



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:57 AM UTC

PDB ID : 8W9Z / pdb_00008w9z
EMDB ID : EMD-37386
Title : The cryo-EM structure of the Nicotiana tabacum PEP-PAP
Authors : Wu, X.X.; Zhang, Y.
Deposited on : 2023-09-06
Resolution : 3.00 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:

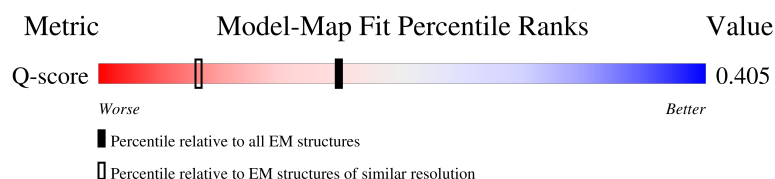
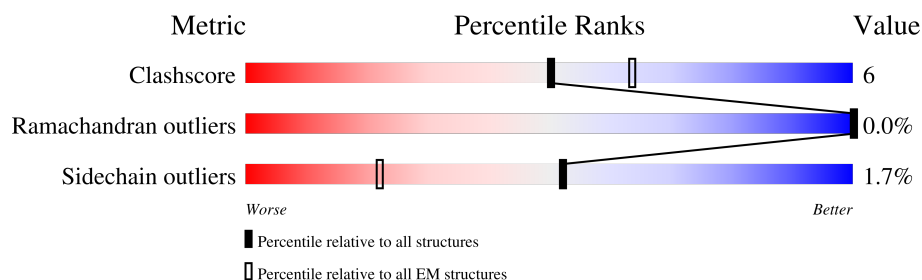
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



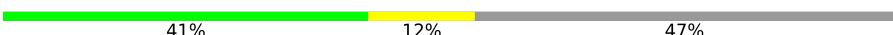
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	337	
1	a	337	
2	B	1070	
3	C	688	

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Mol	Chain	Length	Quality of chain
4	c	1388	
5	D	892	
6	E	860	
7	F	682	
8	G	266	
9	H	531	
10	I	486	
11	i	648	
12	J	507	
13	K	331	
14	L	303	
15	M	178	
15	m	178	
16	N	770	
17	O	167	
18	P	143	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 60525 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 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	293	Total	C	N	O	S	0	0
			2202	1397	382	411	12		
1	a	318	Total	C	N	O	S	0	0
			2441	1555	424	452	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	909	Total	C	N	O	S	0	0
			6820	4328	1216	1253	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	592	Total	C	N	O	S	0	0
			4431	2832	783	799	17		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta”.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	1174	Total	C	N	O	S	0	0
			8086	5072	1482	1503	29		

- Molecule 5 is a protein called PAP1(pTAC3).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	645	Total	C	N	O	S	0	0
			5088	3228	878	956	26		

- Molecule 6 is a protein called Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	700	Total	C	N	O	S	0	0
			4534	2823	822	866	23		

- Molecule 7 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	544	Total	C	N	O	S	0	0
			4233	2678	756	780	19		

- Molecule 8 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	218	Total	C	N	O	S	0	0
			1727	1122	291	309	5		

- Molecule 9 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	260	Total	C	N	O	S	0	0
			2110	1338	371	393	8		

- Molecule 10 is a protein called Fructokinase-like 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	374	Total	C	N	O	S	0	0
			2897	1856	512	517	12		

- Molecule 11 is a protein called Fructokinase-like 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	383	Total	C	N	O	S	0	0
			2983	1902	508	557	16		

- Molecule 12 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	422	Total	C	N	O	S	0	0
			3368	2157	578	612	21		

- Molecule 13 is a protein called PAP8(pTAC6).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	214	Total	C	N	O	S	0	0
			1779	1127	307	337	8		

- Molecule 14 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	234	Total	C	N	O	S	0	0
			1475	943	261	270	1		

- Molecule 15 is a protein called Thioredoxin-like protein CITRX1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	116	Total	C	N	O	S	0	0
			935	598	150	180	7		
15	m	109	Total	C	N	O	S	0	0
			851	545	135	164	7		

- Molecule 16 is a protein called UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	537	Total	C	N	O	S	0	0
			2982	1814	579	583	6		

- Molecule 17 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	88	Total	C	N	O	S	0	0
			692	434	124	131	3		

- Molecule 18 is a protein called PAP13(pTAC18).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	105	Total	C	N	O	S	0	0
			887	576	148	158	5		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Zn	0
			1	1	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total 1	Mg 1	0

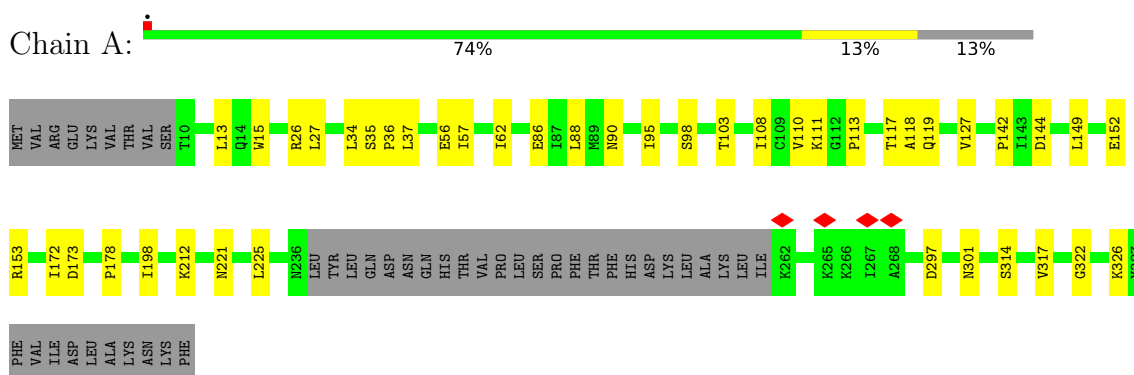
- Molecule 21 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
21	G	1	Total 1	Fe 1	0
21	L	1	Total 1	Fe 1	0

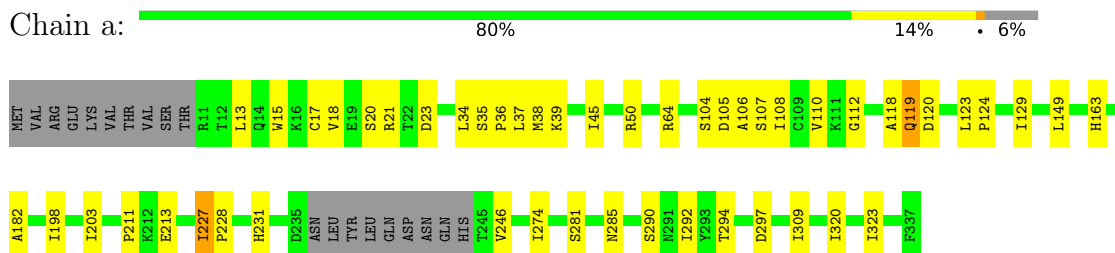
3 Residue-property plots

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.

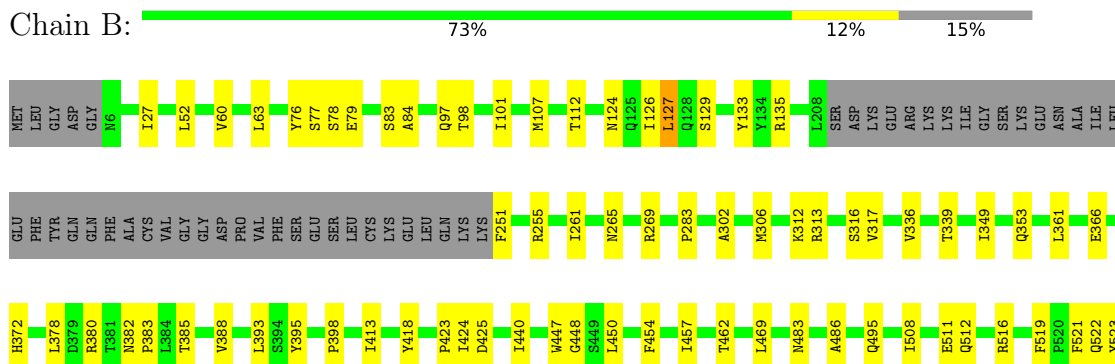
- Molecule 1: DNA-directed RNA polymerase subunit alpha

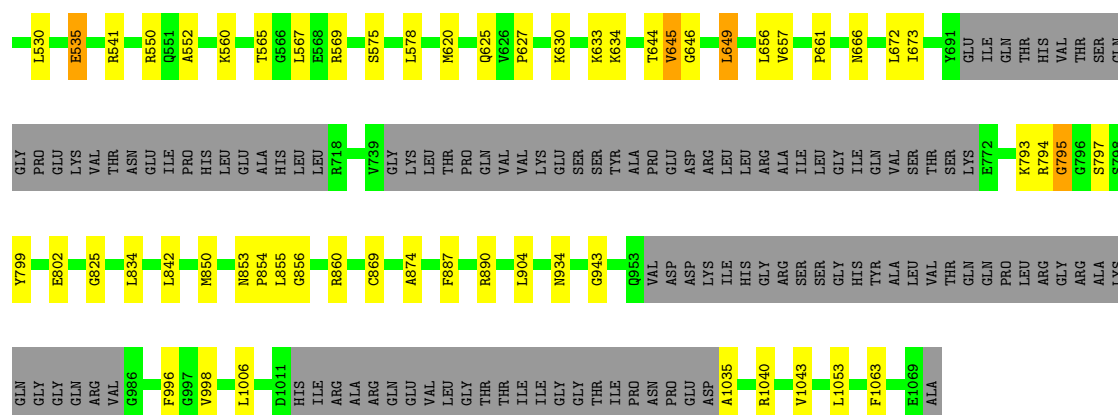


- Molecule 1: DNA-directed RNA polymerase subunit alpha



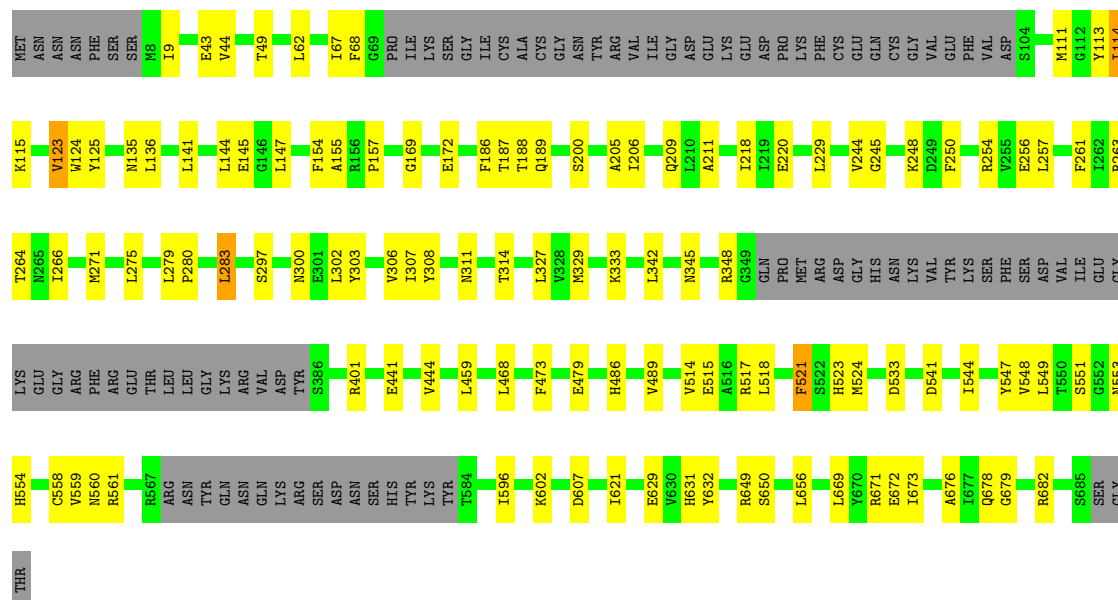
- Molecule 2: DNA-directed RNA polymerase subunit beta





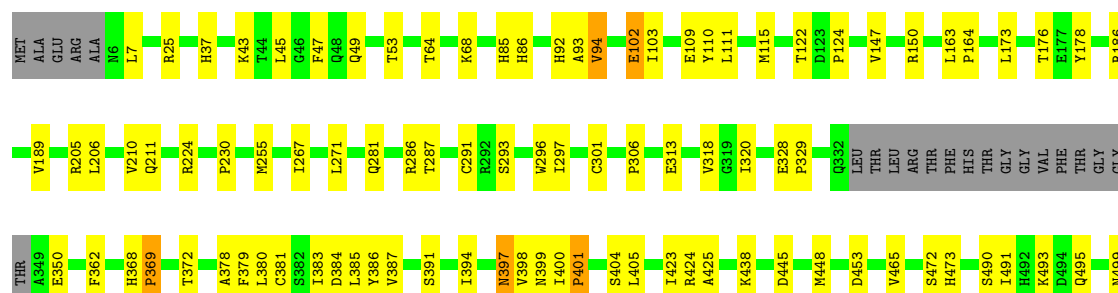
• Molecule 3: DNA-directed RNA polymerase subunit gamma

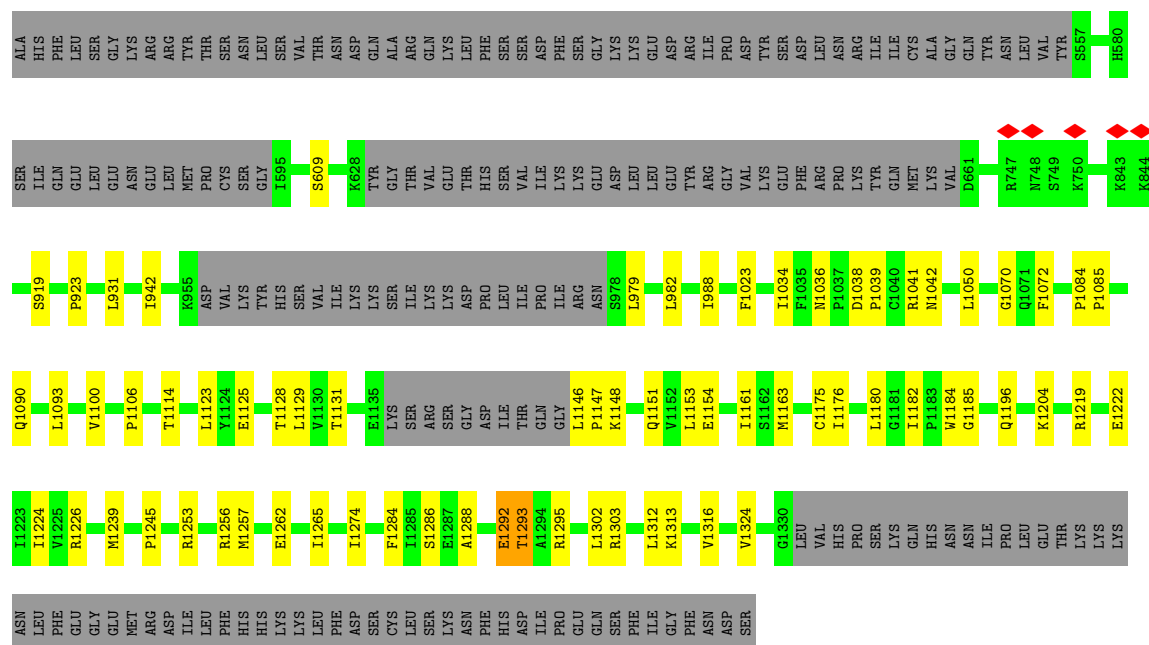
Chain C: 69% 16% 14%



• Molecule 4: DNA-directed RNA polymerase subunit beta"

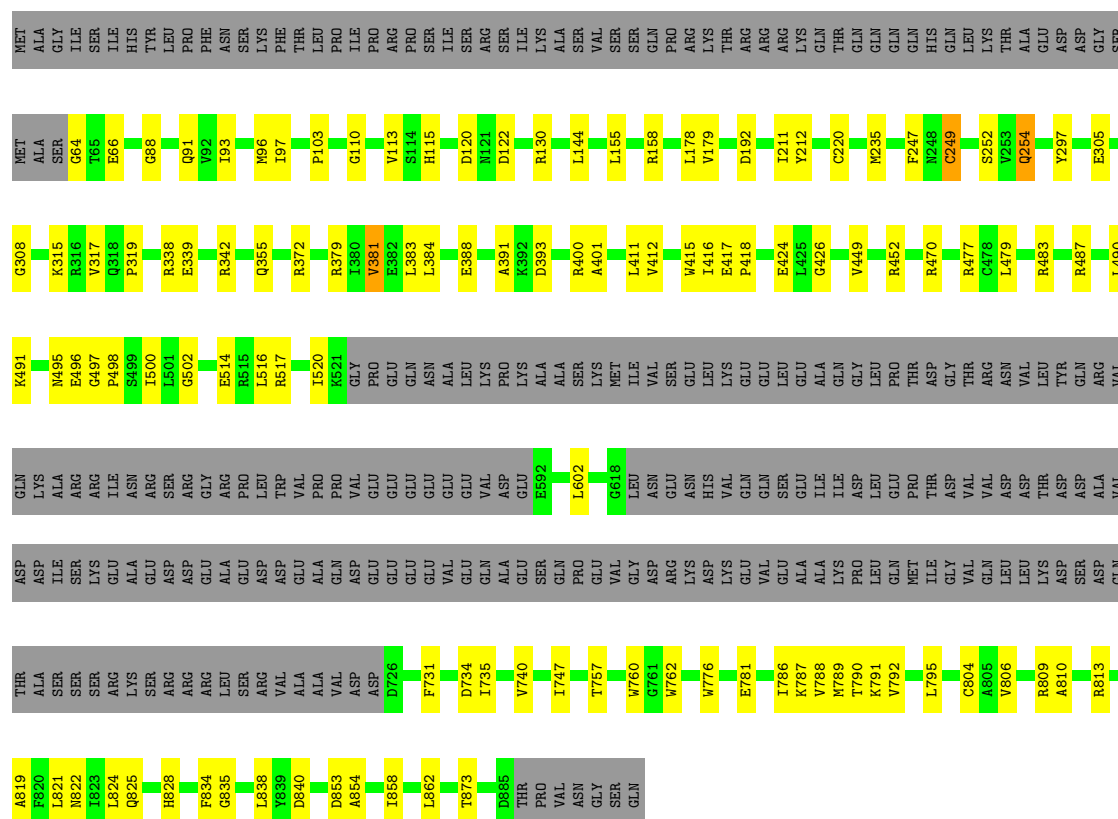
Chain c: 73% 11% 15%





• Molecule 5: PAP1(pTAC3)

