



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:05 AM UTC

PDB ID : 8WA1 / pdb_00008wa1
EMDB ID : EMD-37388
Title : The cryo-EM structure of the Nicotiana tabacum PEP-PAP-TEC2
Authors : Wu, X.X.; Zhang, Y.
Deposited on : 2023-09-06
Resolution : 2.80 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:

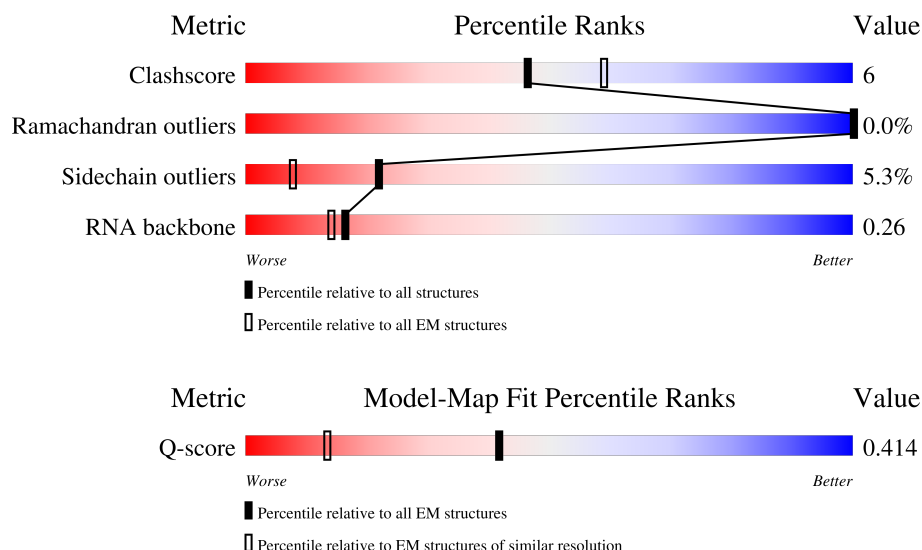
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.80 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.



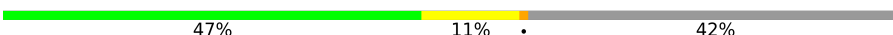
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	

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Mol	Chain	Length	Quality of chain
3	C	688	
4	D	892	
5	E	860	
6	F	682	
7	G	266	
8	H	531	
9	I	486	
10	J	507	
11	K	331	
12	L	303	
13	M	178	
13	m	178	
14	N	770	
15	O	167	
16	P	143	
17	Q	24	
18	R	24	
19	S	27	
20	c	1388	
21	i	648	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 62699 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	288	Total	C	N	O	S	0	0
			2190	1392	378	409	11		
1	a	303	Total	C	N	O	S	0	0
			2358	1508	405	434	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	998	Total	C	N	O	S	0	0
			7604	4823	1367	1391	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	653	Total	C	N	O	S	0	0
			4899	3131	873	875	20		

- Molecule 4 is a protein called PAP1(pTAC3).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	645	Total	C	N	O	S	0	0
			5063	3202	885	950	26		

- Molecule 5 is a protein called Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	700	Total	C	N	O	S	0	0
			4563	2840	829	872	22		

- Molecule 6 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	544	Total	C	N	O	S	0	0
			4259	2692	763	785	19		

- Molecule 7 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1742	1134	291	310	7		

- Molecule 8 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like.

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

- Molecule 9 is a protein called Fructokinase-like 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	376	Total	C	N	O	S	0	0
			2946	1886	519	528	13		

- Molecule 10 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	421	Total	C	N	O	S	0	0
			3410	2184	577	627	22		

- Molecule 11 is a protein called PAP8(pTAC6).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	204	Total	C	N	O	S	0	0
			1705	1077	298	322	8		

- Molecule 12 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	229	Total	C	N	O	S	0	0
			1776	1141	306	324	5		

- Molecule 13 is a protein called Thioredoxin-like protein CITRX1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	116	Total	C	N	O	S	0	0
			935	598	150	180	7		
13	m	109	Total	C	N	O	S	0	0
			855	548	136	164	7		

- Molecule 14 is a protein called UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	537	Total	C	N	O	S	0	0
			2995	1825	582	582	6		

- Molecule 15 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	97	Total	C	N	O	S	0	0
			780	490	140	146	4		

- Molecule 16 is a protein called PAP13(pTAC18).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	102	Total	C	N	O	S	0	0
			843	547	142	151	3		

- Molecule 17 is a DNA chain called DNA (24-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	4	Total	C	N	O	P	0	0
			82	40	11	27	4		

- Molecule 18 is a DNA chain called DNA (24-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	14	Total	C	N	O	P	0	0
			285	136	53	82	14		

- Molecule 19 is a RNA chain called RNA (27-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

- Molecule 20 is a protein called DNA-directed RNA polymerase subunit beta”.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	1176	Total	C	N	O	S	0	0
			8166	5119	1500	1517	30		

- Molecule 21 is a protein called Fructokinase-like 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	375	Total	C	N	O	S	0	0
			2937	1873	500	548	16		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

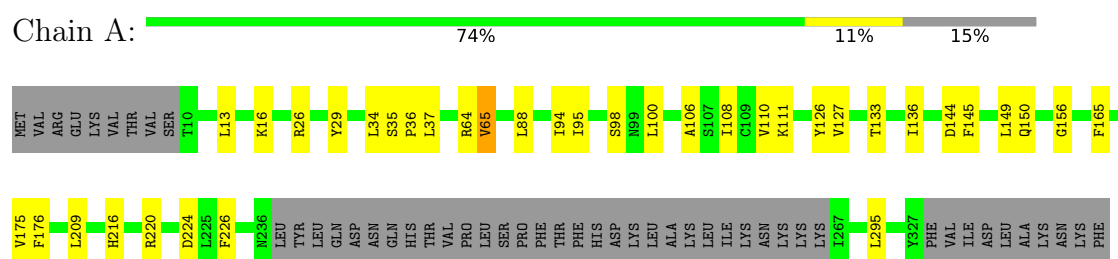
- Molecule 24 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

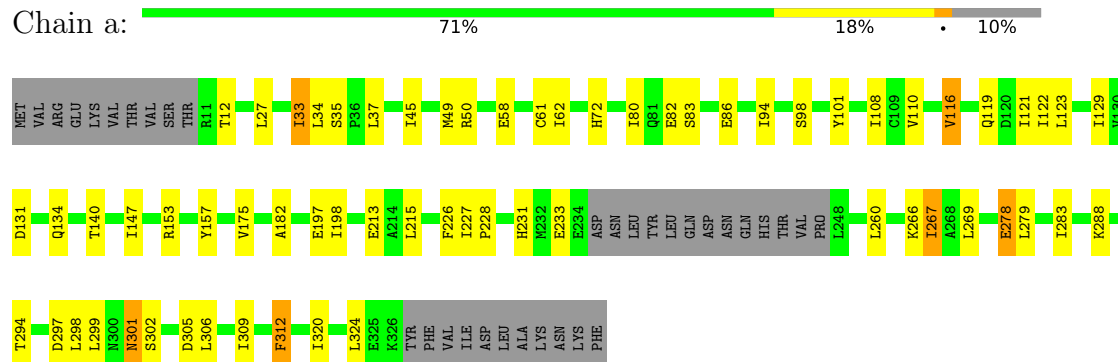
3 Residue-property plots

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.

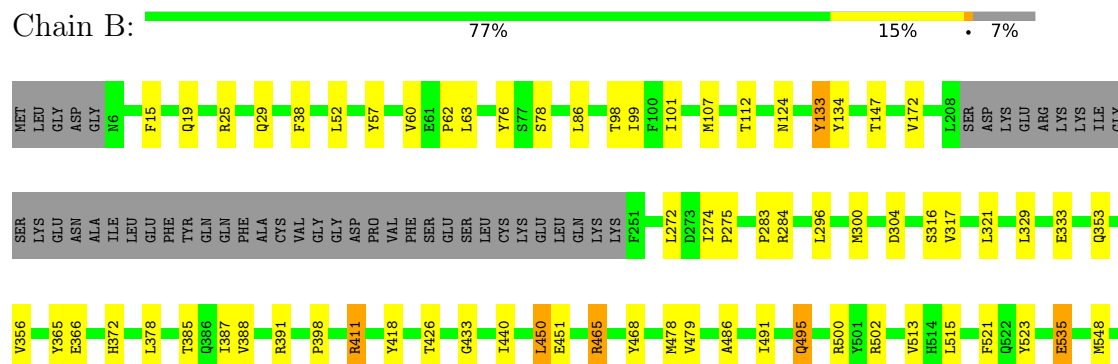
- Molecule 1: DNA-directed RNA polymerase subunit alpha

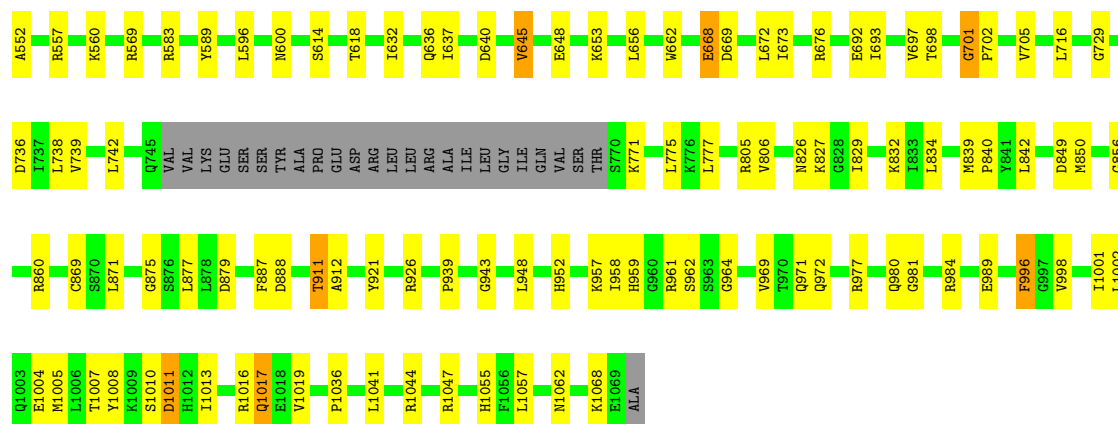


- Molecule 1: DNA-directed RNA polymerase subunit alpha



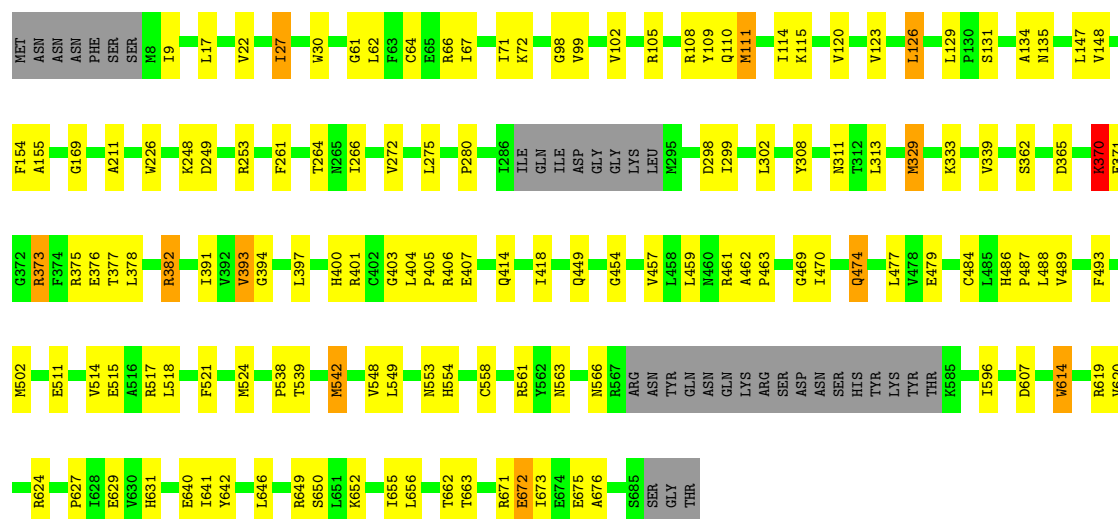
- Molecule 2: DNA-directed RNA polymerase subunit beta





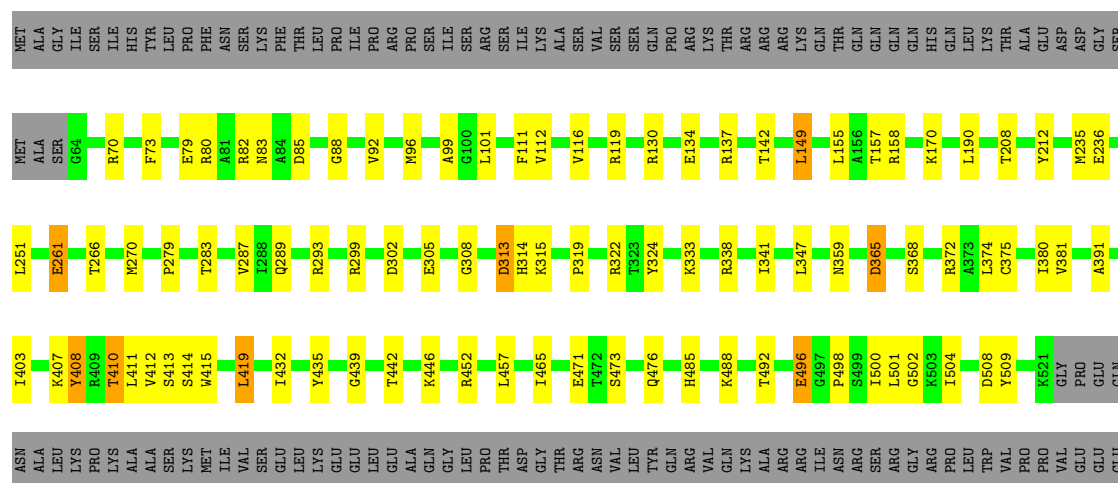
• Molecule 3: DNA-directed RNA polymerase subunit gamma

Chain C: 75% 18% 5%

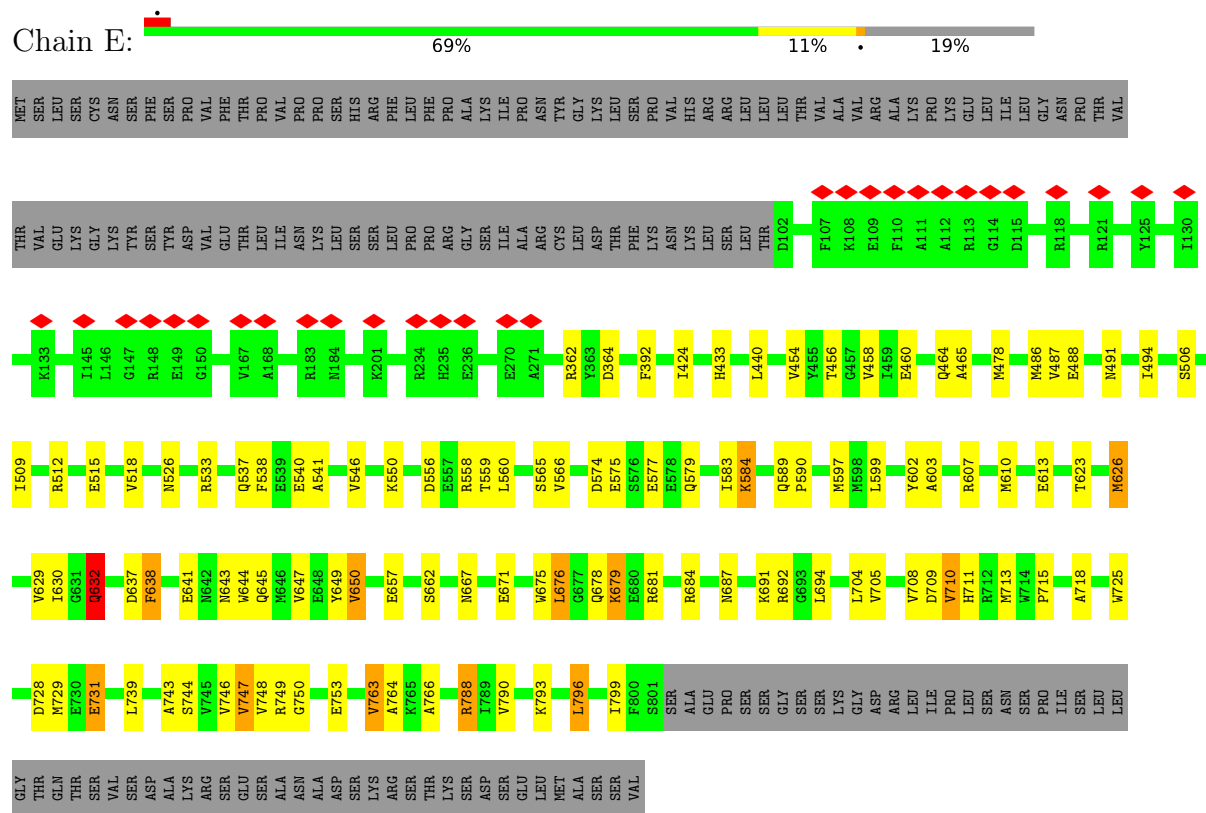


• Molecule 4: PAP1(pTAC3)

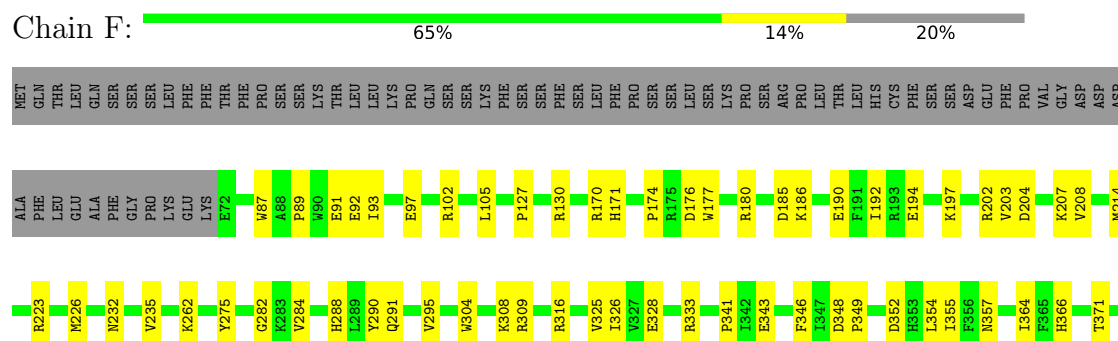
Chain D: 58% 13% 28%

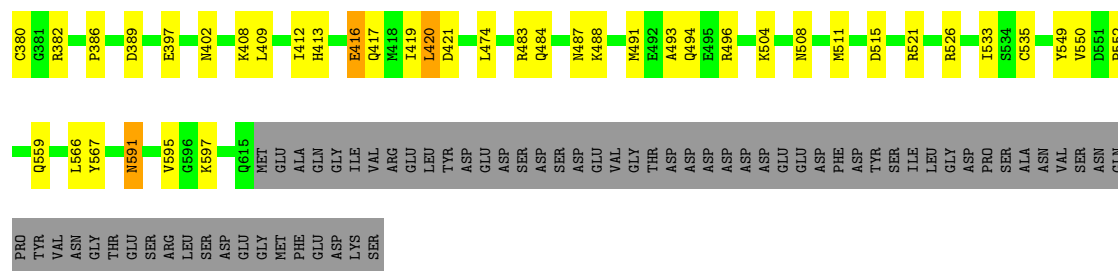


- Molecule 5: Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like



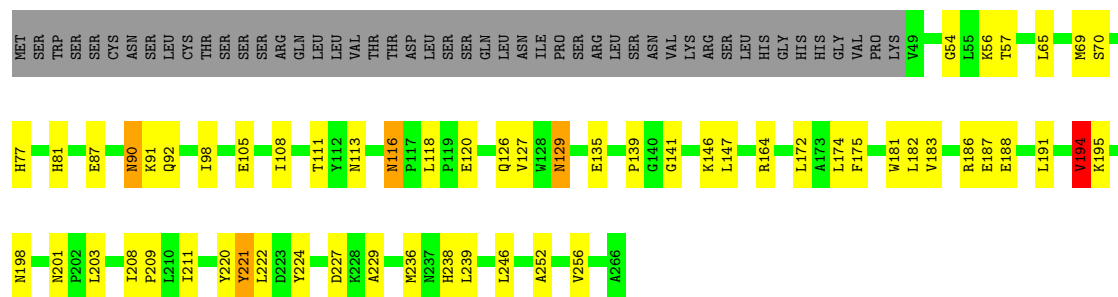
- Molecule 6: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like





