



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:39 PM UTC

PDB ID : 8W9D / pdb_00008w9d
EMDB ID : EMD-37365
Title : Cryo-EM structure of the Rpd3S-nucleosome complex from budding yeast in State 1
Authors : Wang, C.; Zhan, X.
Deposited on : 2023-09-05
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

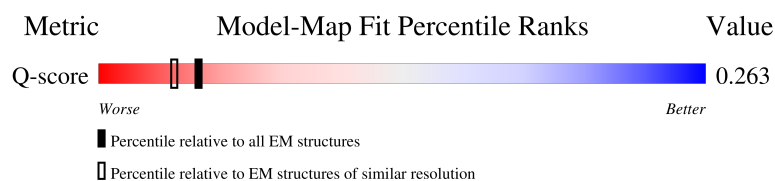
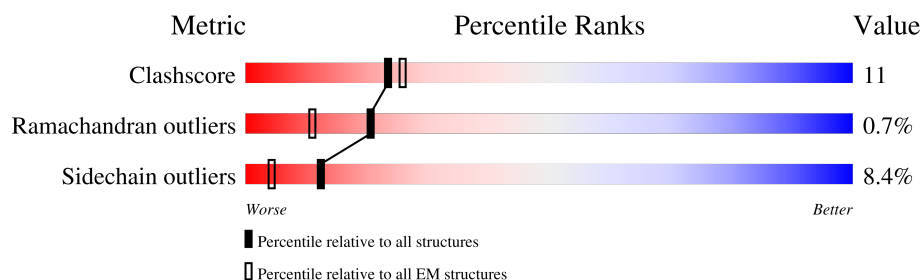
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1536	
2	E	684	
2	F	684	
3	B	433	

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Mol	Chain	Length	Quality of chain
4	C	401	
4	D	401	
4	G	401	
5	a	136	
5	e	136	
6	b	103	
6	f	103	
7	c	130	
7	g	130	
8	d	126	
8	h	126	
9	i	147	
10	j	147	
11	H	5	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 27990 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			5066	3253	860	938	15		

- Molecule 2 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	353	Total	C	N	O	S	0	0
			2884	1837	493	536	18		
2	F	156	Total	C	N	O	S	0	0
			1282	822	211	239	10		

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	385	Total	C	N	O	S	0	0
			3057	1948	513	571	25		

- Molecule 4 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	183	Total	C	N	O	S	0	0
			1483	950	239	285	9		
4	D	185	Total	C	N	O	S	0	0
			1497	959	241	288	9		
4	G	69	Total	C	N	O	S	0	0
			570	371	98	97	4		

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	104	Total	C	N	O	S	0	0
			857	538	168	147	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
6	f	82	Total	C	N	O	S	0	0
			653	412	127	113	1		

- Molecule 7 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	106	Total	C	N	O		0	0
			812	513	157	142			
7	g	108	Total	C	N	O		0	0
			828	522	162	144			

- Molecule 8 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
8	h	95	Total	C	N	O	S	0	0
			744	467	136	139	2		

- Molecule 9 is a DNA chain called 5-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	147	Total	C	N	O	P	0	0
			3011	1440	546	879	146		

- Molecule 10 is a DNA chain called 3-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	147	Total	C	N	O	P	0	0
			3010	1440	543	881	146		

- Molecule 11 is a protein called Unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	H	5	Total	C	N	O	0	0
			29	18	6	5		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

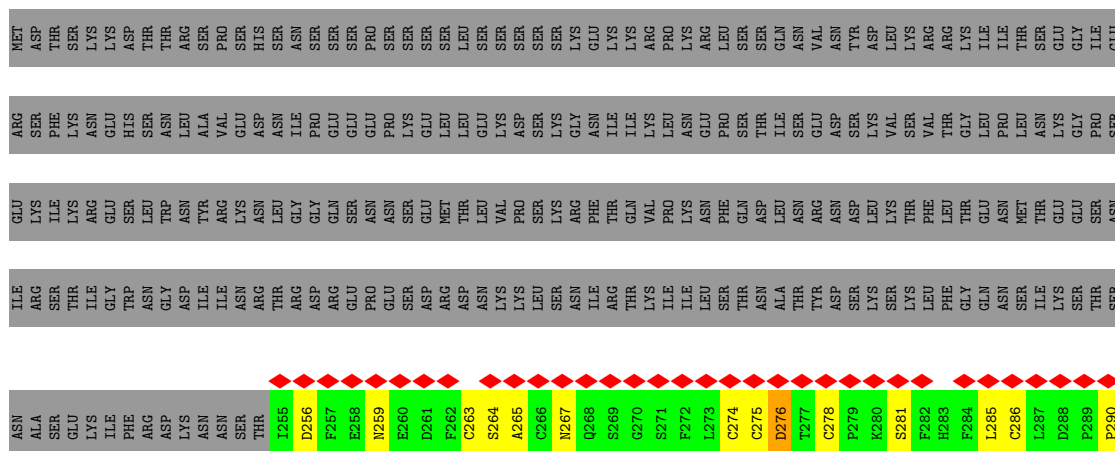
Mol	Chain	Residues	Atoms		AltConf
12	E	4	Total	Zn	0
			4	4	
12	B	1	Total	Zn	0
			1	1	
12	F	2	Total	Zn	0
			2	2	

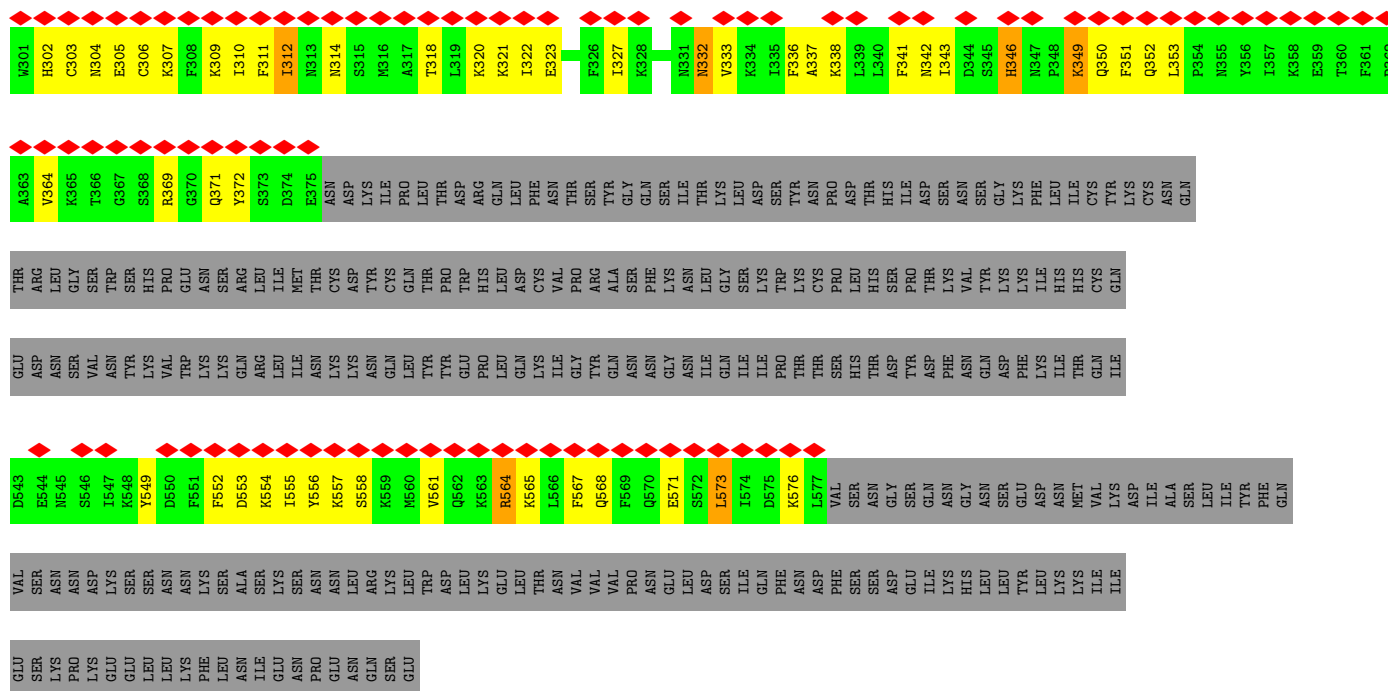
- Molecule 13 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
13	B	2	Total	K	0
			2	2	

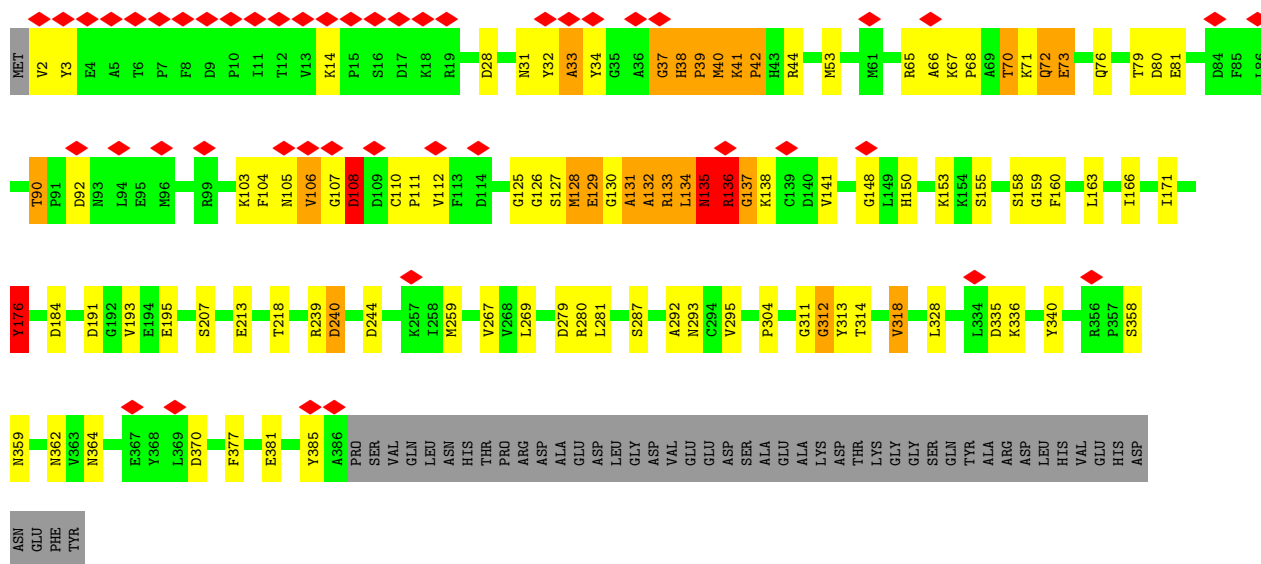


Chain F: 20% 13% 9% 77%

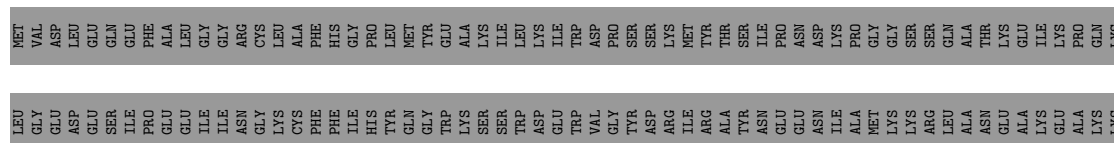
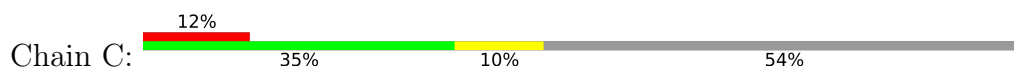