Chain D: 60% 12% 28%



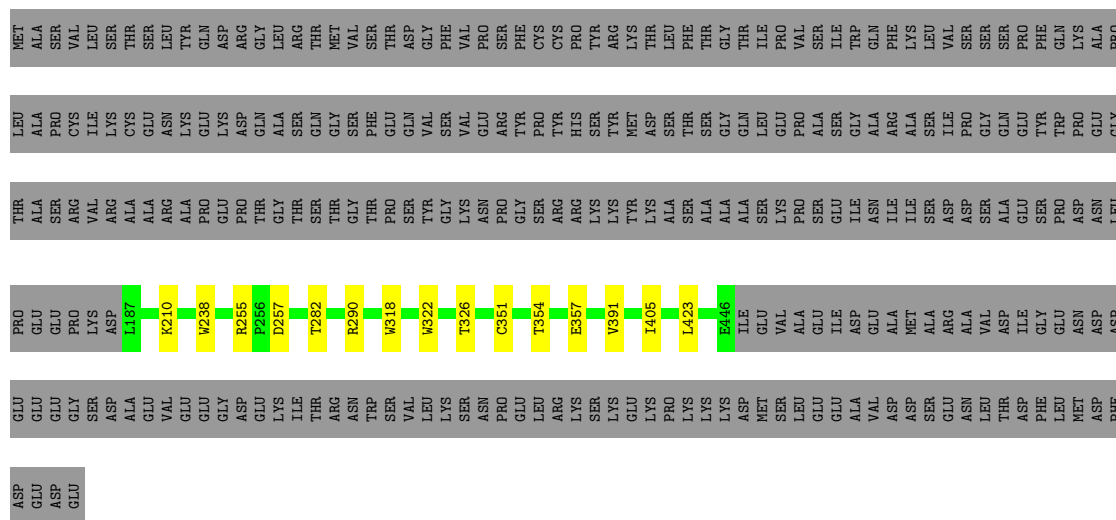
• Molecule 6: Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like

Chain E: 65% 16% 19%



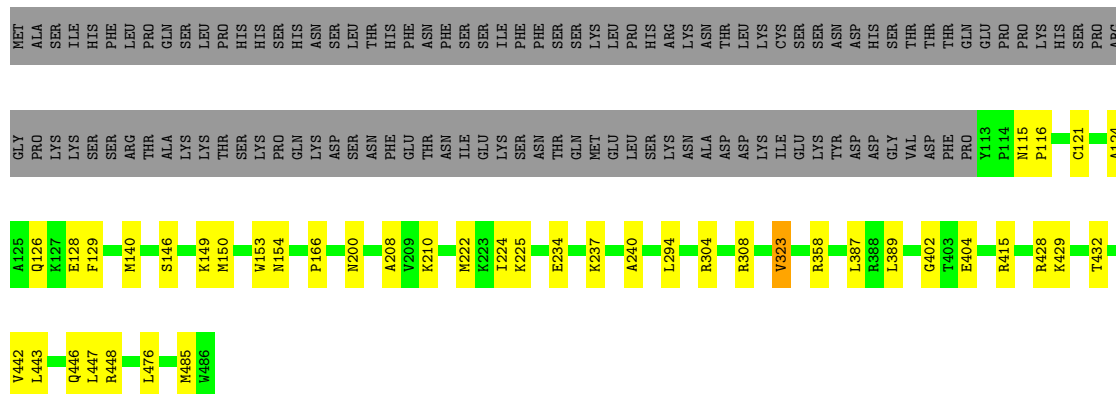
• Molecule 9: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like

Chain H: 46% 51%



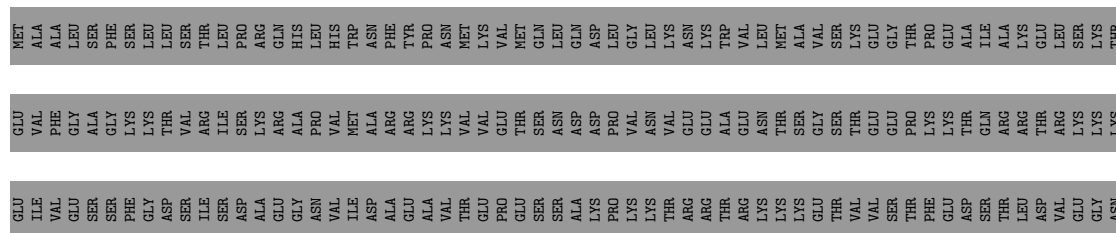
• Molecule 10: Fructokinase-like 1, chloroplastic

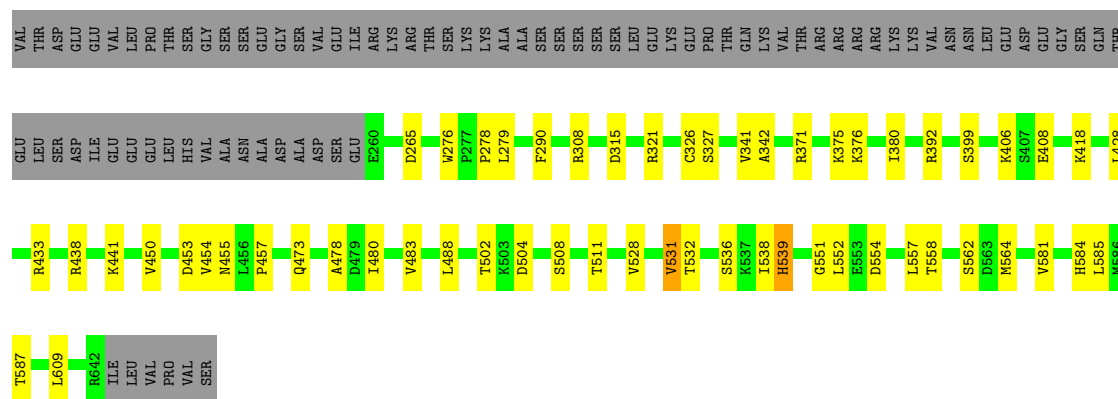
Chain I: 68% 9% 23%



• Molecule 11: Fructokinase-like 2, chloroplastic

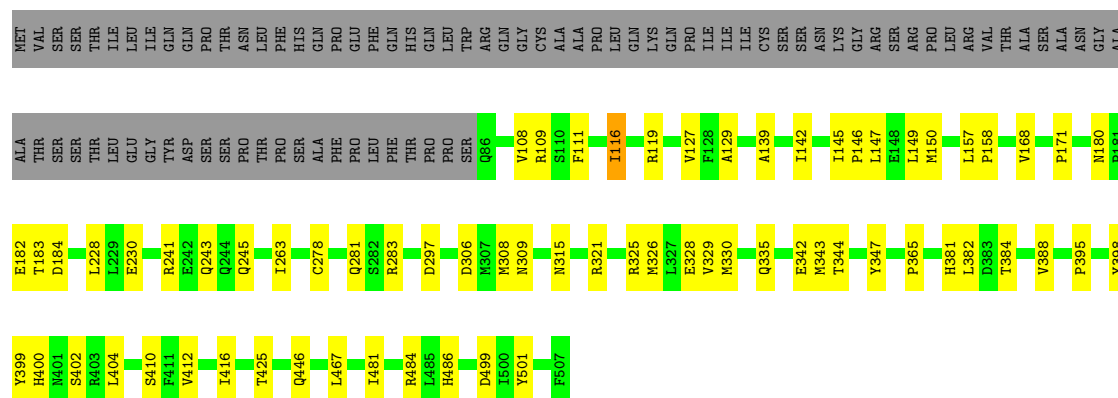
Chain i: 50% 8% 41%





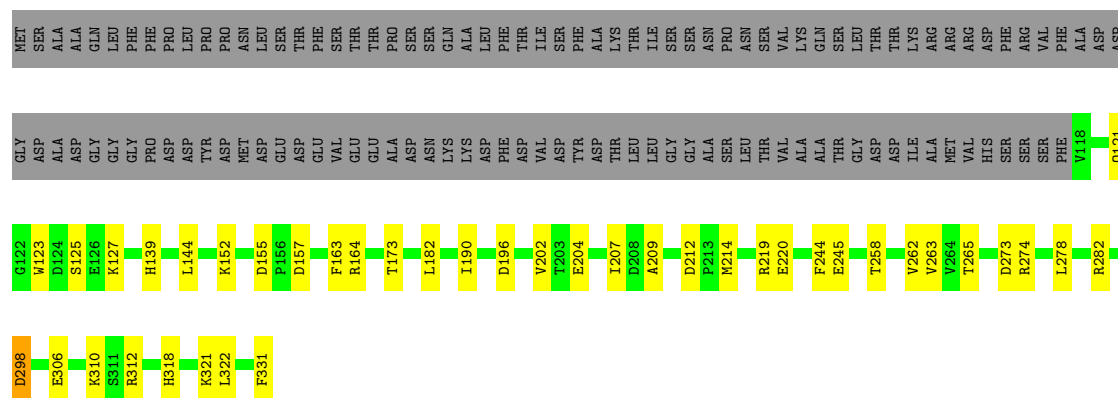
- Molecule 12: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2

Chain J: 70% 13% 17%



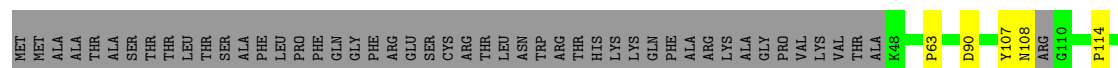
- Molecule 13: PAP8(pTAC6)

Chain K: 52% 12% 35%

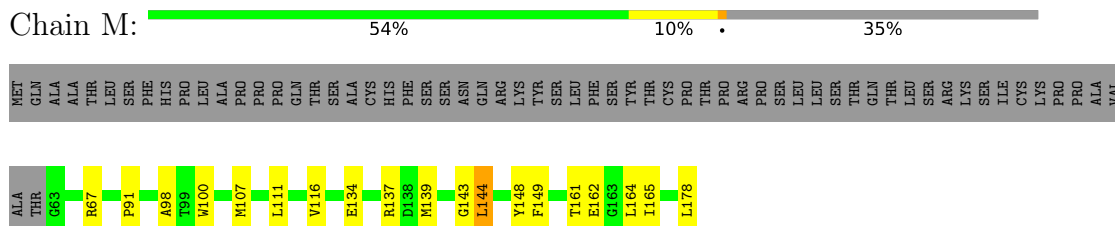


- Molecule 14: superoxide dismutase

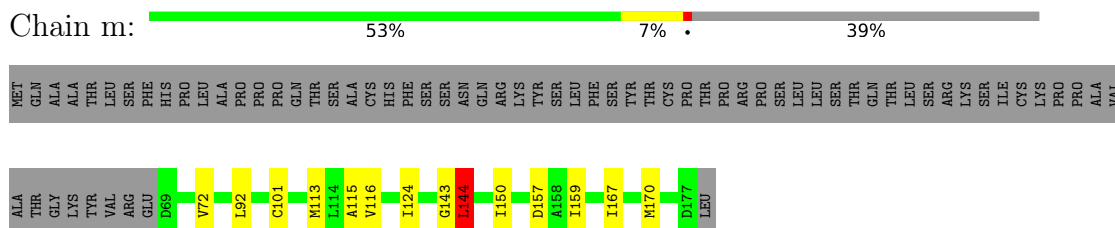
Chain L: 64% 11% 23%



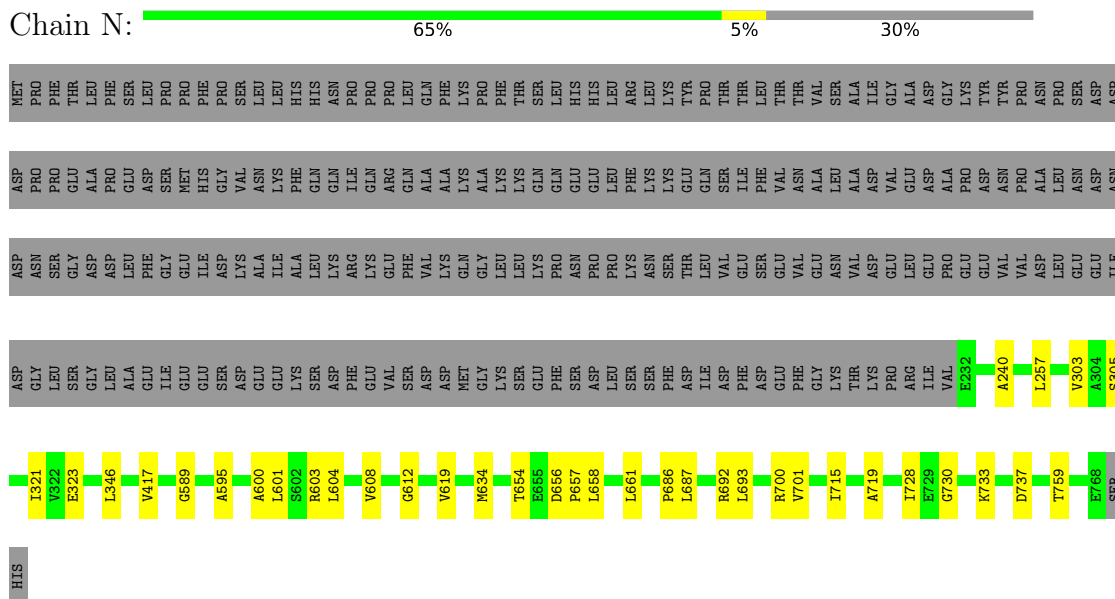
- Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic



- Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic



- Molecule 16: UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like



- Molecule 17: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X1



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

ASP
GLU
THR
LEU
ASP
ALA
LYS
MET
GLU
R54
I55
P56
R57
L58
Q61
I65
G68
G69
K70
L71
L72
T73
H74
N85
V90
I93
E96
N104
A110
R121
E131
A132
D137
P141
GLY
PRO
GLY
TYR
MET
LYS
ASP
GLU
LEU
LEU

● Molecule 18: PAP13(pTAC18)

Chain P: 59% 15% 27%

MET
ALA
SER
PHE
TLE
THR
MET
PRO
ALA
LEU
SER
TYR
LEU
SER
THR
ASN
THR
SER
SER
LEU
GLU
ARG
THR
ASN
PHE
ARG
PRO
SER
SER
ARG
GLY
TYR
GLN
GLY
VAL
ARG
ALA
R38
E41
V50
R51
V52
D59
R60
L61
V66
W72
K73
W83
L88
V96

