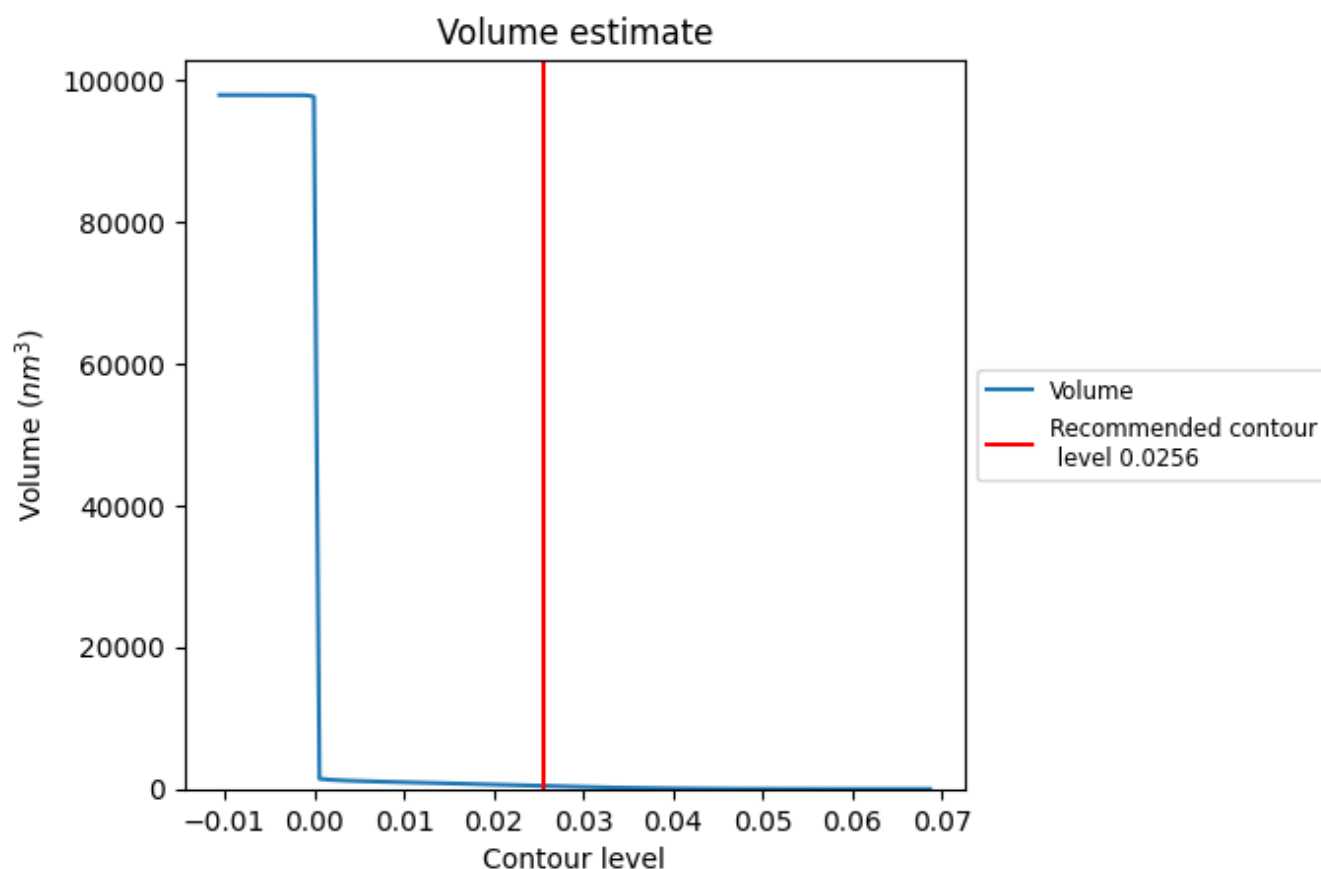
This section contains the results of statistical analysis of the map.

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.