• Molecule 3: Histone deacetylase RPD3

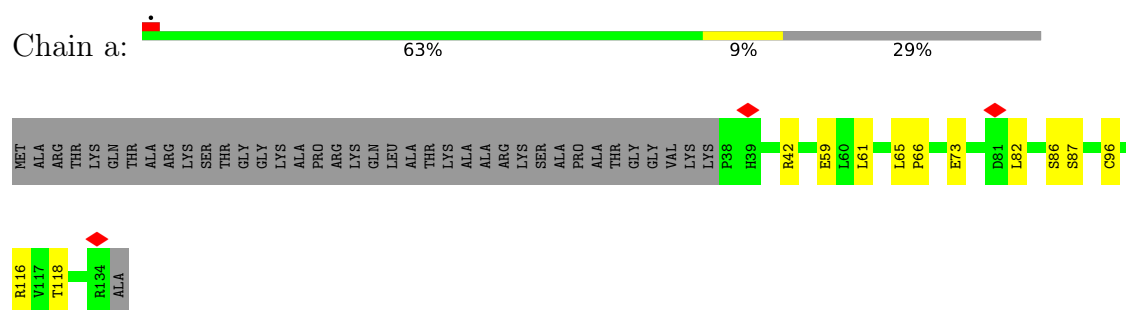


• Molecule 4: Chromatin modification-related protein EAF3

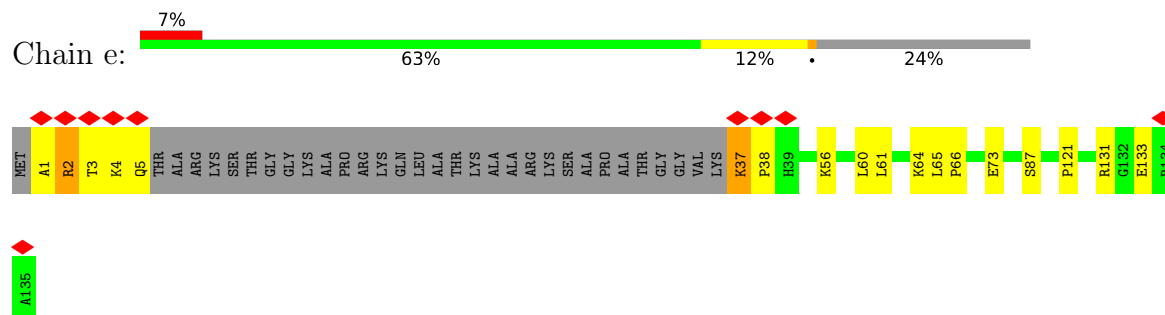




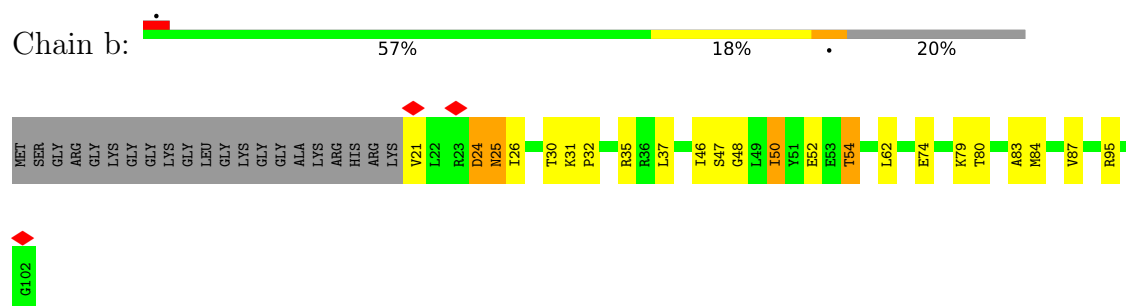
- Molecule 5: Histone H3.1



- Molecule 5: Histone H3.1



- Molecule 6: Histone H4

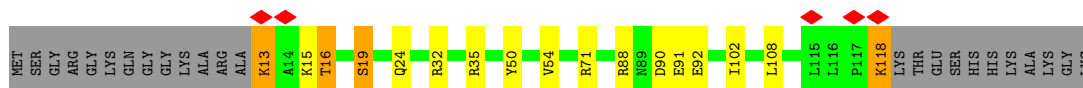


- Molecule 6: Histone H4

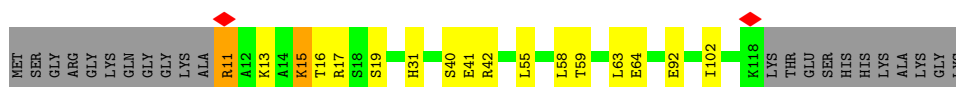




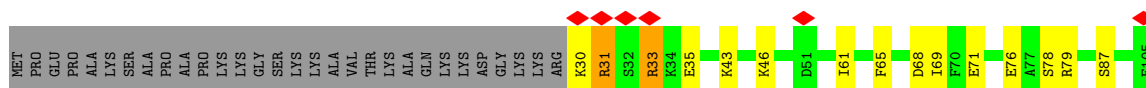
- Molecule 7: Histone H2A type 1-B/E



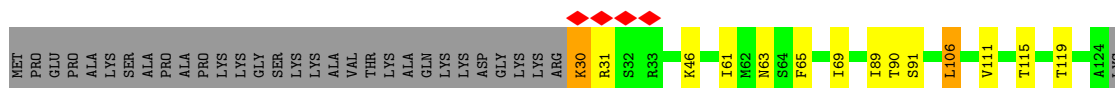
- Molecule 7: Histone H2A type 1-B/E



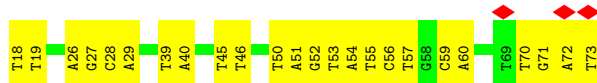
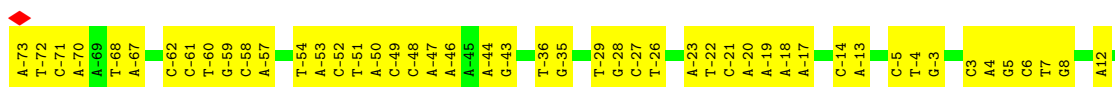
- Molecule 8: Histone H2B type 1-K



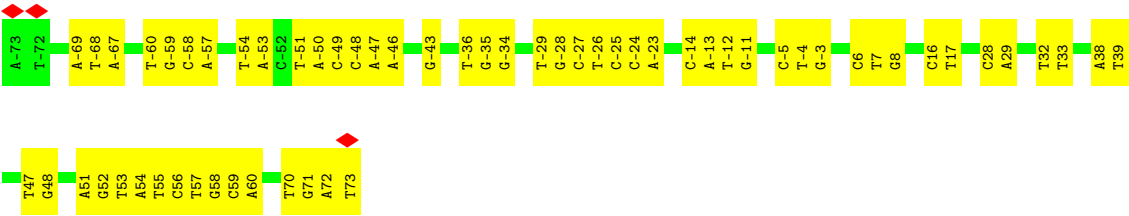
- Molecule 8: Histone H2B type 1-K



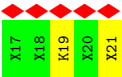
- Molecule 9: 5-DNA



- Molecule 10: 3-DNA



• Molecule 11: Unclear peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	422198	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	304.36002, 304.36002, 304.36002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	9/5180 (0.2%)	0.60	15/6984 (0.2%)
2	E	0.92	21/2952 (0.7%)	1.37	57/3978 (1.4%)
2	F	0.17	0/1313	0.50	0/1763
3	B	1.42	49/3137 (1.6%)	1.11	47/4246 (1.1%)
4	C	0.22	0/1509	0.48	0/2039
4	D	0.17	0/1524	0.46	0/2061
4	G	0.70	0/583	1.13	0/777
5	a	0.34	0/813	0.40	0/1090
5	e	0.44	0/868	0.66	2/1160 (0.2%)
6	b	0.42	0/660	0.53	0/883
6	f	0.45	0/660	0.75	2/883 (0.2%)
7	c	0.50	1/822 (0.1%)	0.55	0/1109
7	g	0.41	0/838	0.53	1/1130 (0.1%)
8	d	0.37	0/755	0.54	0/1014
8	h	0.36	0/755	0.54	0/1014
9	i	0.32	0/3378	0.45	0/5212
10	j	0.33	0/3376	0.45	0/5209
11	H	1.28	0/8	1.88	0/8
All	All	0.66	80/29131 (0.3%)	0.74	124/40560 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
3	B	0	6
All	All	0	10