V99
Q104
R105
F106
M107
V110
A111
G112
L125
Y135
R138
D142
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	410910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.856	Depositor
Minimum map value	-0.729	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.32	0/2237	0.39	0/3034
1	a	0.34	0/2487	0.43	2/3374 (0.1%)
2	B	0.22	2/6945 (0.0%)	0.35	3/9418 (0.0%)
3	C	0.16	0/4518	0.36	2/6148 (0.0%)
4	c	0.38	0/8213	0.49	10/11205 (0.1%)
5	D	0.29	1/5191 (0.0%)	0.37	3/7029 (0.0%)
6	E	0.55	0/4604	0.73	20/6285 (0.3%)
7	F	0.40	0/4339	0.55	7/5885 (0.1%)
8	G	0.55	0/1777	0.53	2/2417 (0.1%)
9	H	0.26	0/2167	0.34	0/2942
10	I	0.43	0/2970	0.41	2/4026 (0.0%)
11	i	0.40	0/3056	0.44	0/4141
12	J	0.31	1/3454 (0.0%)	0.38	2/4689 (0.0%)
13	K	0.18	0/1824	0.28	0/2468
14	L	1.11	2/1514 (0.1%)	1.33	22/2100 (1.0%)
15	M	0.60	0/951	0.60	3/1286 (0.2%)
15	m	0.51	0/865	0.68	3/1175 (0.3%)
16	N	0.08	0/3011	0.23	0/4163
17	O	0.09	0/702	0.24	0/945
18	P	0.09	0/915	0.28	0/1241
All	All	0.39	6/61740 (0.0%)	0.49	81/83971 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	249	CYS	C-O	6.53	1.31	1.24
14	L	155	PHE	CA-C	-5.46	1.45	1.52
2	B	76	TYR	CA-C	-5.30	1.46	1.52
2	B	77	SER	CA-C	-5.16	1.46	1.52
12	J	399	TYR	CA-C	-5.05	1.46	1.52
14	L	144	LEU	CA-C	-5.05	1.46	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	152	PHE	N-CA-C	-11.11	92.30	109.52
6	E	364	ASP	N-CA-C	-10.35	100.96	114.31
6	E	365	GLN	N-CA-C	-10.15	100.30	111.36
14	L	114	PRO	N-CA-C	9.89	122.77	110.70
4	c	401	PRO	N-CA-C	9.74	122.58	110.70
7	F	583	GLN	N-CA-C	-9.69	101.46	113.28
6	E	304	GLU	N-CA-C	9.25	121.44	111.36
15	m	157	ASP	N-CA-C	9.20	122.37	109.31
14	L	198	ASP	N-CA-C	-9.04	102.38	113.50
14	L	153	GLY	N-CA-C	8.61	122.91	112.49
10	I	153	TRP	N-CA-C	-8.54	102.79	113.55
6	E	421	GLU	N-CA-C	8.09	119.72	111.07
7	F	555	PHE	N-CA-C	-8.04	98.11	110.10
6	E	294	GLU	N-CA-C	-7.94	101.35	113.89
7	F	165	GLY	CA-C-N	-7.76	112.01	119.85
7	F	165	GLY	C-N-CA	-7.76	112.01	119.85
14	L	229	ALA	N-CA-C	7.70	119.31	111.07
6	E	326	GLY	N-CA-C	-7.57	103.43	115.08
14	L	193	HIS	CA-C-N	-7.56	111.67	119.83
14	L	193	HIS	C-N-CA	-7.56	111.67	119.83
14	L	196	ASP	N-CA-C	-7.45	100.50	110.55
15	M	100	TRP	N-CA-C	7.43	119.38	111.28
6	E	362	ARG	N-CA-C	-7.36	103.26	111.28
6	E	420	TYR	N-CA-C	-7.18	103.53	111.36
12	J	404	LEU	N-CA-C	-7.09	101.83	112.04
2	B	795	GLY	N-CA-C	-7.08	106.01	115.21
14	L	209	ALA	N-CA-C	7.03	121.22	111.74
6	E	758	THR	N-CA-C	6.93	118.84	111.28
7	F	567	TYR	N-CA-C	-6.89	104.84	113.18
10	I	208	ALA	N-CA-C	6.81	118.70	111.28
4	c	398	VAL	N-CA-C	6.49	116.92	108.35
6	E	277	VAL	N-CA-C	6.49	116.75	111.62
2	B	794	ARG	N-CA-C	6.44	118.38	111.36
14	L	233	ASP	N-CA-C	6.38	118.03	111.14
5	D	254	GLN	N-CA-C	6.35	118.20	111.28
14	L	133	LYS	O-C-N	-6.31	116.59	121.14
14	L	192	PRO	N-CA-C	-6.30	101.99	111.57
1	a	112	GLY	CA-C-N	-6.19	113.58	120.14
1	a	112	GLY	C-N-CA	-6.19	113.58	120.14
14	L	178	ALA	N-CA-C	6.16	118.44	109.07
15	M	144	LEU	CA-C-N	-5.99	112.36	119.84
15	M	144	LEU	C-N-CA	-5.99	112.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	90	ASP	N-CA-C	5.94	118.81	109.96
3	C	125	TYR	N-CA-C	-5.91	106.23	113.50
8	G	221	TYR	N-CA-C	5.91	118.50	111.71
12	J	410	SER	N-CA-C	-5.87	106.16	113.38
4	c	102	GLU	N-CA-C	5.87	117.76	111.36
2	B	802	GLU	N-CA-C	-5.84	104.92	111.28
7	F	556	GLY	N-CA-C	5.82	121.71	110.66
15	m	144	LEU	CA-C-N	-5.81	112.58	119.84
15	m	144	LEU	C-N-CA	-5.81	112.58	119.84
6	E	336	ARG	N-CA-C	-5.75	105.01	111.28
4	c	147	VAL	N-CA-C	5.74	118.41	112.90
6	E	329	LYS	N-CA-C	-5.72	105.05	111.28
7	F	581	SER	N-CA-C	-5.71	103.77	111.54
14	L	63	PRO	N-CA-C	-5.71	106.10	113.57
14	L	238	ARG	CA-C-N	-5.70	112.72	119.05
14	L	238	ARG	C-N-CA	-5.70	112.72	119.05
14	L	248	LYS	N-CA-C	5.70	119.85	113.01
4	c	397	ASN	N-CA-C	5.59	117.52	108.34
6	E	406	HIS	N-CA-C	-5.58	105.19	111.28
6	E	338	MET	N-CA-C	-5.56	105.22	111.28
14	L	114	PRO	CA-C-N	-5.56	114.52	120.47
14	L	114	PRO	C-N-CA	-5.56	114.52	120.47
6	E	324	HIS	N-CA-C	-5.55	105.23	111.28
3	C	145	GLU	N-CA-C	-5.53	105.25	111.28
4	c	369	PRO	CA-C-O	-5.51	115.13	121.36
6	E	316	ASN	N-CA-C	5.47	117.24	111.28
8	G	222	LEU	N-CA-C	5.30	118.21	111.69
6	E	382	ALA	N-CA-C	-5.23	105.00	111.33
6	E	321	ALA	N-CA-C	-5.21	105.78	111.82
6	E	414	GLU	N-CA-C	5.21	117.27	110.08
6	E	296	VAL	N-CA-C	5.20	115.42	110.42
4	c	378	ALA	N-CA-C	5.09	114.97	108.24
5	D	252	SER	CA-C-N	-5.09	113.48	120.46
5	D	252	SER	C-N-CA	-5.09	113.48	120.46
14	L	191	ASN	CA-C-N	-5.08	115.33	120.31
14	L	191	ASN	C-N-CA	-5.08	115.33	120.31
4	c	368	HIS	CA-C-N	5.08	125.08	119.90
4	c	368	HIS	C-N-CA	5.08	125.08	119.90
4	c	379	PHE	N-CA-C	-5.05	100.47	109.06