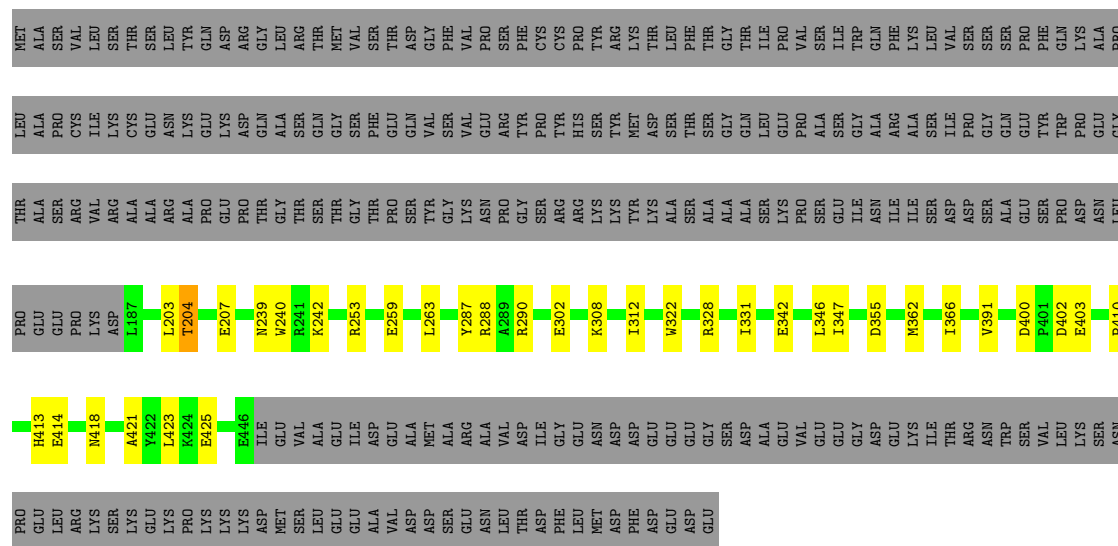
- Molecule 7: superoxide dismutase

Chain G: 60% 20% 18%



- Molecule 8: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like

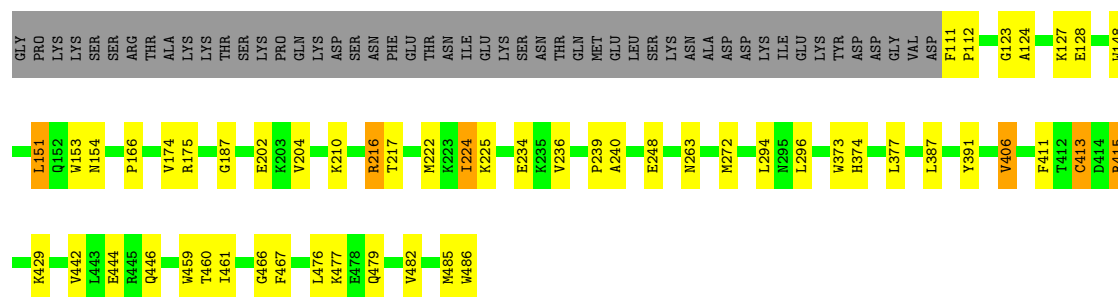
Chain H: 42% 6% 51%



- Molecule 9: Fructokinase-like 1, chloroplastic

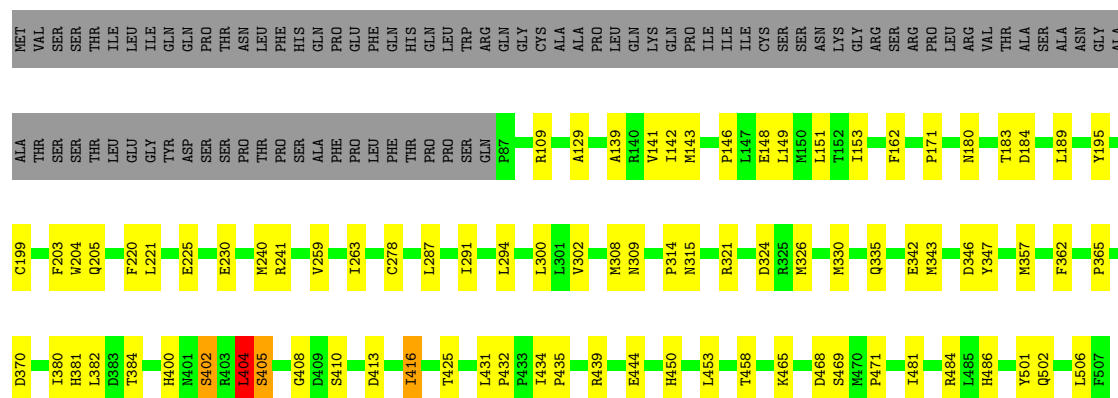
Chain I: 66% 10% 23%





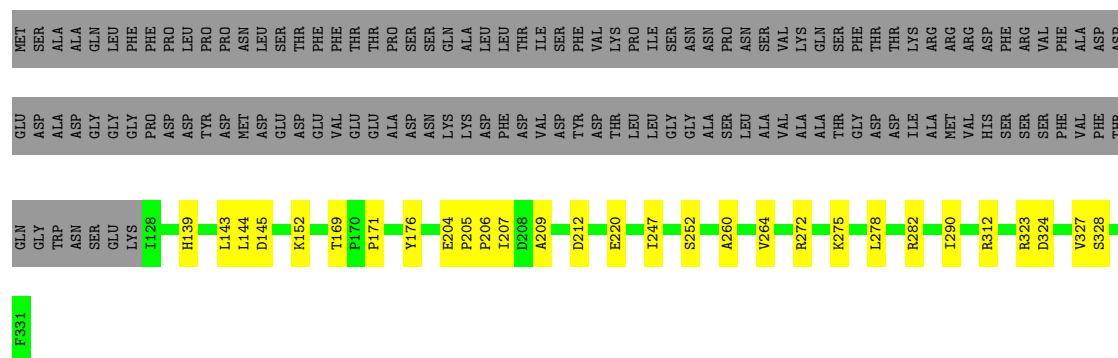
- Molecule 10: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2

Chain J: 66% 16% 17%



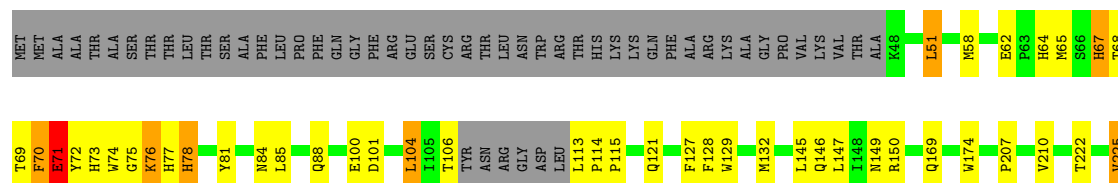
- Molecule 11: PAP8(pTAC6)

Chain K: 53% 9% 38%

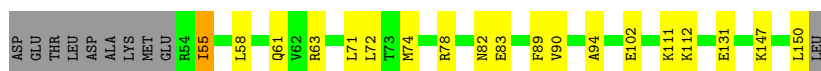


- Molecule 12: superoxide dismutase

Chain L: 54% 19% 24%

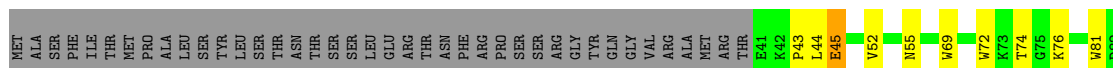






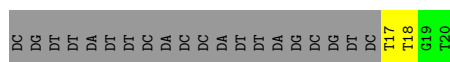
• Molecule 16: PAP13(pTAC18)

Chain P: 55% 15% 29%



• Molecule 17: DNA (24-mer)

Chain Q: 8% 8% 83%



• Molecule 18: DNA (24-mer)

Chain R: 33% 25% 42%



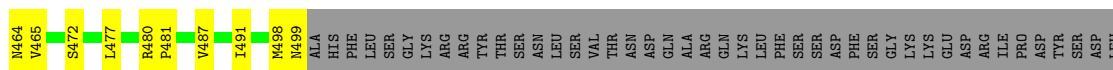
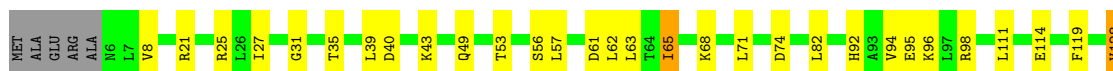
• Molecule 19: RNA (27-mer)

Chain S: 26% 7% 67%



• Molecule 20: DNA-directed RNA polymerase subunit beta''

Chain c: 71% 13% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88607	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 ($e^-/\text{\AA}^2$)	57.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.362	Depositor
Minimum map value	-0.380	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FE, 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	0.30	0/2227	0.40	0/3019
1	a	0.12	0/2403	0.32	1/3256 (0.0%)
2	B	0.56	3/7751 (0.0%)	0.65	6/10510 (0.1%)
3	C	0.38	1/4998 (0.0%)	0.53	7/6792 (0.1%)
4	D	0.20	0/5161	0.41	4/6986 (0.1%)
5	E	0.16	0/4633	0.39	5/6321 (0.1%)
6	F	0.22	0/4366	0.40	3/5918 (0.1%)
7	G	0.55	0/1793	0.75	8/2437 (0.3%)
8	H	0.31	0/2167	0.32	0/2942
9	I	0.20	0/3021	0.43	4/4092 (0.1%)
10	J	0.20	0/3498	0.39	2/4742 (0.0%)
11	K	0.14	0/1747	0.30	0/2362
12	L	0.62	3/1828 (0.2%)	0.82	12/2488 (0.5%)
13	M	0.52	0/951	0.63	3/1286 (0.2%)
13	m	0.42	0/869	0.54	0/1179
14	N	0.23	0/3024	0.48	8/4180 (0.2%)
15	O	0.11	0/793	0.30	0/1065
16	P	0.11	0/870	0.29	0/1182
17	Q	0.35	0/90	0.72	0/137
18	R	0.34	0/319	0.62	0/489
19	S	0.39	0/214	0.63	0/331
20	c	0.32	0/8294	0.44	4/11306 (0.0%)
21	i	0.21	0/3009	0.47	3/4078 (0.1%)
All	All	0.34	7/64026 (0.0%)	0.49	70/87098 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	110	GLN	CA-C	-6.53	1.44	1.52
2	B	911	THR	CA-C	-5.65	1.45	1.52
2	B	668	GLU	CA-C	-5.57	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	74	TRP	CA-C	-5.52	1.45	1.52
12	L	67	HIS	C-O	-5.37	1.17	1.24
12	L	71	GLU	CA-C	-5.11	1.46	1.52
2	B	912	ALA	CA-C	-5.11	1.47	1.53

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	964	GLY	N-CA-C	21.04	136.91	112.50
20	c	1002	GLN	N-CA-C	-10.36	98.77	111.40
2	B	911	THR	N-CA-C	-10.08	92.10	108.52
14	N	683	TYR	N-CA-C	9.30	121.02	111.07
21	i	276	TRP	CA-C-N	-9.18	110.92	120.38
21	i	276	TRP	C-N-CA	-9.18	110.92	120.38
5	E	638	PHE	N-CA-C	-9.06	101.54	112.59
5	E	364	ASP	N-CA-C	-8.75	102.19	113.12
7	G	57	THR	CA-C-N	-8.07	112.07	120.38
7	G	57	THR	C-N-CA	-8.07	112.07	120.38
2	B	133	TYR	N-CA-C	7.91	124.10	113.97
10	J	404	LEU	N-CA-C	-7.69	103.69	113.23
4	D	442	THR	N-CA-C	-7.61	103.56	112.92
20	c	1003	ILE	N-CA-C	7.42	118.21	110.72
3	C	105	ARG	N-CA-C	-7.41	104.49	113.97
3	C	394	GLY	N-CA-C	-7.15	97.75	112.34
2	B	134	TYR	N-CA-C	6.99	121.03	111.39
12	L	113	LEU	CA-C-N	-6.97	113.20	120.38
12	L	113	LEU	C-N-CA	-6.97	113.20	120.38
12	L	84	ASN	N-CA-C	-6.72	103.88	111.14
13	M	100	TRP	N-CA-C	6.66	118.53	111.28
6	F	354	LEU	N-CA-C	6.56	118.51	111.36
14	N	656	ASP	CA-C-N	-6.52	111.81	119.05
14	N	656	ASP	C-N-CA	-6.52	111.81	119.05
9	I	411	PHE	N-CA-C	6.48	118.34	111.28
14	N	680	GLU	N-CA-C	-6.43	104.27	111.28
10	J	410	SER	N-CA-C	-6.34	104.11	113.61
13	M	144	LEU	N-CA-C	6.30	123.74	109.81
3	C	397	LEU	N-CA-C	-6.27	99.77	109.24
7	G	147	LEU	N-CA-C	6.16	117.67	111.07
12	L	68	THR	N-CA-C	-6.12	104.53	111.07
7	G	54	GLY	N-CA-C	6.06	118.45	111.36
6	F	355	ILE	N-CA-C	6.04	116.81	108.84
9	I	413	CYS	N-CA-C	5.92	119.56	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	109	TYR	CA-C-N	-5.87	114.71	122.99
3	C	109	TYR	C-N-CA	-5.87	114.71	122.99
12	L	226	TRP	N-CA-C	-5.86	100.44	109.52
21	i	274	TYR	N-CA-C	5.79	117.67	111.36
9	I	154	ASN	CA-C-N	-5.74	114.47	120.38
9	I	154	ASN	C-N-CA	-5.74	114.47	120.38
14	N	678	HIS	N-CA-C	-5.70	105.06	111.28
6	F	352	ASP	N-CA-C	5.69	118.25	111.71
12	L	235	ARG	N-CA-C	-5.68	102.62	110.35
7	G	127	VAL	CB-CA-C	-5.66	104.72	111.97
5	E	362	ARG	N-CA-C	-5.65	105.20	111.36
12	L	114	PRO	CA-C-N	-5.64	112.79	119.84
12	L	114	PRO	C-N-CA	-5.64	112.79	119.84
12	L	101	ASP	N-CA-C	-5.62	105.06	111.07
5	E	637	ASP	N-CA-C	5.58	118.34	108.24
4	D	763	THR	N-CA-C	5.56	117.42	111.36
7	G	198	ASN	CB-CA-C	-5.56	110.18	116.63
4	D	760	TRP	N-CA-C	-5.55	106.28	113.16
12	L	127	PHE	N-CA-C	-5.53	105.25	111.28
7	G	220	TYR	N-CA-C	5.52	120.89	113.72
13	M	155	ASN	N-CA-C	-5.48	107.14	113.88
3	C	393	VAL	CB-CA-C	-5.41	103.65	111.34
2	B	701	GLY	CA-C-N	-5.41	115.01	120.31
2	B	701	GLY	C-N-CA	-5.41	115.01	120.31
1	a	267	ILE	N-CA-C	-5.32	107.59	111.90
12	L	237	ARG	N-CA-C	-5.30	98.62	107.99
4	D	439	GLY	N-CA-C	-5.27	100.68	113.18
20	c	212	HIS	N-CA-C	5.27	117.03	111.28
14	N	631	ARG	N-CA-C	5.25	119.89	112.75
3	C	370	LYS	N-CA-C	-5.23	105.66	111.36
12	L	236	ASN	N-CA-C	5.16	117.60	109.39
7	G	194	VAL	N-CA-C	5.14	115.31	108.11
14	N	631	ARG	CA-C-N	-5.06	113.43	119.05
14	N	631	ARG	C-N-CA	-5.06	113.43	119.05
5	E	632	GLN	N-CA-C	-5.05	105.87	112.23
20	c	213	ILE	N-CA-C	5.01	116.14	109.37