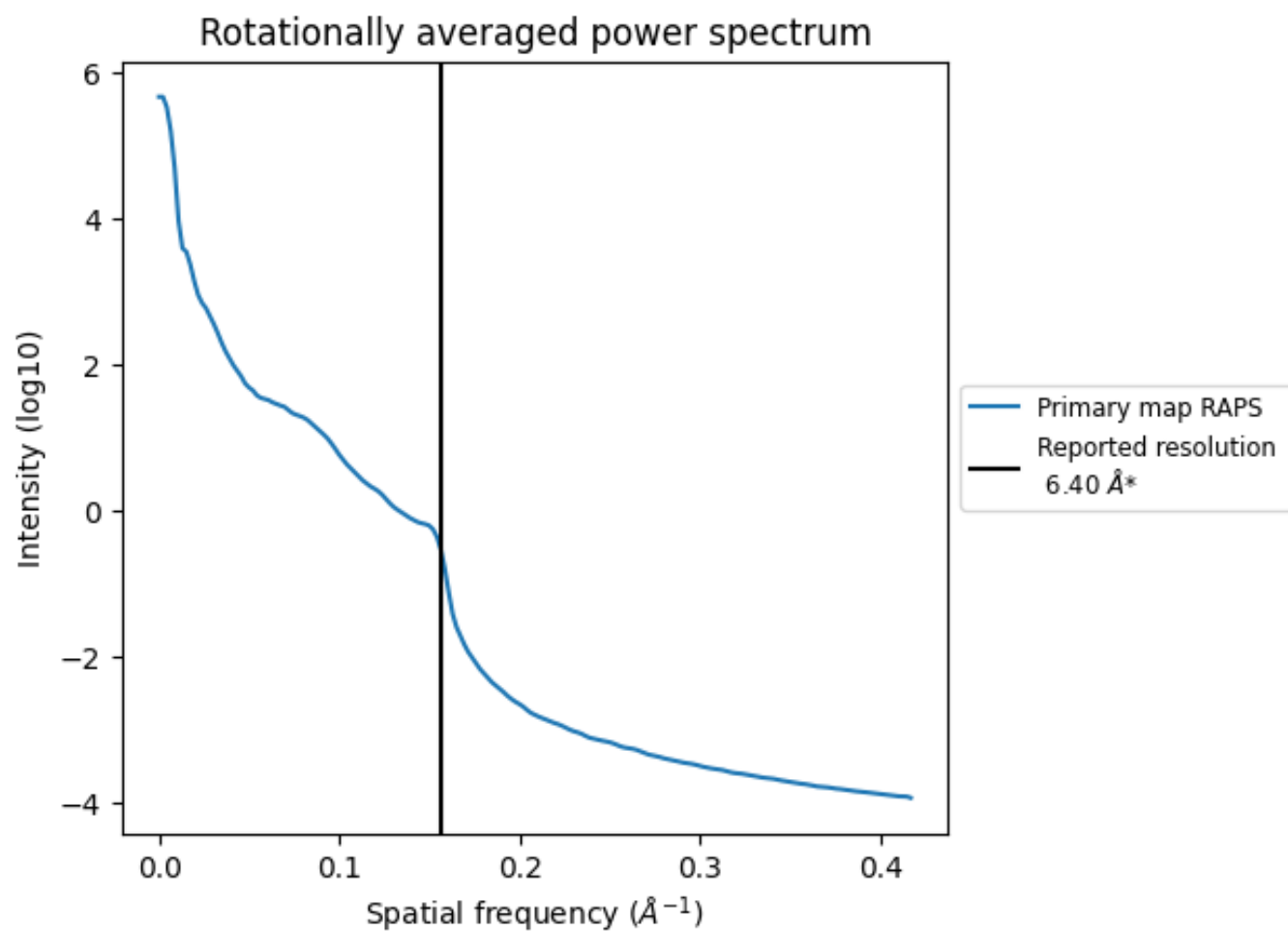
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm^3 ; this corresponds to an approximate mass of 375 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 ⓘ