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	2202	0	2108	23	0
1	a	2441	0	2390	29	0
2	B	6820	0	6495	77	0
3	C	4431	0	4202	86	0
4	c	8086	0	7028	99	0
5	D	5088	0	4957	77	0
6	E	4534	0	3525	68	0
7	F	4233	0	3825	48	0
8	G	1727	0	1648	15	0
9	H	2110	0	1974	11	0
10	I	2897	0	2752	25	0
11	i	2983	0	2896	30	0
12	J	3368	0	3240	38	0
13	K	1779	0	1730	31	0
14	L	1475	0	1046	15	0
15	M	935	0	934	14	0
15	m	851	0	837	7	0
16	N	2982	0	1849	18	0
17	O	692	0	660	18	0
18	P	887	0	826	11	0
19	B	1	0	0	0	0
20	C	1	0	0	0	0
21	G	1	0	0	0	0
21	L	1	0	0	0	0
All	All	60525	0	54922	651	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 (651) 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)
5:D:379:ARG:HH21	5:D:477:ARG:HH21	1.02	0.93
5:D:379:ARG:NH2	5:D:477:ARG:HH21	1.74	0.85
5:D:379:ARG:HH21	5:D:477:ARG:NH2	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:625:GLN:HE22	2:B:646:GLY:H	1.35	0.73
8:G:235:PHE:HA	8:G:239:LEU:HB2	1.70	0.73
3:C:548:VAL:HG11	4:c:53:THR:HG21	1.72	0.70
1:A:225:LEU:HD12	1:a:45:ILE:HD11	1.73	0.70
2:B:1063:PHE:HZ	5:D:254:GLN:HG2	1.55	0.70
5:D:834:PHE:HB3	5:D:838:LEU:HD21	1.74	0.69
5:D:381:VAL:HA	5:D:384:LEU:HD12	1.75	0.69
6:E:655:ASN:HB3	6:E:692:ARG:HH21	1.58	0.68
3:C:147:LEU:HD21	3:C:205:ALA:HB3	1.76	0.68
6:E:502:LEU:HD22	6:E:505:GLU:H	1.59	0.68
3:C:114:ILE:HD12	3:C:307:ILE:HG22	1.76	0.68
5:D:388:GLU:HG3	5:D:791:LYS:HE2	1.74	0.67
5:D:212:TYR:HB3	5:D:235:MET:HE2	1.75	0.67
3:C:672:GLU:HG2	4:c:45:LEU:HD22	1.77	0.67
2:B:1063:PHE:CZ	5:D:254:GLN:HG2	2.31	0.66
3:C:679:GLY:HA3	17:O:61:GLN:HE21	1.59	0.66
4:c:205:ARG:NH2	4:c:1154:GLU:OE1	2.29	0.66
11:i:371:ARG:HD3	11:i:408:GLU:HB3	1.76	0.66
5:D:824:LEU:HD21	5:D:858:ILE:HD12	1.78	0.66
7:F:328:GLU:HB2	7:F:347:ILE:HD11	1.76	0.66
7:F:204:ASP:HB3	7:F:207:LYS:HG2	1.77	0.66
7:F:397:GLU:HG3	7:F:526:ARG:HH21	1.60	0.65
4:c:384:ASP:HB3	4:c:401:PRO:HG3	1.79	0.65
4:c:297:ILE:HD11	4:c:318:VAL:HG21	1.76	0.65
4:c:453:ASP:HB2	4:c:472:SER:HB3	1.78	0.65
11:i:321:ARG:HG3	11:i:564:MET:HB3	1.79	0.65
7:F:180:ARG:NH1	18:P:41:GLU:O	2.29	0.64
4:c:92:HIS:CD2	4:c:94:VAL:HG22	2.33	0.64
7:F:480:PHE:O	7:F:484:GLN:NE2	2.29	0.64
2:B:793:LYS:HA	2:B:799:TYR:HA	1.78	0.64
3:C:263:ARG:NH1	5:D:297:TYR:O	2.31	0.64
5:D:825:GLN:HA	5:D:828:HIS:CD2	2.33	0.64
1:A:103:THR:HG22	1:A:152:GLU:HG2	1.80	0.64
6:E:498:ALA:O	6:E:534:GLN:NE2	2.31	0.64
1:A:26:ARG:HG3	1:A:95:ILE:HD13	1.78	0.64
4:c:979:LEU:HD22	7:F:282:GLY:HA2	1.79	0.64
7:F:79:ARG:HA	8:G:263:ILE:HD13	1.79	0.63
7:F:514:TYR:OH	18:P:73:LYS:NZ	2.31	0.63
9:H:210:LYS:O	13:K:312:ARG:NH1	2.30	0.63
1:a:21:ARG:NH1	1:a:23:ASP:OD1	2.31	0.63
5:D:372:ARG:HH11	5:D:401:ALA:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:VAL:HG22	2:B:850:MET:HB2	1.79	0.63
4:c:491:ILE:O	7:F:382:ARG:NH1	2.32	0.63
2:B:661:PRO:HA	2:B:666:ASN:HD21	1.64	0.63
13:K:207:ILE:HG23	13:K:212:ASP:HB3	1.80	0.62
2:B:795:GLY:C	2:B:797:SER:H	2.08	0.62
3:C:113:TYR:HB2	3:C:275:LEU:HD21	1.81	0.62
4:c:291:CYS:HB3	4:c:1226:ARG:HH12	1.64	0.62
3:C:157:PRO:HG2	3:C:200:SER:HB2	1.81	0.62
15:m:115:ALA:HB2	15:m:124:ILE:HD12	1.80	0.62
3:C:473:PHE:HZ	3:C:489:VAL:HG11	1.64	0.62
3:C:157:PRO:O	3:C:209:GLN:NE2	2.34	0.61
1:A:56:GLU:O	1:A:221:ASN:ND2	2.33	0.61
4:c:1093:LEU:HB3	4:c:1100:VAL:HB	1.82	0.61
14:L:137:GLY:HA3	14:L:247:GLU:O	2.00	0.61
2:B:541:ARG:NH2	2:B:825:GLY:O	2.30	0.61
4:c:1023:PHE:O	4:c:1042:ASN:ND2	2.34	0.61
11:i:488:LEU:HD22	11:i:531:VAL:HG11	1.80	0.61
4:c:328:GLU:HG3	4:c:329:PRO:HD3	1.82	0.61
13:K:245:GLU:OE1	13:K:274:ARG:NH2	2.34	0.61
2:B:998:VAL:HG12	3:C:515:GLU:HB3	1.83	0.61
12:J:446:GLN:NE2	12:J:499:ASP:OD1	2.34	0.61
1:A:98:SER:O	1:A:153:ARG:NH1	2.35	0.60
7:F:173:PRO:HD2	7:F:195:THR:HG21	1.82	0.60
13:K:182:LEU:HB2	13:K:258:THR:HG22	1.83	0.60
4:c:109:GLU:O	4:c:110:TYR:C	2.42	0.60
3:C:279:LEU:HD12	3:C:280:PRO:HD2	1.84	0.60
6:E:568:CYS:SG	6:E:569:PHE:N	2.75	0.60
2:B:869:CYS:HB3	2:B:943:GLY:HA3	1.84	0.60
8:G:108:ILE:HD13	8:G:201:ASN:HD21	1.67	0.60
14:L:123:TRP:O	14:L:126:GLN:HG3	2.00	0.60
3:C:135:ASN:O	3:C:254:ARG:NH1	2.35	0.60
17:O:71:LEU:HA	17:O:74:MET:HE2	1.84	0.60
6:E:755:SER:HB3	6:E:757:ILE:HG13	1.84	0.59
2:B:135:ARG:NH1	2:B:306:MET:SD	2.75	0.59
4:c:25:ARG:NH2	13:K:214:MET:O	2.34	0.59
7:F:482:GLU:O	7:F:486:HIS:ND1	2.34	0.59
16:N:303:VAL:HA	16:N:321:ILE:HA	1.83	0.59
13:K:298:ASP:OD1	13:K:298:ASP:N	2.33	0.59
7:F:175:ARG:NH1	8:G:102:CYS:O	2.36	0.59
10:I:404:GLU:OE2	10:I:415:ARG:NH2	2.32	0.59
13:K:121:GLN:NE2	13:K:164:ARG:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:PHE:O	2:B:890:ARG:NH1	2.36	0.59
6:E:478:MET:HE1	6:E:489:THR:HG21	1.85	0.59
15:m:92:LEU:HD23	15:m:150:ILE:HD11	1.84	0.59
10:I:294:LEU:HD12	10:I:323:VAL:HG13	1.85	0.58
6:E:568:CYS:HB2	6:E:601:ILE:HD11	1.85	0.58
2:B:269:ARG:NH1	2:B:302:ALA:O	2.33	0.58
4:c:206:LEU:HD22	4:c:1224:ILE:HD13	1.86	0.58
6:E:723:SER:O	6:E:727:ASN:ND2	2.37	0.58
4:c:1284:PHE:HA	4:c:1288:ALA:HB3	1.86	0.58
2:B:666:ASN:HD22	2:B:853:ASN:HD22	1.52	0.58
7:F:91:GLU:OE2	7:F:316:ARG:NH2	2.37	0.57
10:I:234:GLU:OE1	10:I:237:LYS:NZ	2.36	0.57
9:H:255:ARG:NH1	9:H:257:ASP:OD1	2.37	0.57
4:c:1175:CYS:HB3	5:D:735:ILE:HD13	1.86	0.57
6:E:746:VAL:HG13	6:E:788:ARG:HH21	1.68	0.57
15:M:161:THR:HG21	15:M:165:ILE:HD13	1.86	0.57
4:c:609:SER:HA	7:F:590:HIS:CE1	2.40	0.57
5:D:483:ARG:NH1	5:D:520:ILE:O	2.38	0.57
4:c:1286:SER:HB2	4:c:1313:LYS:HD2	1.87	0.57
4:c:400:ILE:HG13	4:c:423:ILE:HD12	1.87	0.57
4:c:499:ASN:ND2	4:c:919:SER:O	2.38	0.57
11:i:450:VAL:HB	11:i:478:ALA:HA	1.87	0.57
12:J:108:VAL:HG23	12:J:109:ARG:HD2	1.87	0.57
18:P:110:VAL:HG13	18:P:112:GLY:H	1.70	0.57
6:E:671:GLU:OE2	6:E:717:GLY:N	2.31	0.57
2:B:560:LYS:HG3	2:B:645:VAL:HG13	1.87	0.56
2:B:627:PRO:HD2	2:B:630:LYS:HD2	1.87	0.56
11:i:532:THR:HG22	11:i:538:ILE:HG23	1.85	0.56
12:J:315:ASN:OD1	12:J:335:GLN:NE2	2.37	0.56
4:c:1034:ILE:HD13	7:F:208:VAL:HG13	1.87	0.56
1:a:320:ILE:HD12	1:a:323:ILE:HD11	1.85	0.56
3:C:554:HIS:HB3	3:C:558:CYS:HB2	1.88	0.56
4:c:923:PRO:HB2	4:c:942:ILE:HG21	1.85	0.56
8:G:128:TRP:HH2	8:G:209:PRO:HG2	1.70	0.56
12:J:129:ALA:HB2	12:J:343:MET:HE2	1.85	0.56
1:A:297:ASP:O	1:A:301:ASN:ND2	2.32	0.56
2:B:129:SER:OG	2:B:265:ASN:ND2	2.38	0.56
2:B:450:LEU:HD23	2:B:450:LEU:H	1.70	0.56
5:D:819:ALA:HA	5:D:822:ASN:HD21	1.70	0.56
6:E:709:ASP:HA	6:E:746:VAL:HB	1.88	0.56
9:H:290:ARG:NH2	13:K:331:PHE:OXT	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:595:ALA:HB2	16:N:604:LEU:HD12	1.88	0.56
3:C:141:LEU:HD12	3:C:144:LEU:HD11	1.88	0.56
4:c:391:SER:OG	4:c:394:ILE:O	2.20	0.56
2:B:1035:ALA:O	2:B:1040:ARG:NH1	2.39	0.56
3:C:517:ARG:HD3	17:O:72:LEU:HD21	1.88	0.56
6:E:633:MET:O	6:E:681:ARG:NH1	2.34	0.56
5:D:388:GLU:CG	5:D:791:LYS:HE2	2.36	0.56
10:I:442:VAL:O	10:I:446:GLN:NE2	2.35	0.55
5:D:155:LEU:HD13	5:D:158:ARG:HD2	1.88	0.55
6:E:577:GLU:OE2	6:E:602:TYR:OH	2.24	0.55
2:B:1043:VAL:HG23	2:B:1053:LEU:HB2	1.89	0.55
3:C:308:TYR:HA	3:C:311:ASN:HD21	1.70	0.55
3:C:553:ASN:HB2	3:C:607:ASP:HB3	1.87	0.55
6:E:678:GLN:NE2	6:E:680:GLU:OE1	2.39	0.55
15:M:149:PHE:HB3	15:M:178:LEU:HD11	1.87	0.55
4:c:64:THR:HG21	4:c:68:LYS:HD2	1.89	0.55
8:G:208:ILE:HG21	8:G:252:ALA:HB2	1.87	0.55
2:B:112:THR:HG21	2:B:378:LEU:HD22	1.88	0.55
13:K:245:GLU:HA	13:K:262:VAL:HG21	1.88	0.55
2:B:97:GLN:HB3	2:B:353:GLN:HE22	1.70	0.55
2:B:483:ASN:ND2	2:B:890:ARG:O	2.39	0.55
6:E:628:GLN:O	6:E:632:GLN:NE2	2.40	0.55
5:D:810:ALA:HA	5:D:813:ARG:HE	1.72	0.55
4:c:306:PRO:HD3	4:c:1219:ARG:HH22	1.71	0.55
11:i:375:LYS:HG3	11:i:376:LYS:HG3	1.89	0.55
4:c:1163:MET:SD	4:c:1163:MET:N	2.81	0.54
5:D:479:LEU:HD13	5:D:483:ARG:HH21	1.72	0.54
1:A:111:LYS:NZ	1:A:144:ASP:OD1	2.38	0.54
4:c:1114:THR:OG1	4:c:1131:THR:OG1	2.26	0.54
12:J:230:GLU:OE2	12:J:484:ARG:NH1	2.40	0.54
6:E:604:LYS:HA	6:E:675:TRP:HE1	1.71	0.54
11:i:502:THR:OG1	11:i:504:ASP:OD1	2.25	0.54
12:J:184:ASP:OD1	12:J:184:ASP:N	2.40	0.54
15:M:134:GLU:OE1	15:M:137:ARG:NH2	2.36	0.54
1:a:294:THR:HG23	1:a:297:ASP:H	1.72	0.54
1:A:113:PRO:HA	1:A:142:PRO:HG3	1.89	0.54
4:c:313:GLU:HB3	17:O:85:ASN:HD22	1.72	0.54
5:D:355:GLN:NE2	5:D:393:ASP:O	2.40	0.54
11:i:290:PHE:CZ	15:m:143:GLY:HA3	2.42	0.54
18:P:99:VAL:HG22	18:P:106:PHE:HB3	1.89	0.54
10:I:128:GLU:HB2	15:M:164:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:i:276:TRP:HZ2	11:i:581:VAL:HG13	1.72	0.54
3:C:307:ILE:O	3:C:311:ASN:ND2	2.41	0.54
6:E:499:LYS:HG3	6:E:712:ARG:HD2	1.89	0.54
6:E:592:ILE:HD11	6:E:627:HIS:HA	1.90	0.53
2:B:382:ASN:HD22	2:B:552:ALA:HB3	1.73	0.53
16:N:589:GLY:HA3	16:N:715:ILE:HG22	1.88	0.53
6:E:651:PHE:O	6:E:692:ARG:NH1	2.37	0.53
4:c:1148:LYS:HD2	4:c:1151:GLN:HE21	1.73	0.53
4:c:380:LEU:HD13	4:c:424:ARG:NH2	2.24	0.53
6:E:607:ARG:HG3	6:E:610:MET:HE2	1.91	0.53
10:I:121:CYS:HB3	10:I:166:PRO:HB2	1.91	0.53
11:i:552:LEU:HG	11:i:554:ASP:H	1.73	0.53
12:J:382:LEU:HB2	12:J:425:THR:HB	1.90	0.53
4:c:230:PRO:HD2	4:c:281:GLN:HG3	1.91	0.53
2:B:336:VAL:HA	2:B:339:THR:HG22	1.91	0.53
2:B:424:ILE:HD11	4:c:178:TYR:HE2	1.74	0.53
3:C:631:HIS:HB3	13:K:278:LEU:HD11	1.91	0.53
4:c:206:LEU:HD21	4:c:1153:LEU:HD23	1.90	0.53
5:D:821:LEU:HD23	5:D:821:LEU:H	1.73	0.53
6:E:572:LEU:HB3	6:E:575:GLU:HB2	1.91	0.53
2:B:578:LEU:HD11	2:B:644:THR:HG21	1.91	0.53
3:C:549:LEU:HG	4:c:49:GLN:HG2	1.90	0.53
8:G:147:LEU:HD12	8:G:147:LEU:H	1.74	0.53
12:J:283:ARG:HH11	12:J:306:ASP:HB3	1.74	0.53
2:B:672:LEU:HD21	2:B:834:LEU:HD12	1.91	0.52
4:c:385:LEU:HB3	4:c:399:ASN:HD22	1.74	0.52
5:D:491:LYS:O	5:D:495:ASN:ND2	2.43	0.52
5:D:734:ASP:OD1	5:D:734:ASP:N	2.37	0.52
6:E:732:LEU:HG	6:E:735:LYS:HD2	1.92	0.52
3:C:256:GLU:OE2	4:c:1303:ARG:NH2	2.42	0.52
11:i:380:ILE:HG23	15:m:159:ILE:HG23	1.91	0.52
17:O:110:ALA:HB3	17:O:132:ALA:HB3	1.91	0.52
3:C:297:SER:OG	3:C:300:ASN:ND2	2.42	0.52
6:E:684:ARG:HH11	6:E:687:ASN:HB2	1.75	0.52
7:F:329:ILE:HA	7:F:344:MET:HG2	1.92	0.52
4:c:465:VAL:HG13	4:c:1114:THR:HB	1.92	0.52
6:E:702:ASN:OD1	6:E:703:LYS:N	2.41	0.52
6:E:731:GLU:O	6:E:735:LYS:NZ	2.42	0.52
2:B:383:PRO:HB2	2:B:649:LEU:HD11	1.92	0.52
2:B:569:ARG:HG2	9:H:405:ILE:HG13	1.92	0.52
6:E:639:ASP:HA	6:E:644:TRP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:17:CYS:SG	1:a:20:SER:OG	2.68	0.52
3:C:111:MET:HG2	3:C:280:PRO:HD3	1.92	0.52
9:H:322:TRP:HZ3	9:H:326:THR:HG22	1.74	0.52
4:c:372:THR:HG23	4:c:405:LEU:HD21	1.92	0.52
5:D:384:LEU:HD23	5:D:791:LYS:HZ3	1.74	0.52
12:J:381:HIS:HD2	12:J:384:THR:H	1.58	0.52
7:F:151:ILE:HG21	7:F:317:HIS:HE1	1.75	0.52
10:I:146:SER:O	10:I:149:LYS:NZ	2.43	0.52
11:i:278:PRO:HB3	11:i:418:LYS:HD3	1.92	0.52
2:B:83:SER:HA	2:B:98:THR:HA	1.91	0.51
2:B:856:GLY:O	2:B:860:ARG:HG2	2.09	0.51
3:C:218:ILE:HD12	3:C:254:ARG:HH21	1.75	0.51
12:J:388:VAL:HG11	12:J:501:TYR:HD1	1.75	0.51
2:B:855:LEU:HD21	3:C:544:ILE:HG13	1.92	0.51
5:D:776:TRP:NE1	5:D:781:GLU:OE2	2.36	0.51
6:E:497:PHE:HD2	6:E:509:ILE:HD13	1.73	0.51
7:F:128:ASN:HA	7:F:131:LYS:HG2	1.93	0.51
5:D:514:GLU:HA	5:D:517:ARG:HG2	1.92	0.51
6:E:724:VAL:HA	6:E:727:ASN:HD21	1.76	0.51
7:F:288:HIS:HD2	7:F:291:GLN:H	1.59	0.51
1:a:104:SER:HB2	1:a:124:PRO:HG2	1.92	0.51
3:C:279:LEU:HD21	3:C:283:LEU:HD22	1.91	0.51
17:O:96:GLU:OE1	17:O:121:ARG:NH2	2.44	0.51
1:A:86:GLU:OE1	1:A:90:ASN:ND2	2.44	0.51
5:D:220:CYS:SG	5:D:249:CYS:HB3	2.51	0.51
13:K:209:ALA:HB3	13:K:212:ASP:HB2	1.93	0.51
3:C:302:LEU:HD23	3:C:342:LEU:HA	1.93	0.51
3:C:561:ARG:HA	9:H:290:ARG:HH11	1.76	0.51
6:E:525:PHE:HB3	6:E:548:MET:HE2	1.92	0.51
12:J:325:ARG:HH21	13:K:209:ALA:HA	1.76	0.51
1:a:37:LEU:HD21	1:a:45:ILE:HD12	1.92	0.50
2:B:656:LEU:HD21	2:B:842:LEU:HD11	1.92	0.50
3:C:264:THR:HG23	3:C:266:ILE:H	1.76	0.50
3:C:329:MET:O	3:C:333:LYS:HG2	2.11	0.50
5:D:97:ILE:HG22	5:D:103:PRO:HD3	1.93	0.50
5:D:411:LEU:HD21	5:D:792:VAL:HG21	1.92	0.50
7:F:410:TRP:O	7:F:414:ASN:ND2	2.31	0.50
11:i:453:ASP:OD2	11:i:455:ASN:ND2	2.44	0.50
3:C:9:ILE:HG12	5:D:247:PHE:CZ	2.47	0.50
3:C:220:GLU:OE2	5:D:470:ARG:NE	2.44	0.50
7:F:303:GLY:HA3	7:F:344:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:109:ARG:HG2	12:J:149:LEU:HD11	1.93	0.50
5:D:424:GLU:H	5:D:809:ARG:HH21	1.59	0.50
6:E:487:VAL:O	6:E:491:ASN:ND2	2.45	0.50
2:B:530:LEU:HA	2:B:565:THR:HG21	1.93	0.50
13:K:123:TRP:HE1	13:K:127:LYS:HE3	1.76	0.50
5:D:417:GLU:HB2	5:D:418:PRO:HD3	1.94	0.50
5:D:412:VAL:HA	5:D:415:TRP:HE1	1.77	0.50
11:i:536:SER:O	11:i:551:GLY:N	2.43	0.50
3:C:154:PHE:HB2	3:C:157:PRO:HG3	1.93	0.50
3:C:271:MET:HE2	4:c:1302:LEU:HD11	1.94	0.50
6:E:706:TRP:HB3	6:E:740:PRO:HG3	1.94	0.50
12:J:412:VAL:HA	12:J:416:ILE:HG21	1.94	0.50
6:E:491:ASN:HA	6:E:494:ILE:HG22	1.94	0.49
1:A:118:ALA:O	1:A:119:GLN:HG3	2.12	0.49
2:B:874:ALA:HB2	2:B:904:LEU:HD23	1.94	0.49
3:C:547:TYR:O	3:C:551:SER:HB3	2.12	0.49
5:D:122:ASP:OD1	5:D:122:ASP:N	2.44	0.49
3:C:147:LEU:HD23	3:C:206:ILE:HG12	1.93	0.49
3:C:518:LEU:HD21	17:O:93:ILE:HD12	1.94	0.49
3:C:649:ARG:HH12	13:K:219:ARG:HH22	1.60	0.49
11:i:315:ASP:OD1	11:i:315:ASP:N	2.46	0.49
14:L:155:PHE:CZ	14:L:252:TRP:CZ2	3.00	0.49
2:B:634:LYS:NZ	15:M:67:ARG:O	2.43	0.49
4:c:267:ILE:HA	4:c:271:LEU:HD12	1.95	0.49
12:J:171:PRO:HB2	12:J:263:ILE:HD11	1.93	0.49
6:E:707:SER:OG	6:E:708:VAL:N	2.45	0.49
10:I:387:LEU:O	10:I:402:GLY:N	2.46	0.49
12:J:147:LEU:HA	12:J:150:MET:HE2	1.95	0.49
3:C:155:ALA:HB2	3:C:169:GLY:H	1.78	0.49
5:D:192:ASP:OD1	5:D:192:ASP:N	2.45	0.49
16:N:737:ASP:OD1	16:N:737:ASP:N	2.44	0.49
4:c:490:SER:O	4:c:493:LYS:NZ	2.46	0.49
5:D:787:LYS:HA	5:D:790:THR:HG22	1.94	0.49
13:K:139:HIS:CD2	13:K:152:LYS:HB3	2.48	0.49
4:c:163:LEU:HD12	4:c:164:PRO:HD2	1.95	0.49
2:B:508:ILE:HD12	2:B:512:GLN:HB2	1.95	0.48
4:c:37:HIS:CE1	17:O:65:ILE:HD11	2.48	0.48
13:K:306:GLU:HG2	13:K:310:LYS:HZ2	1.77	0.48
1:A:98:SER:HB2	1:A:127:VAL:HA	1.95	0.48
3:C:514:VAL:HG12	17:O:90:VAL:HG13	1.95	0.48
3:C:669:LEU:O	3:C:672:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:1161:ILE:HB	4:c:1204:LYS:HE2	1.95	0.48
6:E:609:ASN:HA	6:E:612:HIS:HD2	1.78	0.48
15:M:139:MET:O	15:M:148:TYR:OH	2.31	0.48
2:B:60:VAL:O	2:B:78:SER:OG	2.28	0.48
11:i:433:ARG:HD3	11:i:473:GLN:HE22	1.79	0.48
12:J:116:ILE:HG13	12:J:127:VAL:CG1	2.43	0.48
2:B:385:THR:HA	2:B:388:VAL:HG22	1.96	0.48
3:C:649:ARG:NH1	13:K:196:ASP:OD1	2.46	0.48
3:C:186:PHE:O	3:C:187:THR:OG1	2.27	0.48
12:J:228:LEU:HD23	12:J:241:ARG:HG3	1.95	0.48
2:B:457:ILE:HD13	2:B:516:ARG:HB2	1.96	0.48
5:D:88:GLY:O	5:D:91:GLN:HG3	2.13	0.48
5:D:372:ARG:NH1	5:D:400:ARG:O	2.47	0.48
6:E:711:HIS:CE1	6:E:749:ARG:H	2.32	0.48
17:O:65:ILE:HG23	17:O:70:LYS:HB2	1.96	0.48
2:B:126:ILE:HD11	2:B:393:LEU:HD13	1.95	0.48
7:F:348:ASP:HB3	7:F:349:PRO:HD3	1.95	0.48
12:J:146:PRO:HA	12:J:326:MET:HG2	1.95	0.48
16:N:595:ALA:HB3	16:N:719:ALA:HB1	1.95	0.48
16:N:608:VAL:O	16:N:612:GLY:N	2.31	0.47
2:B:313:ARG:HG2	2:B:448:GLY:HA3	1.95	0.47
3:C:632:TYR:HD1	13:K:244:PHE:HE1	1.62	0.47
6:E:488:GLU:HA	6:E:491:ASN:HD21	1.79	0.47
6:E:544:ALA:O	6:E:548:MET:HG3	2.14	0.47
12:J:146:PRO:HG2	12:J:149:LEU:HD13	1.95	0.47
2:B:283:PRO:HB2	7:F:566:LEU:HD23	1.96	0.47
4:c:1072:PHE:HB2	7:F:92:GLU:HA	1.95	0.47
3:C:186:PHE:O	16:N:700:ARG:NH2	2.36	0.47
5:D:93:ILE:HG12	5:D:96:MET:HE2	1.96	0.47
14:L:155:PHE:HZ	14:L:252:TRP:CZ2	2.32	0.47
3:C:229:LEU:HD21	3:C:244:VAL:HG13	1.97	0.47
11:i:531:VAL:HG23	11:i:539:HIS:HB2	1.97	0.47
1:a:64:ARG:HH12	1:a:163:HIS:HA	1.78	0.47
3:C:676:ALA:HA	17:O:61:GLN:HE22	1.79	0.47
5:D:64:GLY:N	5:D:66:GLU:OE1	2.48	0.47
6:E:715:PRO:HG3	6:E:763:VAL:HA	1.97	0.47
9:H:282:THR:HG22	13:K:322:LEU:HD12	1.96	0.47
11:i:508:SER:O	11:i:511:THR:OG1	2.33	0.47
1:A:13:LEU:HA	1:A:36:PRO:HG2	1.97	0.47
2:B:462:THR:O	10:I:154:ASN:ND2	2.48	0.47
5:D:96:MET:HE3	5:D:103:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:822:ASN:HA	5:D:825:GLN:HG2	1.96	0.47
10:I:222:MET:HE2	10:I:234:GLU:HG2	1.96	0.47
2:B:127:LEU:HD11	2:B:313:ARG:HE	1.80	0.47
3:C:311:ASN:HA	3:C:314:THR:HG22	1.96	0.47
4:c:424:ARG:O	4:c:425:ALA:C	2.58	0.47
5:D:144:LEU:HD11	5:D:179:VAL:HG21	1.96	0.47
5:D:496:GLU:C	5:D:498:PRO:HD3	2.40	0.47
16:N:728:ILE:HA	16:N:733:LYS:HA	1.97	0.47
5:D:315:LYS:HB3	5:D:317:VAL:HG23	1.97	0.47
6:E:522:ARG:NH2	6:E:554:ASP:O	2.49	0.47