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	920	GLU	C-O	-19.40	1.01	1.24
2	E	380	PRO	N-CA	18.59	1.69	1.47
3	B	42	PRO	C-O	-16.51	1.01	1.24
3	B	68	PRO	C-O	-16.31	1.05	1.23
3	B	158	SER	C-O	-16.02	1.04	1.23
3	B	131	ALA	C-O	-15.54	1.04	1.24
3	B	111	PRO	C-O	-15.43	1.03	1.24
3	B	314	THR	C-O	-14.04	1.07	1.24
3	B	130	GLY	C-O	-13.47	1.07	1.23
1	A	923	VAL	C-O	-13.21	1.04	1.23
3	B	73	GLU	C-O	-13.14	1.06	1.24
3	B	71	LYS	C-O	-13.11	1.07	1.24
3	B	128	MET	C-O	-12.71	1.09	1.24
3	B	176	TYR	C-O	-12.57	1.08	1.24
3	B	41	LYS	C-O	-12.31	1.09	1.25
1	A	915	VAL	C-O	-11.57	1.10	1.24
3	B	127	SER	C-O	-11.50	1.10	1.24
3	B	105	ASN	C-O	-11.29	1.09	1.23
3	B	132	ALA	C-O	-11.13	1.10	1.24
3	B	72	GLN	C-O	-11.11	1.08	1.24
1	A	921	GLN	C-O	-11.05	1.11	1.24
3	B	112	VAL	C-O	-10.97	1.12	1.24
1	A	917	ARG	C-O	-10.83	1.11	1.24
3	B	135	ASN	C-O	-10.81	1.11	1.24
3	B	133	ARG	C-O	-10.62	1.10	1.24
3	B	67	LYS	C-O	-10.31	1.10	1.24
3	B	159	GLY	C-O	-10.21	1.09	1.24
3	B	127	SER	CA-CB	-10.16	1.37	1.53
3	B	110	CYS	C-O	-9.88	1.13	1.24
3	B	280	ARG	C-O	-9.50	1.11	1.24
3	B	136	ARG	C-O	-9.45	1.12	1.24
1	A	922	LYS	C-O	-9.39	1.13	1.24
3	B	106	VAL	C-O	-9.21	1.13	1.24
3	B	32	TYR	C-O	-8.98	1.13	1.24
2	E	177	GLU	C-O	-8.25	1.14	1.24
3	B	66	ALA	C-O	-7.99	1.14	1.23
3	B	312	GLY	C-O	-7.88	1.13	1.23
2	E	184	THR	C-O	-7.83	1.13	1.23
3	B	33	ALA	C-O	-7.74	1.14	1.24
2	E	114	PRO	C-O	-7.73	1.14	1.23
3	B	129	GLU	C-O	-7.65	1.15	1.24
2	E	179	SER	CA-CB	-7.28	1.43	1.53
3	B	38	HIS	CE1-NE2	-7.12	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	379	ILE	C-N	7.10	1.42	1.33
2	E	182	ARG	C-O	-7.08	1.15	1.24
7	c	16	THR	C-O	-7.04	1.14	1.23
1	A	916	TRP	C-O	-6.94	1.16	1.24
3	B	42	PRO	N-CA	-6.61	1.39	1.47
3	B	39	PRO	C-O	-6.46	1.14	1.23
3	B	281	LEU	C-O	-6.42	1.14	1.23
3	B	158	SER	CA-CB	-6.36	1.42	1.53
1	A	914	LYS	C-O	-6.27	1.16	1.24
2	E	111	THR	C-O	-6.25	1.16	1.24
3	B	133	ARG	CD-NE	-6.17	1.37	1.46
2	E	178	GLU	C-O	-6.13	1.16	1.23
1	A	918	GLU	C-O	-6.11	1.17	1.24
3	B	138	LYS	N-CA	5.97	1.53	1.46
2	E	109	SER	C-O	-5.91	1.16	1.24
2	E	301	TRP	C-O	-5.88	1.16	1.24
2	E	302	HIS	C-O	-5.86	1.16	1.23
3	B	128	MET	CG-SD	-5.85	1.66	1.80
3	B	38	HIS	CG-ND1	-5.75	1.31	1.38
3	B	111	PRO	N-CD	-5.75	1.39	1.47
2	E	123	ILE	C-O	-5.69	1.17	1.24
2	E	110	VAL	C-O	-5.53	1.17	1.24
3	B	37	GLY	C-O	-5.49	1.16	1.24
2	E	387	PHE	N-CA	5.45	1.52	1.46
2	E	385	GLN	C-O	5.45	1.30	1.24
3	B	126	GLY	C-N	-5.44	1.26	1.33
3	B	132	ALA	CA-CB	-5.44	1.44	1.53
3	B	129	GLU	CD-OE1	-5.41	1.15	1.25
2	E	108	VAL	C-O	-5.38	1.17	1.24
2	E	274	CYS	C-O	-5.36	1.17	1.23
3	B	131	ALA	CA-CB	-5.34	1.44	1.53
3	B	130	GLY	CA-C	-5.28	1.46	1.52
3	B	73	GLU	CD-OE2	-5.14	1.15	1.25
2	E	128	LEU	C-O	-5.10	1.19	1.24
2	E	275	CYS	C-O	-5.08	1.17	1.24
3	B	133	ARG	NE-CZ	-5.07	1.27	1.33
2	E	109	SER	CA-CB	-5.05	1.45	1.53

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	384	ARG	CB-CA-C	18.60	142.01	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	379	ILE	O-C-N	-15.93	102.94	121.10
3	B	136	ARG	CA-C-N	11.85	139.52	121.51
3	B	136	ARG	C-N-CA	11.85	139.52	121.51
3	B	129	GLU	CB-CA-C	-10.54	92.93	110.85
2	E	393	GLN	CA-C-N	10.40	139.58	123.04
2	E	393	GLN	C-N-CA	10.40	139.58	123.04
2	E	394	SER	CA-C-N	10.27	136.35	120.13
2	E	394	SER	C-N-CA	10.27	136.35	120.13
3	B	138	LYS	CA-C-N	10.18	139.20	121.80
3	B	138	LYS	C-N-CA	10.18	139.20	121.80
3	B	137	GLY	CA-C-N	-10.06	106.39	122.79
3	B	137	GLY	C-N-CA	-10.06	106.39	122.79
2	E	379	ILE	CA-C-N	9.92	130.54	119.92
2	E	379	ILE	C-N-CA	9.92	130.54	119.92
1	A	922	LYS	CB-CA-C	-9.88	95.29	110.90
3	B	135	ASN	O-C-N	-9.69	111.62	122.09
3	B	105	ASN	CB-CA-C	9.60	124.73	111.86
3	B	73	GLU	N-CA-C	-9.56	101.98	114.31
3	B	280	ARG	CB-CG-CD	-9.20	90.15	111.30
3	B	138	LYS	N-CA-C	9.14	124.76	111.87
2	E	389	THR	CB-CA-C	9.04	125.19	110.90
3	B	135	ASN	CB-CA-C	-9.00	96.67	110.90
2	E	380	PRO	CB-CA-C	8.91	122.61	111.12
2	E	383	ASP	CB-CA-C	8.86	125.56	110.94
3	B	314	THR	OG1-CB-CG2	-8.86	91.57	109.30
2	E	387	PHE	CA-CB-CG	8.70	122.50	113.80
2	E	181	ILE	N-CA-C	-8.56	104.10	113.43
3	B	105	ASN	CA-CB-CG	8.55	121.15	112.60
2	E	387	PHE	N-CA-CB	8.49	122.60	110.12
1	A	917	ARG	CB-CA-C	-8.44	97.57	110.90
1	A	917	ARG	CB-CG-CD	-8.27	92.28	111.30
2	E	182	ARG	CB-CG-CD	-8.23	92.37	111.30
3	B	133	ARG	CG-CD-NE	-8.16	94.05	112.00
2	E	184	THR	OG1-CB-CG2	-8.03	93.23	109.30
2	E	385	GLN	N-CA-C	-7.98	102.67	111.36
3	B	313	TYR	CA-C-O	-7.74	110.62	119.14
1	A	923	VAL	CA-C-O	-7.74	111.45	119.89
2	E	386	LEU	CA-C-N	7.71	130.61	120.28
2	E	386	LEU	C-N-CA	7.71	130.61	120.28
3	B	313	TYR	CB-CA-C	7.65	123.22	109.29
2	E	172	THR	CA-CB-OG1	7.62	121.03	109.60
2	E	388	ASN	N-CA-C	-7.59	103.09	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	34	TYR	CB-CA-C	-7.44	96.87	110.63
2	E	169	THR	CB-CA-C	7.28	122.86	111.13
2	E	180	ASN	CA-C-N	7.23	131.28	122.16
2	E	180	ASN	C-N-CA	7.23	131.28	122.16
2	E	380	PRO	N-CA-C	-7.20	100.17	111.34
3	B	67	LYS	CA-C-O	-7.19	112.61	119.80
3	B	68	PRO	N-CA-C	7.16	122.76	111.38
3	B	66	ALA	CA-C-O	-6.99	113.51	121.19
3	B	130	GLY	CA-C-O	-6.86	113.59	121.00
3	B	112	VAL	CA-C-O	-6.74	113.32	120.53
1	A	921	GLN	CB-CA-C	-6.70	99.67	110.79
2	E	123	ILE	N-CA-CB	6.66	119.09	110.57
3	B	160	PHE	CA-CB-CG	6.63	120.44	113.80
5	e	3	THR	CA-C-N	6.56	133.20	120.99
5	e	3	THR	C-N-CA	6.56	133.20	120.99
2	E	170	PHE	CA-C-N	6.56	134.07	121.54
2	E	170	PHE	C-N-CA	6.56	134.07	121.54
2	E	169	THR	CA-C-N	6.55	129.05	120.28
2	E	169	THR	C-N-CA	6.55	129.05	120.28
1	A	913	ASN	O-C-N	-6.54	114.57	122.22
2	E	125	ARG	CB-CA-C	-6.43	97.62	110.42
3	B	134	LEU	O-C-N	-6.40	115.34	122.12
3	B	42	PRO	CA-C-N	6.38	130.01	120.31
3	B	42	PRO	C-N-CA	6.38	130.01	120.31
2	E	181	ILE	N-CA-CB	-6.36	105.21	112.21
2	E	388	ASN	CA-C-N	-6.36	111.79	120.44
2	E	388	ASN	C-N-CA	-6.36	111.79	120.44
3	B	132	ALA	CA-C-O	-6.30	112.73	119.97
2	E	384	ARG	N-CA-C	-6.25	105.69	113.38
2	E	384	ARG	CB-CG-CD	6.19	125.53	111.30
2	E	129	TRP	N-CA-C	-6.11	105.73	113.43
2	E	114	PRO	N-CA-CB	-6.09	98.21	103.32
3	B	133	ARG	CB-CA-C	-6.08	97.98	110.38
7	g	15	LYS	CB-CA-C	-6.05	98.76	109.70
1	A	914	LYS	CA-C-N	5.98	128.66	120.46
1	A	914	LYS	C-N-CA	5.98	128.66	120.46
3	B	68	PRO	N-CA-CB	-5.92	97.82	103.33
2	E	393	GLN	CB-CA-C	5.87	121.44	112.00
6	f	25	ASN	CA-C-N	-5.86	111.03	120.64
6	f	25	ASN	C-N-CA	-5.86	111.03	120.64
3	B	176	TYR	CA-C-O	-5.83	112.17	120.51
3	B	159	GLY	CA-C-N	5.81	132.88	123.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	159	GLY	C-N-CA	5.81	132.88	123.93
2	E	381	LEU	CA-C-N	5.79	128.31	120.44
2	E	381	LEU	C-N-CA	5.79	128.31	120.44
1	A	919	LEU	N-CA-CB	-5.78	101.60	110.16
2	E	257	PHE	CB-CA-C	-5.78	98.44	110.40
2	E	380	PRO	O-C-N	-5.78	115.92	122.91
1	A	920	GLU	CA-C-O	-5.78	114.30	120.42
3	B	137	GLY	N-CA-C	-5.73	106.84	115.32
1	A	917	ARG	CA-C-O	-5.69	114.84	120.70
3	B	41	LYS	CA-C-O	-5.68	115.16	119.59
2	E	185	ILE	CA-C-N	5.63	126.19	120.00
2	E	185	ILE	C-N-CA	5.63	126.19	120.00
2	E	184	THR	CA-C-O	-5.63	114.90	122.44
3	B	108	ASP	CB-CA-C	-5.56	100.44	110.23
3	B	133	ARG	CA-C-O	-5.56	113.23	119.79
2	E	395	ILE	CA-C-O	-5.55	116.53	121.97
1	A	914	LYS	CB-CA-C	-5.54	102.14	110.90
3	B	176	TYR	N-CA-CB	-5.50	101.20	110.49
3	B	131	ALA	CA-C-O	-5.47	113.68	119.97
2	E	126	GLU	CA-C-N	5.46	130.70	122.67
2	E	126	GLU	C-N-CA	5.46	130.70	122.67
3	B	176	TYR	CB-CA-C	5.45	121.26	110.42
3	B	68	PRO	CB-CA-C	5.37	118.02	110.98
3	B	127	SER	CA-C-N	5.37	127.48	120.28
3	B	127	SER	C-N-CA	5.37	127.48	120.28
3	B	42	PRO	N-CA-CB	-5.33	97.86	103.19
1	A	921	GLN	CA-C-O	-5.29	114.94	120.55
3	B	127	SER	N-CA-CB	-5.17	102.50	110.16
2	E	182	ARG	CB-CA-C	-5.17	100.13	110.42
2	E	110	VAL	CA-C-N	5.15	128.83	120.60
2	E	110	VAL	C-N-CA	5.15	128.83	120.60
2	E	169	THR	OG1-CB-CG2	5.14	119.59	109.30
3	B	129	GLU	CB-CG-CD	-5.12	103.90	112.60
2	E	174	ASN	CB-CA-C	-5.11	100.26	110.42
1	A	922	LYS	N-CA-C	5.10	116.65	111.14
2	E	386	LEU	CA-C-O	-5.07	114.37	120.10
2	E	178	GLU	CB-CA-C	-5.05	100.58	109.62
2	E	108	VAL	CA-C-O	-5.03	116.55	121.58
1	A	915	VAL	N-CA-CB	-5.02	103.71	110.54