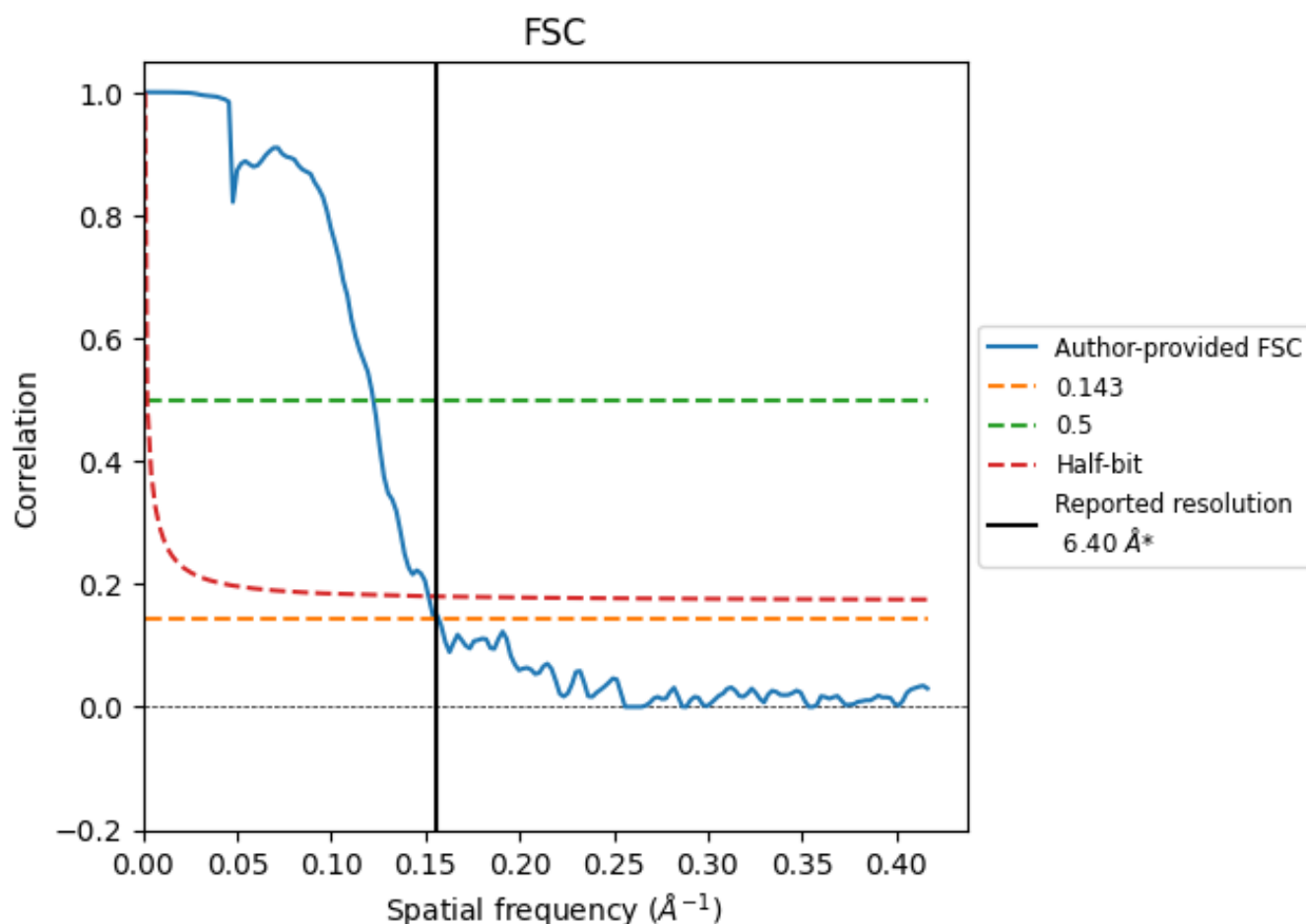


*Reported resolution corresponds to spatial frequency of 0.156 Å⁻¹

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 0.156 Å⁻¹

8.2 Resolution estimates [i](#)

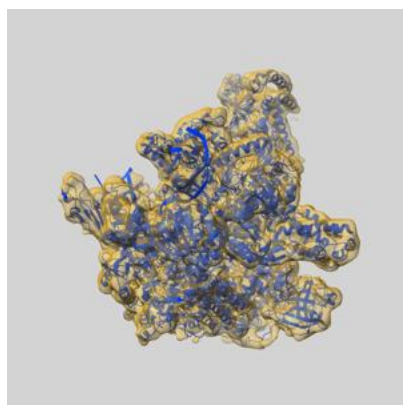
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	6.37	8.18	6.60
Unmasked-calculated*	-	-	-

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

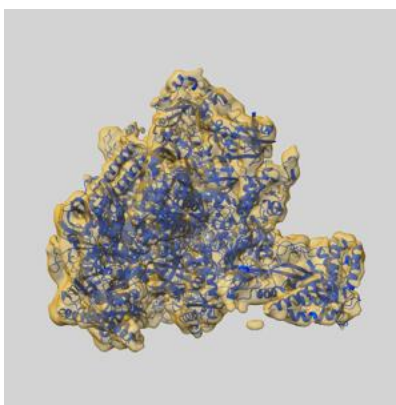
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8737 and PDB model 5VVS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