17:O:137:ASP:OD1	17:O:137:ASP:N	2.43	0.47
3:C:673:ILE:HG21	4:c:7:LEU:HD22	1.95	0.46
4:c:445:ASP:OD1	4:c:1125:GLU:N	2.48	0.46
12:J:297:ASP:OD1	12:J:297:ASP:N	2.47	0.46
2:B:1006:LEU:HD21	4:c:1316:VAL:HG13	1.96	0.46
3:C:621:ILE:HA	13:K:202:VAL:HG21	1.96	0.46
9:H:391:VAL:HG11	10:I:476:LEU:HD13	1.97	0.46
4:c:205:ARG:HH21	4:c:1274:ILE:HB	1.80	0.46
4:c:931:LEU:HB3	7:F:84:ASP:O	2.16	0.46
6:E:607:ARG:HG3	6:E:610:MET:HB2	1.96	0.46
7:F:286:ALA:HB3	7:F:294:PHE:HB2	1.96	0.46
7:F:370:ASP:OD1	7:F:370:ASP:N	2.44	0.46
4:c:473:HIS:HD2	4:c:1106:PRO:HB2	1.80	0.46
4:c:1036:ASN:ND2	4:c:1038:ASP:O	2.48	0.46
5:D:500:ILE:HG23	5:D:502:GLY:H	1.80	0.46
7:F:159:LEU:HD13	7:F:318:HIS:CE1	2.50	0.46
16:N:656:ASP:N	16:N:656:ASP:OD1	2.48	0.46
2:B:486:ALA:O	2:B:495:GLN:NE2	2.47	0.46
4:c:291:CYS:HB3	4:c:1226:ARG:NH1	2.30	0.46
6:E:459:ILE:HD12	6:E:493:LEU:HG	1.96	0.46
12:J:395:PRO:HA	12:J:398:TYR:CZ	2.51	0.46
18:P:88:LEU:HD12	18:P:138:ARG:HE	1.80	0.46
5:D:853:ASP:OD1	5:D:853:ASP:N	2.49	0.46
6:E:433:HIS:HB2	6:E:462:TYR:CE1	2.50	0.46
12:J:116:ILE:HD11	12:J:343:MET:HG3	1.98	0.46
10:I:389:LEU:HD23	10:I:447:LEU:HB3	1.98	0.46
2:B:440:ILE:HD12	2:B:521:PHE:HB3	1.98	0.46
3:C:459:LEU:HD23	3:C:473:PHE:HD2	1.81	0.46
4:c:211:GLN:HG2	4:c:320:ILE:HD11	1.97	0.46
6:E:574:ASP:OD1	6:E:574:ASP:N	2.49	0.46
1:A:88:LEU:HD22	1:A:172:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:290:SER:HB2	1:a:309:ILE:HD12	1.97	0.46
2:B:383:PRO:HB3	2:B:575:SER:HB2	1.98	0.46
4:c:122:THR:O	4:c:124:PRO:HD3	2.15	0.46
5:D:602:LEU:H	5:D:602:LEU:HD23	1.81	0.46
10:I:304:ARG:O	10:I:308:ARG:HB2	2.15	0.46
1:a:123:LEU:HD11	1:a:129:ILE:HG23	1.98	0.46
4:c:287:THR:OG1	4:c:1222:GLU:OE1	2.34	0.46
6:E:701:ARG:NH1	6:E:702:ASN:O	2.49	0.46
11:i:557:LEU:HD11	11:i:562:SER:HA	1.98	0.46
15:M:98:ALA:HB3	15:M:144:LEU:HD21	1.97	0.46
2:B:934:ASN:HB3	3:C:602:LYS:HZ1	1.81	0.45
5:D:426:GLY:HA3	5:D:835:GLY:HA3	1.98	0.45
15:M:91:PRO:HB3	15:M:178:LEU:HD13	1.98	0.45
15:m:144:LEU:HA	15:m:144:LEU:HD13	1.73	0.45
2:B:312:LYS:HE2	2:B:395:TYR:HE2	1.81	0.45
5:D:497:GLY:N	5:D:498:PRO:HD3	2.31	0.45
14:L:173:GLY:O	14:L:225:VAL:HG22	2.16	0.45
2:B:101:ILE:HG22	2:B:361:LEU:HD12	1.97	0.45
1:a:35:SER:HA	1:a:198:ILE:HG23	1.98	0.45
2:B:425:ASP:OD1	2:B:550:ARG:NH2	2.39	0.45
3:C:345:ASN:HA	3:C:348:ARG:HG2	1.98	0.45
3:C:441:GLU:O	3:C:444:VAL:HG12	2.16	0.45
14:L:126:GLN:HA	14:L:129:TRP:CD1	2.51	0.45
18:P:83:TRP:HH2	18:P:125:LEU:HD11	1.80	0.45
1:a:213:GLU:OE2	11:i:308:ARG:NH1	2.50	0.45
5:D:391:ALA:HB2	5:D:795:LEU:HD13	1.97	0.45
3:C:135:ASN:HA	3:C:250:PHE:HE1	1.82	0.45
11:i:406:LYS:HD2	11:i:438:ARG:HG3	1.98	0.45
1:A:34:LEU:HD23	1:A:37:LEU:HD11	1.98	0.45
3:C:211:ALA:HB1	5:D:452:ARG:HD3	1.98	0.45
4:c:255:MET:HE3	12:J:168:VAL:HG11	1.99	0.45
6:E:562:ALA:O	6:E:566:VAL:HG23	2.17	0.45
7:F:371:THR:OG1	18:P:104:GLN:NE2	2.50	0.45
10:I:129:PHE:CE1	15:M:143:GLY:HA3	2.52	0.45
16:N:686:PRO:HB3	16:N:692:ARG:HE	1.82	0.45
2:B:52:LEU:HA	2:B:84:ALA:HB1	1.99	0.45
4:c:386:TYR:HB3	4:c:397:ASN:HD22	1.82	0.45
3:C:650:SER:HB3	3:C:656:LEU:HD11	1.98	0.44
6:E:747:VAL:HG13	6:E:748:VAL:HG12	1.99	0.44
4:c:1182:ILE:HG23	4:c:1184:TRP:HB2	1.98	0.44
5:D:115:HIS:HB3	5:D:120:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:i:428:LEU:HD11	11:i:457:PRO:HG3	1.99	0.44
1:A:322:GLY:O	1:A:326:LYS:N	2.50	0.44
2:B:129:SER:O	2:B:133:TYR:OH	2.27	0.44
5:D:786:ILE:O	5:D:789:MET:HG3	2.17	0.44
6:E:573:VAL:HG13	6:E:601:ILE:HG22	1.99	0.44
6:E:742:LEU:HD11	6:E:790:VAL:HB	1.99	0.44
12:J:309:ASN:ND2	12:J:342:GLU:OE2	2.51	0.44
13:K:273:ASP:OD1	13:K:273:ASP:N	2.50	0.44
4:c:68:LYS:HG3	4:c:111:LEU:HD21	2.00	0.44
14:L:158:PHE:HD1	14:L:158:PHE:HA	1.60	0.44
18:P:50:VAL:HG21	18:P:107:MET:HE1	1.98	0.44
18:P:72:TRP:HB2	18:P:135:TYR:HE1	1.82	0.44
1:a:203:ILE:HB	1:a:211:PRO:HB3	1.99	0.44
2:B:535:GLU:HG2	2:B:887:PHE:HA	1.99	0.44
4:c:1239:MET:HG3	4:c:1245:PRO:HD3	2.00	0.44
11:i:438:ARG:HD2	11:i:441:LYS:HD2	1.99	0.44
16:N:346:LEU:HA	16:N:417:VAL:HA	1.99	0.44
6:E:697:GLU:O	6:E:709:ASP:HB3	2.18	0.44
12:J:309:ASN:HB2	12:J:344:THR:HG22	1.99	0.44
16:N:305:SER:HA	16:N:323:GLU:HA	2.00	0.44
16:N:654:THR:H	16:N:730:GLY:HA2	1.83	0.44
2:B:261:ILE:HG22	2:B:447:TRP:HE3	1.83	0.44
3:C:43:GLU:OE2	3:C:115:LYS:N	2.51	0.44
7:F:487:ASN:OD1	7:F:488:LYS:N	2.51	0.44
1:A:27:LEU:HD21	17:O:56:PRO:HB3	1.99	0.44
2:B:79:GLU:OE1	2:B:79:GLU:N	2.49	0.44
18:P:61:LEU:HD22	18:P:66:VAL:HG21	1.98	0.44
3:C:308:TYR:HA	3:C:311:ASN:ND2	2.33	0.44
4:c:1256:ARG:HB3	5:D:308:GLY:HA3	2.00	0.44
5:D:490:LEU:HB3	5:D:516:LEU:HD23	1.98	0.44
6:E:440:LEU:HD11	6:E:458:VAL:HG21	1.98	0.44
8:G:227:ASP:OD1	8:G:227:ASP:N	2.36	0.44
12:J:382:LEU:HD13	12:J:425:THR:HG21	1.98	0.44
13:K:157:ASP:OD1	13:K:157:ASP:N	2.46	0.44
10:I:126:GLN:NE2	15:M:162:GLU:OE1	2.50	0.43
14:L:144:LEU:HD23	14:L:144:LEU:HA	1.79	0.43
3:C:123:VAL:HG13	3:C:124:TRP:CD1	2.54	0.43
4:c:1253:ARG:HG2	4:c:1257:MET:HE2	2.00	0.43
6:E:250:SER:O	6:E:251:ALA:C	2.60	0.43
12:J:321:ARG:NE	12:J:328:GLU:OE2	2.40	0.43
1:a:13:LEU:HA	1:a:36:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:185:ASP:OD1	7:F:185:ASP:N	2.50	0.43
3:C:67:ILE:HG13	3:C:68:PHE:CD2	2.54	0.43
4:c:1070:GLY:HA2	4:c:1090:GLN:HE21	1.81	0.43
5:D:416:ILE:HG23	5:D:418:PRO:HD2	2.00	0.43
6:E:427:CYS:O	6:E:431:GLY:N	2.51	0.43
7:F:176:ASP:HB3	8:G:101:GLY:HA3	2.00	0.43
3:C:136:LEU:HD11	3:C:261:PHE:HE2	1.83	0.43
4:c:293:SER:OG	4:c:296:TRP:O	2.34	0.43
4:c:381:CYS:HB2	4:c:404:SER:HB3	2.00	0.43
4:c:448:MET:HE2	4:c:1123:LEU:HD11	2.00	0.43
6:E:747:VAL:HG12	6:E:788:ARG:HA	1.99	0.43
12:J:111:PHE:HE1	12:J:145:ILE:HG12	1.84	0.43
1:a:15:TRP:HB3	1:a:34:LEU:HD13	2.00	0.43
1:a:231:HIS:CD2	11:i:609:LEU:HD22	2.54	0.43
2:B:418:TYR:HB3	2:B:523:TYR:HE2	1.84	0.43
3:C:303:TYR:HA	3:C:306:VAL:HG22	2.00	0.43
4:c:186:ARG:HA	4:c:189:VAL:HG22	2.01	0.43
10:I:429:LYS:HD2	10:I:446:GLN:HG3	2.01	0.43
3:C:245:GLY:HA2	3:C:248:LYS:HG2	2.00	0.43
3:C:280:PRO:HG2	3:C:283:LEU:HB2	2.00	0.43
4:c:1292:GLU:O	4:c:1293:THR:HG22	2.18	0.43
5:D:487:ARG:O	5:D:490:LEU:HG	2.19	0.43
4:c:224:ARG:NH2	5:D:747:ILE:O	2.51	0.43
8:G:136:SER:HA	8:G:248:ARG:HH22	1.83	0.43
11:i:279:LEU:HD11	11:i:342:ALA:HB2	2.00	0.43
11:i:326:CYS:SG	11:i:327:SER:N	2.91	0.43
15:M:107:MET:HG3	15:M:111:LEU:HD23	2.00	0.43
2:B:519:PHE:HB2	2:B:522:GLN:HB2	2.00	0.43
3:C:678:GLN:HE22	17:O:54:ARG:HA	1.83	0.43
7:F:372:ASN:HD22	7:F:375:GLU:HG3	1.84	0.43
12:J:467:LEU:HA	12:J:481:ILE:HD12	2.01	0.43
16:N:240:ALA:HB2	16:N:257:LEU:H	1.83	0.43
1:A:57:ILE:HG22	1:A:178:PRO:HG2	2.01	0.43
4:c:25:ARG:NH1	13:K:204:GLU:OE1	2.33	0.43
7:F:177:TRP:CH2	7:F:231:TYR:HA	2.54	0.43
4:c:1292:GLU:HG2	4:c:1295:ARG:HE	1.85	0.42
5:D:477:ARG:HD2	5:D:477:ARG:HA	1.90	0.42
6:E:706:TRP:CD1	6:E:725:TRP:HE1	2.37	0.42
14:L:175:ALA:O	14:L:222:THR:HA	2.18	0.42
15:m:167:ILE:HA	15:m:170:MET:HE2	2.00	0.42
2:B:511:GLU:OE2	10:I:358:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:PHE:HZ	3:C:468:LEU:HD12	1.83	0.42
3:C:629:GLU:HG2	13:K:282:ARG:HG2	2.01	0.42
4:c:286:ARG:HG2	4:c:301:CYS:HA	2.00	0.42
5:D:384:LEU:HD22	5:D:787:LYS:HZ2	1.84	0.42
6:E:433:HIS:HB2	6:E:462:TYR:HE1	1.83	0.42
7:F:565:PRO:O	7:F:566:LEU:HB2	2.18	0.42
11:i:265:ASP:N	11:i:265:ASP:OD1	2.50	0.42
2:B:633:LYS:HG2	15:M:116:VAL:HG21	2.02	0.42
4:c:93:ALA:C	4:c:438:LYS:HZ1	2.27	0.42
4:c:982:LEU:HB2	7:F:279:ILE:HG13	2.02	0.42
10:I:115:ASN:HB3	10:I:116:PRO:HD3	2.00	0.42
10:I:448:ARG:NH2	10:I:485:MET:SD	2.92	0.42
17:O:110:ALA:HB2	17:O:131:GLU:HG3	2.01	0.42
3:C:188:THR:O	3:C:189:GLN:HB2	2.18	0.42
3:C:541:ASP:HB3	4:c:47:PHE:HE1	1.85	0.42
6:E:637:ASP:O	6:E:681:ARG:NH2	2.50	0.42
6:E:670:ILE:HD11	6:E:685:VAL:HB	1.99	0.42
12:J:365:PRO:HD3	12:J:486:HIS:CE1	2.54	0.42
13:K:123:TRP:HD1	13:K:125:SER:HB2	1.83	0.42
4:c:1084:PRO:HA	4:c:1085:PRO:HD3	1.91	0.42
4:c:1196:GLN:HE21	5:D:731:PHE:HD1	1.68	0.42
5:D:319:PRO:HG3	5:D:760:TRP:CD2	2.54	0.42
14:L:107:TYR:O	14:L:108:ASN:C	2.63	0.42
14:L:231:TYR:O	14:L:232:LEU:C	2.61	0.42
3:C:401:ARG:NH2	17:O:68:GLY:O	2.42	0.42
4:c:380:LEU:HD22	4:c:424:ARG:HH22	1.84	0.42
5:D:412:VAL:HG12	5:D:788:VAL:HG12	2.00	0.42
5:D:416:ILE:HD12	5:D:416:ILE:HA	1.92	0.42
6:E:716:GLY:O	6:E:720:THR:HG23	2.20	0.42
14:L:133:LYS:O	14:L:134:PRO:C	2.62	0.42
2:B:795:GLY:C	2:B:797:SER:N	2.74	0.42
3:C:682:ARG:NH2	17:O:58:LEU:HB3	2.35	0.42
4:c:1176:ILE:HD12	4:c:1176:ILE:HA	1.94	0.42
4:c:1256:ARG:HE	5:D:305:GLU:CD	2.28	0.42
5:D:178:LEU:HD22	5:D:211:ILE:HD12	2.00	0.42
6:E:600:ALA:HB2	6:E:672:ALA:HA	2.01	0.42
13:K:318:HIS:O	13:K:321:LYS:HG2	2.19	0.42
1:a:119:GLN:H	1:a:119:GLN:HG3	1.62	0.42
2:B:413:ILE:HD13	2:B:423:PRO:HB3	2.02	0.42
2:B:854:PRO:HG2	2:B:855:LEU:HD12	2.02	0.42
3:C:479:GLU:OE1	3:C:479:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:559:VAL:HG13	3:C:560:ASN:HD22	1.85	0.42
6:E:543:LYS:O	6:E:546:VAL:HG12	2.19	0.42
8:G:184:LEU:HD22	8:G:256:VAL:HG11	2.02	0.42
2:B:251:PHE:HA	2:B:255:ARG:HD3	2.02	0.42
3:C:147:LEU:HD22	3:C:154:PHE:CE2	2.55	0.42
3:C:596:ILE:HD12	3:C:671:ARG:NH1	2.34	0.42
10:I:140:MET:HE3	10:I:150:MET:HB2	2.01	0.42
4:c:115:MET:HE2	4:c:115:MET:HB3	1.92	0.42
7:F:539:LEU:HD23	7:F:539:LEU:HA	1.92	0.41
16:N:600:ALA:HA	16:N:603:ARG:HG2	2.01	0.41
18:P:59:ASP:OD1	18:P:60:ARG:N	2.52	0.41
3:C:49:THR:HB	3:C:62:LEU:H	1.85	0.41
3:C:486:HIS:HE2	4:c:43:LYS:HE2	1.84	0.41
4:c:495:GLN:O	7:F:363:PRO:HB3	2.20	0.41
12:J:157:LEU:HB3	12:J:158:PRO:HD3	2.03	0.41
14:L:147:LEU:HD22	14:L:147:LEU:HA	1.93	0.41
1:A:15:TRP:HH2	1:A:212:LYS:HE2	1.84	0.41
1:a:105:ASP:OD1	1:a:105:ASP:N	2.54	0.41
1:a:274:ILE:HD11	1:a:292:ILE:HG22	2.02	0.41
2:B:27:ILE:HD13	9:H:423:LEU:HD23	2.03	0.41
3:C:621:ILE:HD13	13:K:202:VAL:HG11	2.03	0.41
5:D:110:GLY:HA2	5:D:113:VAL:HG12	2.02	0.41
6:E:565:SER:HA	6:E:568:CYS:HB3	2.02	0.41
7:F:180:ARG:HH21	8:G:98:ILE:HD11	1.85	0.41
8:G:65:LEU:HD13	8:G:239:LEU:HD22	2.02	0.41
10:I:224:ILE:HG13	10:I:225:LYS:H	1.85	0.41
15:M:144:LEU:HD12	15:M:144:LEU:HA	1.69	0.41
1:a:320:ILE:HA	1:a:323:ILE:HG12	2.01	0.41
3:C:261:PHE:HA	3:C:264:THR:HG22	2.01	0.41
4:c:1039:PRO:HA	7:F:212:VAL:HG11	2.02	0.41
4:c:1180:LEU:O	4:c:1185:GLY:HA3	2.20	0.41
5:D:416:ILE:HG21	5:D:806:VAL:HG21	2.02	0.41
6:E:331:ALA:O	6:E:335:PHE:N	2.49	0.41
7:F:550:VAL:O	7:F:552:PRO:HD3	2.21	0.41
1:A:35:SER:HA	1:A:198:ILE:HG12	2.02	0.41
1:a:18:VAL:HG13	9:H:351:CYS:HA	2.01	0.41
2:B:107:MET:HE1	2:B:317:VAL:HG11	2.01	0.41
2:B:124:ASN:HD22	2:B:316:SER:HA	1.86	0.41
4:c:473:HIS:ND1	7:F:102:ARG:HD2	2.35	0.41
1:A:314:SER:O	1:A:317:VAL:HG12	2.20	0.41
1:a:227:ILE:HD13	1:a:227:ILE:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:1274:ILE:HD13	4:c:1274:ILE:HA	1.94	0.41
4:c:1312:LEU:HD21	4:c:1324:VAL:HG21	2.01	0.41
12:J:180:ASN:ND2	12:J:182:GLU:OE2	2.54	0.41
4:c:85:HIS:O	4:c:86:HIS:C	2.63	0.41
6:E:556:ASP:N	6:E:559:THR:OG1	2.54	0.41
7:F:420:LEU:HD22	7:F:483:ARG:HG2	2.03	0.41
10:I:124:ALA:HB1	10:I:240:ALA:HB1	2.02	0.41
3:C:596:ILE:HD12	3:C:671:ARG:HH11	1.85	0.41
7:F:151:ILE:HG21	7:F:317:HIS:CE1	2.52	0.41
12:J:180:ASN:HD22	12:J:183:THR:HG22	1.85	0.41
12:J:243:GLN:HE22	12:J:281:GLN:HE22	1.69	0.41
13:K:163:PHE:CE1	13:K:190:ILE:HD11	2.56	0.41
14:L:155:PHE:HZ	14:L:252:TRP:CE2	2.39	0.41
1:a:106:ALA:HB3	1:a:149:LEU:HB2	2.02	0.41
1:a:118:ALA:C	1:a:120:ASP:N	2.79	0.41
2:B:372:HIS:CE1	2:B:398:PRO:HG2	2.56	0.41
2:B:565:THR:HG23	2:B:567:LEU:H	1.85	0.41
3:C:302:LEU:HB3	3:C:342:LEU:HD13	2.03	0.41
5:D:854:ALA:O	5:D:858:ILE:HG12	2.21	0.41
6:E:416:ASN:H	6:E:419:THR:CB	2.34	0.41
6:E:560:LEU:HB3	6:E:583:ILE:HD11	2.03	0.41
7:F:400:LEU:HD23	7:F:402:ASN:H	1.86	0.41
8:G:55:LEU:HD21	8:G:83:ARG:HB2	2.03	0.41
10:I:428:ARG:NH1	10:I:432:THR:HG21	2.36	0.41
11:i:480:ILE:HG23	11:i:528:VAL:HG23	2.03	0.41
13:K:155:ASP:OD1	13:K:155:ASP:N	2.52	0.41
16:N:657:PRO:HB2	16:N:658:LEU:HD12	2.02	0.41
1:a:38:MET:HG2	1:a:39:LYS:H	1.86	0.41
2:B:63:LEU:H	2:B:63:LEU:HD23	1.85	0.41
4:c:362:PHE:HB3	4:c:387:VAL:HG12	2.02	0.41
4:c:1146:LEU:HB2	4:c:1147:PRO:HD3	2.03	0.41
6:E:490:PHE:CD2	6:E:518:VAL:HG21	2.55	0.41
8:G:180:ILE:CG2	8:G:213:LEU:HB3	2.51	0.41
12:J:116:ILE:HD12	12:J:116:ILE:HA	1.85	0.41
17:O:104:ASN:OD1	17:O:104:ASN:N	2.54	0.41
1:A:62:ILE:HD13	1:A:149:LEU:HD23	2.02	0.40
1:a:37:LEU:HD12	1:a:37:LEU:HA	1.92	0.40
1:a:227:ILE:N	1:a:228:PRO:HD2	2.35	0.40
12:J:142:ILE:HG12	12:J:329:VAL:O	2.21	0.40
3:C:521:PHE:HD1	3:C:521:PHE:HA	1.79	0.40
3:C:523:HIS:HD2	3:C:524:MET:HE3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:533:ASP:OD1	3:C:533:ASP:N	2.53	0.40
4:c:150:ARG:HD3	4:c:173:LEU:HD21	2.04	0.40
4:c:163:LEU:HD23	4:c:176:THR:HG21	2.03	0.40
10:I:128:GLU:HG3	15:M:164:LEU:HD22	2.02	0.40
14:L:173:GLY:C	14:L:225:VAL:HG22	2.47	0.40
15:m:113:MET:O	15:m:116:VAL:HG12	2.21	0.40
16:N:687:LEU:HD21	16:N:693:LEU:HB2	2.04	0.40
1:A:173:ASP:OD1	1:A:173:ASP:N	2.51	0.40
1:a:281:SER:O	1:a:285:ASN:ND2	2.55	0.40
2:B:454:PHE:HB2	2:B:469:LEU:HD23	2.04	0.40
4:c:1038:ASP:HB3	4:c:1041:ARG:HB2	2.02	0.40
5:D:130:ARG:HH12	6:E:470:GLU:HG3	1.86	0.40
5:D:757:THR:HG23	5:D:762:TRP:CD1	2.57	0.40
5:D:840:ASP:HB2	5:D:873:THR:HG21	2.02	0.40
7:F:420:LEU:HD11	7:F:480:PHE:HA	2.03	0.40
7:F:580:LYS:O	7:F:581:SER:C	2.65	0.40
10:I:210:LYS:HD3	10:I:210:LYS:HA	1.88	0.40
11:i:584:HIS:CD2	11:i:585:LEU:HG	2.57	0.40
7:F:216:THR:OG1	7:F:217:ASP:N	2.54	0.40
9:H:318:TRP:O	9:H:357:GLU:HB3	2.22	0.40
12:J:139:ALA:HB1	12:J:330:MET:HB3	2.03	0.40
12:J:308:MET:O	12:J:347:TYR:OH	2.32	0.40
13:K:144:LEU:HD13	13:K:220:GLU:HG2	2.03	0.40
13:K:263:VAL:HG12	13:K:265:THR:HG23	2.02	0.40
1:A:110:VAL:HG11	1:A:117:THR:HG22	2.04	0.40
1:a:50:ARG:NH1	1:a:182:ALA:O	2.54	0.40
2:B:380:ARG:HD2	2:B:620:MET:HE1	2.04	0.40
2:B:673:ILE:HG22	2:B:850:MET:HG2	2.03	0.40
4:c:1262:GLU:HB2	5:D:342:ARG:NH2	2.36	0.40
5:D:338:ARG:HG3	5:D:339:GLU:OE1	2.21	0.40
6:E:630:ILE:HD13	6:E:665:PHE:HZ	1.87	0.40
11:i:392:ARG:HD3	11:i:392:ARG:HA	1.91	0.40
16:N:601:LEU:HD22	16:N:634:MET:HE3	2.03	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	289/337 (86%)	277 (96%)	12 (4%)	0	100	100
1	a	314/337 (93%)	303 (96%)	11 (4%)	0	100	100
2	B	897/1070 (84%)	862 (96%)	35 (4%)	0	100	100
3	C	584/688 (85%)	555 (95%)	29 (5%)	0	100	100
4	c	1160/1388 (84%)	1124 (97%)	36 (3%)	0	100	100
5	D	639/892 (72%)	620 (97%)	19 (3%)	0	100	100
6	E	698/860 (81%)	680 (97%)	18 (3%)	0	100	100
7	F	542/682 (80%)	529 (98%)	13 (2%)	0	100	100
8	G	216/266 (81%)	211 (98%)	5 (2%)	0	100	100
9	H	258/531 (49%)	254 (98%)	4 (2%)	0	100	100
10	I	372/486 (76%)	349 (94%)	23 (6%)	0	100	100
11	i	381/648 (59%)	365 (96%)	16 (4%)	0	100	100
12	J	420/507 (83%)	404 (96%)	16 (4%)	0	100	100
13	K	212/331 (64%)	207 (98%)	5 (2%)	0	100	100
14	L	230/303 (76%)	220 (96%)	9 (4%)	1 (0%)	30	65
15	M	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
15	m	107/178 (60%)	100 (94%)	7 (6%)	0	100	100
16	N	535/770 (70%)	521 (97%)	14 (3%)	0	100	100
17	O	86/167 (52%)	84 (98%)	2 (2%)	0	100	100
18	P	103/143 (72%)	99 (96%)	4 (4%)	0	100	100
All	All	8157/10762 (76%)	7876 (97%)	280 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	L	134	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/308 (72%)	222 (100%)	1 (0%)	84	90
1	a	257/308 (83%)	251 (98%)	6 (2%)	44	74
2	B	667/924 (72%)	661 (99%)	6 (1%)	70	85
3	C	429/612 (70%)	421 (98%)	8 (2%)	50	76
4	c	679/1238 (55%)	665 (98%)	14 (2%)	47	75
5	D	528/770 (69%)	522 (99%)	6 (1%)	65	83
6	E	300/741 (40%)	291 (97%)	9 (3%)	36	69
7	F	395/615 (64%)	392 (99%)	3 (1%)	73	86
8	G	172/232 (74%)	169 (98%)	3 (2%)	53	78
9	H	212/472 (45%)	210 (99%)	2 (1%)	70	85
10	I	287/437 (66%)	284 (99%)	3 (1%)	68	84
11	i	316/567 (56%)	308 (98%)	8 (2%)	42	72
12	J	352/449 (78%)	346 (98%)	6 (2%)	53	78
13	K	199/300 (66%)	197 (99%)	2 (1%)	68	84
14	L	83/258 (32%)	74 (89%)	9 (11%)	6	26
15	M	103/160 (64%)	103 (100%)	0	100	100
15	m	92/160 (58%)	89 (97%)	3 (3%)	33	67
16	N	95/659 (14%)	91 (96%)	4 (4%)	26	61
17	O	69/144 (48%)	69 (100%)	0	100	100
18	P	91/129 (70%)	89 (98%)	2 (2%)	45	74
All	All	5549/9483 (58%)	5454 (98%)	95 (2%)	52	78