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	2190	0	2116	20	0
1	a	2358	0	2354	35	0
2	B	7604	0	7393	92	0
3	C	4899	0	4598	81	0
4	D	5063	0	4944	71	0
5	E	4563	0	3584	61	0
6	F	4259	0	3864	70	0
7	G	1742	0	1676	30	0
8	H	2110	0	1974	22	0
9	I	2946	0	2821	31	0
10	J	3410	0	3316	52	0
11	K	1705	0	1668	16	0
12	L	1776	0	1608	36	0
13	M	935	0	934	11	0
13	m	855	0	848	12	0
14	N	2995	0	1888	17	0
15	O	780	0	754	12	0
16	P	843	0	758	16	0
17	Q	82	0	48	1	0
18	R	285	0	158	6	0
19	S	192	0	97	2	0
20	c	8166	0	7164	111	0
21	i	2937	0	2878	32	0
22	B	1	0	0	0	0
23	C	1	0	0	0	0
24	G	1	0	0	0	0
24	L	1	0	0	0	0
All	All	62699	0	57443	736	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 (736) 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)
10:J:402:SER:HA	10:J:405:SER:OG	1.04	1.20
4:D:137:ARG:HH22	10:J:404:LEU:CD1	1.55	1.20
10:J:402:SER:CA	10:J:405:SER:OG	1.91	1.18
4:D:137:ARG:NH2	10:J:404:LEU:HD21	1.58	1.17
4:D:137:ARG:HH21	10:J:404:LEU:HD21	1.08	1.12
4:D:137:ARG:NH2	10:J:404:LEU:CD2	2.19	1.03
4:D:137:ARG:NH2	10:J:404:LEU:HD11	1.72	1.02
4:D:137:ARG:HH22	10:J:404:LEU:HD11	0.87	1.02
10:J:402:SER:HA	10:J:405:SER:HG	1.21	1.01
4:D:137:ARG:NH2	10:J:404:LEU:CD1	2.30	0.93
21:i:376:LYS:HB3	21:i:400:ALA:HB2	1.62	0.82
7:G:174:LEU:HD12	7:G:195:LYS:HB3	1.65	0.78
4:D:73:PHE:HD2	4:D:96:MET:HG2	1.50	0.76
7:G:146:LYS:HB3	7:G:246:LEU:HD22	1.68	0.76
3:C:548:VAL:HG11	20:c:53:THR:HG21	1.68	0.75
4:D:824:LEU:HD21	4:D:858:ILE:HD12	1.68	0.75
3:C:614:TRP:HZ3	3:C:619:ARG:H	1.36	0.73
9:I:153:TRP:CD1	9:I:413:CYS:HG	2.08	0.72
4:D:432:ILE:HG22	14:N:632:PRO:HB2	1.71	0.72
3:C:391:ILE:HD13	3:C:502:MET:HE3	1.69	0.72
20:c:400:ILE:HG22	20:c:402:PRO:HD2	1.74	0.70
21:i:457:PRO:HD2	21:i:460:LEU:HD12	1.74	0.69
20:c:1236:GLU:HA	20:c:1245:PRO:HB3	1.75	0.69
3:C:596:ILE:HD12	3:C:671:ARG:HH11	1.59	0.68
4:D:492:THR:O	4:D:496:GLU:HB2	1.93	0.68
10:J:221:LEU:HB2	10:J:278:CYS:SG	2.32	0.68
6:F:202:ARG:NH1	20:c:988:ILE:O	2.26	0.68
2:B:869:CYS:HB3	2:B:943:GLY:HA3	1.76	0.68
15:O:83:GLU:HG2	15:O:89:PHE:HB2	1.76	0.68
6:F:92:GLU:OE1	6:F:102:ARG:NH1	2.26	0.68
3:C:131:SER:O	3:C:135:ASN:ND2	2.22	0.67
1:a:123:LEU:HD11	1:a:129:ILE:HG23	1.75	0.67
21:i:450:VAL:HB	21:i:478:ALA:HA	1.77	0.67
20:c:453:ASP:HB2	20:c:472:SER:HB3	1.76	0.67
4:D:82:ARG:HD2	10:J:434:ILE:HD11	1.77	0.66
3:C:66:ARG:HG3	3:C:98:GLY:HA3	1.76	0.66
3:C:486:HIS:HE1	3:C:488:LEU:HD12	1.60	0.66
8:H:308:LYS:O	8:H:328:ARG:NH2	2.29	0.66
2:B:998:VAL:HG12	3:C:515:GLU:HB3	1.78	0.66
11:K:323:ARG:HG2	20:c:416:SER:HB3	1.78	0.66
4:D:80:ARG:HG3	4:D:85:ASP:HB3	1.77	0.65
5:E:739:LEU:HD22	5:E:796:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:LEU:HD13	20:c:1309:LEU:HD11	1.79	0.65
4:D:313:ASP:N	4:D:313:ASP:OD1	2.30	0.65
3:C:61:GLY:H	3:C:64:CYS:HB2	1.60	0.64
5:E:709:ASP:HA	5:E:746:VAL:HB	1.80	0.64
10:J:309:ASN:ND2	10:J:342:GLU:OE2	2.30	0.64
5:E:509:ILE:HG22	5:E:512:ARG:HH12	1.63	0.64
3:C:71:ILE:HG23	3:C:72:LYS:HG3	1.80	0.64
4:D:116:VAL:HG22	4:D:149:LEU:HD12	1.79	0.64
10:J:402:SER:C	10:J:405:SER:OG	2.41	0.64
16:P:44:LEU:HB3	16:P:107:MET:HE2	1.79	0.64
16:P:44:LEU:HD11	16:P:105:ARG:HB3	1.79	0.63
2:B:283:PRO:HB2	6:F:566:LEU:HD23	1.81	0.63
6:F:382:ARG:NH1	20:c:491:ILE:O	2.32	0.63
9:I:187:GLY:H	9:I:217:THR:HG1	1.47	0.63
20:c:1073:ILE:HG22	20:c:1077:VAL:HG21	1.81	0.63
6:F:208:VAL:HG13	20:c:1034:ILE:HD13	1.81	0.63
2:B:440:ILE:HD12	2:B:521:PHE:HB3	1.80	0.62
20:c:1182:ILE:HG23	20:c:1183:PRO:HD3	1.80	0.62
2:B:1004:GLU:HB2	2:B:1008:TYR:CZ	2.35	0.62
16:P:110:VAL:HG13	16:P:112:GLY:H	1.63	0.62
2:B:560:LYS:HG3	2:B:645:VAL:HG13	1.80	0.62
5:E:793:LYS:HA	5:E:796:LEU:HD23	1.81	0.62
12:L:147:LEU:HG	12:L:150:ARG:HH12	1.64	0.62
3:C:649:ARG:HG2	3:C:655:ILE:HA	1.81	0.62
5:E:644:TRP:HA	5:E:647:VAL:HG22	1.82	0.62
6:F:409:LEU:HD12	6:F:412:ILE:HD11	1.82	0.62
4:D:333:LYS:HB3	4:D:465:ILE:HD13	1.80	0.62
12:L:145:LEU:O	12:L:149:ASN:ND2	2.32	0.62
6:F:93:ILE:HD12	20:c:1073:ILE:HG12	1.82	0.62
4:D:112:VAL:HG11	4:D:142:THR:HG23	1.81	0.62
7:G:105:GLU:HG3	7:G:203:LEU:HD13	1.82	0.62
9:I:224:ILE:HD12	9:I:225:LYS:H	1.64	0.62
3:C:538:PRO:HB3	3:C:542:MET:HB2	1.81	0.62
4:D:410:THR:HG22	4:D:411:LEU:HD23	1.81	0.62
6:F:180:ARG:HH21	7:G:98:ILE:HD11	1.65	0.61
13:M:140:GLN:O	13:M:160:ARG:NH1	2.33	0.61
14:N:595:ALA:HB3	14:N:719:ALA:HB1	1.82	0.61
14:N:662:ASP:HB2	14:N:672:MET:HG3	1.82	0.61
7:G:208:ILE:HG21	7:G:252:ALA:HB2	1.82	0.61
5:E:487:VAL:HG22	5:E:518:VAL:HB	1.83	0.61
6:F:282:GLY:HA2	20:c:979:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:149:PHE:HB3	13:M:178:LEU:HD11	1.82	0.61
12:L:58:MET:HE3	12:L:71:GLU:HA	1.83	0.61
5:E:456:THR:HG21	5:E:488:GLU:HG3	1.81	0.60
18:R:-2:DA:H2'	18:R:-1:DA:C8	2.36	0.60
20:c:1038:ASP:HB3	20:c:1041:ARG:HB2	1.83	0.60
21:i:626:VAL:HG12	21:i:631:HIS:HB3	1.83	0.60
5:E:739:LEU:HB3	5:E:796:LEU:HD21	1.83	0.60
20:c:95:GLU:OE1	20:c:371:ARG:NH1	2.33	0.60
2:B:112:THR:HG21	2:B:378:LEU:HD22	1.83	0.60
2:B:450:LEU:HD23	2:B:450:LEU:H	1.67	0.60
6:F:288:HIS:HD2	6:F:291:GLN:H	1.50	0.60
7:G:77:HIS:HA	7:G:81:HIS:HD2	1.67	0.60
10:J:162:PHE:HZ	10:J:294:LEU:HD23	1.67	0.59
13:m:84:ILE:HD13	13:m:150:ILE:HD13	1.84	0.59
10:J:431:LEU:HD12	10:J:432:PRO:HD2	1.84	0.59
13:M:92:LEU:HB3	13:M:150:ILE:HB	1.83	0.59
3:C:378:LEU:HD13	20:c:1317:VAL:HG13	1.84	0.59
4:D:375:CYS:SG	4:D:414:SER:OG	2.61	0.59
1:a:35:SER:HA	1:a:198:ILE:HG23	1.83	0.59
6:F:483:ARG:O	6:F:487:ASN:ND2	2.35	0.59
14:N:592:VAL:HG12	14:N:722:GLY:HA2	1.84	0.59
3:C:454:GLY:O	3:C:517:ARG:NH2	2.35	0.59
4:D:391:ALA:HB2	4:D:795:LEU:HD21	1.84	0.59
10:J:315:ASN:OD1	10:J:335:GLN:NE2	2.35	0.59
13:m:167:ILE:HA	13:m:170:MET:HE2	1.85	0.59
10:J:321:ARG:HD2	10:J:324:ASP:HB2	1.84	0.59
20:c:1093:LEU:HB3	20:c:1100:VAL:HB	1.83	0.59
9:I:210:LYS:HG3	9:I:248:GLU:HG3	1.83	0.59
10:J:381:HIS:HD2	10:J:384:THR:H	1.49	0.59
4:D:403:ILE:HD12	4:D:407:LYS:HG2	1.85	0.58
7:G:183:VAL:HG12	7:G:209:PRO:HA	1.85	0.58
9:I:429:LYS:HD2	9:I:446:GLN:HG3	1.85	0.58
21:i:485:LYS:NZ	21:i:489:GLU:OE2	2.35	0.58
20:c:247:ARG:HG3	20:c:285:ILE:HD12	1.83	0.58
4:D:819:ALA:HA	4:D:822:ASN:HD21	1.67	0.58
13:m:140:GLN:O	13:m:160:ARG:NH1	2.37	0.58
4:D:137:ARG:NH2	10:J:404:LEU:CG	2.67	0.58
5:E:704:LEU:H	5:E:704:LEU:HD23	1.68	0.58
5:E:589:GLN:HG3	5:E:623:THR:HG21	1.85	0.58
14:N:303:VAL:HA	14:N:321:ILE:HA	1.85	0.58
10:J:148:GLU:HG3	10:J:149:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:THR:O	2:B:353:GLN:NE2	2.37	0.57
2:B:411:ARG:HB2	2:B:433:GLY:HA3	1.86	0.57
2:B:632:ILE:HG23	2:B:636:GLN:HB2	1.86	0.57
1:a:301:ASN:HD22	1:a:305:ASP:HB2	1.69	0.57
1:a:301:ASN:HD21	1:a:306:LEU:HG	1.69	0.57
7:G:141:GLY:HA2	7:G:238:HIS:O	2.04	0.57
9:I:187:GLY:N	9:I:217:THR:OG1	2.31	0.57
12:L:225:VAL:HG12	12:L:238:ARG:HD2	1.86	0.57
16:P:87:GLN:HE21	16:P:135:TYR:HB2	1.67	0.57
20:c:82:LEU:HD21	20:c:96:LYS:HA	1.85	0.57
2:B:15:PHE:HA	2:B:391:ARG:HH21	1.70	0.57
12:L:207:PRO:HG2	12:L:210:VAL:HG21	1.87	0.57
6:F:591:ASN:OD1	6:F:597:LYS:NZ	2.38	0.57
10:J:314:PRO:HG3	10:J:346:ASP:HB2	1.86	0.57
4:D:80:ARG:HG2	4:D:88:GLY:HA3	1.86	0.57
5:E:424:ILE:HG21	5:E:454:VAL:HA	1.86	0.57
11:K:264:VAL:HG22	11:K:290:ILE:HD12	1.87	0.57
12:L:245:PHE:HA	12:L:249:LEU:HG	1.87	0.56
2:B:557:ARG:O	2:B:653:LYS:NZ	2.35	0.56
10:J:180:ASN:HD22	10:J:183:THR:HG22	1.69	0.56
18:R:-3:DC:H2'	18:R:-2:DA:C8	2.40	0.56
2:B:959:HIS:NE2	2:B:981:GLY:O	2.37	0.56
4:D:473:SER:OG	4:D:476:GLN:OE1	2.22	0.56
21:i:618:PRO:HB2	21:i:622:MET:HB3	1.88	0.56
2:B:716:LEU:HD22	2:B:736:ASP:HA	1.88	0.56
12:L:121:GLN:HE22	12:L:174:TRP:HE1	1.53	0.56
3:C:563:ASN:O	3:C:566:ASN:ND2	2.38	0.56
4:D:302:ASP:OD1	20:c:1253:ARG:NH2	2.39	0.56
9:I:460:THR:HB	9:I:466:GLY:HA3	1.87	0.56
3:C:511:GLU:HG3	15:O:94:ALA:HB1	1.87	0.56
7:G:186:ARG:HH21	7:G:208:ILE:HD11	1.71	0.56
14:N:623:ALA:HB3	14:N:626:SER:HB3	1.88	0.56
15:O:78:ARG:NH1	15:O:82:ASN:OD1	2.37	0.56
20:c:1265:ILE:HG12	20:c:1267:TYR:HD2	1.71	0.56
5:E:753:GLU:OE1	5:E:788:ARG:NH1	2.39	0.55
3:C:27:ILE:HD11	3:C:275:LEU:HB2	1.87	0.55
20:c:1286:SER:HB3	20:c:1314:GLU:HG3	1.88	0.55
5:E:486:MET:HE3	5:E:488:GLU:HB3	1.89	0.55
10:J:225:GLU:OE2	10:J:241:ARG:NH2	2.39	0.55
2:B:385:THR:HA	2:B:388:VAL:HG22	1.88	0.55
6:F:408:LYS:HZ2	16:P:76:LYS:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:308:MET:O	10:J:347:TYR:OH	2.23	0.55
9:I:391:TYR:OH	9:I:444:GLU:OE2	2.25	0.55
11:K:207:ILE:HG23	11:K:212:ASP:HB3	1.88	0.55
1:a:80:ILE:HG22	1:a:82:GLU:H	1.72	0.55
4:D:79:GLU:O	4:D:83:ASN:ND2	2.40	0.55
5:E:711:HIS:CE1	5:E:749:ARG:H	2.25	0.54
13:M:117:GLU:OE2	13:M:171:ARG:NH2	2.39	0.54
20:c:304:ARG:O	20:c:1219:ARG:NH1	2.40	0.54
3:C:561:ARG:HA	8:H:290:ARG:HH12	1.72	0.54
4:D:212:TYR:HB3	4:D:235:MET:HE2	1.88	0.54
6:F:171:HIS:NE2	20:c:982:LEU:O	2.39	0.54
17:Q:17:DT:H2''	17:Q:18:DT:H5'	1.89	0.54
7:G:187:GLU:HG3	7:G:188:GLU:HG2	1.89	0.54
20:c:930:LEU:HD11	20:c:941:ILE:HG12	1.89	0.54
6:F:504:LYS:HG3	6:F:508:ASN:HB2	1.89	0.54
10:J:139:ALA:HB1	10:J:330:MET:HB3	1.90	0.54
10:J:402:SER:CA	10:J:405:SER:HG	2.02	0.54
6:F:202:ARG:HD3	20:c:989:GLU:HA	1.88	0.54
2:B:972:GLN:HG2	2:B:1011:ASP:OD2	2.08	0.54
6:F:493:ALA:HA	6:F:496:ARG:HD3	1.90	0.54
2:B:697:VAL:HG13	2:B:702:PRO:HB3	1.90	0.54
9:I:216:ARG:NH2	13:M:177:ASP:OD2	2.41	0.54
20:c:387:VAL:O	20:c:397:ASN:ND2	2.41	0.54
2:B:656:LEU:HD21	2:B:842:LEU:HD11	1.90	0.54
2:B:672:LEU:HD12	2:B:832:LYS:HB3	1.90	0.54
2:B:729:GLY:HA2	1:a:72:HIS:HB3	1.90	0.54
9:I:123:GLY:HA3	9:I:166:PRO:HG2	1.89	0.54
9:I:127:LYS:HG3	9:I:128:GLU:HG2	1.89	0.54
19:S:-4:C:H2'	19:S:-3:G:C8	2.43	0.54
2:B:1044:ARG:HA	2:B:1047:ARG:HG2	1.89	0.53
6:F:386:PRO:HD2	20:c:487:VAL:HA	1.90	0.53
8:H:253:ARG:HH11	9:I:479:GLN:HG3	1.73	0.53
2:B:834:LEU:HB2	2:B:839:MET:HE2	1.91	0.53
3:C:111:MET:SD	3:C:280:PRO:HD3	2.49	0.53
7:G:146:LYS:CB	7:G:246:LEU:HD22	2.37	0.53
10:J:171:PRO:HB2	10:J:263:ILE:HD11	1.90	0.53
20:c:437:ARG:HG2	20:c:1133:ILE:HG23	1.89	0.53
3:C:400:HIS:HB2	3:C:521:PHE:HE2	1.74	0.53
6:F:409:LEU:HB3	6:F:511:MET:HE2	1.90	0.53
2:B:329:LEU:O	2:B:333:GLU:HG2	2.06	0.53
4:D:308:GLY:HA3	20:c:1256:ARG:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:129:ALA:HB2	10:J:343:MET:HE2	1.91	0.53
11:K:144:LEU:HD13	11:K:220:GLU:HG3	1.91	0.53
5:E:629:VAL:HG23	5:E:630:ILE:HG23	1.91	0.52
12:L:245:PHE:CD2	12:L:249:LEU:HD11	2.44	0.52
21:i:476:ASP:O	21:i:525:ASN:ND2	2.39	0.52
11:K:139:HIS:CD2	11:K:152:LYS:HB3	2.44	0.52
20:c:65:ILE:HD13	20:c:65:ILE:H	1.74	0.52
3:C:553:ASN:HD22	3:C:607:ASP:HB3	1.73	0.52
6:F:346:PHE:HB3	6:F:349:PRO:HD2	1.90	0.52
11:K:169:THR:HG22	11:K:176:TYR:HA	1.91	0.52
20:c:68:LYS:HG3	20:c:111:LEU:HD21	1.91	0.52
3:C:640:GLU:OE2	3:C:649:ARG:NH2	2.42	0.52
5:E:603:ALA:HB1	5:E:675:TRP:HD1	1.74	0.52
12:L:106:THR:HG21	12:L:115:PRO:HB2	1.91	0.52
1:A:29:TYR:OH	15:O:63:ARG:NH2	2.40	0.52
6:F:290:TYR:HD1	6:F:309:ARG:HG2	1.75	0.52
5:E:584:LYS:HE3	5:E:590:PRO:HG3	1.92	0.52
5:E:632:GLN:HB2	5:E:638:PHE:HB2	1.92	0.52
14:N:698:ILE:HB	14:N:701:VAL:HG22	1.91	0.52
4:D:854:ALA:O	4:D:858:ILE:HG12	2.09	0.52
5:E:533:ARG:NH2	5:E:538:PHE:O	2.43	0.52
5:E:796:LEU:HA	5:E:799:ILE:HG22	1.90	0.52
7:G:227:ASP:OD1	7:G:227:ASP:N	2.42	0.52
21:i:523:HIS:ND1	21:i:525:ASN:OD1	2.34	0.52
5:E:645:GLN:NE2	5:E:649:TYR:OH	2.42	0.52
1:a:49:MET:HE2	1:a:215:LEU:HD12	1.91	0.52
12:L:62:GLU:HG3	12:L:64:HIS:H	1.75	0.51
16:P:69:TRP:O	16:P:134:ARG:NH2	2.43	0.51
6:F:421:ASP:OD1	6:F:483:ARG:NH1	2.43	0.51
15:O:71:LEU:HA	15:O:74:MET:HE2	1.92	0.51
6:F:348:ASP:HB3	6:F:349:PRO:HD3	1.91	0.51
20:c:150:ARG:HD3	20:c:173:LEU:HD21	1.93	0.51
2:B:856:GLY:O	2:B:860:ARG:HG2	2.11	0.51
5:E:678:GLN:HB3	5:E:681:ARG:HB2	1.92	0.51
20:c:229:SER:HB3	20:c:282:PRO:HG3	1.91	0.51
6:F:309:ARG:NH2	20:c:929:THR:O	2.41	0.51
2:B:614:SER:OG	2:B:618:THR:OG1	2.25	0.51
2:B:676:ARG:NH2	2:B:849:ASP:OD2	2.34	0.51
4:D:435:TYR:CD2	14:N:632:PRO:HG3	2.46	0.51
6:F:416:GLU:HG3	6:F:474:LEU:HB3	1.93	0.51
14:N:656:ASP:HB2	14:N:659:ASP:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:1001:ASN:HB3	20:c:1004:LEU:H	1.75	0.51