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	131	ALA	Mainchain
3	B	132	ALA	Mainchain
3	B	135	ASN	Mainchain
3	B	176	TYR	Mainchain
3	B	33	ALA	Mainchain
3	B	70	THR	Mainchain
2	E	379	ILE	Mainchain
2	E	428	TRP	Peptide
2	E	470	SER	Peptide
2	E	492	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5066	0	5024	127	0
2	E	2884	0	2833	127	0
2	F	1282	0	1245	47	0
3	B	3057	0	2934	57	0
4	C	1483	0	1510	23	0
4	D	1497	0	1524	52	0
4	G	570	0	563	3	0
5	a	801	0	839	9	0
5	e	857	0	904	17	0
6	b	653	0	696	17	0
6	f	653	0	696	16	0
7	c	812	0	867	15	0
7	g	828	0	885	11	0
8	d	744	0	768	15	0
8	h	744	0	769	21	0
9	i	3011	0	1662	64	0
10	j	3010	0	1663	48	0
11	H	29	0	19	4	0
12	B	1	0	0	0	0
12	E	4	0	0	0	0
12	F	2	0	0	0	0
13	B	2	0	0	1	0
All	All	27990	0	25401	585	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 11.

All (585) 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)
2:E:258:GLU:OE1	5:e:4:LYS:HD3	1.14	1.31
2:E:380:PRO:N	2:E:380:PRO:CA	1.69	1.31
8:d:31:ARG:NH2	10:j:51:DA:OP1	1.59	1.30
2:E:178:GLU:OE1	3:B:65:ARG:NH1	1.67	1.26
8:h:65:PHE:CE1	8:h:69:ILE:HD11	1.71	1.25
8:d:65:PHE:CE1	8:d:69:ILE:HD11	1.72	1.22
2:E:258:GLU:OE1	5:e:4:LYS:CD	1.90	1.18
2:E:184:THR:OG1	3:B:73:GLU:OE1	1.68	1.08
8:d:65:PHE:CZ	8:d:69:ILE:HD11	1.98	0.98
8:h:65:PHE:CZ	8:h:69:ILE:HD11	2.00	0.95
8:d:65:PHE:CZ	8:d:69:ILE:CD1	2.51	0.94
8:h:65:PHE:CE1	8:h:69:ILE:CD1	2.50	0.94
2:E:167:LEU:HD21	3:B:340:TYR:CE1	2.03	0.93
8:h:65:PHE:CZ	8:h:69:ILE:CD1	2.53	0.91
8:d:65:PHE:CE1	8:d:69:ILE:CD1	2.52	0.91
1:A:912:TRP:HH2	2:E:113:LEU:HD13	1.36	0.88
3:B:38:HIS:HA	11:H:21:UNK:C	2.05	0.87
4:C:240:THR:O	4:C:242:ASP:N	2.09	0.86
3:B:184:ASP:OD2	13:B:1001:K:K	1.87	0.85
2:E:381:LEU:HB3	2:E:384:ARG:HB2	1.59	0.85
1:A:918:GLU:OE1	2:E:128:LEU:HD12	1.78	0.84
2:E:447:TRP:NE1	2:E:466:CYS:SG	2.51	0.84
2:E:271:SER:OG	5:e:5:GLN:NE2	2.12	0.82
9:i:12:DA:OP1	4:G:80:HIS:CE1	2.32	0.82
3:B:39:PRO:HD2	11:H:21:UNK:C	2.10	0.82
2:E:495:GLN:H	2:E:519:ASN:HD21	1.27	0.80
1:A:794:GLY:HA2	2:E:460:LEU:HD13	1.64	0.80
3:B:108:ASP:OD2	3:B:108:ASP:N	2.13	0.79
2:E:259:ASN:ND2	2:E:274:CYS:HB3	1.97	0.79
6:f:50:ILE:HD12	6:f:50:ILE:H	1.47	0.79
6:b:50:ILE:HD12	6:b:50:ILE:H	1.47	0.78
5:e:2:ARG:HG2	5:e:4:LYS:HB2	1.66	0.78
2:E:384:ARG:HA	2:E:387:PHE:HB3	1.65	0.77
2:E:301:TRP:H	5:e:1:ALA:HB2	1.50	0.77
3:B:38:HIS:HA	11:H:21:UNK:O	1.84	0.77
9:i:12:DA:P	4:G:80:HIS:CE1	2.79	0.76
2:E:189:GLY:HA2	3:B:72:GLN:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:96:CYS:SG	6:b:62:LEU:HD21	2.26	0.74
1:A:767:CYS:SG	1:A:770:ARG:NH1	2.61	0.74
4:C:318:LYS:HE3	4:C:319:PRO:HD2	1.69	0.74
2:E:257:PHE:HZ	2:E:276:ASP:O	1.72	0.73
1:A:828:ILE:HD11	1:A:899:LYS:HD3	1.69	0.72
2:E:362:PRO:HG3	2:E:499:ASN:HB3	1.72	0.72
2:E:259:ASN:ND2	2:E:274:CYS:CB	2.52	0.72
7:c:35:ARG:NH2	10:j:39:DT:OP2	2.20	0.72
4:D:240:THR:HG21	2:F:372:TYR:H	1.53	0.71
1:A:831:LEU:HB3	1:A:895:LEU:HD13	1.72	0.71
2:E:259:ASN:ND2	2:E:274:CYS:SG	2.63	0.71
2:E:258:GLU:HA	2:E:258:GLU:OE2	1.88	0.71
4:D:303:ARG:NH1	2:F:286:CYS:SG	2.64	0.70
2:E:113:LEU:HD12	2:E:113:LEU:N	2.07	0.70
2:E:167:LEU:HD21	3:B:340:TYR:CD1	2.26	0.70
1:A:885:GLU:OE1	1:A:886:HIS:ND1	2.24	0.70
7:g:92:GLU:HG3	8:h:106:LEU:HD13	1.73	0.70
4:C:300:ARG:NH2	4:C:399:LEU:O	2.25	0.69
4:D:371:ASP:O	4:D:377:LYS:NZ	2.24	0.69
2:E:380:PRO:N	2:E:380:PRO:C	2.49	0.69
1:A:919:LEU:HD12	1:A:919:LEU:O	1.92	0.69
2:E:187:TRP:HE3	2:E:187:TRP:N	1.91	0.69
2:E:257:PHE:CZ	2:E:276:ASP:O	2.45	0.69
4:D:243:LYS:HE3	4:D:301:LEU:HD23	1.75	0.69
9:i:-52:DC:H2'	9:i:-51:DT:H71	1.73	0.69
2:F:275:CYS:SG	2:F:276:ASP:N	2.66	0.68
2:F:320:LYS:HA	2:F:323:GLU:HG2	1.75	0.68
2:E:381:LEU:HD22	2:E:384:ARG:HE	1.58	0.68
7:c:13:LYS:HB2	7:c:13:LYS:NZ	2.09	0.68
3:B:90:THR:HG23	3:B:92:ASP:H	1.59	0.68
4:C:222:LEU:HD12	4:C:356:ILE:HG23	1.77	0.67
9:i:12:DA:P	4:G:80:HIS:HE1	2.17	0.67
1:A:929:ASP:HB3	1:A:1234:ASN:HB3	1.76	0.67
2:E:384:ARG:HG3	2:E:387:PHE:HB3	1.75	0.66
2:E:367:GLY:HA3	2:E:371:GLN:HG3	1.78	0.66
6:b:50:ILE:O	6:b:54:THR:OG1	2.14	0.66
2:E:395:ILE:HD12	2:E:399:ASP:HB2	1.78	0.66
2:E:180:ASN:C	2:E:180:ASN:HD22	2.00	0.66
5:e:37:LYS:N	5:e:38:PRO:CD	2.59	0.66
4:D:287:LEU:HB3	4:D:291:LYS:HE3	1.77	0.65
2:F:318:THR:O	2:F:322:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:384:ARG:HB3	2:E:387:PHE:HD2	1.61	0.65
1:A:912:TRP:CH2	2:E:113:LEU:HD13	2.25	0.65
1:A:912:TRP:HH2	2:E:113:LEU:CD1	2.07	0.65
2:E:189:GLY:HA2	3:B:72:GLN:CB	2.27	0.65
2:E:180:ASN:HB2	2:E:185:ILE:HD12	1.78	0.65
6:f:50:ILE:O	6:f:54:THR:OG1	2.14	0.65
2:E:184:THR:HG21	3:B:76:GLN:HE22	1.61	0.64
4:D:247:ARG:NH2	4:D:382:SER:O	2.29	0.64
2:E:121:GLU:O	2:E:125:ARG:HG2	1.98	0.64
4:D:226:ILE:HA	4:D:229:LYS:HE2	1.78	0.64
2:E:371:GLN:HA	4:C:240:THR:HG21	1.79	0.64
5:a:42:ARG:NH1	9:i:72:DA:OP1	2.31	0.64
1:A:695:ASP:OD1	2:E:554:LYS:NZ	2.31	0.64
7:g:11:ARG:O	7:g:11:ARG:HG3	1.96	0.64