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
1	a	107	SER
1	a	108	ILE

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Mol	Chain	Res	Type
1	a	110	VAL
1	a	119	GLN
1	a	227	ILE
1	a	246	VAL
2	B	127	LEU
2	B	349	ILE
2	B	366	GLU
2	B	535	GLU
2	B	645	VAL
2	B	649	LEU
3	C	44	VAL
3	C	114	ILE
3	C	123	VAL
3	C	172	GLU
3	C	257	LEU
3	C	283	LEU
3	C	327	LEU
3	C	521	PHE
4	c	94	VAL
4	c	102	GLU
4	c	103	ILE
4	c	210	VAL
4	c	350	GLU
4	c	369	PRO
4	c	383	ILE
4	c	988	ILE
4	c	1050	LEU
4	c	1128	THR
4	c	1129	LEU
4	c	1265	ILE
4	c	1292	GLU
4	c	1293	THR
5	D	381	VAL
5	D	383	LEU
5	D	449	VAL
5	D	740	VAL
5	D	804	CYS
5	D	862	LEU
6	E	424	ILE
6	E	502	LEU
6	E	634	ILE
6	E	653	LYS

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Mol	Chain	Res	Type
6	E	673	LEU
6	E	676	LEU
6	E	697	GLU
6	E	708	VAL
6	E	757	ILE
7	F	420	LEU
7	F	499	VAL
7	F	594	ILE
8	G	135	GLU
8	G	174	LEU
8	G	256	VAL
9	H	238	TRP
9	H	354	THR
10	I	200	ASN
10	I	323	VAL
10	I	443	LEU
11	i	341	VAL
11	i	399	SER
11	i	454	VAL
11	i	483	VAL
11	i	531	VAL
11	i	539	HIS
11	i	558	THR
11	i	587	THR
12	J	116	ILE
12	J	119	ARG
12	J	245	GLN
12	J	278	CYS
12	J	400	HIS
12	J	402	SER
13	K	173	THR
13	K	298	ASP
14	L	144	LEU
14	L	145	LEU
14	L	147	LEU
14	L	158	PHE
14	L	208	ASN
14	L	225	VAL
14	L	251	SER
14	L	255	VAL
14	L	282	GLU
15	m	72	VAL

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Mol	Chain	Res	Type
15	m	101	CYS
15	m	144	LEU
16	N	619	VAL
16	N	661	LEU
16	N	701	VAL
16	N	759	THR
18	P	52	VAL
18	P	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	196	GLN
1	A	221	ASN
1	A	276	GLN
1	A	285	ASN
1	a	41	GLN
1	a	85	HIS
1	a	150	GLN
1	a	187	HIS
1	a	231	HIS
2	B	58	GLN
2	B	124	ASN
2	B	128	GLN
2	B	276	GLN
2	B	322	GLN
2	B	334	ASN
2	B	372	HIS
2	B	386	GLN
2	B	503	GLN
2	B	522	GLN
2	B	551	GLN
2	B	621	HIS
2	B	622	GLN
2	B	625	GLN
2	B	636	GLN
2	B	666	ASN
2	B	810	GLN
2	B	910	GLN
2	B	934	ASN
2	B	938	GLN

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Mol	Chain	Res	Type
2	B	1000	HIS
3	C	110	GLN
3	C	135	ASN
3	C	209	GLN
3	C	300	ASN
3	C	311	ASN
3	C	331	GLN
3	C	400	HIS
3	C	449	GLN
3	C	453	GLN
3	C	455	HIS
3	C	460	ASN
3	C	471	GLN
3	C	474	GLN
3	C	501	GLN
3	C	505	HIS
3	C	513	GLN
3	C	523	HIS
3	C	525	ASN
3	C	560	ASN
4	c	11	ASN
4	c	73	GLN
4	c	77	GLN
4	c	90	ASN
4	c	145	GLN
4	c	374	HIS
4	c	376	HIS
4	c	397	ASN
4	c	399	ASN
4	c	464	ASN
4	c	497	GLN
4	c	924	GLN
4	c	1007	ASN
4	c	1019	GLN
4	c	1049	ASN
4	c	1071	GLN
4	c	1095	GLN
4	c	1118	HIS
4	c	1151	GLN
4	c	1196	GLN
4	c	1207	GLN
4	c	1212	GLN

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Mol	Chain	Res	Type
4	c	1215	GLN
5	D	175	GLN
5	D	194	ASN
5	D	343	HIS
5	D	420	GLN
5	D	882	GLN
6	E	464	GLN
6	E	476	ASN
6	E	491	ASN
6	E	579	GLN
6	E	612	HIS
6	E	643	ASN
6	E	711	HIS
6	E	727	ASN
6	E	792	GLN
7	F	81	ASN
7	F	128	ASN
7	F	148	GLN
7	F	196	HIS
7	F	251	GLN
7	F	288	HIS
7	F	317	HIS
7	F	318	HIS
7	F	372	ASN
7	F	402	ASN
7	F	518	HIS
7	F	591	ASN
8	G	82	HIS
8	G	96	ASN
8	G	116	ASN
8	G	151	GLN
8	G	226	ASN
8	G	238	HIS
8	G	253	GLN
9	H	195	GLN
9	H	216	HIS
9	H	247	GLN
9	H	271	GLN
9	H	300	GLN
9	H	320	GLN
9	H	332	GLN
9	H	334	HIS

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Mol	Chain	Res	Type
9	H	345	GLN
9	H	353	GLN
9	H	399	GLN
10	I	139	GLN
10	I	142	GLN
10	I	193	GLN
10	I	200	ASN
10	I	317	GLN
10	I	346	GLN
10	I	390	HIS
10	I	440	GLN
11	i	287	GLN
11	i	354	GLN
11	i	361	ASN
11	i	363	ASN
11	i	539	HIS
11	i	607	GLN
12	J	243	GLN
12	J	244	GLN
12	J	254	ASN
12	J	288	GLN
12	J	299	ASN
12	J	313	GLN
12	J	381	HIS
12	J	400	HIS
12	J	496	GLN
13	K	121	GLN
13	K	313	GLN
15	M	109	GLN
15	M	155	ASN
15	M	176	ASN
15	m	81	GLN
16	N	691	HIS
17	O	61	GLN
17	O	77	HIS
17	O	85	ASN
17	O	99	GLN
18	P	104	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](#)

Of 4 ligands modelled in this entry, 4 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.

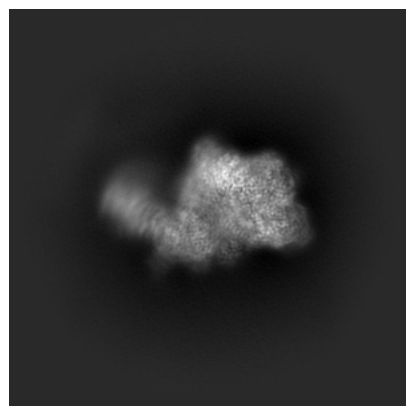
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37386. These allow visual inspection of the internal detail of the map and identification of artifacts.

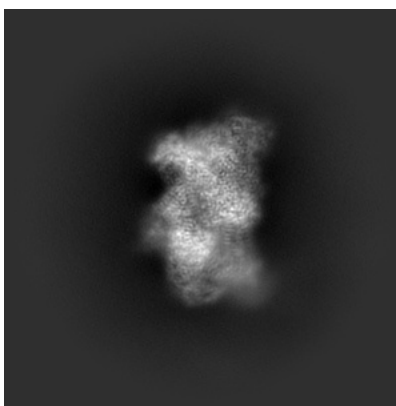
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

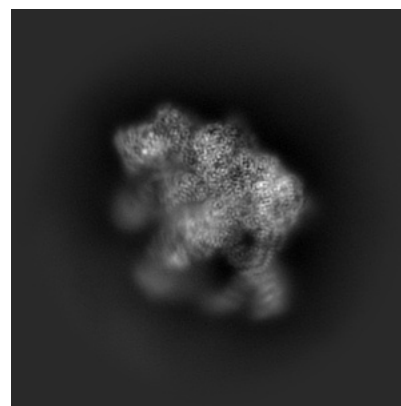
6.1.1 Primary map



X

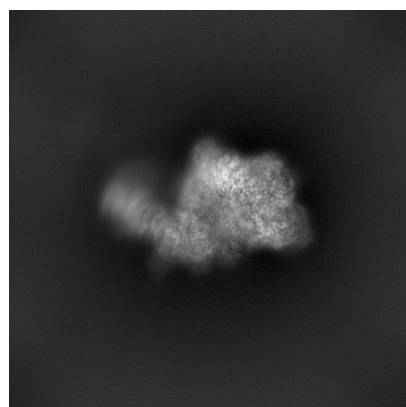


Y

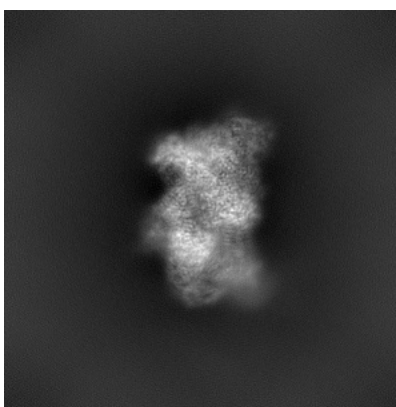


Z

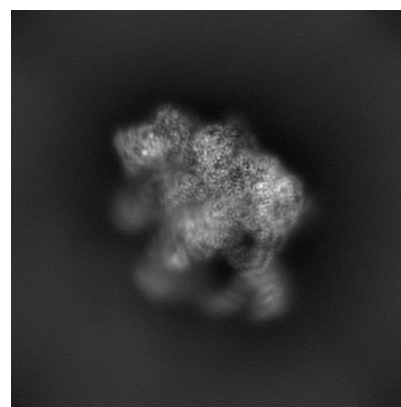
6.1.2 Raw map



X



Y

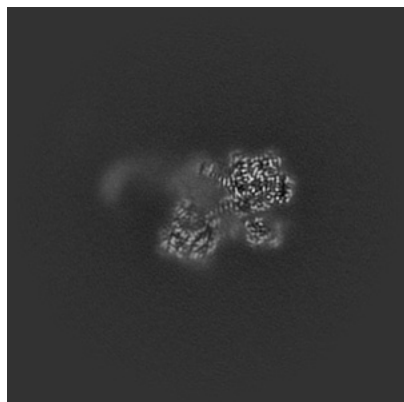


Z

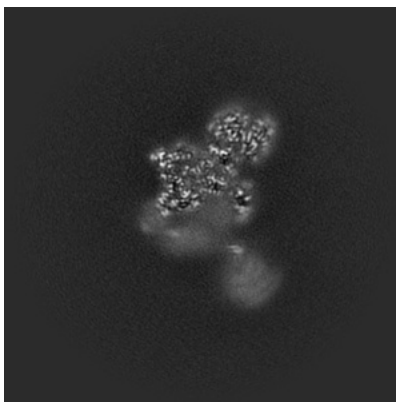
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