10:J:153:ILE:HD12	10:J:189:LEU:HD12	1.92	0.51
15:O:111:LYS:NZ	15:O:131:GLU:OE2	2.40	0.51
3:C:650:SER:HB3	3:C:656:LEU:HD11	1.92	0.51
13:M:87:GLU:N	13:M:87:GLU:OE1	2.42	0.51
2:B:60:VAL:O	2:B:78:SER:OG	2.22	0.50
20:c:362:PHE:HB3	20:c:387:VAL:HG12	1.94	0.50
21:i:298:ASN:ND2	21:i:498:GLU:OE1	2.43	0.50
3:C:676:ALA:HA	15:O:61:GLN:HE22	1.76	0.50
3:C:131:SER:HB2	3:C:134:ALA:HB3	1.93	0.50
3:C:553:ASN:ND2	3:C:607:ASP:O	2.45	0.50
8:H:240:TRP:NE1	20:c:407:LEU:O	2.44	0.50
3:C:373:ARG:HH21	3:C:377:THR:HG21	1.77	0.50
3:C:641:ILE:HG13	3:C:646:LEU:HD13	1.93	0.50
5:E:488:GLU:HA	5:E:491:ASN:ND2	2.27	0.50
1:A:64:ARG:HB3	1:A:150:GLN:HB3	1.94	0.50
6:F:366:HIS:HB2	20:c:498:MET:HA	1.93	0.50
9:I:148:TRP:HE3	13:M:105:ILE:HG12	1.76	0.50
12:L:272:GLU:HG2	12:L:275:ARG:HH21	1.77	0.50
20:c:211:GLN:NE2	20:c:1313:LYS:HG3	2.27	0.50
20:c:1239:MET:HG3	20:c:1245:PRO:HD3	1.93	0.50
3:C:631:HIS:HB3	11:K:278:LEU:HD11	1.93	0.50
5:E:565:SER:OG	5:E:597:MET:SD	2.58	0.50
5:E:710:VAL:HG11	5:E:718:ALA:HA	1.93	0.50
12:L:85:LEU:HA	12:L:88:GLN:HE21	1.77	0.50
4:D:413:SER:HB2	4:D:803:ASP:HB2	1.93	0.50
1:A:226:PHE:HE2	1:a:226:PHE:HE2	1.58	0.50
3:C:662:THR:OG1	3:C:663:THR:N	2.45	0.50
4:D:763:THR:O	4:D:766:LYS:HG3	2.11	0.50
6:F:402:ASN:HD22	20:c:571:ARG:HG3	1.76	0.50
9:I:442:VAL:O	9:I:446:GLN:NE2	2.41	0.50
1:A:13:LEU:HA	1:A:36:PRO:HG2	1.94	0.49
5:E:537:GLN:HG3	5:E:540:GLU:HB2	1.94	0.49
16:P:83:TRP:HH2	16:P:125:LEU:HD11	1.77	0.49
4:D:170:LYS:HB2	10:J:404:LEU:HD23	1.94	0.49
7:G:224:TYR:HB3	7:G:227:ASP:OD1	2.11	0.49
20:c:1036:ASN:ND2	20:c:1038:ASP:O	2.44	0.49
21:i:438:ARG:HD2	21:i:441:LYS:HD2	1.94	0.49
21:i:541:TYR:HA	21:i:546:ASN:HD22	1.78	0.49
7:G:181:TRP:HB2	7:G:194:VAL:HG23	1.94	0.49
20:c:211:GLN:HE22	20:c:1313:LYS:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:443:ASP:OD1	20:c:1107:TYR:OH	2.30	0.49
1:a:37:LEU:HD21	1:a:45:ILE:HD12	1.94	0.49
2:B:272:LEU:HB3	2:B:274:ILE:HG12	1.93	0.49
4:D:251:LEU:HD21	4:D:266:THR:HB	1.93	0.49
8:H:259:GLU:OE2	8:H:288:ARG:NE	2.39	0.49
8:H:331:ILE:HG21	8:H:342:GLU:HG2	1.94	0.49
14:N:665:LEU:HD11	14:N:695:LEU:HD22	1.94	0.49
21:i:567:SER:OG	21:i:607:GLN:NE2	2.46	0.49
2:B:971:GLN:HG3	3:C:108:ARG:NH1	2.27	0.49
5:E:657:GLU:OE2	5:E:662:SER:N	2.39	0.49
19:S:-4:C:H2'	19:S:-3:G:H8	1.77	0.49
1:A:144:ASP:OD1	1:A:144:ASP:N	2.45	0.49
3:C:249:ASP:OD2	3:C:253:ARG:NH1	2.46	0.49
20:c:578:PRO:HA	20:c:867:PHE:HA	1.95	0.49
1:A:34:LEU:HD23	1:A:37:LEU:HD11	1.95	0.49
2:B:63:LEU:HD23	2:B:63:LEU:H	1.76	0.49
3:C:514:VAL:HG12	15:O:90:VAL:HG13	1.94	0.49
3:C:629:GLU:HG3	11:K:282:ARG:HG2	1.95	0.49
3:C:461:ARG:HG3	3:C:502:MET:HG2	1.93	0.49
9:I:217:THR:HA	9:I:239:PRO:HD2	1.95	0.49
5:E:603:ALA:HB1	5:E:676:LEU:HB2	1.95	0.48
8:H:410:PRO:HD3	13:M:109:GLN:HE22	1.78	0.48
20:c:1040:CYS:SG	20:c:1041:ARG:NH1	2.86	0.48
2:B:500:ARG:NH1	2:B:523:TYR:OH	2.46	0.48
3:C:627:PRO:HG3	3:C:642:TYR:CZ	2.48	0.48
11:K:204:GLU:OE1	20:c:25:ARG:NH1	2.45	0.48
16:P:83:TRP:NE1	16:P:87:GLN:OE1	2.33	0.48
21:i:428:LEU:HD11	21:i:457:PRO:HG2	1.94	0.48
13:m:92:LEU:HB3	13:m:150:ILE:HB	1.95	0.48
2:B:989:GLU:HB3	3:C:470:ILE:HD11	1.94	0.48
3:C:461:ARG:HD3	3:C:493:PHE:HB3	1.95	0.48
10:J:146:PRO:HA	10:J:326:MET:HG2	1.95	0.48
10:J:220:PHE:HB2	10:J:240:MET:HE2	1.95	0.48
4:D:823:ILE:O	4:D:827:THR:HG23	2.13	0.48
7:G:182:LEU:HG	7:G:191:LEU:HD11	1.95	0.48
9:I:166:PRO:HG3	9:I:263:ASN:HD22	1.79	0.48
15:O:55:ILE:HG22	15:O:58:LEU:HB2	1.96	0.48
20:c:62:LEU:HB2	20:c:170:ARG:HD3	1.94	0.48
3:C:406:ARG:NH2	3:C:479:GLU:OE2	2.47	0.48
2:B:583:ARG:HD3	2:B:600:ASN:HD21	1.79	0.48
4:D:766:LYS:HD2	4:D:767:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:533:ARG:NH2	5:E:566:VAL:HG13	2.28	0.48
5:E:638:PHE:CD2	5:E:643:ASN:HB3	2.49	0.48
7:G:90:ASN:HD22	7:G:91:LYS:N	2.11	0.48
8:H:366:ILE:HD13	1:a:197:GLU:HG2	1.94	0.48
2:B:959:HIS:HE1	2:B:980:GLN:HA	1.78	0.48
3:C:329:MET:O	3:C:333:LYS:HG2	2.14	0.48
3:C:549:LEU:HG	20:c:49:GLN:HG2	1.94	0.48
9:I:124:ALA:HB1	9:I:240:ALA:HB1	1.96	0.48
1:a:269:LEU:HD21	1:a:299:LEU:HD12	1.95	0.48
1:A:98:SER:HB2	1:A:127:VAL:HG13	1.95	0.48
3:C:454:GLY:HA3	15:O:112:LYS:HG3	1.95	0.48
8:H:391:VAL:HG11	9:I:476:LEU:HD13	1.96	0.48
9:I:482:VAL:HG22	9:I:485:MET:HE2	1.95	0.48
1:a:213:GLU:OE1	21:i:308:ARG:NH1	2.47	0.48
3:C:403:GLY:HA3	3:C:484:CYS:HB2	1.96	0.47
6:F:105:LEU:HD13	20:c:1110:THR:HG22	1.96	0.47
2:B:275:PRO:HD3	6:F:559:GLN:HG3	1.96	0.47
5:E:560:LEU:HD23	5:E:583:ILE:HG12	1.95	0.47
18:R:-2:DA:H2'	18:R:-1:DA:H8	1.79	0.47
1:a:86:GLU:N	1:a:86:GLU:OE1	2.48	0.47
21:i:380:ILE:HG23	13:m:159:ILE:HG23	1.96	0.47
1:A:65:VAL:HG11	1:A:88:LEU:HD21	1.95	0.47
4:D:498:PRO:O	4:D:509:TYR:OH	2.28	0.47
14:N:737:ASP:OD1	14:N:737:ASP:N	2.48	0.47
20:c:297:ILE:HD11	20:c:318:VAL:HG21	1.96	0.47
2:B:124:ASN:HD22	2:B:316:SER:HA	1.79	0.47
6:F:87:TRP:CH2	6:F:89:PRO:HG3	2.49	0.47
16:P:43:PRO:HB2	16:P:45:GLU:HG2	1.97	0.47
1:A:64:ARG:HH22	1:A:165:PHE:H	1.63	0.47
2:B:479:VAL:HG22	2:B:515:LEU:HB2	1.96	0.47
1:A:156:GLY:HA2	1:A:176:PHE:HB2	1.96	0.47
3:C:487:PRO:HG2	20:c:43:LYS:HD2	1.96	0.47
6:F:186:LYS:O	6:F:190:GLU:HG2	2.14	0.47
8:H:400:ASP:HB3	8:H:403:GLU:HB2	1.97	0.47
8:H:413:HIS:ND1	8:H:414:GLU:O	2.41	0.47
20:c:1225:VAL:O	20:c:1229:THR:HG22	2.14	0.47
1:A:35:SER:HB2	1:A:36:PRO:HD3	1.95	0.47
2:B:321:LEU:HD22	2:B:365:TYR:HE1	1.79	0.47
4:D:809:ARG:HA	4:D:812:VAL:HG22	1.96	0.47
5:E:533:ARG:HH21	5:E:541:ALA:HB3	1.80	0.47
5:E:728:ASP:HA	5:E:731:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:371:THR:OG1	16:P:104:GLN:NE2	2.48	0.47
6:F:521:ARG:HH11	16:P:87:GLN:HE22	1.62	0.47
10:J:439:ARG:NE	10:J:502:GLN:OE1	2.47	0.47
12:L:259:LEU:HG	12:L:263:LYS:HE3	1.95	0.47
1:a:260:LEU:HG	1:a:267:ILE:HG22	1.97	0.47
3:C:298:ASP:O	3:C:299:ILE:C	2.57	0.47
4:D:365:ASP:OD1	4:D:365:ASP:N	2.48	0.47
6:F:284:VAL:HG22	6:F:295:VAL:HG22	1.95	0.47
21:i:523:HIS:CE1	21:i:526:LEU:HB2	2.50	0.47
2:B:569:ARG:HG2	2:B:648:GLU:HG2	1.96	0.47
9:I:151:LEU:HD12	9:I:151:LEU:HA	1.79	0.47
21:i:346:LYS:HB2	21:i:404:LEU:HD13	1.97	0.47
1:A:13:LEU:HD22	1:a:228:PRO:HG2	1.97	0.47
1:A:98:SER:HB2	1:A:127:VAL:HA	1.97	0.47
3:C:111:MET:HE3	3:C:111:MET:HB3	1.65	0.47
3:C:126:LEU:HD11	3:C:148:VAL:HG21	1.97	0.47
4:D:757:THR:HA	4:D:762:TRP:CD1	2.50	0.47
5:E:607:ARG:HB2	5:E:610:MET:HB2	1.97	0.47
6:F:192:ILE:HD11	6:F:226:MET:HB3	1.96	0.47
20:c:384:ASP:OD1	20:c:384:ASP:N	2.48	0.47
20:c:385:LEU:HB3	20:c:399:ASN:HD22	1.80	0.47
2:B:372:HIS:CE1	2:B:398:PRO:HG2	2.50	0.46
2:B:1047:ARG:HB2	3:C:30:TRP:CZ3	2.49	0.46
5:E:526:ASN:HB2	5:E:559:THR:HG22	1.98	0.46
6:F:535:CYS:HA	12:L:207:PRO:HG3	1.97	0.46
8:H:204:THR:HG23	8:H:207:GLU:HB2	1.97	0.46
16:P:81:TRP:HA	20:c:883:ARG:HA	1.97	0.46
20:c:139:ASN:OD1	20:c:140:ALA:N	2.46	0.46
2:B:961:ARG:HE	2:B:981:GLY:HA2	1.79	0.46
6:F:91:GLU:OE2	6:F:316:ARG:NH2	2.48	0.46
9:I:128:GLU:HG3	13:M:164:LEU:HD22	1.98	0.46
9:I:175:ARG:NH2	9:I:202:GLU:OE2	2.49	0.46
1:A:106:ALA:HB3	1:A:149:LEU:HB2	1.96	0.46
6:F:288:HIS:CD2	6:F:291:GLN:H	2.32	0.46
2:B:693:ILE:HD11	2:B:739:VAL:HB	1.98	0.46
6:F:389:ASP:HB2	6:F:549:TYR:HB3	1.97	0.46
7:G:87:GLU:O	7:G:90:ASN:ND2	2.47	0.46
3:C:400:HIS:O	3:C:474:GLN:N	2.40	0.46
6:F:326:ILE:HB	6:F:348:ASP:HB2	1.96	0.46
7:G:172:LEU:HD11	7:G:229:ALA:HA	1.98	0.46
12:L:58:MET:CE	12:L:71:GLU:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:408:TYR:HB2	4:D:802:GLY:HA3	1.97	0.46
4:D:419:LEU:HB2	4:D:471:GLU:OE2	2.16	0.46
20:c:222:THR:HB	20:c:292:ARG:HG3	1.97	0.46
2:B:984:ARG:HA	3:C:382:ARG:HA	1.98	0.46
3:C:554:HIS:HB3	3:C:558:CYS:HB2	1.98	0.46
6:F:409:LEU:HD23	6:F:511:MET:HB2	1.97	0.46
7:G:65:LEU:HD21	7:G:139:PRO:HA	1.97	0.46
2:B:101:ILE:HD13	2:B:356:VAL:HG11	1.96	0.46
3:C:308:TYR:HA	3:C:311:ASN:ND2	2.31	0.46
11:K:143:LEU:HB3	11:K:252:SER:HB3	1.98	0.46
14:N:623:ALA:HB1	14:N:653:LYS:HE2	1.98	0.46
20:c:390:GLU:HA	20:c:395:LEU:HD23	1.98	0.46
21:i:321:ARG:NH1	21:i:533:ASN:OD1	2.42	0.46
13:m:115:ALA:HB2	13:m:124:ILE:HD12	1.98	0.46
2:B:284:ARG:HG2	6:F:567:TYR:HE1	1.81	0.46
16:P:55:ASN:N	16:P:112:GLY:O	2.46	0.46
20:c:92:HIS:NE2	20:c:95:GLU:HG3	2.31	0.46
2:B:1017:GLN:HE21	2:B:1017:GLN:HB3	1.50	0.46
5:E:556:ASP:N	5:E:559:THR:OG1	2.49	0.46
20:c:65:ILE:HD11	20:c:111:LEU:HG	1.98	0.46
5:E:747:VAL:HG23	5:E:763:VAL:HG13	1.99	0.45
9:I:174:VAL:HG21	9:I:204:VAL:HG22	1.98	0.45
20:c:465:VAL:HG13	20:c:1114:THR:HB	1.99	0.45
21:i:350:ASP:OD1	21:i:378:THR:OG1	2.33	0.45
5:E:750:GLY:H	5:E:753:GLU:HG3	1.81	0.45
5:E:626:MET:O	5:E:630:ILE:HG12	2.16	0.45
6:F:413:HIS:NE2	6:F:417:GLN:OE1	2.50	0.45
7:G:222:LEU:HG	12:L:231:TYR:CE2	2.51	0.45
10:J:413:ASP:H	10:J:416:ILE:HG23	1.81	0.45
4:D:411:LEU:HD23	4:D:411:LEU:H	1.80	0.45
5:E:506:SER:O	5:E:509:ILE:HG13	2.15	0.45
6:F:420:LEU:HD11	6:F:483:ARG:HG2	1.99	0.45
7:G:111:THR:HA	7:G:118:LEU:HD12	1.97	0.45
11:K:324:ASP:O	11:K:328:SER:OG	2.32	0.45
21:i:278:PRO:HB3	21:i:418:LYS:HD3	1.99	0.45
21:i:405:LEU:HB2	21:i:408:GLU:HG3	1.98	0.45
2:B:589:TYR:HB3	2:B:596:LEU:HB2	1.98	0.45
2:B:673:ILE:HG22	2:B:850:MET:HG2	1.99	0.45
4:D:289:GLN:OE1	4:D:322:ARG:NH2	2.49	0.45
4:D:293:ARG:HH22	4:D:359:ASN:HD22	1.64	0.45
3:C:404:LEU:HD12	3:C:405:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:MET:HE2	7:G:239:LEU:HD13	1.98	0.45
10:J:357:MET:HE3	10:J:357:MET:HB3	1.74	0.45
4:D:849:LEU:HD11	4:D:851:GLU:HB2	1.98	0.45
5:E:667:ASN:O	5:E:671:GLU:HG2	2.16	0.45
12:L:104:LEU:HD13	12:L:104:LEU:HA	1.69	0.45
14:N:305:SER:HA	14:N:323:GLU:HA	1.98	0.45
14:N:687:LEU:N	14:N:691:HIS:O	2.49	0.45
7:G:92:GLN:HB3	7:G:120:GLU:HG2	1.99	0.45
9:I:374:HIS:CE1	9:I:377:LEU:HB2	2.52	0.45
1:a:294:THR:HG23	1:a:297:ASP:H	1.81	0.45
6:F:397:GLU:OE2	6:F:526:ARG:NH2	2.50	0.45
1:a:110:VAL:HG11	1:a:116:VAL:HB	1.98	0.45
1:a:279:LEU:HD21	1:a:320:ILE:HD13	1.98	0.45
2:B:133:TYR:O	2:B:304:ASP:HB2	2.17	0.45
3:C:461:ARG:NH1	3:C:469:GLY:O	2.41	0.45
12:L:73:HIS:HD2	12:L:77:HIS:CD2	2.34	0.45
12:L:132:MET:HE3	12:L:249:LEU:HB2	1.99	0.45
20:c:360:ILE:HD11	20:c:420:ILE:HD12	1.99	0.45
21:i:381:THR:HG21	13:m:160:ARG:HH21	1.81	0.45
2:B:668:GLU:HB3	2:B:669:ASP:H	1.65	0.44
4:D:319:PRO:HG3	4:D:760:TRP:CD2	2.53	0.44
5:E:744:SER:HA	5:E:790:VAL:HA	1.99	0.44
5:E:747:VAL:HG21	5:E:764:ALA:HB2	1.98	0.44
8:H:239:ASN:HD22	20:c:376:HIS:HB3	1.82	0.44
8:H:418:ASN:HD22	8:H:421:ALA:H	1.63	0.44
9:I:111:PHE:HB2	9:I:112:PRO:HD3	1.98	0.44
10:J:230:GLU:O	10:J:484:ARG:HD2	2.16	0.44
4:D:504:ILE:O	4:D:508:ASP:HB2	2.17	0.44
5:E:460:GLU:O	5:E:464:GLN:HG2	2.17	0.44
12:L:71:GLU:O	12:L:72:TYR:C	2.59	0.44
3:C:155:ALA:HB3	3:C:169:GLY:H	1.82	0.44
18:R:4:DG:H2'	18:R:5:DA:H8	1.82	0.44
2:B:486:ALA:HB3	2:B:495:GLN:HG2	1.98	0.44
3:C:64:CYS:HB3	3:C:67:ILE:HG12	2.00	0.44
12:L:75:GLY:O	12:L:76:LYS:C	2.60	0.44
2:B:300:MET:SD	20:c:463:GLY:HA2	2.58	0.44
2:B:1055:HIS:HD2	2:B:1068:LYS:HD2	1.82	0.44
3:C:308:TYR:HA	3:C:311:ASN:HD21	1.82	0.44
3:C:370:LYS:HA	3:C:375:ARG:HD3	1.99	0.44
4:D:283:THR:O	4:D:287:VAL:HG23	2.18	0.44
5:E:710:VAL:HG12	5:E:713:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:i:523:HIS:NE2	21:i:526:LEU:HB2	2.32	0.44
1:A:224:ASP:OD1	21:i:601:SER:OG	2.34	0.44
2:B:888:ASP:OD1	2:B:888:ASP:N	2.50	0.44
2:B:959:HIS:CG	2:B:977:ARG:HG3	2.52	0.44
3:C:211:ALA:HB1	4:D:452:ARG:HD3	1.98	0.44
6:F:174:PRO:HB3	6:F:275:TYR:HB2	1.99	0.44
12:L:245:PHE:CE2	12:L:249:LEU:HD11	2.53	0.44
12:L:260:GLU:HA	12:L:263:LYS:HZ2	1.82	0.44
3:C:461:ARG:HE	3:C:502:MET:CE	2.31	0.44
4:D:155:LEU:HD13	4:D:158:ARG:HD2	1.99	0.44
4:D:305:GLU:HB2	20:c:1253:ARG:HG3	1.99	0.44
10:J:382:LEU:HB2	10:J:425:THR:HB	1.98	0.44
20:c:480:ARG:HH11	20:c:481:PRO:HD2	1.83	0.44
1:A:26:ARG:HG2	1:A:95:ILE:HD11	1.99	0.44
1:A:94:ILE:HD11	1:A:136:ILE:HG12	2.00	0.44
2:B:451:GLU:HB3	2:B:468:TYR:HB3	1.99	0.44
4:D:341:ILE:HD11	4:D:374:LEU:HD21	1.99	0.44
9:I:477:LYS:HE2	9:I:486:TRP:HB2	2.00	0.44
12:L:128:PHE:HE1	12:L:245:PHE:HE2	1.66	0.44
20:c:62:LEU:HB3	20:c:147:VAL:HG12	1.99	0.44
6:F:333:ARG:N	6:F:341:PRO:O	2.48	0.44
10:J:365:PRO:HD3	10:J:486:HIS:CE1	2.53	0.44