2:E:259:ASN:HD21	2:E:274:CYS:HB3	1.62	0.64
7:c:32:ARG:NH1	9:i:-44:DA:OP1	2.30	0.64
1:A:1069:LEU:HD11	1:A:1266:MET:HB2	1.80	0.63
8:d:33:ARG:NH1	8:d:35:GLU:OE2	2.31	0.63
2:E:124:LYS:O	2:E:124:LYS:HG3	1.98	0.63
9:i:-49:DC:H4'	9:i:-48:DC:H5'	1.79	0.63
6:b:24:ASP:O	6:b:26:ILE:N	2.31	0.63
1:A:1066:LEU:HB2	1:A:1270:VAL:HG11	1.81	0.63
9:i:-54:DT:H1'	9:i:-53:DA:H5'	1.81	0.63
4:C:378:ASP:OD2	4:C:381:ARG:NH2	2.32	0.62
2:E:496:ARG:NH2	4:C:234:ASP:OD1	2.31	0.62
7:g:16:THR:HA	10:j:-43:DG:H5''	1.81	0.62
1:A:919:LEU:HD12	1:A:919:LEU:C	2.22	0.62
3:B:72:GLN:O	3:B:72:GLN:HG2	1.98	0.62
10:j:16:DC:H2''	10:j:17:DT:H71	1.81	0.62
7:c:13:LYS:O	7:c:13:LYS:HG3	1.98	0.62
1:A:851:LEU:HG	1:A:887:PRO:HG3	1.82	0.62
4:D:266:SER:O	4:D:275:GLN:NE2	2.34	0.61
9:i:-22:DT:H2''	9:i:-21:DC:H5''	1.81	0.61
2:E:506:TYR:OH	4:D:348:ASP:OD2	2.18	0.61
8:d:76:GLU:OE1	8:d:79:ARG:NH1	2.34	0.61
2:E:517:ASN:ND2	2:E:519:ASN:OD1	2.33	0.61
1:A:1199:VAL:O	1:A:1201:GLU:N	2.34	0.61
1:A:828:ILE:HD12	1:A:898:LEU:HB3	1.81	0.61
1:A:1302:ARG:NH1	1:A:1315:GLN:OE1	2.34	0.61
2:E:543:ASP:OD1	2:E:543:ASP:N	2.34	0.61
10:j:-54:DT:H2''	10:j:-53:DA:H5''	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:-48:DC:H2''	10:j:-47:DA:N7	2.15	0.60
2:E:189:GLY:HA3	3:B:70:THR:HB	1.83	0.60
1:A:826:ARG:HG3	3:B:31:ASN:HD21	1.67	0.60
1:A:1066:LEU:HA	1:A:1069:LEU:HB2	1.83	0.60
2:F:565:LYS:HA	2:F:568:GLN:HE21	1.65	0.60
3:B:39:PRO:CD	11:H:21:UNK:C	2.80	0.60
10:j:-47:DA:H2''	10:j:-46:DA:H2'	1.82	0.60
2:F:321:LYS:NZ	2:F:321:LYS:O	2.33	0.60
8:d:65:PHE:CZ	8:d:69:ILE:HD12	2.37	0.60
1:A:851:LEU:HD13	1:A:855:LEU:HG	1.84	0.59
5:e:121:PRO:HB3	6:f:53:GLU:HG3	1.83	0.59
6:f:23:ARG:HG2	6:f:23:ARG:HH11	1.66	0.59
3:B:106:VAL:HG12	3:B:106:VAL:O	2.01	0.59
9:i:-68:DT:H2''	9:i:-67:DA:C8	2.36	0.59
1:A:812:GLU:OE2	3:B:37:GLY:HA2	2.02	0.59
8:h:30:LYS:HZ3	8:h:30:LYS:HB2	1.67	0.59
3:B:312:GLY:HA3	3:B:318:VAL:HG21	1.85	0.59
9:i:-29:DT:H2''	9:i:-28:DG:C8	2.37	0.59
2:E:187:TRP:N	2:E:187:TRP:CE3	2.71	0.59
6:f:50:ILE:HD12	6:f:50:ILE:N	2.17	0.59
2:E:171:LEU:O	2:E:173:GLU:N	2.36	0.58
2:E:180:ASN:ND2	2:E:180:ASN:O	2.35	0.58
9:i:-53:DA:H2''	9:i:-52:DC:H5''	1.83	0.58
1:A:921:GLN:HG2	1:A:1188:SER:HB2	1.84	0.58
2:E:167:LEU:CD2	3:B:340:TYR:CD1	2.86	0.58
2:E:184:THR:OG1	2:E:184:THR:O	2.15	0.58
2:F:312:ILE:HG23	2:F:314:ASN:H	1.67	0.58
5:a:61:LEU:HD12	6:b:37:LEU:HD23	1.85	0.58
6:b:50:ILE:HD12	6:b:50:ILE:N	2.17	0.58
9:i:72:DA:H2''	9:i:73:DT:H5''	1.86	0.58
10:j:-51:DT:O4	10:j:-50:DA:N6	2.37	0.58
1:A:1254:HIS:HD2	1:A:1257:MET:HE2	1.69	0.58
10:j:-5:DC:H2''	10:j:-4:DT:H71	1.85	0.58
2:F:573:LEU:HA	2:F:576:LYS:HG3	1.84	0.58
8:h:65:PHE:CZ	8:h:69:ILE:HD12	2.38	0.58
2:E:437:ILE:HG12	2:E:448:HIS:CD2	2.39	0.57
4:D:327:GLY:H	4:D:330:HIS:CE1	2.22	0.57
7:g:17:ARG:HH12	7:g:31:HIS:HD2	1.50	0.57
9:i:-5:DC:H2''	9:i:-4:DT:H71	1.85	0.57
10:j:51:DA:C6	10:j:52:DG:C6	2.92	0.57
1:A:765:MET:HE3	1:A:766:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:107:LYS:HG3	2:E:107:LYS:O	2.05	0.57
2:E:387:PHE:CD1	2:E:387:PHE:C	2.82	0.57
4:D:394:TYR:O	4:D:398:ALA:HB2	2.04	0.57
8:h:115:THR:O	8:h:119:THR:HG23	2.04	0.57
4:D:236:TRP:CG	4:D:299:TYR:HH	2.23	0.57
5:a:96:CYS:SG	6:b:62:LEU:CD2	2.93	0.57
7:g:41:GLU:HG3	7:g:42:ARG:HG3	1.86	0.57
8:h:30:LYS:HZ2	8:h:30:LYS:HA	1.70	0.57
1:A:768:SER:OG	3:B:80:ASP:OD1	2.23	0.57
1:A:826:ARG:NH2	3:B:28:ASP:OD1	2.38	0.57
10:j:72:DA:H2''	10:j:73:DT:H5''	1.86	0.57
2:E:372:TYR:OH	2:E:496:ARG:NH1	2.37	0.56
2:E:452:VAL:O	2:E:454:ARG:N	2.38	0.56
4:D:310:LEU:HD13	2:F:290:PRO:HD2	1.86	0.56
2:F:263:CYS:O	2:F:267:ASN:N	2.38	0.56
1:A:1005:PRO:O	1:A:1009:ARG:HG3	2.06	0.56
1:A:1071:ARG:O	1:A:1075:GLN:HG2	2.05	0.56
3:B:292:ALA:HB1	3:B:328:LEU:HD21	1.86	0.56
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.87	0.56
3:B:135:ASN:O	3:B:137:GLY:N	2.38	0.56
1:A:981:ASP:O	1:A:1155:TYR:OH	2.21	0.56
3:B:244:ASP:OD2	3:B:287:SER:OG	2.23	0.56
9:i:28:DC:H2''	9:i:29:DA:C8	2.41	0.56
4:D:272:PRO:HB3	2:F:549:TYR:HB3	1.88	0.56
6:b:24:ASP:C	6:b:26:ILE:H	2.14	0.56
1:A:682:TYR:OH	2:E:544:GLU:OE2	2.20	0.55
3:B:44:ARG:NH1	3:B:311:GLY:O	2.39	0.55
1:A:986:TYR:HE1	1:A:1029:ILE:HD13	1.71	0.55
1:A:1002:TYR:HB3	1:A:1006:ASP:HB2	1.89	0.55
9:i:50:DT:H1'	9:i:51:DA:H5'	1.88	0.55
10:j:32:DT:H1'	10:j:33:DT:H5''	1.89	0.55
6:b:31:LYS:HE2	6:b:35:ARG:HH21	1.71	0.55
6:f:31:LYS:HE2	6:f:35:ARG:HH21	1.71	0.55
6:f:23:ARG:HH11	6:f:23:ARG:CG	2.20	0.55
2:F:553:ASP:OD1	2:F:557:LYS:NZ	2.33	0.55
9:i:-50:DA:H1'	9:i:-49:DC:H5'	1.88	0.55
4:C:383:ASP:OD1	4:C:384:ASP:N	2.40	0.55
8:d:109:HIS:O	8:d:113:GLU:HG2	2.07	0.55
1:A:1335:LYS:HA	1:A:1338:VAL:HG22	1.87	0.55
3:B:240:ASP:OD1	3:B:240:ASP:N	2.40	0.55
2:F:306:CYS:O	2:F:310:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:-60:DT:H2''	9:i:-59:DG:C8	2.41	0.55
10:j:55:DT:H2''	10:j:56:DC:C5	2.42	0.55