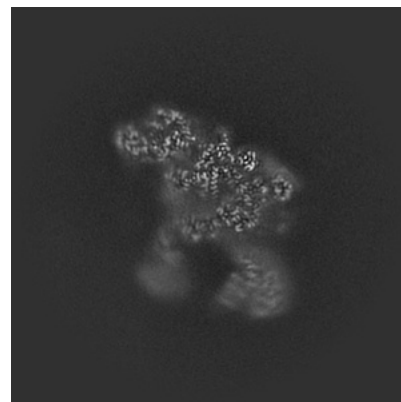
6.2.1 Primary map



X Index: 200

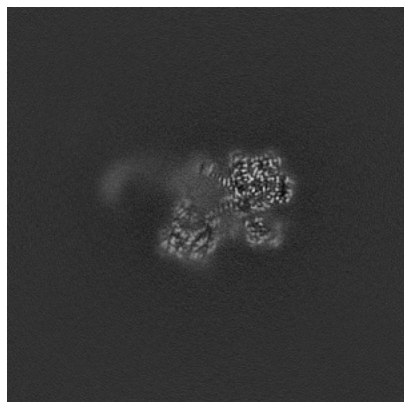


Y Index: 200

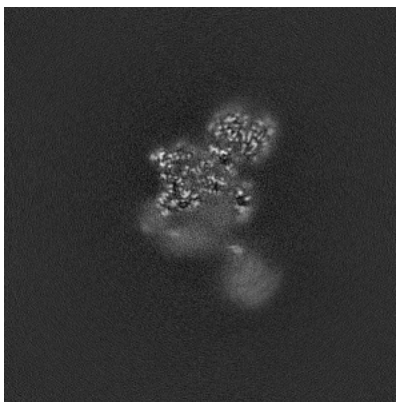


Z Index: 200

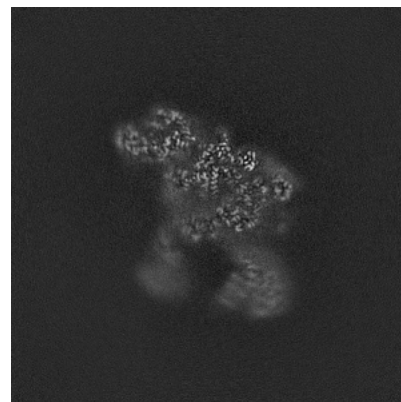
6.2.2 Raw map



X Index: 200



Y Index: 200

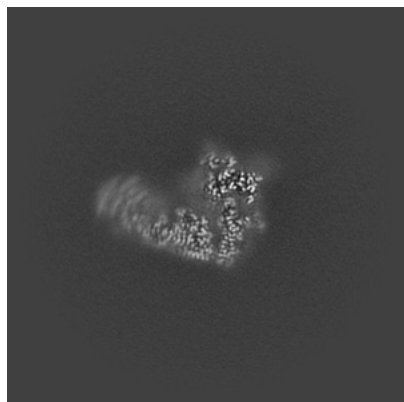


Z Index: 200

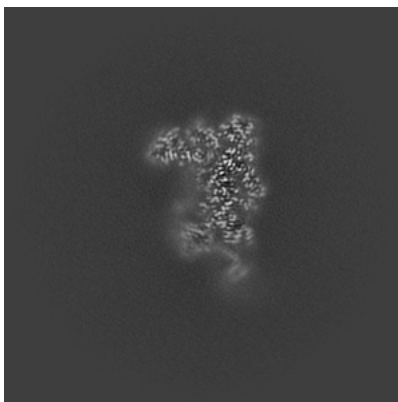
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

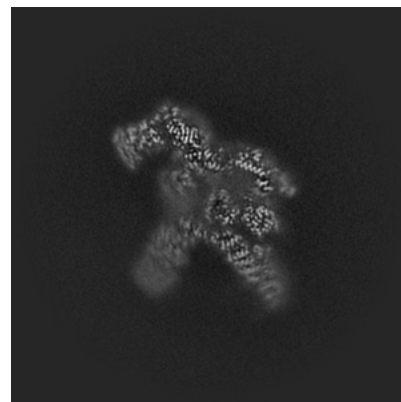
6.3.1 Primary map



X Index: 250

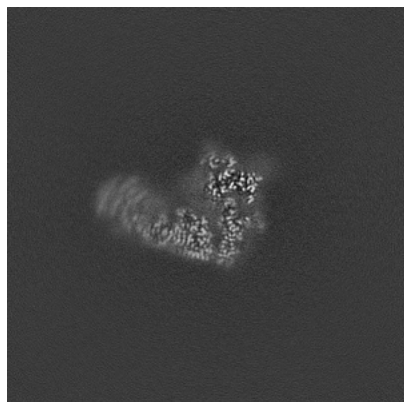


Y Index: 223

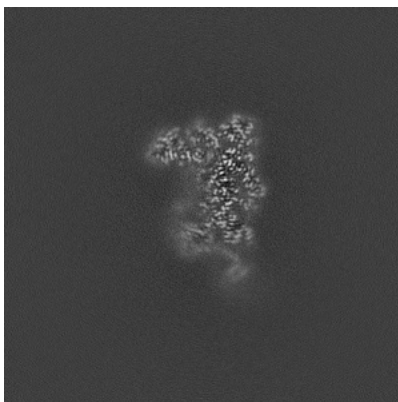


Z Index: 184

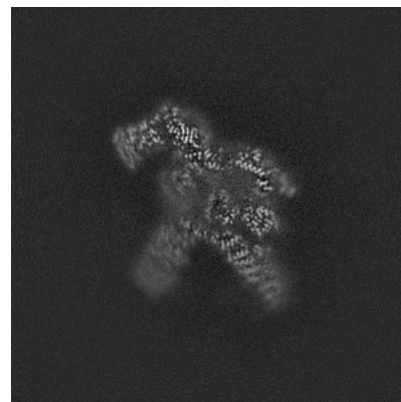
6.3.2 Raw map



X Index: 250



Y Index: 223

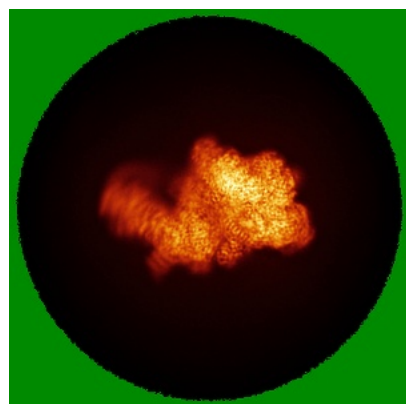


Z Index: 184

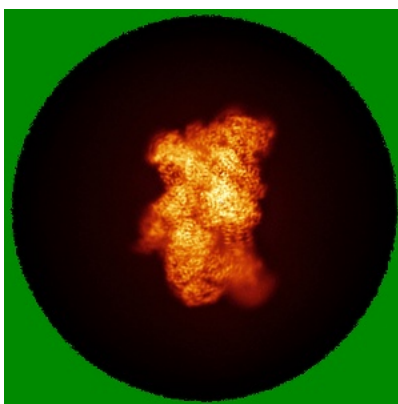
The images above show the largest variance slices of the map in three orthogonal directions.

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

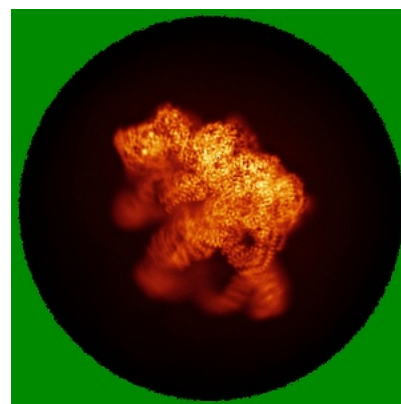
6.4.1 Primary map



X

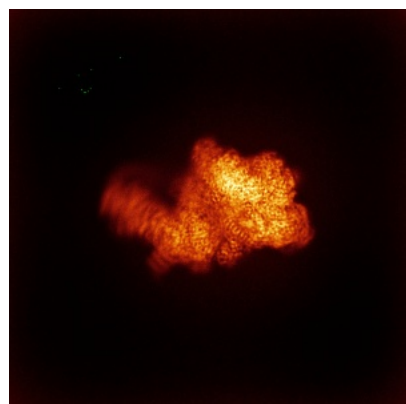


Y

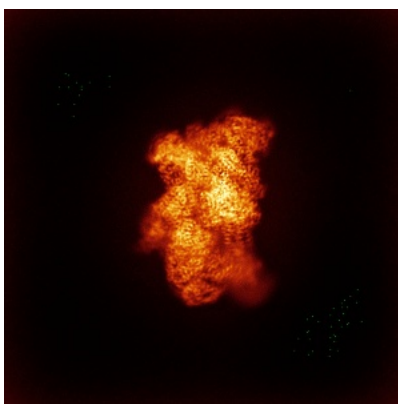


Z

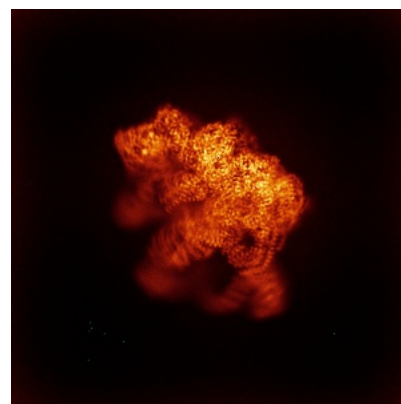
6.4.2 Raw map



X



Y

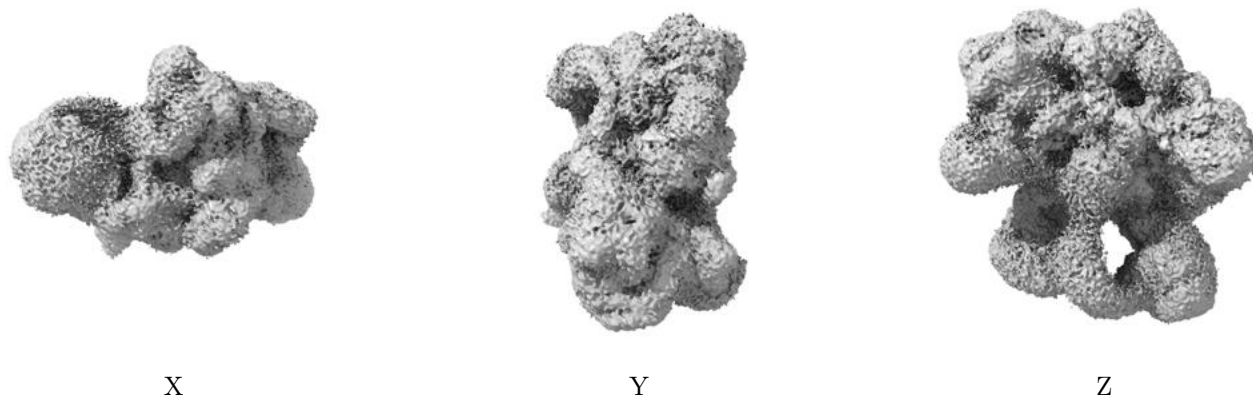


Z

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.

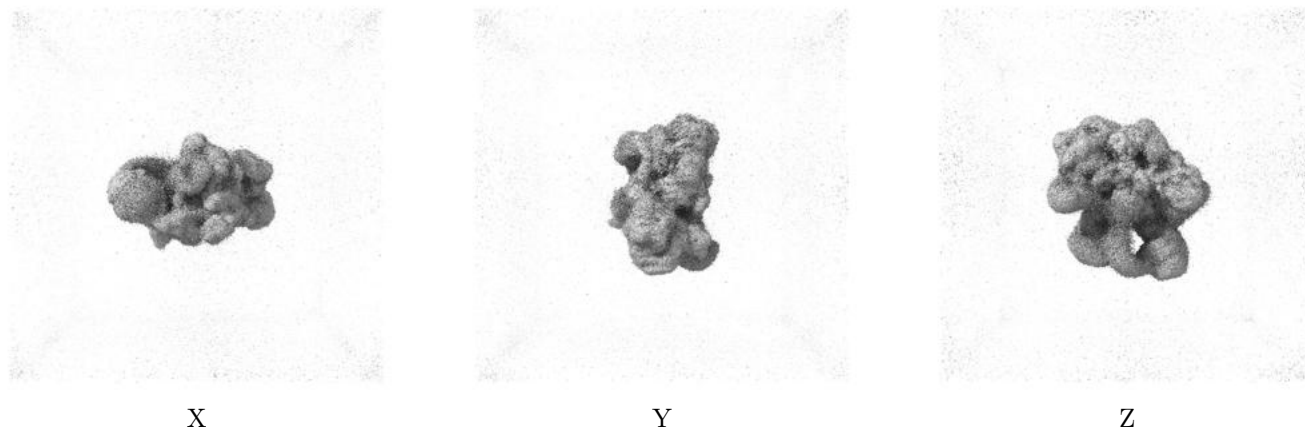
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

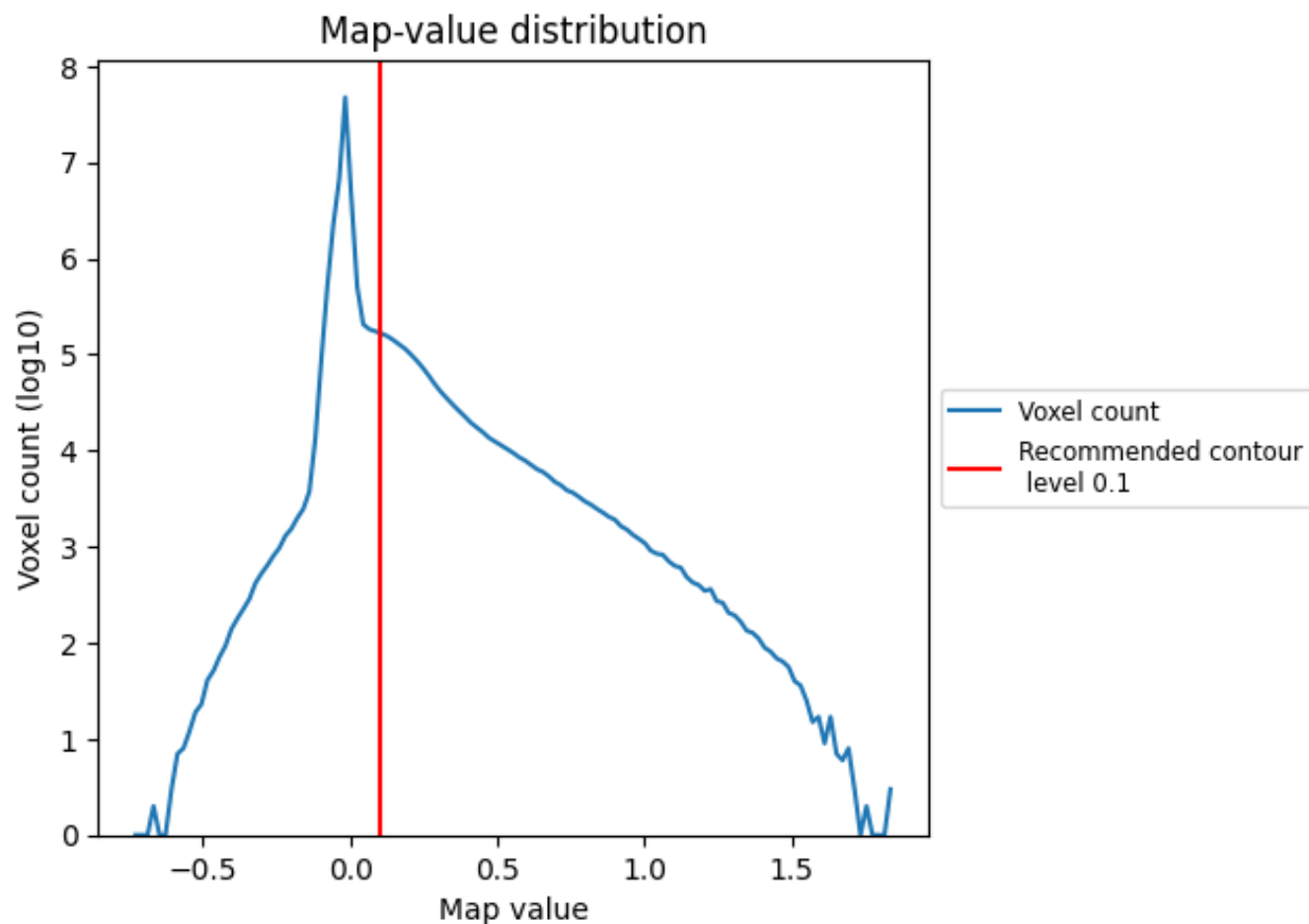
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

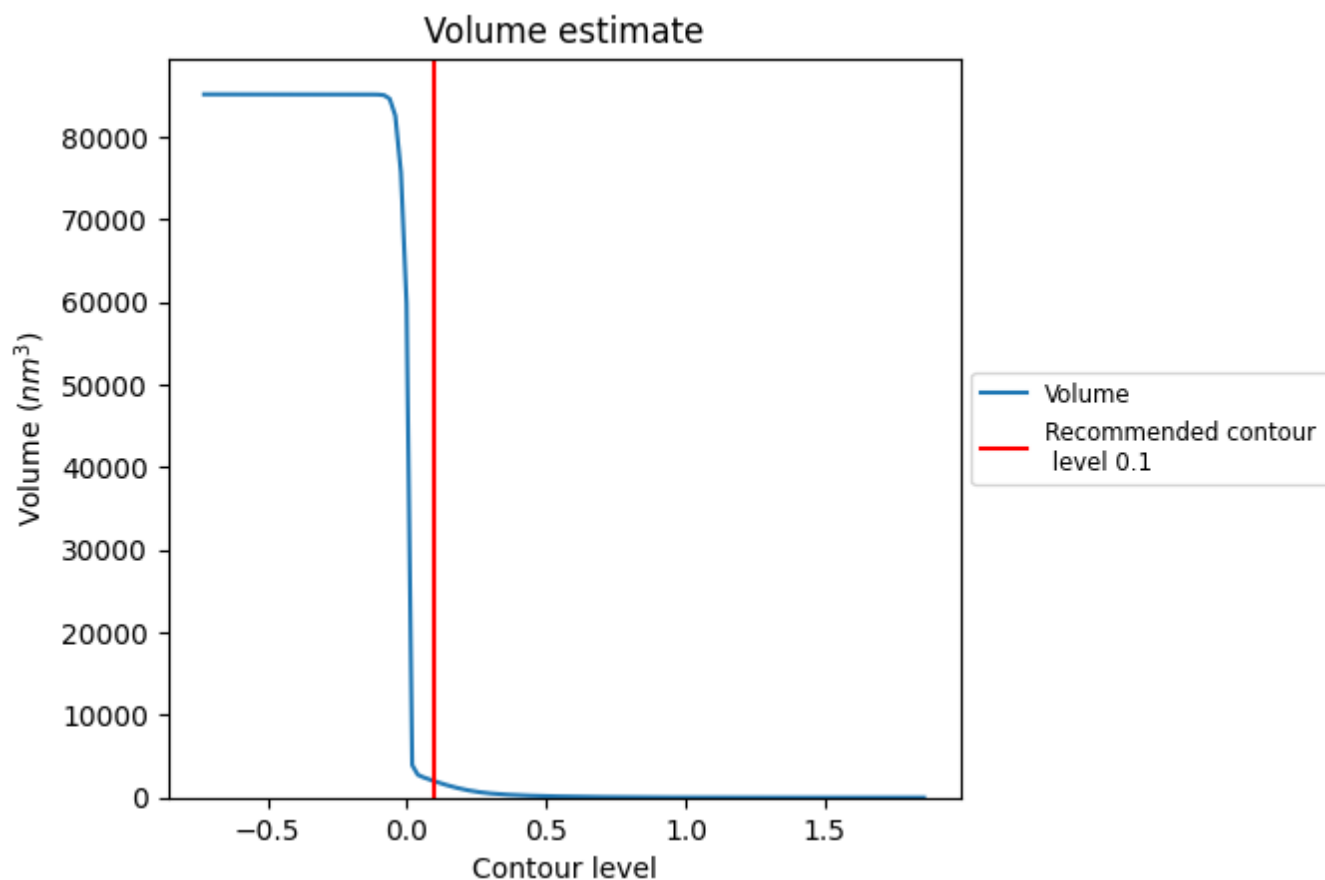
This section contains the results of statistical analysis of the map.