2:B:535:GLU:HG2	2:B:887:PHE:HA	2.00	0.43
2:B:1005:MET:O	2:B:1010:SER:OG	2.31	0.43
20:c:1109:ALA:HA	20:c:1132:PHE:HZ	1.82	0.43
3:C:449:GLN:HE21	3:C:477:LEU:HD23	1.82	0.43
16:P:91:ILE:HD11	16:P:94:GLY:O	2.18	0.43
20:c:281:GLN:HB3	20:c:282:PRO:HD2	1.98	0.43
20:c:477:LEU:HD23	20:c:1104:ALA:HB2	2.00	0.43
21:i:532:THR:HG22	21:i:538:ILE:HG23	1.99	0.43
21:i:538:ILE:HD11	21:i:571:ILE:HD13	1.99	0.43
13:m:128:ASP:OD1	13:m:128:ASP:N	2.51	0.43
2:B:984:ARG:HB2	3:C:382:ARG:NH1	2.33	0.43
3:C:115:LYS:HA	3:C:275:LEU:HD22	1.99	0.43
5:E:440:LEU:HD21	5:E:458:VAL:HG21	2.01	0.43
10:J:142:ILE:HG13	10:J:143:MET:HG3	2.01	0.43
20:c:1079:ILE:HG22	20:c:1085:PRO:HD3	2.01	0.43
2:B:1007:THR:HG22	2:B:1036:PRO:HG3	1.99	0.43
3:C:362:SER:OG	3:C:365:ASP:OD1	2.36	0.43
5:E:488:GLU:HA	5:E:491:ASN:HD21	1.83	0.43
7:G:126:GLN:HA	7:G:129:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:222:MET:HE2	9:I:234:GLU:HG2	2.00	0.43
21:i:555:VAL:HG21	21:i:607:GLN:HG2	2.00	0.43
2:B:1001:ILE:O	2:B:1004:GLU:HG2	2.18	0.43
4:D:261:GLU:OE2	4:D:299:ARG:NH2	2.51	0.43
6:F:308:LYS:HD3	6:F:357:ASN:HB3	2.00	0.43
14:N:624:GLY:HA3	14:N:652:PRO:O	2.17	0.43
20:c:27:ILE:HG13	20:c:35:THR:HG21	2.01	0.43
20:c:401:PRO:HG2	20:c:402:PRO:HD3	2.01	0.43
2:B:952:HIS:HB3	2:B:957:LYS:HE2	2.01	0.43
2:B:961:ARG:HG2	2:B:962:SER:N	2.34	0.43
4:D:412:VAL:HG22	4:D:792:VAL:HG21	1.99	0.43
8:H:391:VAL:HG12	9:I:459:TRP:HZ3	1.84	0.43
2:B:548:MET:SD	2:B:827:LYS:HB2	2.59	0.43
5:E:629:VAL:HG21	5:E:650:VAL:HG21	2.01	0.43
6:F:408:LYS:HB3	6:F:408:LYS:HE2	1.84	0.43
8:H:288:ARG:HD3	20:c:63:LEU:HD13	1.99	0.43
20:c:384:ASP:HB3	20:c:401:PRO:HB3	2.00	0.43
2:B:996:PHE:HD1	2:B:996:PHE:HA	1.78	0.43
11:K:247:ILE:HB	11:K:260:ALA:HB3	2.01	0.43
12:L:81:TYR:CE2	12:L:121:GLN:HB3	2.53	0.43
1:a:50:ARG:NH1	1:a:182:ALA:O	2.52	0.43
20:c:57:LEU:HD13	20:c:128:VAL:HG23	2.01	0.43
2:B:939:PRO:O	20:c:56:SER:OG	2.36	0.43
2:B:971:GLN:HG3	3:C:108:ARG:HH12	1.83	0.43
12:L:265:LYS:O	12:L:268:GLU:HG2	2.18	0.43
1:a:283:ILE:HG23	1:a:312:PHE:HZ	1.83	0.43
5:E:725:TRP:HH2	5:E:743:ALA:HB1	1.84	0.43
8:H:425:GLU:HG3	13:M:66:VAL:HG22	2.01	0.43
1:a:37:LEU:HD12	1:a:37:LEU:HA	1.87	0.43
3:C:9:ILE:H	4:D:236:GLU:CD	2.27	0.42
3:C:538:PRO:HD3	20:c:39:LEU:HD11	2.01	0.42
4:D:368:SER:O	4:D:372:ARG:HG2	2.19	0.42
5:E:715:PRO:HB3	5:E:766:ALA:HB2	2.01	0.42
6:F:87:TRP:HA	20:c:1119:TYR:CZ	2.54	0.42
7:G:164:ARG:HG3	7:G:236:MET:HE2	2.01	0.42
12:L:268:GLU:O	12:L:271:GLU:HG2	2.19	0.42
13:M:147:LEU:HB2	13:M:161:THR:OG1	2.19	0.42
3:C:462:ALA:HB3	3:C:463:PRO:HD3	2.01	0.42
4:D:324:TYR:HB3	4:D:347:LEU:HB2	2.01	0.42
4:D:756:ILE:O	4:D:757:THR:C	2.56	0.42
6:F:232:ASN:HA	6:F:235:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:309:ARG:H	6:F:309:ARG:HG3	1.67	0.42
6:F:364:ILE:HG21	6:F:380:CYS:HB2	2.01	0.42
20:c:438:LYS:HB2	20:c:1134:TYR:HE1	1.83	0.42
1:A:111:LYS:HE3	1:A:144:ASP:HB3	2.01	0.42
3:C:400:HIS:CD2	3:C:401:ARG:HG3	2.55	0.42
4:D:500:ILE:HG23	4:D:502:GLY:H	1.84	0.42
5:E:613:GLU:H	5:E:613:GLU:HG3	1.66	0.42
5:E:687:ASN:O	5:E:691:LYS:HG2	2.19	0.42
6:F:127:PRO:HA	6:F:130:ARG:HE	1.84	0.42
6:F:170:ARG:HB2	20:c:986:LEU:HD21	2.01	0.42
1:a:61:CYS:SG	1:a:62:ILE:N	2.92	0.42
6:F:262:LYS:HE2	6:F:262:LYS:HB2	1.83	0.42
8:H:312:ILE:HG12	8:H:346:LEU:HD13	2.01	0.42
1:a:306:LEU:O	1:a:309:ILE:HG12	2.19	0.42
20:c:953:PRO:HA	20:c:1097:ASP:O	2.19	0.42
21:i:383:MET:HG2	21:i:394:THR:HA	2.00	0.42
2:B:38:PHE:HZ	2:B:52:LEU:H	1.67	0.42
3:C:517:ARG:HD3	15:O:72:LEU:HD21	2.01	0.42
6:F:484:GLN:HA	6:F:487:ASN:HD21	1.85	0.42
7:G:108:ILE:HD13	7:G:201:ASN:HD21	1.84	0.42
9:I:153:TRP:HD1	9:I:413:CYS:HG	1.62	0.42
9:I:294:LEU:HD22	9:I:296:LEU:HD21	2.02	0.42
12:L:78:HIS:CD2	12:L:129:TRP:HE1	2.36	0.42
20:c:57:LEU:HD12	20:c:61:ASP:HB3	2.02	0.42
20:c:385:LEU:HB3	20:c:399:ASN:ND2	2.35	0.42
20:c:1235:SER:HB3	20:c:1266:CYS:SG	2.59	0.42
2:B:693:ILE:HG12	2:B:775:LEU:HD22	2.02	0.42
3:C:147:LEU:HD21	3:C:154:PHE:HB2	2.01	0.42
4:D:408:TYR:CE2	4:D:806:VAL:HG21	2.55	0.42
8:H:402:ASP:OD1	8:H:402:ASP:N	2.51	0.42
10:J:151:LEU:HG	10:J:204:TRP:NE1	2.35	0.42
10:J:404:LEU:HD22	10:J:404:LEU:HA	1.79	0.42
12:L:274:GLU:O	12:L:278:ARG:HG2	2.20	0.42
1:a:278:GLU:OE1	1:a:279:LEU:N	2.52	0.42
13:m:92:LEU:HD23	13:m:150:ILE:HD12	2.00	0.42
4:D:137:ARG:HH22	10:J:404:LEU:CG	2.17	0.42
5:E:577:GLU:OE1	5:E:602:TYR:OH	2.28	0.42
12:L:69:THR:HG21	12:L:233:ASP:HB2	2.01	0.42
1:a:131:ASP:HB3	1:a:134:GLN:HG3	2.01	0.42
1:a:231:HIS:CD2	21:i:609:LEU:HD22	2.55	0.42
20:c:448:MET:HB2	20:c:1123:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:TYR:HB3	2:B:523:TYR:HE2	1.83	0.42
2:B:450:LEU:H	2:B:450:LEU:CD2	2.31	0.42
6:F:194:GLU:OE1	6:F:223:ARG:NH1	2.53	0.42
6:F:366:HIS:O	20:c:499:ASN:N	2.50	0.42
21:i:289:ALA:O	13:m:145:PRO:HG2	2.20	0.42
6:F:170:ARG:HE	20:c:986:LEU:HD11	1.85	0.42
10:J:141:VAL:HG22	10:J:330:MET:HG2	2.02	0.42
12:L:51:LEU:HD23	12:L:51:LEU:H	1.85	0.42
1:a:108:ILE:HG12	1:a:121:ILE:HG12	2.01	0.42
2:B:107:MET:HE1	2:B:317:VAL:HG11	2.02	0.42
4:D:270:MET:HE2	4:D:279:PRO:HA	2.02	0.42
8:H:347:ILE:HG12	1:a:33:ILE:HD13	2.02	0.42
12:L:72:TYR:O	12:L:73:HIS:C	2.62	0.42
20:c:1202:VAL:O	20:c:1203:ASN:C	2.63	0.42
2:B:465:ARG:HA	2:B:465:ARG:HH11	1.85	0.41
6:F:204:ASP:HB3	6:F:207:LYS:HG2	2.02	0.41
10:J:195:TYR:O	10:J:199:CYS:N	2.48	0.41
12:L:67:HIS:HA	12:L:70:PHE:HB2	2.02	0.41
14:N:678:HIS:HB3	14:N:685:PRO:HD2	2.01	0.41
1:a:58:GLU:OE2	1:a:101:TYR:OH	2.31	0.41
20:c:1105:LYS:HA	20:c:1106:PRO:HD3	1.91	0.41
2:B:478:MET:HB2	2:B:513:VAL:HA	2.02	0.41
3:C:226:TRP:CD1	3:C:248:LYS:HG3	2.55	0.41
4:D:839:TYR:HA	4:D:842:ILE:HG12	2.02	0.41
5:E:692:ARG:NH2	5:E:694:LEU:HD11	2.35	0.41
7:G:221:TYR:HB3	12:L:231:TYR:CD2	2.55	0.41
1:A:16:LYS:HA	1:a:233:GLU:HG3	2.01	0.41
1:A:216:HIS:O	1:A:220:ARG:HG3	2.20	0.41
2:B:692:GLU:HB3	2:B:805:ARG:HG2	2.00	0.41
2:B:875:GLY:O	2:B:879:ASP:N	2.53	0.41
6:F:550:VAL:O	6:F:552:PRO:HD3	2.20	0.41
10:J:465:LYS:HA	10:J:468:ASP:OD2	2.21	0.41
11:K:205:PRO:HA	11:K:206:PRO:HD3	1.96	0.41
11:K:209:ALA:HB3	11:K:212:ASP:HB2	2.01	0.41
20:c:1039:PRO:HD2	20:c:1041:ARG:NH2	2.35	0.41
20:c:1279:LEU:HD13	20:c:1295:ARG:HH22	1.85	0.41
2:B:672:LEU:HD21	2:B:834:LEU:HD12	2.01	0.41
5:E:725:TRP:O	5:E:729:MET:HG3	2.20	0.41
6:F:488:LYS:O	6:F:491:MET:HG3	2.19	0.41
8:H:263:LEU:HD21	8:H:287:TYR:HB2	2.02	0.41
18:R:4:DG:H2'	18:R:5:DA:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:301:ASN:ND2	1:a:302:SER:O	2.53	0.41
20:c:63:LEU:HB2	20:c:119:PHE:HE1	1.84	0.41
20:c:851:ALA:HA	20:c:872:LEU:HA	2.03	0.41
21:i:283:PHE:HZ	21:i:435:THR:HG22	1.85	0.41
21:i:584:HIS:CE1	21:i:585:LEU:HG	2.56	0.41
2:B:99:ILE:HD12	2:B:356:VAL:HG21	2.03	0.41
2:B:698:THR:OG1	2:B:701:GLY:O	2.35	0.41
2:B:1002:LEU:HD23	20:c:1322:ILE:HD13	2.02	0.41
4:D:485:HIS:HA	4:D:488:LYS:HE2	2.03	0.41
10:J:435:PRO:HB3	10:J:506:LEU:HD21	2.01	0.41
20:c:141:SER:O	20:c:145:GLN:HG2	2.20	0.41
2:B:62:PRO:HG2	2:B:76:TYR:CZ	2.55	0.41
2:B:552:ALA:HB2	2:B:948:LEU:HD23	2.02	0.41
3:C:120:VAL:HG11	3:C:339:VAL:HG21	2.03	0.41
3:C:414:GLN:O	3:C:418:ILE:HG12	2.21	0.41
3:C:624:ARG:NH1	11:K:220:GLU:OE2	2.53	0.41
5:E:574:ASP:OD1	5:E:574:ASP:N	2.53	0.41
5:E:679:LYS:HE3	5:E:679:LYS:HB2	1.93	0.41
1:a:94:ILE:HD13	1:a:134:GLN:NE2	2.35	0.41
20:c:21:ARG:O	20:c:25:ARG:HG3	2.21	0.41
20:c:31:GLY:O	20:c:35:THR:OG1	2.29	0.41
20:c:1249:ILE:HG22	20:c:1250:GLY:H	1.85	0.41
20:c:1312:LEU:HD21	20:c:1324:VAL:HG21	2.02	0.41
2:B:662:TRP:CZ3	2:B:840:PRO:HG3	2.56	0.41
5:E:546:VAL:O	5:E:550:LYS:HG2	2.20	0.41
6:F:325:VAL:HG21	6:F:346:PHE:HE1	1.85	0.41
18:R:5:DA:H2'	18:R:6:DT:C6	2.56	0.41
2:B:1004:GLU:HB2	2:B:1008:TYR:CE2	2.55	0.41
3:C:672:GLU:HG3	3:C:673:ILE:N	2.36	0.41
10:J:109:ARG:HD2	10:J:203:PHE:CD1	2.56	0.41
16:P:72:TRP:HB2	16:P:135:TYR:CE1	2.55	0.41
16:P:110:VAL:HG22	16:P:111:ALA:H	1.85	0.41
1:a:83:SER:HB2	1:a:86:GLU:OE1	2.21	0.41
20:c:366:LEU:HB3	20:c:383:ILE:HD11	2.02	0.41
20:c:576:ILE:HA	20:c:869:ARG:HA	2.01	0.41
2:B:25:ARG:O	2:B:29:GLN:HG2	2.21	0.41
2:B:738:LEU:HD13	2:B:806:VAL:HG21	2.02	0.41
2:B:1013:ILE:O	2:B:1016:ARG:HG2	2.20	0.41
6:F:194:GLU:O	6:F:197:LYS:HG2	2.20	0.41
6:F:408:LYS:O	6:F:412:ILE:HG23	2.20	0.41
8:H:362:MET:HE2	8:H:362:MET:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:406:VAL:HG11	9:I:415:ARG:HH12	1.86	0.41
14:N:684:TYR:CD2	14:N:763:PRO:HD3	2.56	0.41
2:B:523:TYR:CD1	20:c:175:LEU:HD21	2.56	0.41
3:C:486:HIS:O	3:C:489:VAL:HG12	2.21	0.41
4:D:92:VAL:O	4:D:96:MET:HG3	2.20	0.41
6:F:420:LEU:HD11	6:F:483:ARG:CB	2.50	0.41
7:G:113:ASN:HB3	7:G:116:ASN:O	2.21	0.41
1:a:157:TYR:HD1	1:a:157:TYR:H	1.68	0.41
20:c:98:ARG:HH21	20:c:1134:TYR:HB2	1.85	0.41
20:c:464:ASN:HD22	20:c:1118:HIS:CE1	2.38	0.41
3:C:672:GLU:HA	3:C:675:GLU:HG2	2.03	0.40
4:D:380:ILE:HG21	4:D:415:TRP:CD2	2.57	0.40
6:F:262:LYS:H	6:F:262:LYS:HD3	1.84	0.40
10:J:469:SER:O	10:J:471:PRO:HD3	2.21	0.40
11:K:145:ASP:O	11:K:171:PRO:HD3	2.21	0.40
1:a:98:SER:O	1:a:153:ARG:NH1	2.54	0.40
13:m:149:PHE:HB2	13:m:159:ILE:HB	2.03	0.40
2:B:284:ARG:HG2	6:F:567:TYR:CE1	2.56	0.40
4:D:737:GLU:HA	4:D:740:VAL:HG22	2.04	0.40
7:G:77:HIS:O	7:G:81:HIS:HB2	2.22	0.40
7:G:175:PHE:HZ	12:L:121:GLN:HG3	1.86	0.40
10:J:481:ILE:HA	10:J:484:ARG:HD3	2.03	0.40
20:c:239:ILE:HD12	20:c:1210:ARG:NH1	2.36	0.40
20:c:381:CYS:O	20:c:403:LYS:HA	2.21	0.40
13:m:173:ILE:HD13	13:m:173:ILE:HA	1.88	0.40
3:C:264:THR:O	3:C:266:ILE:HG12	2.22	0.40
10:J:199:CYS:O	10:J:205:GLN:NE2	2.54	0.40
12:L:146:GLN:HA	12:L:149:ASN:HD21	1.85	0.40
3:C:518:LEU:HD22	15:O:90:VAL:HG22	2.03	0.40
4:D:70:ARG:HD3	4:D:101:LEU:HD13	2.04	0.40
4:D:99:ALA:HB2	5:E:705:VAL:HG21	2.04	0.40
5:E:491:ASN:O	5:E:494:ILE:HG22	2.21	0.40
6:F:304:TRP:HE3	6:F:343:GLU:HG2	1.86	0.40
20:c:71:LEU:HA	20:c:74:ASP:OD2	2.22	0.40
2:B:871:LEU:HD12	2:B:871:LEU:HA	1.88	0.40
5:E:433:HIS:NE2	5:E:465:ALA:HB2	2.37	0.40
10:J:380:ILE:HD11	10:J:501:TYR:CD2	2.56	0.40
20:c:405:LEU:HD13	20:c:405:LEU:HA	1.98	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	284/337 (84%)	276 (97%)	8 (3%)	0	100	100
1	a	299/337 (89%)	291 (97%)	8 (3%)	0	100	100
2	B	992/1070 (93%)	973 (98%)	19 (2%)	0	100	100
3	C	647/688 (94%)	629 (97%)	18 (3%)	0	100	100
4	D	639/892 (72%)	627 (98%)	12 (2%)	0	100	100
5	E	698/860 (81%)	691 (99%)	7 (1%)	0	100	100
6	F	542/682 (80%)	532 (98%)	10 (2%)	0	100	100
7	G	216/266 (81%)	207 (96%)	9 (4%)	0	100	100
8	H	258/531 (49%)	256 (99%)	2 (1%)	0	100	100
9	I	374/486 (77%)	365 (98%)	9 (2%)	0	100	100
10	J	419/507 (83%)	412 (98%)	6 (1%)	1 (0%)	43	72
11	K	202/331 (61%)	200 (99%)	2 (1%)	0	100	100
12	L	225/303 (74%)	215 (96%)	10 (4%)	0	100	100
13	M	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
13	m	107/178 (60%)	107 (100%)	0	0	100	100
14	N	535/770 (70%)	523 (98%)	12 (2%)	0	100	100
15	O	95/167 (57%)	93 (98%)	2 (2%)	0	100	100
16	P	100/143 (70%)	100 (100%)	0	0	100	100
20	c	1162/1388 (84%)	1129 (97%)	33 (3%)	0	100	100
21	i	373/648 (58%)	360 (96%)	13 (4%)	0	100	100
All	All	8281/10762 (77%)	8098 (98%)	182 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	408	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/308 (73%)	216 (96%)	10 (4%)	25	59
1	a	256/308 (83%)	238 (93%)	18 (7%)	14	40
2	B	767/924 (83%)	729 (95%)	38 (5%)	22	54
3	C	465/612 (76%)	433 (93%)	32 (7%)	14	41
4	D	523/770 (68%)	489 (94%)	34 (6%)	15	43
5	E	308/741 (42%)	285 (92%)	23 (8%)	12	37
6	F	401/615 (65%)	386 (96%)	15 (4%)	30	65
7	G	176/232 (76%)	166 (94%)	10 (6%)	18	49
8	H	212/472 (45%)	205 (97%)	7 (3%)	33	69
9	I	298/437 (68%)	287 (96%)	11 (4%)	30	65
10	J	368/449 (82%)	351 (95%)	17 (5%)	24	58
11	K	192/301 (64%)	188 (98%)	4 (2%)	47	79
12	L	167/258 (65%)	153 (92%)	14 (8%)	10	32
13	M	103/160 (64%)	102 (99%)	1 (1%)	68	88
13	m	93/160 (58%)	88 (95%)	5 (5%)	20	51
14	N	99/659 (15%)	90 (91%)	9 (9%)	9	28
15	O	79/144 (55%)	75 (95%)	4 (5%)	21	54
16	P	82/129 (64%)	77 (94%)	5 (6%)	17	46
20	c	697/1238 (56%)	657 (94%)	40 (6%)	18	49
21	i	316/567 (56%)	307 (97%)	9 (3%)	38	73
All	All	5828/9484 (62%)	5522 (95%)	306 (5%)	22	52