1:A:965:HIS:NE2	1:A:967:LEU:HB2	2.22	0.54
1:A:814:ARG:NH1	1:A:913:ASN:OD1	2.39	0.54
9:i:-51:DT:C4	9:i:-50:DA:N6	2.75	0.54
2:E:460:LEU:HD12	3:B:213:GLU:HG2	1.90	0.54
2:E:517:ASN:HB3	2:E:519:ASN:H	1.72	0.54
1:A:1003:SER:O	1:A:1007:LYS:HG3	2.08	0.54
1:A:1067:ASP:O	1:A:1073:ARG:HB2	2.08	0.54
2:E:560:MET:HG2	2:E:564:ARG:HH12	1.73	0.54
7:g:55:LEU:O	7:g:59:THR:HG23	2.07	0.54
1:A:1064:SER:OG	1:A:1065:LEU:N	2.40	0.54
8:h:90:THR:HG22	8:h:91:SER:H	1.73	0.54
9:i:4:DA:H2''	9:i:5:DG:C8	2.43	0.54
10:j:-60:DT:H2''	10:j:-59:DG:N7	2.22	0.54
7:c:102:ILE:HG23	8:d:61:ILE:HD12	1.88	0.54
1:A:874:GLU:CD	1:A:874:GLU:H	2.16	0.53
10:j:-29:DT:H2''	10:j:-28:DG:C8	2.43	0.53
6:f:47:SER:OG	6:f:48:GLY:N	2.42	0.53
9:i:-52:DC:H42	10:j:51:DA:N6	2.06	0.53
2:E:476:LYS:HB2	2:E:490:LYS:HZ2	1.73	0.53
6:b:47:SER:OG	6:b:48:GLY:N	2.42	0.53
2:E:126:GLU:O	2:E:126:GLU:HG3	2.08	0.53
3:B:153:LYS:NZ	3:B:195:GLU:OE2	2.36	0.53
4:D:275:GLN:HE22	2:F:552:PHE:HB3	1.74	0.53
6:b:30:THR:HB	6:b:32:PRO:HD2	1.91	0.53
7:c:91:GLU:CD	7:c:91:GLU:H	2.17	0.52
10:j:-51:DT:C4	10:j:-50:DA:N6	2.77	0.52
7:g:102:ILE:HG23	8:h:61:ILE:HD12	1.91	0.52
8:h:30:LYS:CA	8:h:30:LYS:NZ	2.72	0.52
2:E:491:VAL:HG12	2:E:492:TRP:H	1.74	0.52
8:d:68:ASP:OD2	6:f:98:TYR:OH	2.27	0.52
3:B:335:ASP:OD1	3:B:336:LYS:N	2.43	0.52
7:c:13:LYS:HB2	7:c:13:LYS:HZ2	1.75	0.52
6:f:30:THR:HB	6:f:32:PRO:HD2	1.91	0.52
1:A:1141:ASN:OD1	1:A:1141:ASN:N	2.38	0.52
2:E:402:ASN:N	2:E:403:PRO:HD3	2.24	0.52
4:D:255:GLU:HB2	4:D:323:ILE:HG12	1.91	0.52
1:A:767:CYS:SG	1:A:770:ARG:HD2	2.50	0.52
4:D:256:MET:SD	4:D:256:MET:N	2.83	0.52
5:e:37:LYS:N	5:e:38:PRO:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:LEU:C	1:A:919:LEU:CD1	2.83	0.51
1:A:1281:LYS:NZ	1:A:1343:LEU:HB2	2.24	0.51
2:F:259:ASN:HD21	2:F:281:SER:HB3	1.75	0.51
8:h:111:VAL:O	8:h:115:THR:HG23	2.09	0.51
9:i:-27:DC:H2''	9:i:-26:DT:H71	1.92	0.51
10:j:-48:DC:H2''	10:j:-47:DA:C8	2.46	0.51
4:D:217:THR:N	4:D:345:THR:O	2.43	0.51
5:e:73:GLU:OE1	6:f:25:ASN:ND2	2.40	0.51
9:i:6:DC:H2''	9:i:7:DT:H71	1.91	0.51
10:j:52:DG:C5	10:j:53:DT:C4	2.99	0.51
1:A:1169:THR:HA	1:A:1172:ILE:HG22	1.90	0.51
2:E:178:GLU:CD	3:B:65:ARG:HH11	2.08	0.51
3:B:134:LEU:HD22	3:B:304:PRO:HB3	1.90	0.51
8:h:65:PHE:HE1	8:h:69:ILE:HD11	1.60	0.51
2:F:554:LYS:HA	2:F:557:LYS:HZ3	1.75	0.51
1:A:976:ASP:OD1	1:A:1313:SER:OG	2.24	0.51
2:F:274:CYS:HB2	2:F:281:SER:HB3	1.92	0.51
9:i:39:DT:H2''	9:i:40:DA:C8	2.46	0.51
8:h:30:LYS:HA	8:h:30:LYS:NZ	2.25	0.51
1:A:868:ARG:HD2	1:A:873:LYS:HZ3	1.77	0.50
2:E:259:ASN:HD21	2:E:274:CYS:CB	2.19	0.50
10:j:57:DT:H2''	10:j:58:DG:N7	2.26	0.50
2:F:312:ILE:HG23	2:F:314:ASN:N	2.27	0.50
2:E:384:ARG:HA	2:E:387:PHE:CB	2.38	0.50
2:E:470:SER:HB2	2:E:471:PRO:CD	2.42	0.50
8:d:118:VAL:O	8:d:122:THR:HG23	2.12	0.50
10:j:-4:DT:H2''	10:j:-3:DG:C8	2.47	0.50
1:A:918:GLU:OE1	2:E:128:LEU:CD1	2.54	0.50
8:h:30:LYS:HZ3	8:h:30:LYS:CB	2.24	0.50
9:i:18:DT:H1'	9:i:19:DT:H5'	1.94	0.50
9:i:-4:DT:H2''	9:i:-3:DG:C8	2.47	0.50
2:E:318:THR:O	2:E:322:ILE:HD12	2.12	0.50
3:B:3:TYR:HB3	3:B:370:ASP:OD2	2.10	0.50
3:B:148:GLY:HA2	3:B:166:ILE:HD11	1.94	0.50
2:E:257:PHE:C	2:E:257:PHE:CD2	2.89	0.50
1:A:841:MET:HE1	1:A:849:PHE:CD2	2.46	0.49
1:A:1068:ILE:HA	1:A:1074:TYR:HB2	1.94	0.49
1:A:1233:ASN:HD22	1:A:1235:LYS:HD3	1.76	0.49
4:C:348:ASP:N	4:C:348:ASP:OD1	2.45	0.49
2:E:381:LEU:HD22	2:E:384:ARG:NE	2.26	0.49
9:i:26:DA:H2''	9:i:27:DG:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:ARG:HD3	3:B:128:MET:CE	2.42	0.49
4:C:266:SER:O	4:C:275:GLN:NE2	2.44	0.49
2:E:516:ASN:ND2	2:E:540:THR:OG1	2.46	0.49
7:c:16:THR:HA	9:i:-43:DG:H5''	1.93	0.49
9:i:51:DA:H2''	9:i:52:DG:H5''	1.93	0.49
10:j:56:DC:H2''	10:j:57:DT:C6	2.47	0.49
1:A:1065:LEU:HG	1:A:1069:LEU:HD23	1.94	0.49
2:E:385:GLN:CD	2:E:385:GLN:N	2.71	0.49
2:E:560:MET:SD	2:F:557:LYS:HG2	2.53	0.49
1:A:1343:LEU:HB3	1:A:1345:HIS:ND1	2.28	0.49
2:E:111:THR:HG22	2:E:113:LEU:H	1.77	0.49
2:E:180:ASN:ND2	2:E:180:ASN:N	2.59	0.49
2:E:570:GLN:O	2:E:574:ILE:HG23	2.13	0.49
4:D:321:VAL:HG22	4:D:323:ILE:HG22	1.95	0.49
2:E:181:ILE:HG22	3:B:129:GLU:OE1	2.13	0.49
2:E:385:GLN:OE1	2:E:385:GLN:HA	2.12	0.49
4:C:293:LEU:HD22	4:C:322:PRO:HB3	1.95	0.49
2:F:302:HIS:HB3	2:F:306:CYS:HB2	1.94	0.49
2:F:350:GLN:OE1	2:F:352:GLN:NE2	2.45	0.49
2:F:567:PHE:O	2:F:571:GLU:HG2	2.13	0.49
1:A:1148:PHE:O	1:A:1152:THR:HG23	2.13	0.48
2:E:378:LYS:O	2:E:379:ILE:HG23	2.13	0.48
4:D:239:VAL:C	4:D:243:LYS:HA	2.39	0.48
4:D:394:TYR:O	4:D:398:ALA:CB	2.61	0.48
10:j:-68:DT:H2''	10:j:-67:DA:C8	2.48	0.48
2:E:509:LEU:HD21	2:F:338:LYS:HB2	1.95	0.48
9:i:-23:DA:H5'	9:i:-23:DA:C8	2.48	0.48
9:i:56:DC:H2''	9:i:57:DT:H71	1.94	0.48
8:h:30:LYS:NZ	8:h:30:LYS:CB	2.75	0.48
1:A:828:ILE:CD1	1:A:899:LYS:HD3	2.43	0.48
6:b:84:MET:HA	6:b:87:VAL:HG22	1.96	0.48
6:f:23:ARG:CG	6:f:23:ARG:NH1	2.73	0.48
1:A:665:GLU:HB3	2:E:552:PHE:CZ	2.49	0.48