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.

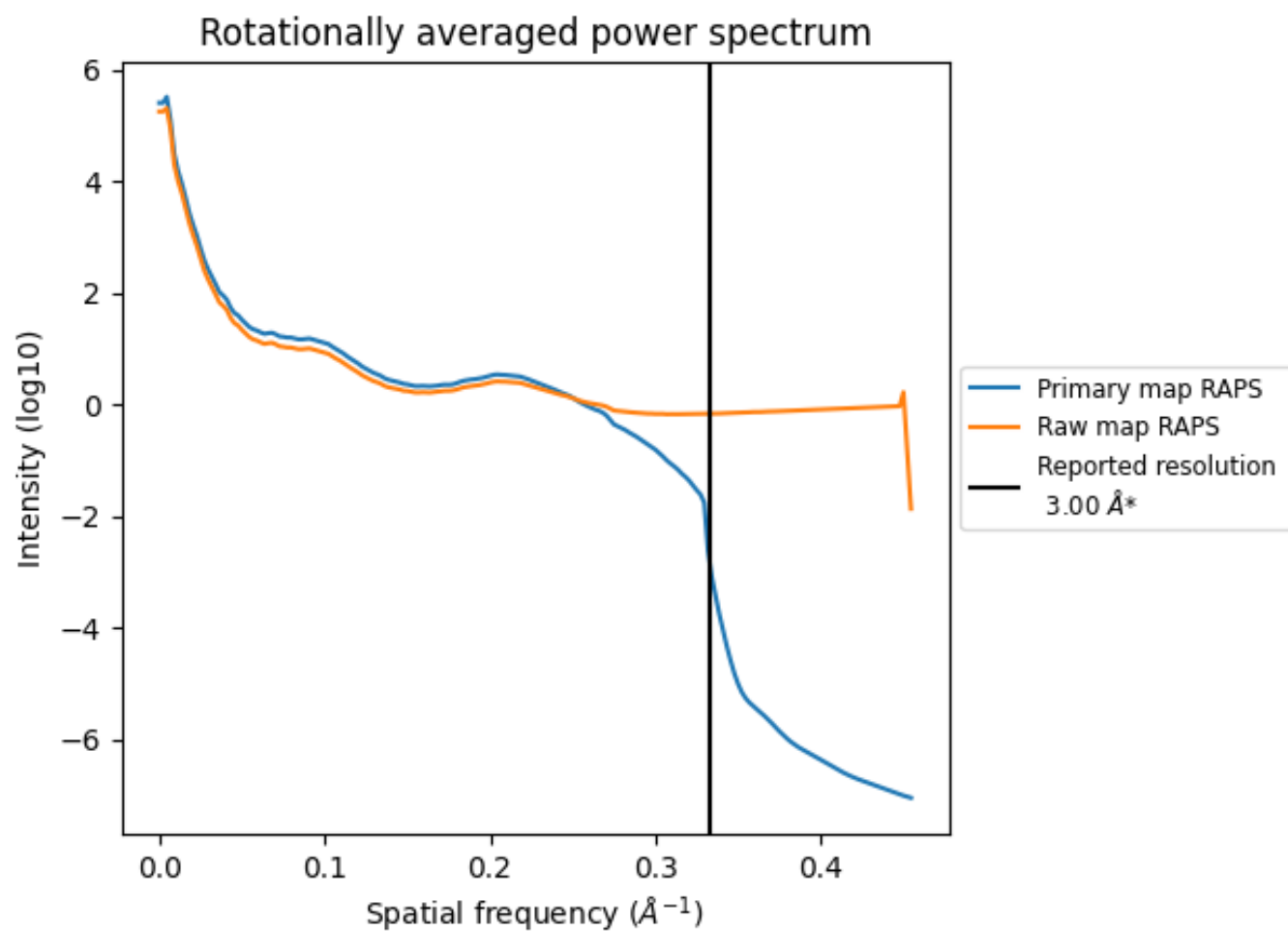
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1962 nm^3 ; this corresponds to an approximate mass of 1772 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 ⓘ

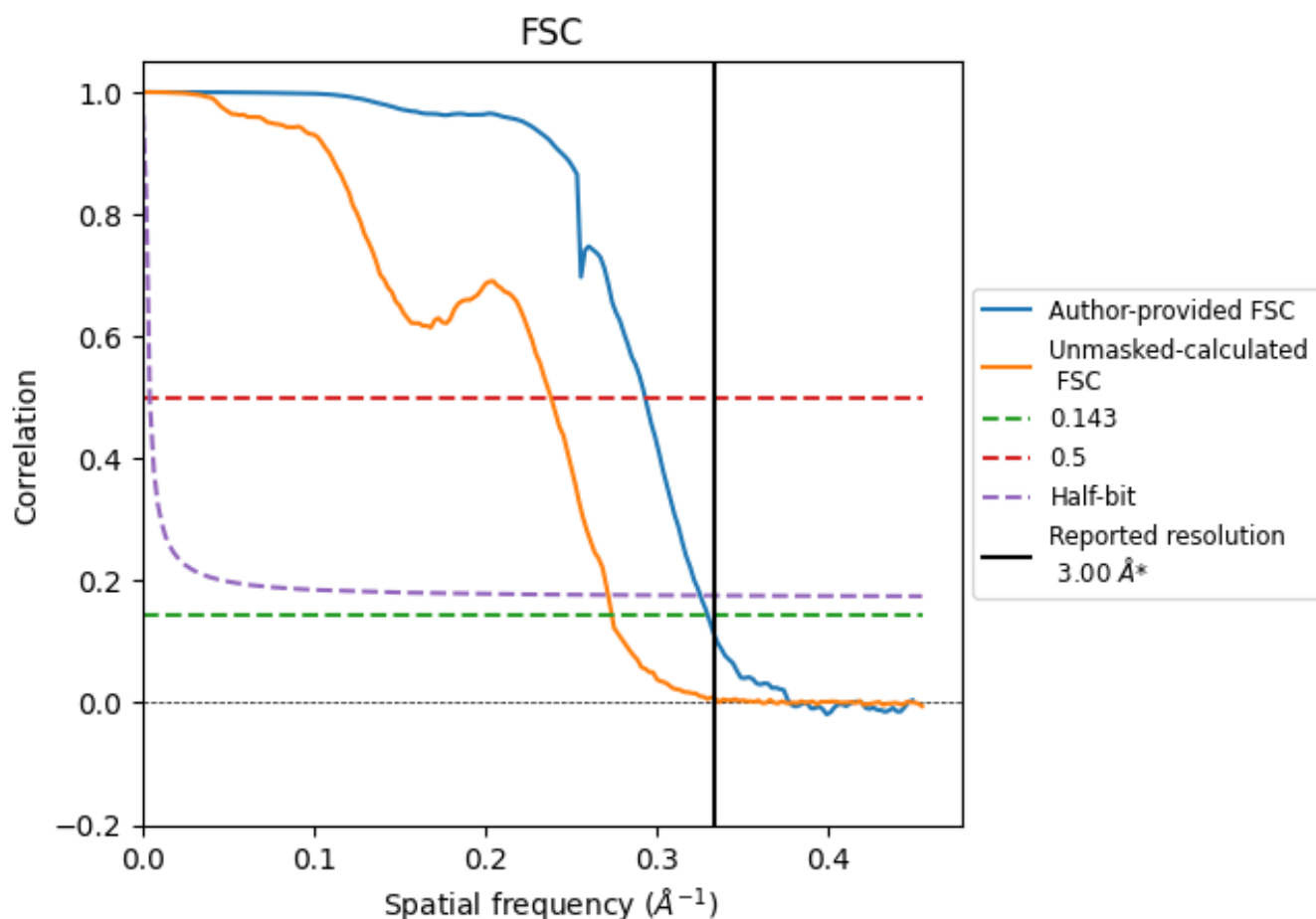


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

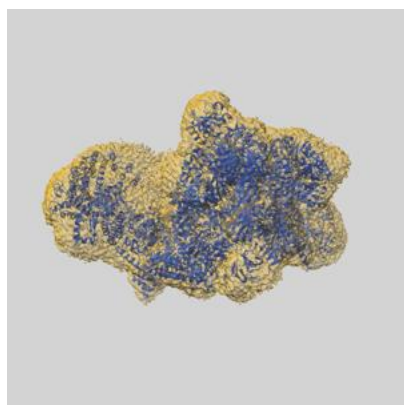
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.41	3.08
Unmasked-calculated*	3.65	4.20	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 3.0 by more than 10 %

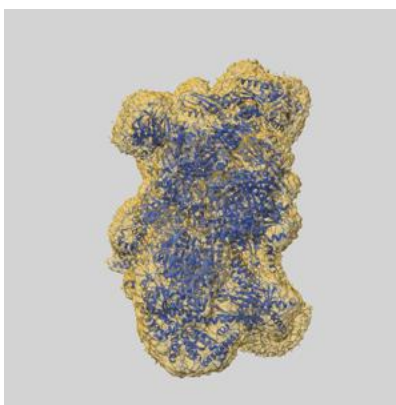
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37386 and PDB model 8W9Z. Per-residue inclusion information can be found in section [3](#) on page [8](#).

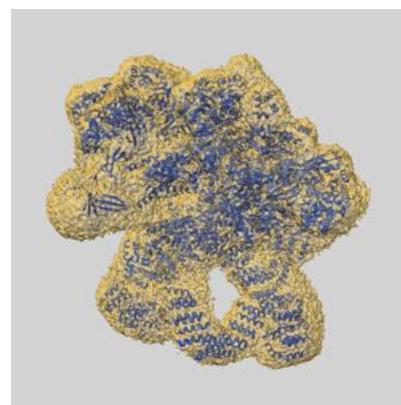
9.1 Map-model overlay [i](#)



X



Y



Z

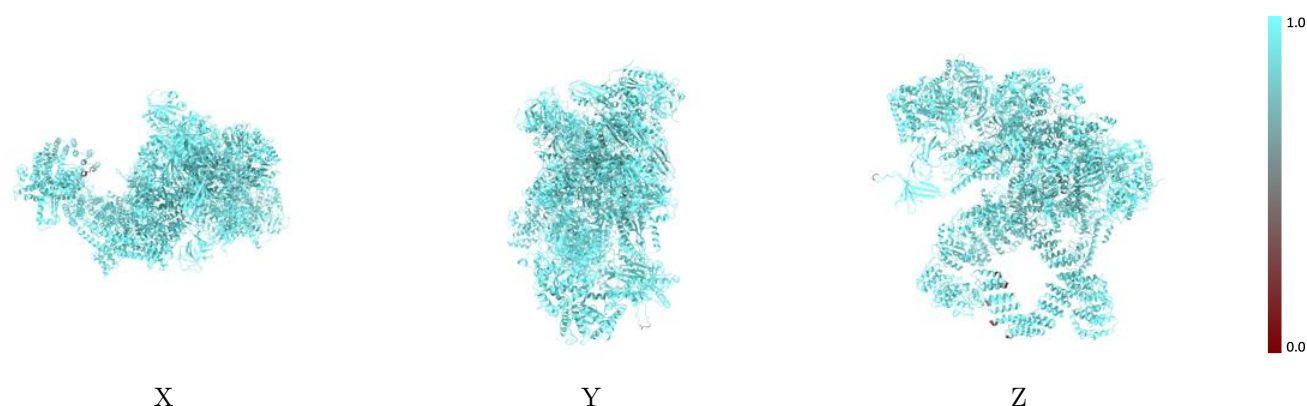
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



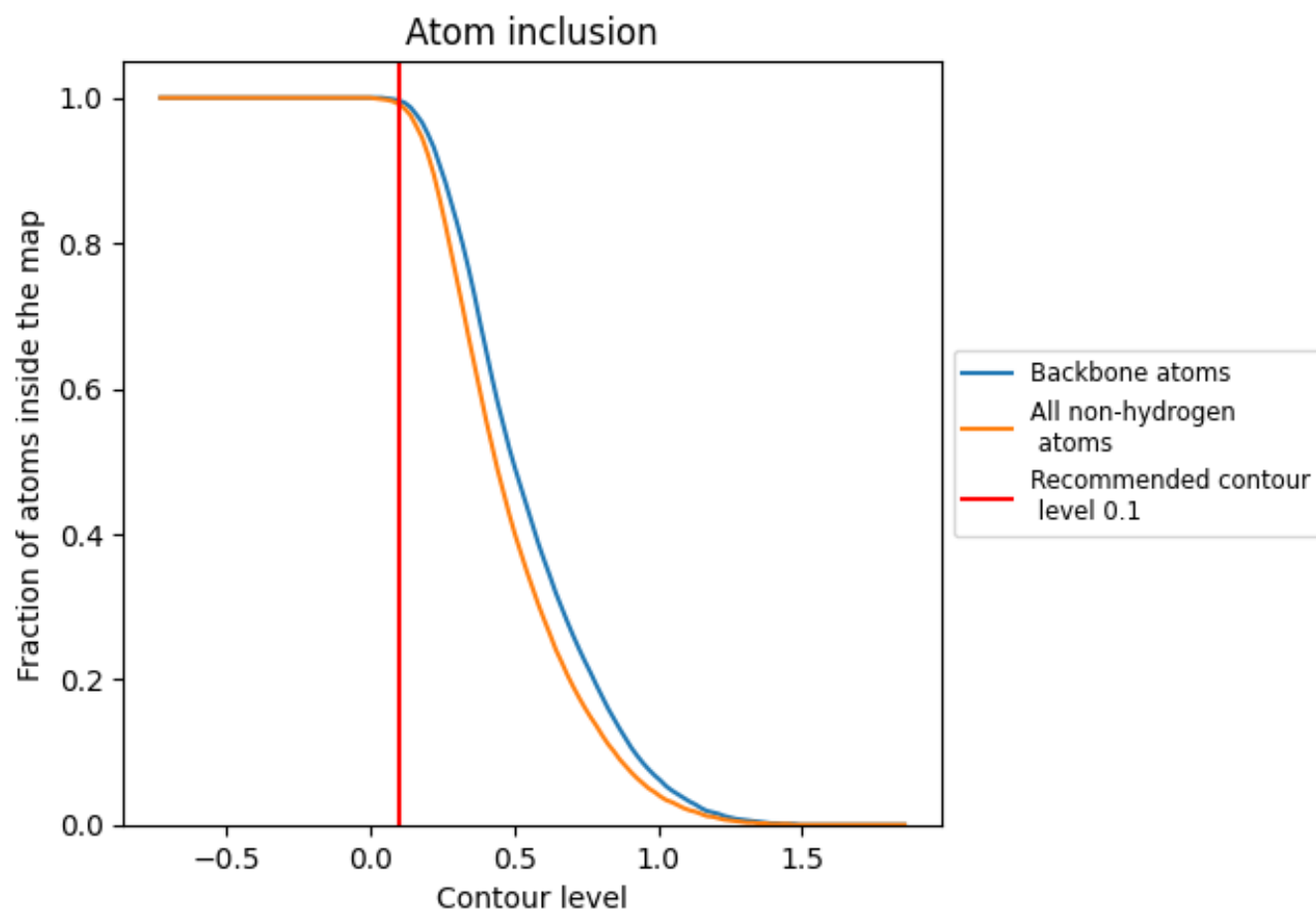
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9910	 0.4050
A	 0.9810	 0.4340
B	 0.9900	 0.4720
C	 0.9950	 0.3800
D	 0.9950	 0.3680
E	 0.9750	 0.1700
F	 0.9960	 0.4270
G	 0.9940	 0.4700
H	 0.9920	 0.5000
I	 0.9930	 0.5180
J	 0.9940	 0.4570
K	 0.9910	 0.4560
L	 1.0000	 0.4250
M	 0.9900	 0.5070
N	 1.0000	 0.1620
O	 0.9930	 0.4450
P	 0.9930	 0.4410
a	 0.9910	 0.4690
c	 0.9910	 0.4090
i	 0.9950	 0.4700
m	 0.9950	 0.4400