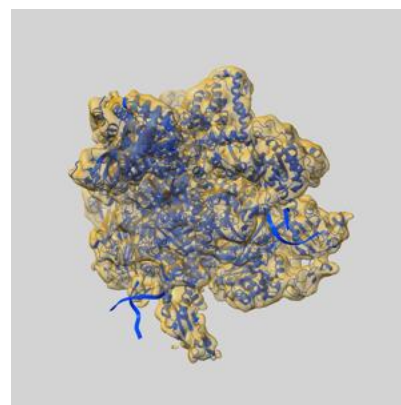
9.1 Map-model overlay [i](#)



X



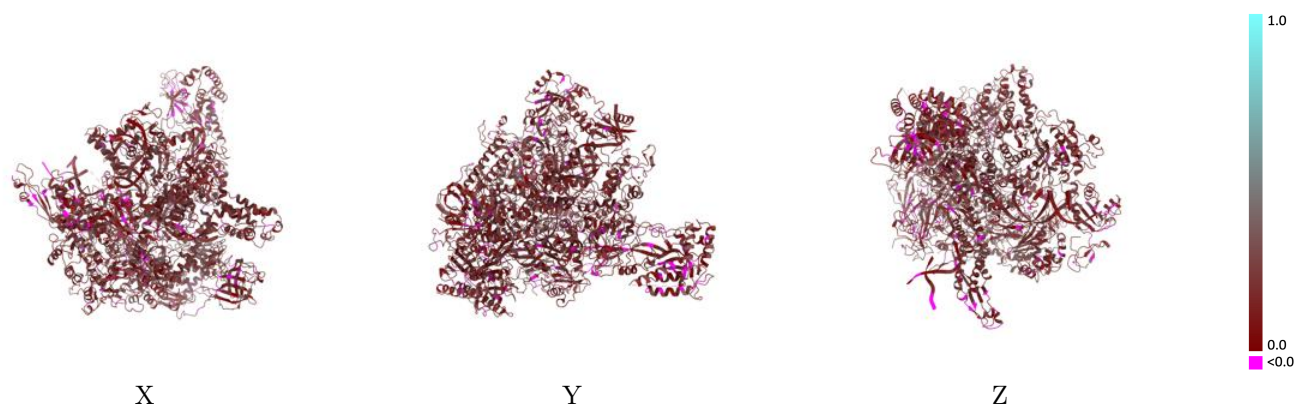
Y



Z

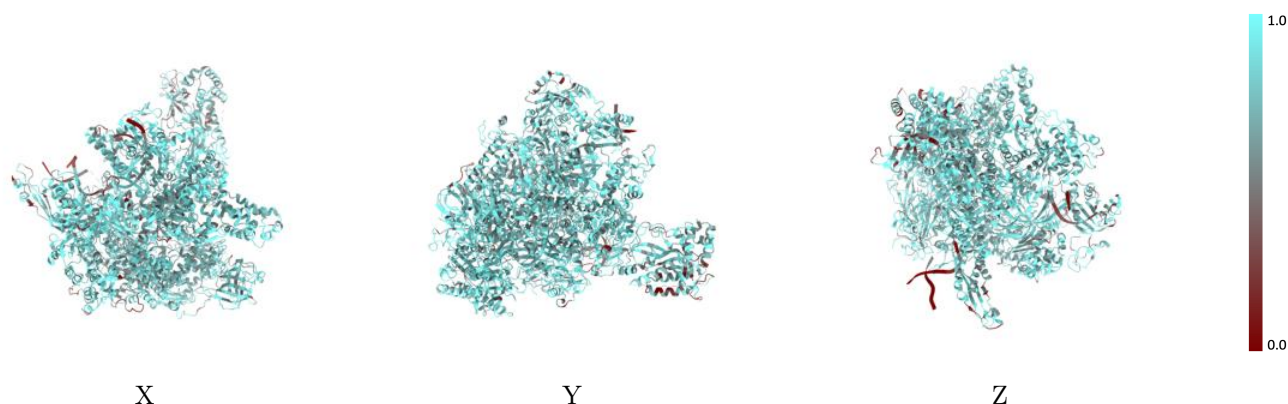
The images above show the 3D surface view of the map at the recommended contour level 0.0256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