1:A:953:SER:O	1:A:957:VAL:HG13	2.13	0.48
2:E:179:SER:OG	3:B:133:ARG:NH1	2.47	0.48
2:E:258:GLU:OE1	5:e:4:LYS:HD2	2.04	0.47
4:D:381:ARG:HE	4:D:382:SER:H	1.61	0.47
10:j:-58:DC:H2''	10:j:-57:DA:N7	2.29	0.47
2:E:560:MET:HG2	2:E:564:ARG:NH1	2.29	0.47
4:C:269:LEU:HD23	4:C:270:GLU:H	1.79	0.47
9:i:-51:DT:O4	9:i:-50:DA:N6	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:3:DC:H2''	9:i:4:DA:C8	2.50	0.47
1:A:956:LYS:O	1:A:960:THR:HG23	2.14	0.47
4:D:360:GLU:HA	4:D:363:LEU:HD23	1.97	0.47
9:i:51:DA:C6	9:i:52:DG:C6	3.02	0.47
1:A:823:SER:O	1:A:827:THR:HG23	2.14	0.47
1:A:1317:ILE:HG23	1:A:1321:ASP:HB2	1.97	0.47
10:j:38:DA:C8	10:j:39:DT:H72	2.50	0.47
2:E:324:SER:O	2:E:328:LYS:HG3	2.14	0.47
2:E:383:ASP:HA	2:E:386:LEU:HB2	1.97	0.47
9:i:51:DA:H2''	9:i:52:DG:H8	1.80	0.47
5:e:37:LYS:NZ	5:e:37:LYS:HB3	2.25	0.47
9:i:-5:DC:H2''	9:i:-4:DT:C7	2.45	0.47
1:A:1309:THR:HG23	1:A:1311:HIS:HB2	1.96	0.47
3:B:79:THR:HG1	3:B:155:SER:HG	1.61	0.47
2:F:333:VAL:HG22	2:F:336:PHE:HB2	1.97	0.47
1:A:679:LYS:HA	1:A:679:LYS:HD3	1.62	0.47
4:C:247:ARG:NH2	4:C:251:ASP:OD1	2.48	0.47
1:A:825:LEU:O	1:A:828:ILE:HG22	2.15	0.46
1:A:1196:LEU:HB3	1:A:1227:SER:OG	2.14	0.46
2:E:489:TYR:OH	4:C:377:LYS:O	2.31	0.46
2:F:303:CYS:O	2:F:307:LYS:HG3	2.15	0.46
5:a:73:GLU:OE1	6:b:25:ASN:HB2	2.14	0.46
4:D:381:ARG:HE	4:D:382:SER:N	2.12	0.46
1:A:1161:ILE:HG21	1:A:1239:LEU:HD11	1.96	0.46
1:A:1325:LYS:HD2	1:A:1325:LYS:HA	1.51	0.46
3:B:191:ASP:OD1	3:B:191:ASP:N	2.48	0.46
9:i:-23:DA:H5'	9:i:-23:DA:H8	1.79	0.46
9:i:7:DT:H2''	9:i:8:DG:C8	2.50	0.46
2:E:395:ILE:H	2:E:395:ILE:HG12	1.30	0.46
2:E:499:ASN:CG	2:E:500:LYS:H	2.23	0.46
6:b:24:ASP:C	6:b:26:ILE:N	2.72	0.46
9:i:-71:DC:H2''	9:i:-70:DA:C8	2.50	0.46
10:j:-69:DA:H2''	10:j:-68:DT:H5''	1.97	0.46
1:A:921:GLN:HG2	1:A:1188:SER:CB	2.45	0.46
10:j:-49:DC:H4'	10:j:-48:DC:H5'	1.97	0.46
2:F:274:CYS:SG	2:F:275:CYS:N	2.89	0.46
6:f:95:ARG:HE	6:f:95:ARG:HB3	1.60	0.46
2:E:107:LYS:HB2	2:E:107:LYS:HZ2	1.81	0.46
9:i:52:DG:C5	9:i:53:DT:C4	3.04	0.46
2:E:169:THR:HG22	3:B:53:MET:CE	2.46	0.46
2:E:395:ILE:CD1	2:E:399:ASP:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:331:LEU:O	4:D:335:ILE:HG12	2.16	0.46
6:f:84:MET:HA	6:f:87:VAL:HG22	1.96	0.46
10:j:-14:DC:H2"	10:j:-13:DA:C8	2.50	0.46
2:E:516:ASN:O	2:E:517:ASN:HB2	2.15	0.46
4:C:247:ARG:NH1	4:C:385:ALA:O	2.46	0.46
4:D:325:ILE:HG13	4:D:326:TYR:CD2	2.51	0.46
1:A:800:LYS:HE2	3:B:279:ASP:O	2.16	0.46
1:A:903:GLU:HG3	1:A:904:GLU:N	2.31	0.46
7:c:35:ARG:HH12	10:j:39:DT:P	2.38	0.46
4:D:290:ASP:OD2	4:D:291:LYS:N	2.50	0.45
1:A:913:ASN:HA	1:A:916:TRP:HE3	1.81	0.45
1:A:983:ASN:HA	1:A:986:TYR:CD2	2.52	0.45
6:f:22:LEU:HD13	6:f:22:LEU:HA	1.75	0.45
1:A:1119:ASN:OD1	1:A:1119:ASN:N	2.49	0.45
2:E:125:ARG:HD3	2:E:125:ARG:HA	1.31	0.45
4:D:261:TYR:O	4:D:265:VAL:HG22	2.17	0.45
5:a:87:SER:HB2	6:b:83:ALA:HB2	1.98	0.45
5:e:60:LEU:HD12	5:e:64:LYS:HE2	1.98	0.45
9:i:-36:DT:H2"	9:i:-35:DG:N7	2.30	0.45
10:j:7:DT:H2"	10:j:8:DG:C8	2.52	0.45
6:b:35:ARG:HG2	6:b:46:ILE:HD12	1.99	0.45
6:f:35:ARG:HG2	6:f:46:ILE:HD12	1.99	0.45
4:D:293:LEU:HA	4:D:297:LEU:HB2	1.98	0.45
3:B:362:ASN:OD1	3:B:364:ASN:ND2	2.43	0.45
4:D:253:THR:HG21	4:D:324:ARG:C	2.42	0.45
1:A:1005:PRO:HA	1:A:1008:GLU:OE2	2.16	0.45
7:c:118:LYS:HA	7:c:118:LYS:HD3	1.55	0.45
2:E:276:ASP:OD1	5:e:1:ALA:HA	2.17	0.45
3:B:269:LEU:HD21	3:B:295:VAL:HG22	1.98	0.45
4:D:299:TYR:O	4:D:303:ARG:HG3	2.17	0.45
10:j:-24:DC:H2"	10:j:-23:DA:C8	2.52	0.45
9:i:-18:DA:H2"	9:i:-17:DA:C8	2.51	0.45
4:D:233:VAL:HG11	2:F:364:VAL:HG21	1.99	0.44
2:F:265:ALA:HA	2:F:349:LYS:HA	1.98	0.44
4:C:252:VAL:HG11	4:C:373:TYR:CE1	2.53	0.44
5:e:56:LYS:HE3	5:e:56:LYS:HB2	1.71	0.44
9:i:59:DC:H2"	9:i:60:DA:N7	2.32	0.44
1:A:1165:ASN:O	1:A:1169:THR:HG22	2.17	0.44
4:D:308:GLU:HA	4:D:311:LYS:HD2	1.99	0.44
2:F:338:LYS:HA	2:F:338:LYS:HD3	1.73	0.44
9:i:-47:DA:H2"	9:i:-46:DA:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:-12:DT:H2''	10:j:-11:DG:C8	2.53	0.44
1:A:755:TYR:HE1	3:B:195:GLU:HG3	1.82	0.44
1:A:960:THR:O	1:A:964:ILE:HG13	2.17	0.44
4:D:365:TRP:HA	4:D:368:MET:HE2	2.00	0.44
1:A:921:GLN:CD	1:A:1188:SER:HB2	2.43	0.44
2:E:288:ASP:HA	2:E:289:PRO:HA	1.86	0.44
3:B:377:PHE:O	3:B:381:GLU:HG2	2.18	0.44
6:b:95:ARG:HE	6:b:95:ARG:HB3	1.60	0.44
8:d:31:ARG:CZ	10:j:51:DA:OP1	2.50	0.44
1:A:1235:LYS:HE2	1:A:1235:LYS:HB2	1.55	0.44
8:h:30:LYS:HZ3	8:h:30:LYS:CA	2.31	0.44
1:A:875:ARG:HA	1:A:878:GLU:CG	2.48	0.44
2:E:563:LYS:O	2:E:566:LEU:HG	2.18	0.44
1:A:1338:VAL:O	1:A:1341:TYR:HB2	2.18	0.44
3:B:79:THR:OG1	3:B:155:SER:OG	2.32	0.44
2:F:307:LYS:O	2:F:311:PHE:HB2	2.18	0.44
9:i:51:DA:C4	9:i:52:DG:C5	3.06	0.44
1:A:921:GLN:CG	1:A:1188:SER:HB2	2.48	0.44
1:A:1168:VAL:HG11	1:A:1232:TYR:CE1	2.53	0.44
2:F:558:SER:HA	2:F:561:VAL:HG22	2.00	0.44
8:d:46:LYS:HA	8:d:46:LYS:HD3	1.76	0.44
10:j:-26:DT:H2''	10:j:-25:DC:C6	2.53	0.44