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	100	LEU
1	A	108	ILE

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Mol	Chain	Res	Type
1	A	110	VAL
1	A	126	TYR
1	A	133	THR
1	A	145	PHE
1	A	175	VAL
1	A	209	LEU
1	A	295	LEU
2	B	19	GLN
2	B	57	TYR
2	B	86	LEU
2	B	147	THR
2	B	172	VAL
2	B	296	LEU
2	B	366	GLU
2	B	387	ILE
2	B	411	ARG
2	B	426	THR
2	B	450	LEU
2	B	465	ARG
2	B	491	ILE
2	B	495	GLN
2	B	502	ARG
2	B	535	GLU
2	B	637	ILE
2	B	640	ASP
2	B	645	VAL
2	B	705	VAL
2	B	742	LEU
2	B	771	LYS
2	B	777	LEU
2	B	826	ASN
2	B	829	ILE
2	B	877	LEU
2	B	911	THR
2	B	921	TYR
2	B	926	ARG
2	B	958	ILE
2	B	969	VAL
2	B	996	PHE
2	B	1011	ASP
2	B	1017	GLN
2	B	1019	VAL

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Mol	Chain	Res	Type
2	B	1041	LEU
2	B	1057	LEU
2	B	1062	ASN
3	C	22	VAL
3	C	27	ILE
3	C	62	LEU
3	C	99	VAL
3	C	102	VAL
3	C	111	MET
3	C	114	ILE
3	C	123	VAL
3	C	126	LEU
3	C	129	LEU
3	C	261	PHE
3	C	272	VAL
3	C	302	LEU
3	C	313	LEU
3	C	329	MET
3	C	370	LYS
3	C	371	GLU
3	C	373	ARG
3	C	376	GLU
3	C	382	ARG
3	C	393	VAL
3	C	407	GLU
3	C	457	VAL
3	C	459	LEU
3	C	474	GLN
3	C	524	MET
3	C	539	THR
3	C	542	MET
3	C	614	TRP
3	C	620	VAL
3	C	652	LYS
3	C	672	GLU
4	D	111	PHE
4	D	119	ARG
4	D	130	ARG
4	D	134	GLU
4	D	149	LEU
4	D	157	THR
4	D	190	LEU

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Mol	Chain	Res	Type
4	D	208	THR
4	D	261	GLU
4	D	313	ASP
4	D	314	HIS
4	D	315	LYS
4	D	338	ARG
4	D	365	ASP
4	D	381	VAL
4	D	408	TYR
4	D	410	THR
4	D	419	LEU
4	D	446	LYS
4	D	457	LEU
4	D	496	GLU
4	D	501	LEU
4	D	758	ASP
4	D	766	LYS
4	D	798	THR
4	D	803	ASP
4	D	806	VAL
4	D	821	LEU
4	D	822	ASN
4	D	828	HIS
4	D	830	LEU
4	D	840	ASP
4	D	847	LEU
4	D	862	LEU
5	E	392	PHE
5	E	478	MET
5	E	515	GLU
5	E	558	ARG
5	E	575	GLU
5	E	579	GLN
5	E	584	LYS
5	E	599	LEU
5	E	626	MET
5	E	632	GLN
5	E	641	GLU
5	E	650	VAL
5	E	676	LEU
5	E	679	LYS
5	E	684	ARG

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Mol	Chain	Res	Type
5	E	708	VAL
5	E	710	VAL
5	E	731	GLU
5	E	747	VAL
5	E	748	VAL
5	E	763	VAL
5	E	788	ARG
5	E	796	LEU
6	F	97	GLU
6	F	176	ASP
6	F	177	TRP
6	F	185	ASP
6	F	203	VAL
6	F	214	MET
6	F	328	GLU
6	F	416	GLU
6	F	419	ILE
6	F	420	LEU
6	F	494	GLN
6	F	515	ASP
6	F	533	ILE
6	F	591	ASN
6	F	595	VAL
7	G	56	LYS
7	G	70	SER
7	G	90	ASN
7	G	116	ASN
7	G	129	ASN
7	G	135	GLU
7	G	194	VAL
7	G	211	ILE
7	G	221	TYR
7	G	256	VAL
8	H	203	LEU
8	H	204	THR
8	H	242	LYS
8	H	302	GLU
8	H	322	TRP
8	H	355	ASP
8	H	423	LEU
9	I	151	LEU
9	I	216	ARG

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Mol	Chain	Res	Type
9	I	224	ILE
9	I	236	VAL
9	I	272	MET
9	I	373	TRP
9	I	387	LEU
9	I	406	VAL
9	I	415	ARG
9	I	461	ILE
9	I	467	PHE
10	J	184	ASP
10	J	259	VAL
10	J	287	LEU
10	J	291	ILE
10	J	300	LEU
10	J	302	VAL
10	J	362	PHE
10	J	370	ASP
10	J	400	HIS
10	J	402	SER
10	J	404	LEU
10	J	405	SER
10	J	416	ILE
10	J	444	GLU
10	J	450	HIS
10	J	453	LEU
10	J	458	THR
11	K	272	ARG
11	K	275	LYS
11	K	312	ARG
11	K	327	VAL
12	L	51	LEU
12	L	65	MET
12	L	70	PHE
12	L	71	GLU
12	L	76	LYS
12	L	78	HIS
12	L	100	GLU
12	L	104	LEU
12	L	169	GLN
12	L	222	THR
12	L	225	VAL
12	L	227	GLU

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Mol	Chain	Res	Type
12	L	232	LEU
12	L	246	MET
13	M	144	LEU
14	N	588	PHE
14	N	596	HIS
14	N	608	VAL
14	N	619	VAL
14	N	633	ILE
14	N	654	THR
14	N	672	MET
14	N	687	LEU
14	N	759	THR
15	O	55	ILE
15	O	102	GLU
15	O	147	LYS
15	O	150	LEU
16	P	45	GLU
16	P	52	VAL
16	P	74	THR
16	P	91	ILE
16	P	95	GLU
1	a	12	THR
1	a	27	LEU
1	a	33	ILE
1	a	34	LEU
1	a	116	VAL
1	a	119	GLN
1	a	122	ILE
1	a	140	THR
1	a	147	ILE
1	a	175	VAL
1	a	227	ILE
1	a	266	LYS
1	a	278	GLU
1	a	288	LYS
1	a	298	LEU
1	a	301	ASN
1	a	312	PHE
1	a	324	LEU
20	c	8	VAL
20	c	40	ASP
20	c	65	ILE

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Mol	Chain	Res	Type
20	c	94	VAL
20	c	114	GLU
20	c	128	VAL
20	c	157	GLN
20	c	191	ASP
20	c	211	GLN
20	c	213	ILE
20	c	312	VAL
20	c	320	ILE
20	c	372	THR
20	c	397	ASN
20	c	422	GLU
20	c	569	LYS
20	c	1010	GLN
20	c	1022	LYS
20	c	1038	ASP
20	c	1044	ILE
20	c	1067	ILE
20	c	1073	ILE
20	c	1099	ILE
20	c	1128	THR
20	c	1129	LEU
20	c	1146	LEU
20	c	1152	VAL
20	c	1153	LEU
20	c	1173	ASN
20	c	1182	ILE
20	c	1194	ILE
20	c	1215	GLN
20	c	1224	ILE
20	c	1233	LEU
20	c	1249	ILE
20	c	1265	ILE
20	c	1270	VAL
20	c	1272	LEU
20	c	1290	PHE
20	c	1321	VAL
21	i	270	ILE
21	i	308	ARG
21	i	341	VAL
21	i	454	VAL
21	i	473	GLN

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Mol	Chain	Res	Type
21	i	549	VAL
21	i	561	THR
21	i	564	MET
21	i	596	LEU
13	m	83	LEU
13	m	101	CYS
13	m	119	GLU
13	m	144	LEU
13	m	172	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	85	HIS
1	A	150	GLN
1	A	196	GLN
1	A	276	GLN
1	A	285	ASN
2	B	6	ASN
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	376	GLN
2	B	386	GLN
2	B	483	ASN
2	B	522	GLN
2	B	600	ASN
2	B	615	ASN
2	B	622	GLN
2	B	636	GLN
2	B	719	ASN
2	B	910	GLN
2	B	934	ASN
2	B	938	GLN
2	B	953	GLN
2	B	1017	GLN
2	B	1062	ASN
2	B	1064	GLN

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Mol	Chain	Res	Type
3	C	80	ASN
3	C	110	GLN
3	C	221	ASN
3	C	331	GLN
3	C	336	GLN
3	C	449	GLN
3	C	453	GLN
3	C	471	GLN
3	C	474	GLN
3	C	513	GLN
3	C	523	HIS
3	C	525	ASN
3	C	553	ASN
4	D	83	ASN
4	D	109	HIS
4	D	126	HIS
4	D	175	GLN
4	D	194	ASN
4	D	269	ASN
4	D	349	ASN
4	D	420	GLN
4	D	778	GLN
4	D	822	ASN
4	D	882	GLN
5	E	476	ASN
5	E	495	HIS
5	E	579	GLN
5	E	581	GLN
5	E	616	ASN
5	E	645	GLN
5	E	792	GLN
6	F	81	ASN
6	F	128	ASN
6	F	148	GLN
6	F	196	HIS
6	F	278	GLN
6	F	288	HIS
6	F	301	HIS
6	F	324	HIS
6	F	366	HIS
6	F	372	ASN
6	F	402	ASN

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Mol	Chain	Res	Type
6	F	484	GLN
6	F	494	GLN
6	F	518	HIS
6	F	559	GLN
7	G	90	ASN
7	G	92	GLN
7	G	116	ASN
7	G	129	ASN
7	G	226	ASN
7	G	253	GLN
8	H	195	GLN
8	H	247	GLN
8	H	300	GLN
8	H	320	GLN
8	H	332	GLN
8	H	343	ASN
8	H	353	GLN
8	H	418	ASN
9	I	139	GLN
9	I	193	GLN
9	I	200	ASN
9	I	263	ASN
9	I	317	GLN
9	I	336	HIS
9	I	346	GLN
9	I	354	GLN
9	I	440	GLN
10	J	180	ASN
10	J	243	GLN
10	J	244	GLN
10	J	254	ASN
10	J	281	GLN
10	J	288	GLN
10	J	313	GLN
10	J	319	HIS
10	J	400	HIS
10	J	446	GLN
10	J	496	GLN
11	K	139	HIS
11	K	313	GLN
12	L	67	HIS
12	L	77	HIS

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Mol	Chain	Res	Type
12	L	78	HIS
12	L	84	ASN
12	L	88	GLN
12	L	121	GLN
12	L	149	ASN
12	L	169	GLN
14	N	678	HIS
14	N	681	ASN
15	O	61	GLN
15	O	99	GLN
15	O	116	HIS
15	O	120	ASN
16	P	104	GLN
16	P	132	GLN
1	a	119	GLN
1	a	187	HIS
1	a	196	GLN
1	a	221	ASN
1	a	231	HIS
1	a	263	ASN
1	a	285	ASN
1	a	301	ASN
20	c	41	GLN
20	c	73	GLN
20	c	77	GLN
20	c	126	ASN
20	c	157	GLN
20	c	264	ASN
20	c	265	GLN
20	c	397	ASN
20	c	449	HIS
20	c	456	HIS
20	c	464	ASN
20	c	495	GLN
20	c	497	GLN
20	c	924	GLN
20	c	1001	ASN
20	c	1007	ASN
20	c	1095	GLN
20	c	1207	GLN
20	c	1212	GLN
20	c	1218	ASN

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Mol	Chain	Res	Type
20	c	1315	ASN
21	i	287	GLN
21	i	288	HIS
21	i	361	ASN
21	i	363	ASN
21	i	410	ASN
21	i	455	ASN
21	i	473	GLN
21	i	546	ASN
21	i	584	HIS
21	i	607	GLN
13	m	121	ASN
13	m	140	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S	8/27 (29%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

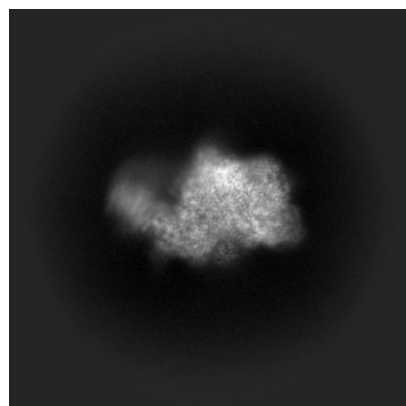
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37388. These allow visual inspection of the internal detail of the map and identification of artifacts.