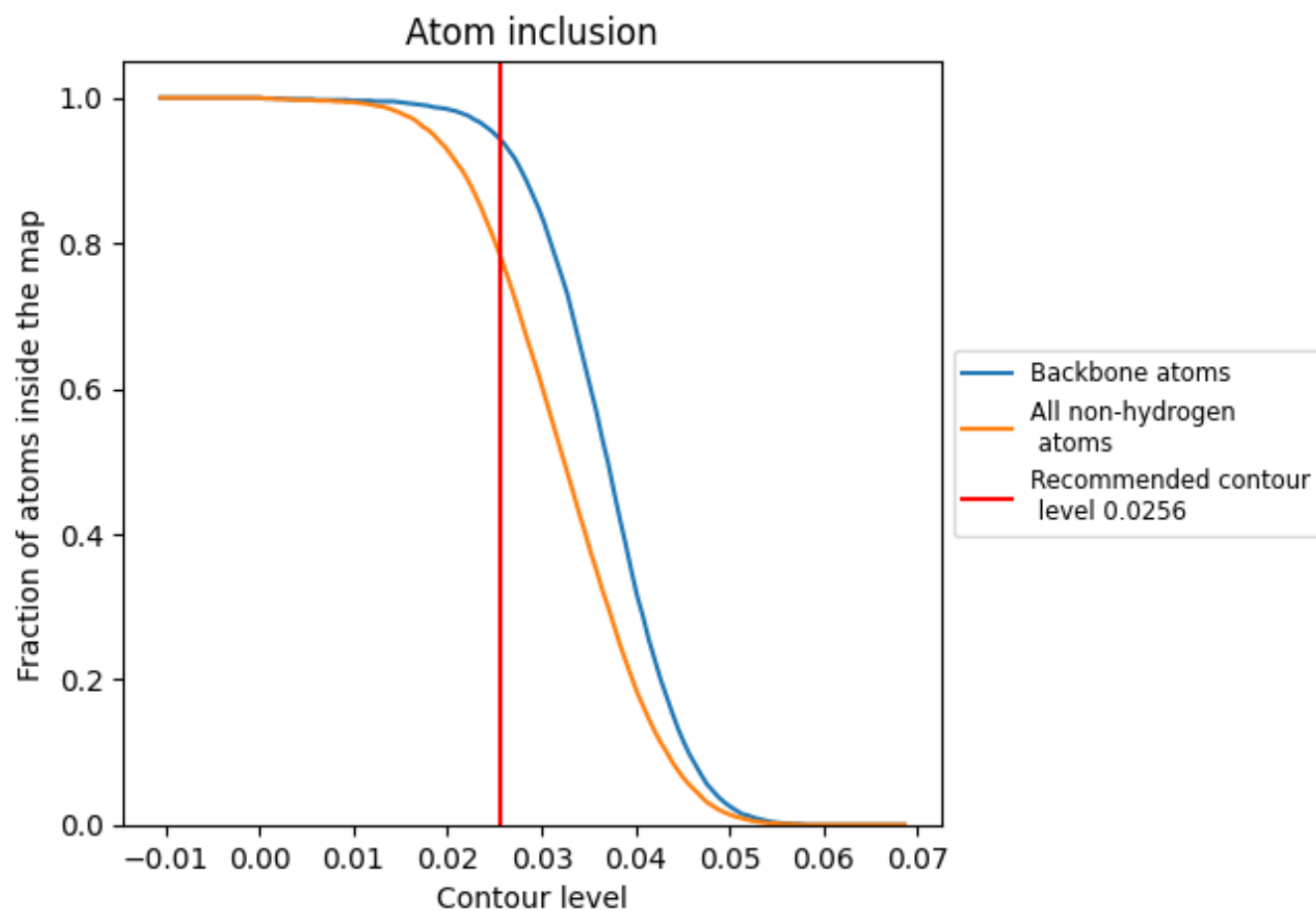
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0256).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 78% 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 (0.0256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.1840
A	0.7930	0.1910
B	0.7850	0.1810
C	0.8260	0.1890
D	0.6960	0.1650
E	0.8360	0.1970
F	0.8310	0.1990
G	0.6880	0.1490
H	0.7830	0.1800
I	0.8090	0.1830
J	0.8110	0.1680
K	0.8310	0.1880
L	0.8410	0.1790
N	0.5800	0.1550
R	0.8100	0.2170
T	0.6240	0.1620

1.0

0.0

<0.0