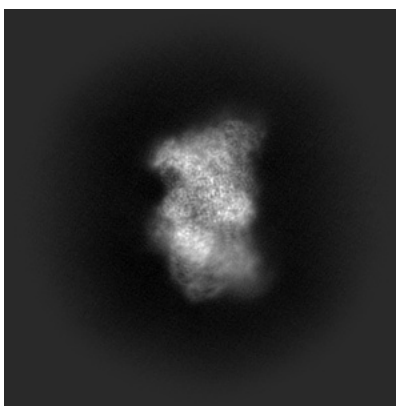
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

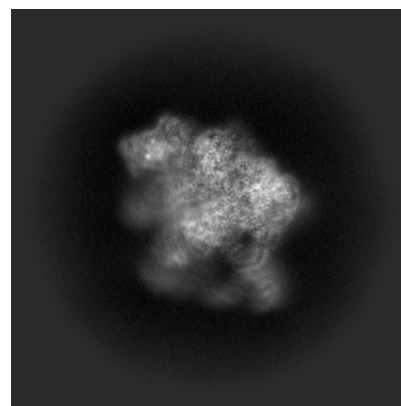
6.1.1 Primary map



X

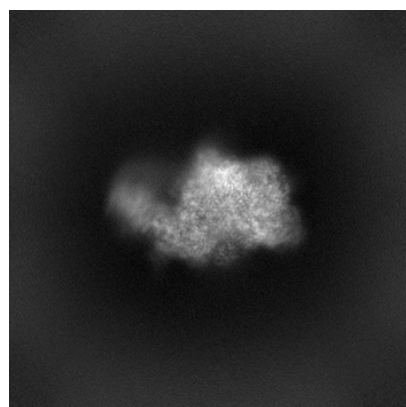


Y

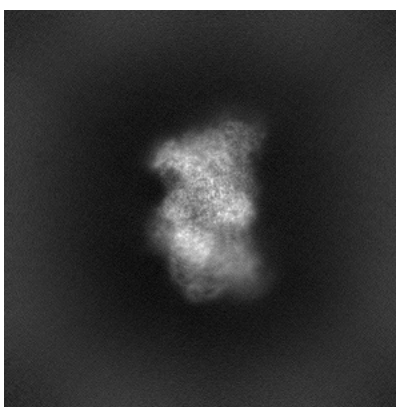


Z

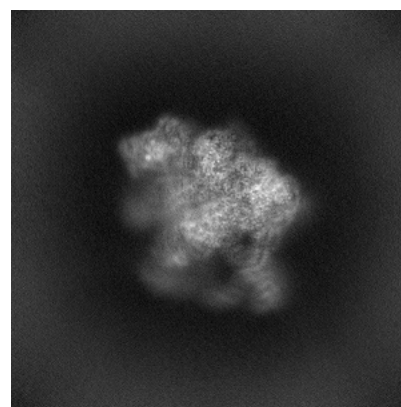
6.1.2 Raw map



X



Y

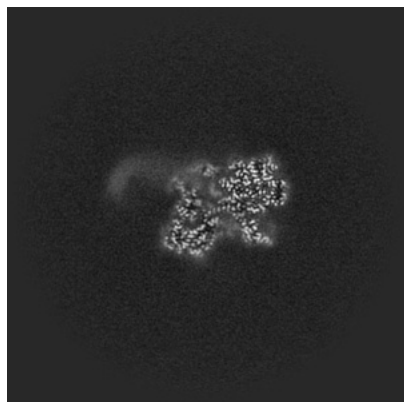


Z

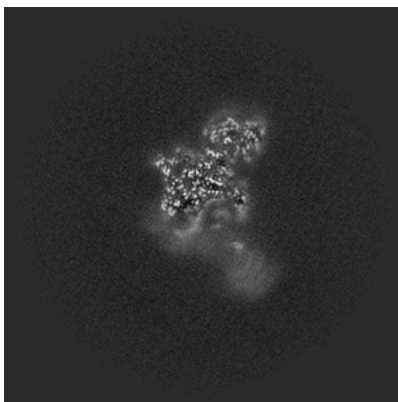
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

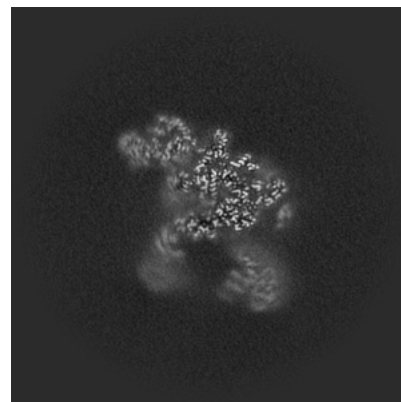
6.2.1 Primary map



X Index: 280

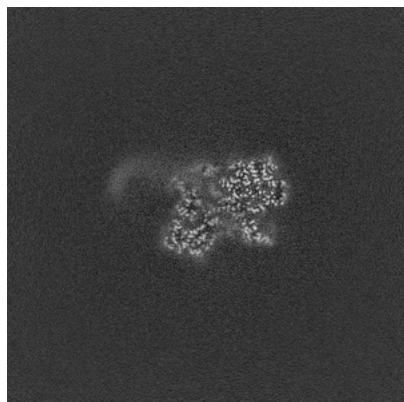


Y Index: 280

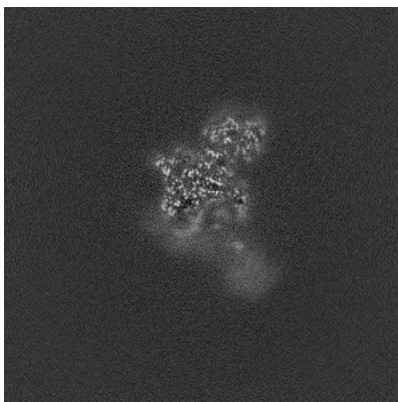


Z Index: 280

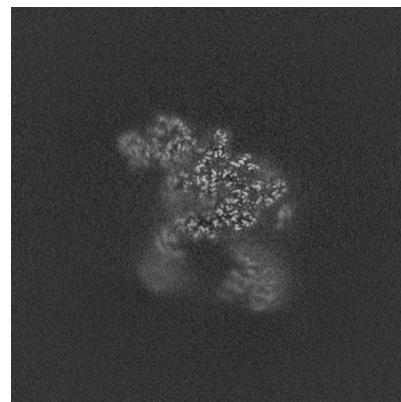
6.2.2 Raw map



X Index: 280



Y Index: 280

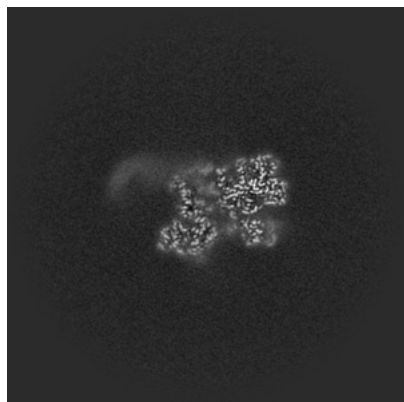


Z Index: 280

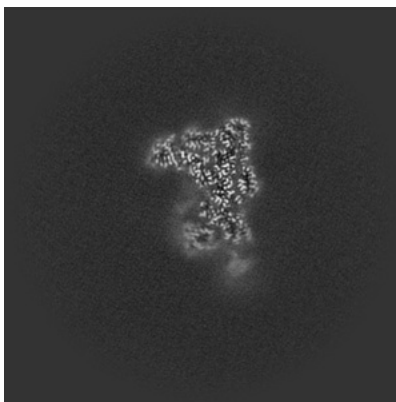
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

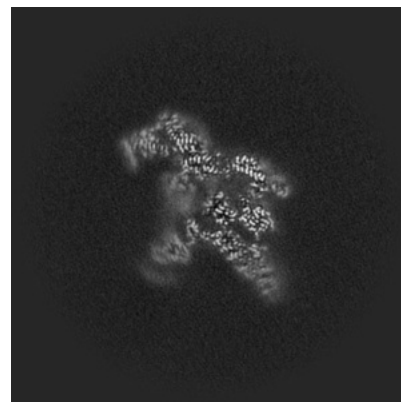
6.3.1 Primary map



X Index: 274

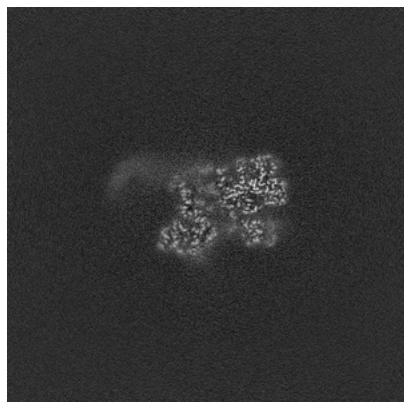


Y Index: 307

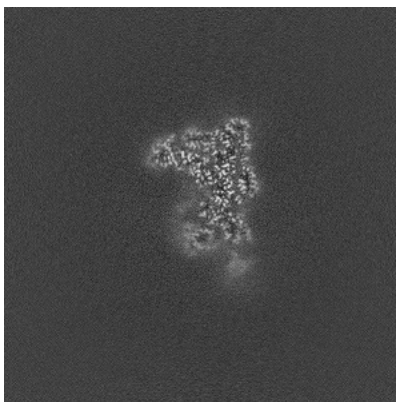


Z Index: 256

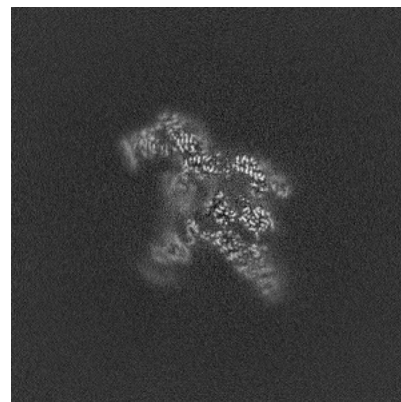
6.3.2 Raw map



X Index: 274



Y Index: 307

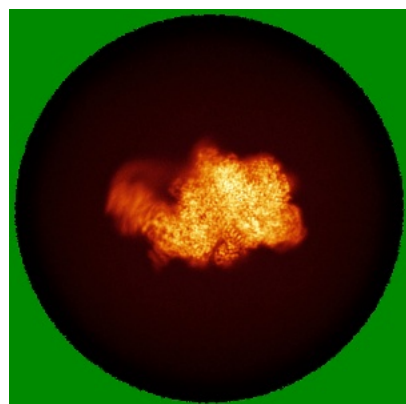


Z Index: 256

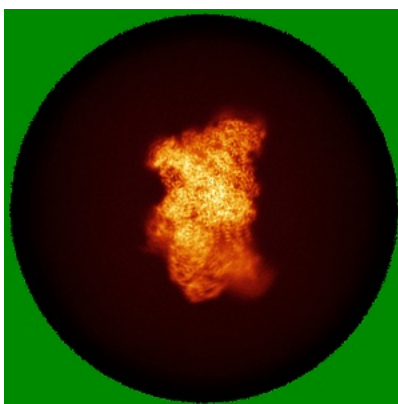
The images above show the largest variance slices of the map in three orthogonal directions.

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

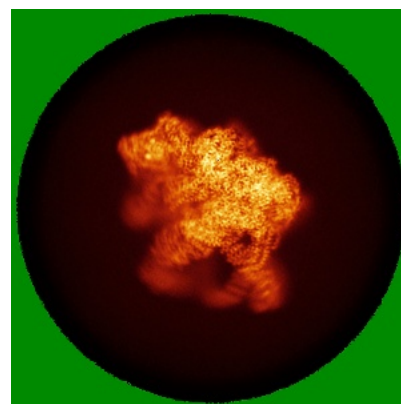
6.4.1 Primary map



X

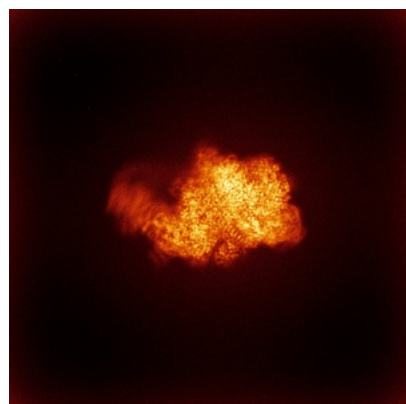


Y

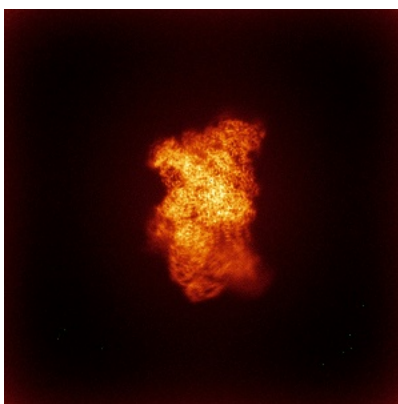


Z

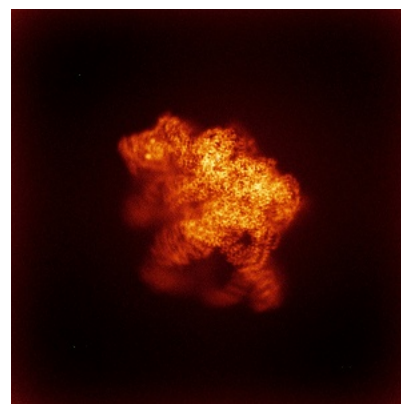
6.4.2 Raw map



X



Y



Z

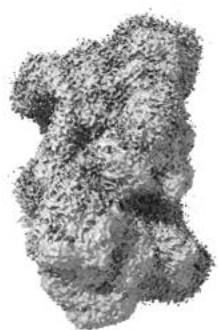
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



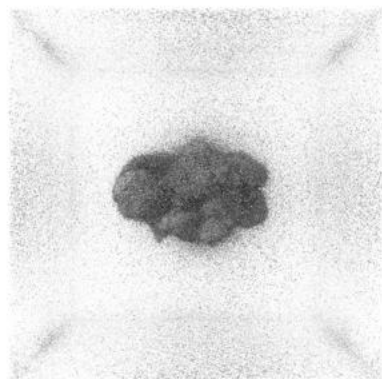
Y



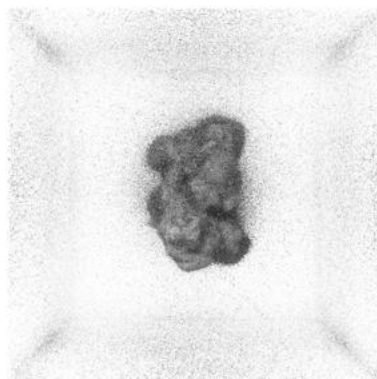
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

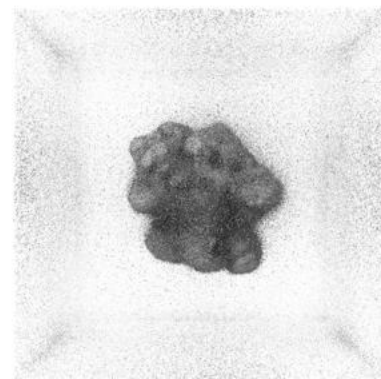
6.5.2 Raw map



X



Y



Z

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

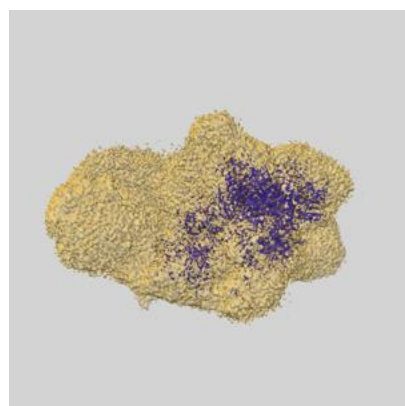
6.6 Mask visualisation [i](#)

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

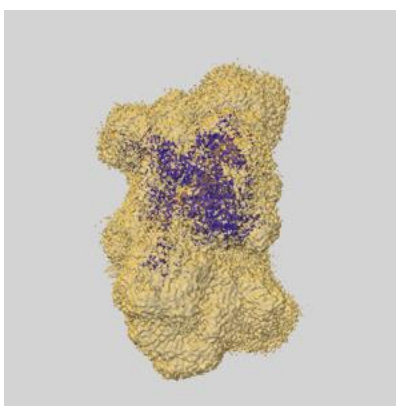
A mask typically either:

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

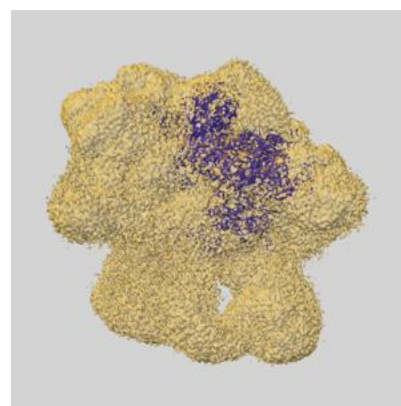
6.6.1 emd_37388_msk_1.map [i](#)



X



Y

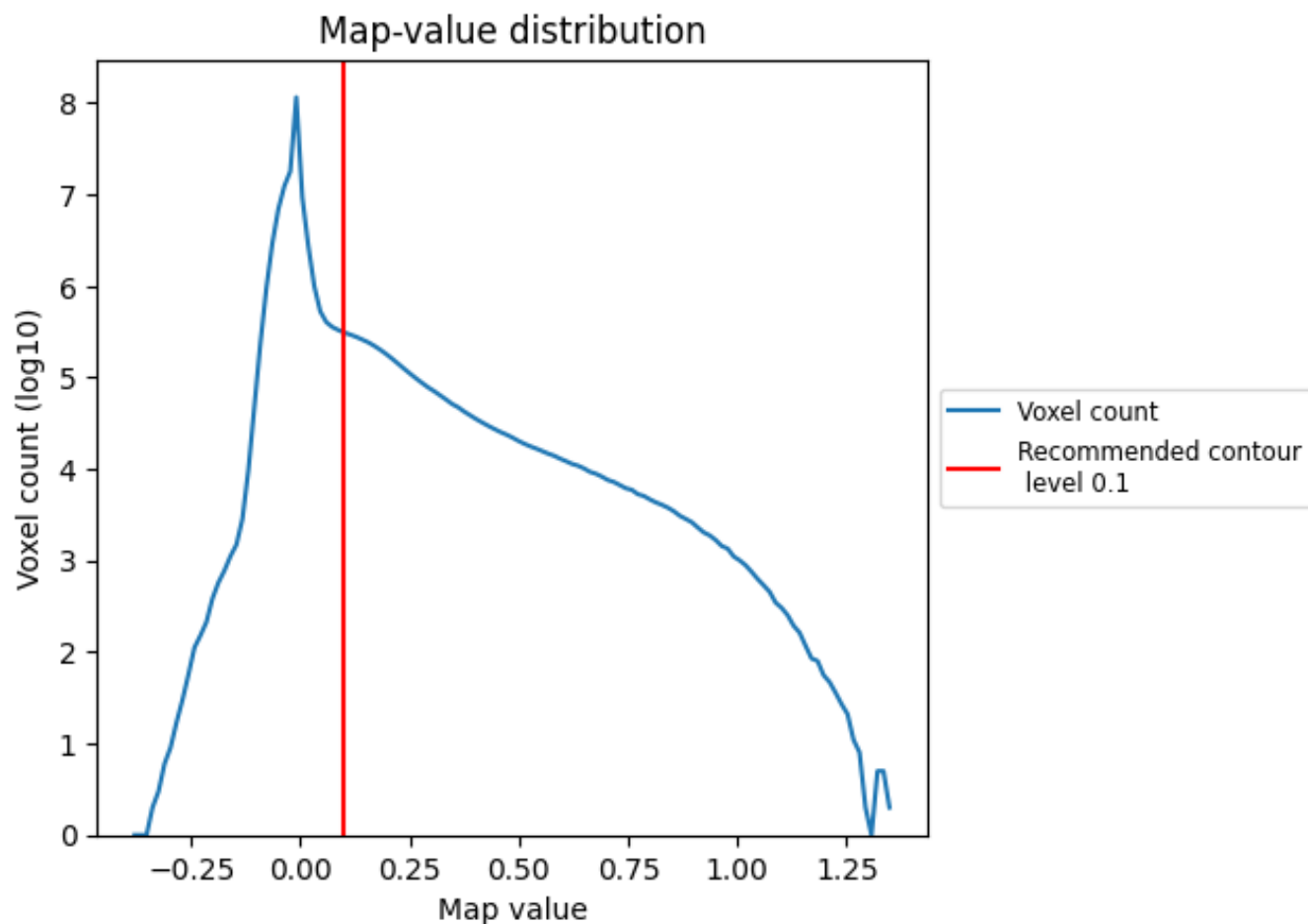


Z

7 Map analysis [i](#)

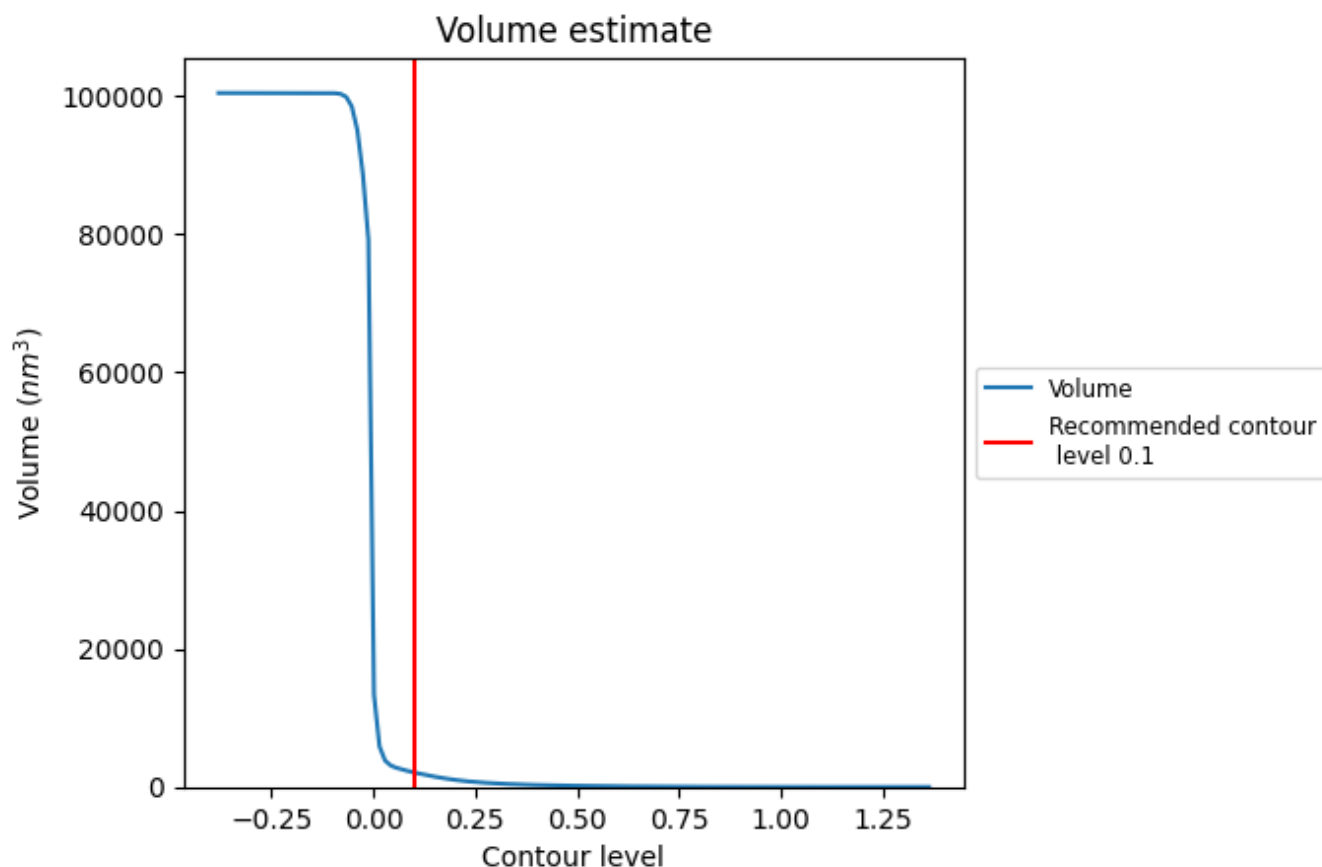
This section contains the results of statistical analysis of the map.

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.

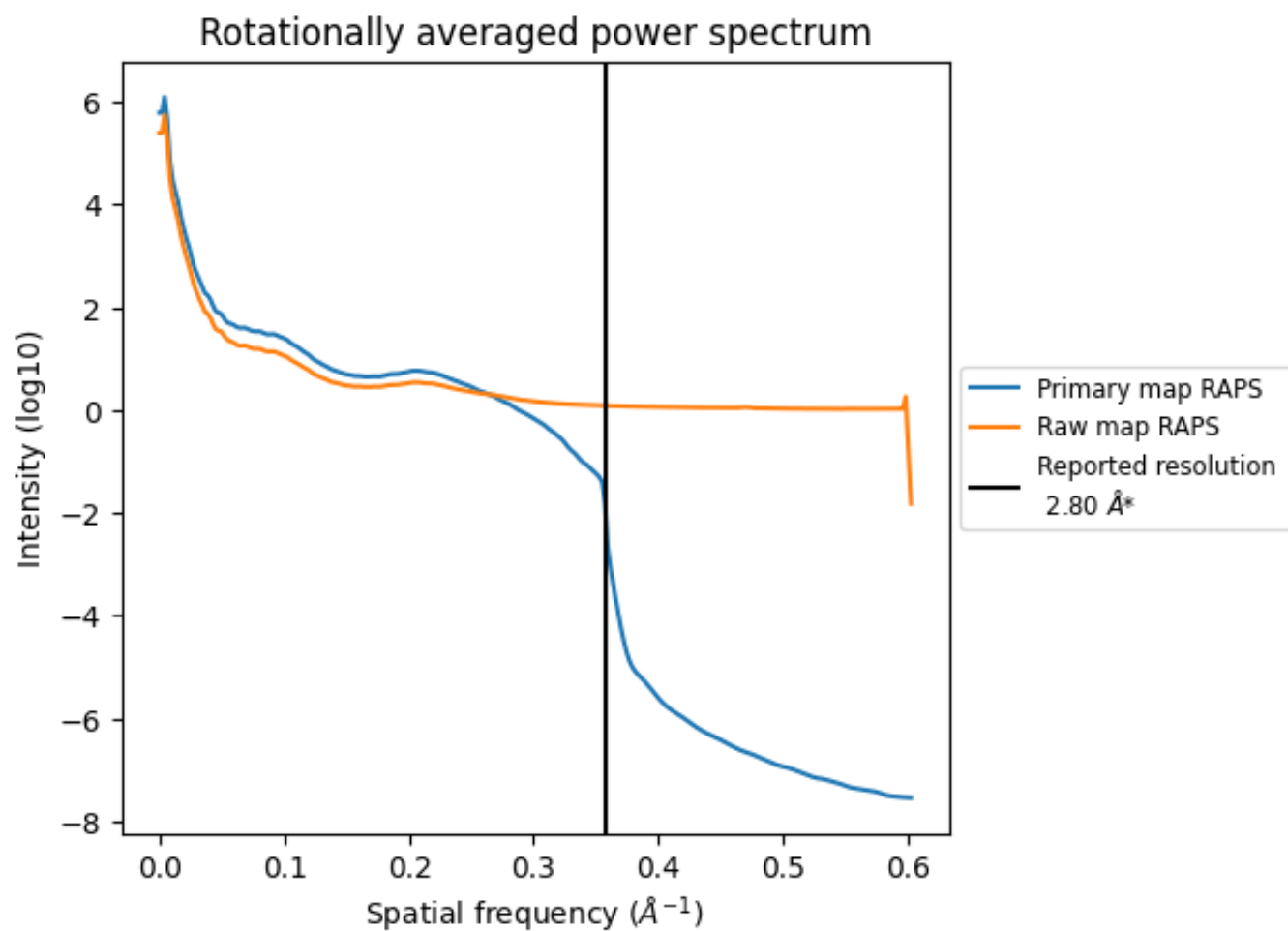
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2097 nm³; this corresponds to an approximate mass of 1894 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 ⓘ

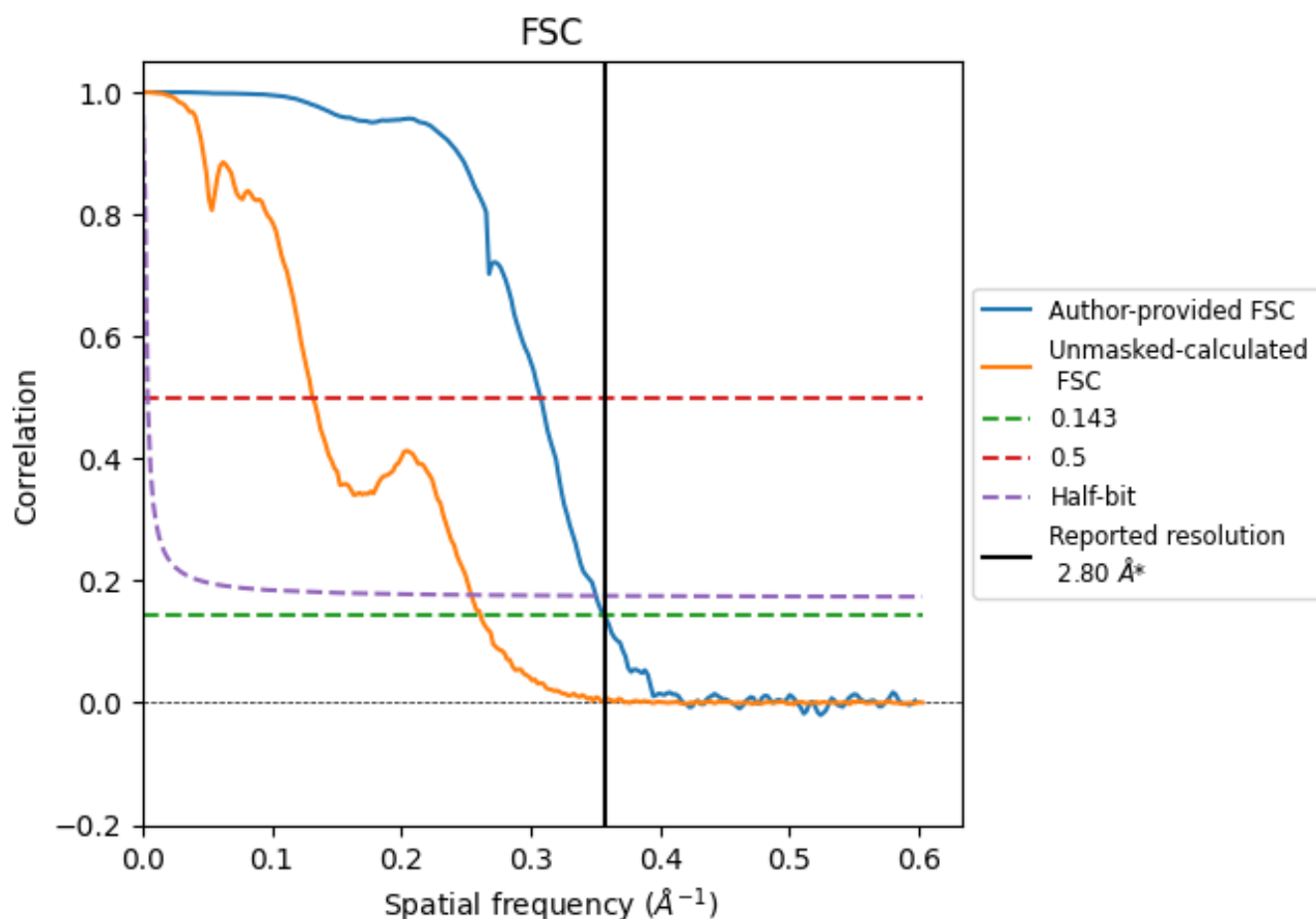


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

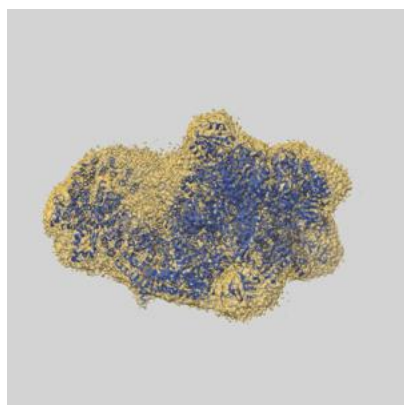
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.81	3.25	2.85
Unmasked-calculated*	3.83	7.59	3.94

*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 3.83 differs from the reported value 2.8 by more than 10 %

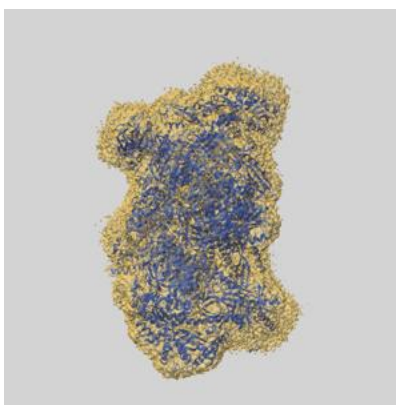
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37388 and PDB model 8WA1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

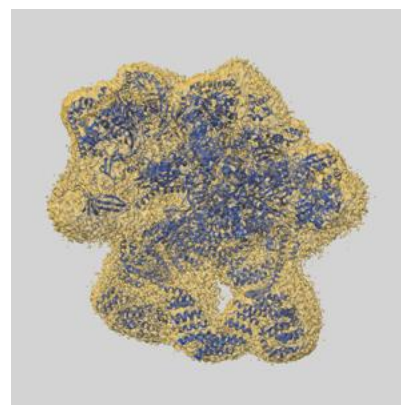
9.1 Map-model overlay [i](#)



X



Y



Z

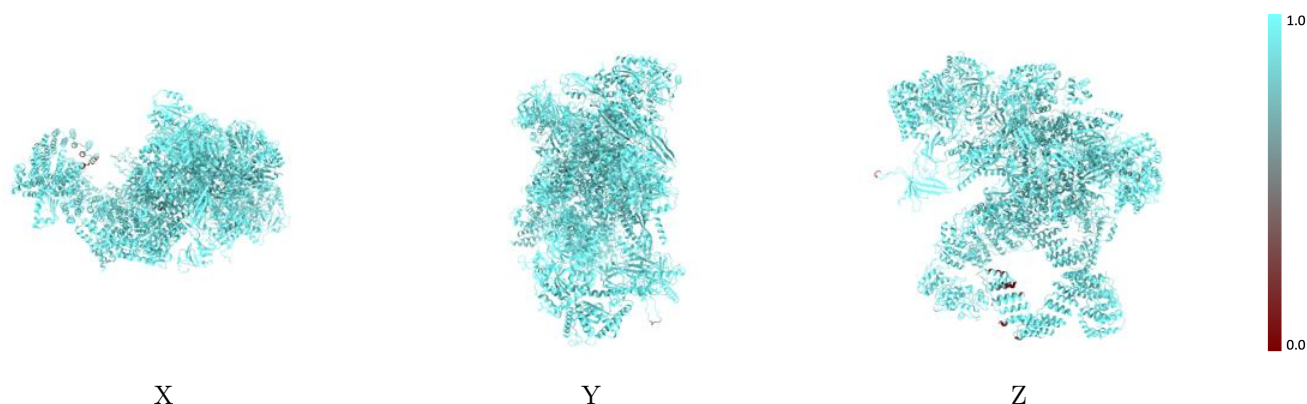
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



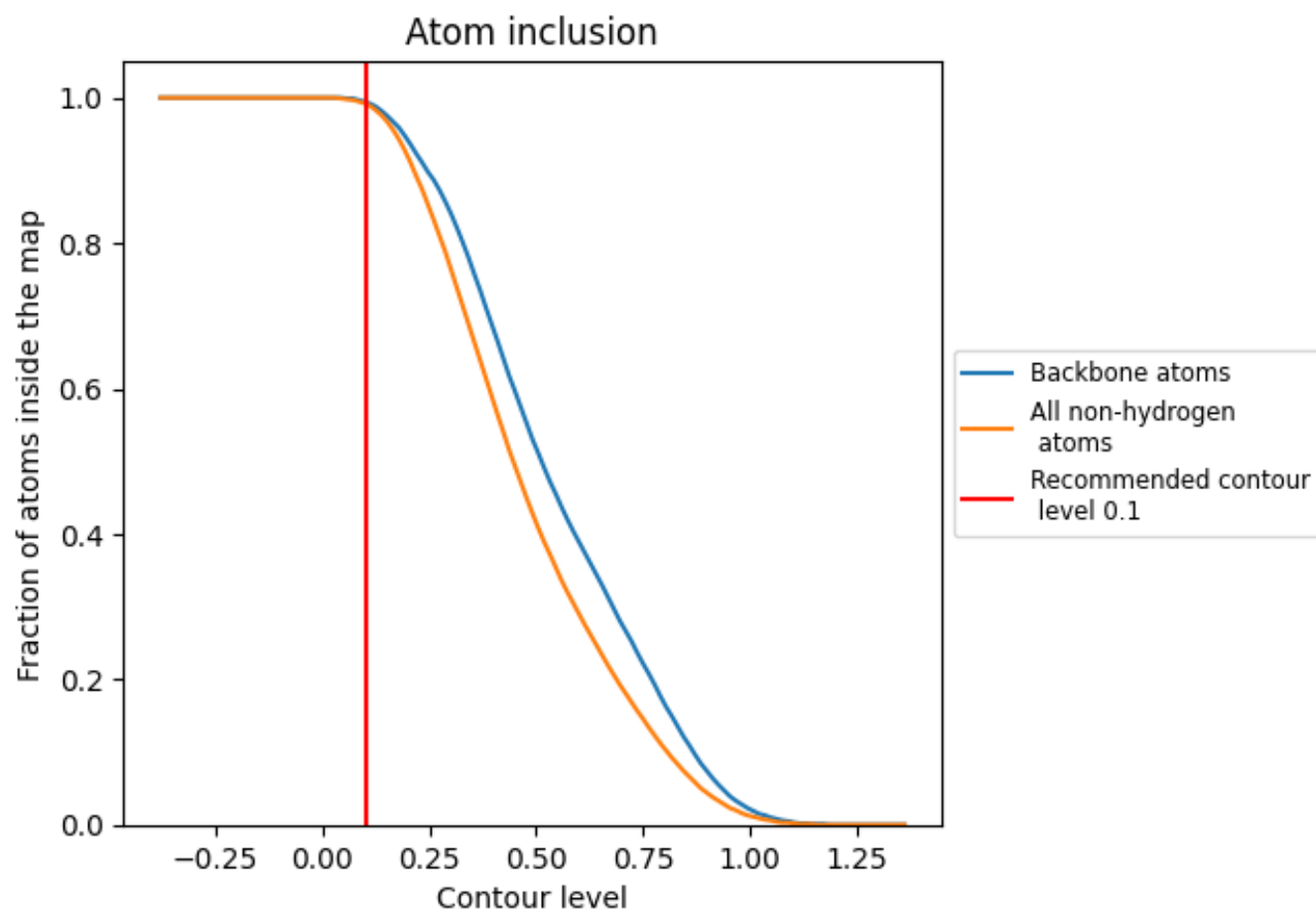
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 99% 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	 0.9920	 0.4140
A	 0.9940	 0.4720
B	 0.9960	 0.4970
C	 0.9920	 0.4530
D	 0.9880	 0.3930
E	 0.9600	 0.1560
F	 0.9970	 0.3910
G	 0.9950	 0.3960
H	 0.9970	 0.5150
I	 0.9980	 0.5290
J	 0.9940	 0.4810
K	 0.9940	 0.4900
L	 0.9990	 0.2920
M	 0.9980	 0.5330
N	 0.9890	 0.1520
O	 0.9960	 0.5040
P	 0.9990	 0.3830
Q	 1.0000	 0.2810
R	 1.0000	 0.3110
S	 1.0000	 0.3220
a	 0.9970	 0.4980
c	 0.9920	 0.4130
i	 0.9970	 0.4850
m	 0.9950	 0.4610