9:i:52:DG:H1'	9:i:53:DT:H5'	2.00	0.43
1:A:841:MET:HE1	1:A:849:PHE:CG	2.54	0.43
1:A:1241:THR:O	1:A:1245:VAL:HG23	2.18	0.43
1:A:1281:LYS:HZ1	1:A:1343:LEU:HB2	1.82	0.43
4:D:312:LYS:HE2	4:D:313:SER:N	2.33	0.43
2:F:555:ILE:HD12	2:F:556:TYR:N	2.33	0.43
9:i:51:DA:H2''	9:i:52:DG:C8	2.54	0.43
1:A:1261:LYS:O	1:A:1265:ILE:HG13	2.18	0.43
2:F:369:ARG:O	2:F:369:ARG:NH1	2.47	0.43
1:A:1120:LEU:HD21	1:A:1338:VAL:HG23	2.00	0.43
2:F:327:ILE:HG22	2:F:337:ALA:HB1	2.01	0.43
5:a:116:ARG:NH1	5:a:118:THR:O	2.52	0.43
8:h:46:LYS:HD3	8:h:46:LYS:HA	1.78	0.43
9:i:-58:DC:H2''	9:i:-57:DA:N7	2.34	0.43
9:i:-28:DG:H2''	9:i:-27:DC:C5	2.54	0.43
9:i:45:DT:H2''	9:i:46:DT:H71	2.01	0.43
2:E:180:ASN:ND2	2:E:180:ASN:H	2.16	0.43
4:C:382:SER:OG	4:C:383:ASP:N	2.50	0.43
4:D:227:LYS:O	4:D:231:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:270:GLU:HB3	2:F:556:TYR:HD1	1.84	0.43
4:D:282:CYS:SG	4:D:283:ALA:N	2.91	0.43
9:i:-50:DA:H2''	9:i:-49:DC:H2'	2.00	0.43
10:j:53:DT:C2	10:j:54:DA:C8	3.06	0.43
1:A:835:VAL:O	1:A:838:ILE:HG22	2.19	0.43
4:D:255:GLU:OE2	4:D:324:ARG:NH1	2.52	0.43
1:A:1331:GLU:O	1:A:1335:LYS:HG2	2.18	0.43
2:E:552:PHE:HD1	2:E:555:ILE:HD11	1.83	0.43
4:D:358:GLN:HE21	4:D:358:GLN:HB3	1.65	0.43
7:c:91:GLU:HG2	7:c:92:GLU:HG2	2.01	0.43
10:j:-49:DC:H2''	10:j:-48:DC:C6	2.53	0.43
1:A:845:GLU:O	1:A:849:PHE:N	2.52	0.43
4:D:304:LEU:HA	4:D:307:ASP:OD2	2.18	0.43
10:j:-36:DT:H2''	10:j:-35:DG:N7	2.34	0.43
10:j:-35:DG:H2''	10:j:-34:DG:C8	2.54	0.43
10:j:6:DC:H2''	10:j:7:DT:H72	2.01	0.43
1:A:965:HIS:O	1:A:968:THR:HG22	2.18	0.43
7:c:16:THR:OG1	7:c:19:SER:HB3	2.18	0.43
1:A:1007:LYS:O	1:A:1011:LYS:HG3	2.19	0.43
1:A:1178:VAL:HG22	1:A:1180:PHE:H	1.83	0.43
1:A:785:HIS:CD2	1:A:786:PRO:HD2	2.54	0.42
2:E:175:MET:HE2	2:E:175:MET:HB3	1.59	0.42
2:E:571:GLU:O	2:E:574:ILE:HG12	2.19	0.42
3:B:80:ASP:OD2	3:B:80:ASP:N	2.52	0.42
4:D:326:TYR:HD1	4:D:330:HIS:NE2	2.17	0.42
10:j:47:DT:H2''	10:j:48:DG:C8	2.54	0.42
2:E:106:SER:O	2:E:106:SER:OG	2.18	0.42
4:D:292:CYS:SG	2:F:343:ILE:HG21	2.59	0.42
10:j:-27:DC:H2''	10:j:-26:DT:C7	2.48	0.42
10:j:70:DT:H2''	10:j:71:DG:C8	2.54	0.42
1:A:842:THR:O	1:A:846:LYS:HD3	2.19	0.42
2:E:388:ASN:HD22	2:E:388:ASN:HA	1.37	0.42
2:E:517:ASN:HB3	2:E:519:ASN:HB2	2.01	0.42
2:F:332:ASN:OD1	2:F:332:ASN:N	2.50	0.42
9:i:70:DT:H2''	9:i:71:DG:C8	2.55	0.42
1:A:1166:GLU:OE1	1:A:1167:ARG:NH1	2.51	0.42
2:E:567:PHE:HD1	2:E:567:PHE:HA	1.77	0.42
10:j:-50:DA:C5	10:j:-49:DC:C4	3.07	0.42
1:A:1124:ALA:HB1	1:A:1335:LYS:HE3	2.00	0.42
4:C:352:CYS:O	4:C:356:ILE:HG12	2.19	0.42
7:c:88:ARG:HA	7:c:88:ARG:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:LYS:HD2	1:A:1333:LYS:HA	1.75	0.42
2:F:322:ILE:HD13	2:F:341:PHE:HZ	1.84	0.42
5:a:82:LEU:HD23	5:a:82:LEU:HA	1.81	0.42
7:c:24:GLN:OE1	8:d:43:LYS:HD3	2.20	0.42
2:E:384:ARG:CG	2:E:387:PHE:HB3	2.44	0.42
4:C:219:LYS:HA	4:C:219:LYS:HD2	1.84	0.42
4:D:377:LYS:HE2	4:D:377:LYS:HB2	1.55	0.42
2:F:333:VAL:HG22	2:F:333:VAL:O	2.19	0.42
9:i:-68:DT:H2''	9:i:-67:DA:H8	1.83	0.42
9:i:-48:DC:H2''	9:i:-47:DA:C8	2.55	0.42
1:A:832:GLU:OE2	1:A:895:LEU:HD21	2.20	0.42
1:A:1037:LYS:HA	1:A:1040:VAL:HG23	2.02	0.42
2:E:177:GLU:H	2:E:177:GLU:HG2	1.52	0.42
2:E:307:LYS:HB3	2:E:307:LYS:HE3	1.85	0.42
2:E:564:ARG:HB3	2:F:564:ARG:NH1	2.34	0.42
4:C:252:VAL:HG11	4:C:373:TYR:HE1	1.85	0.42
4:C:300:ARG:HG2	4:C:399:LEU:HD23	2.01	0.42
2:F:565:LYS:HA	2:F:568:GLN:NE2	2.33	0.42
7:g:16:THR:HG23	7:g:19:SER:H	1.83	0.42
7:g:63:LEU:HD23	7:g:63:LEU:HA	1.90	0.42
10:j:55:DT:H2''	10:j:56:DC:C6	2.55	0.42
9:i:-50:DA:C5	9:i:-49:DC:C4	3.08	0.42
10:j:59:DC:H2''	10:j:60:DA:C8	2.55	0.42
2:F:275:CYS:HB3	2:F:278:CYS:HB3	2.01	0.42
10:j:28:DC:H2''	10:j:29:DA:C8	2.54	0.42
1:A:995:PHE:CE2	1:A:1247:GLN:HG2	2.55	0.41
1:A:1234:ASN:O	3:B:359:ASN:ND2	2.46	0.41
3:B:150:HIS:CD2	3:B:150:HIS:H	2.38	0.41
4:D:290:ASP:OD2	4:D:291:LYS:HG3	2.20	0.41
1:A:936:LYS:NZ	1:A:1225:GLU:OE2	2.46	0.41
1:A:1006:ASP:OD2	1:A:1006:ASP:N	2.52	0.41
2:E:565:LYS:O	2:E:568:GLN:HG3	2.19	0.41
2:F:564:ARG:HA	2:F:567:PHE:HB2	2.02	0.41
10:j:52:DG:C6	10:j:53:DT:N3	2.87	0.41
1:A:831:LEU:O	1:A:834:ILE:HG13	2.20	0.41
3:B:38:HIS:CD2	3:B:40:MET:HB2	2.55	0.41
4:D:393:GLN:O	4:D:397:VAL:HG23	2.20	0.41
5:a:65:LEU:HB3	5:a:66:PRO:HD3	2.02	0.41
5:e:37:LYS:HB3	5:e:37:LYS:HZ3	1.84	0.41
1:A:1318:ALA:O	1:A:1321:ASP:N	2.53	0.41
5:e:131:ARG:NH1	5:e:133:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:-62:DC:H1'	9:i:-61:DC:H5'	2.01	0.41
1:A:878:GLU:H	1:A:878:GLU:HG2	1.71	0.41
2:E:455:ALA:HA	3:B:239:ARG:HH11	1.85	0.41
9:i:39:DT:H2''	9:i:40:DA:H8	1.84	0.41
1:A:835:VAL:HA	1:A:838:ILE:HG22	2.03	0.41
3:B:125:GLY:O	3:B:129:GLU:HB2	2.19	0.41
1:A:664:GLU:O	1:A:667:THR:OG1	2.34	0.41
1:A:1336:TYR:O	1:A:1339:THR:HG22	2.20	0.41
2:E:277:THR:HG21	2:E:306:CYS:SG	2.61	0.41
1:A:942:LEU:HD21	2:E:403:PRO:HG2	2.02	0.41
1:A:1139:PHE:CE1	1:A:1302:ARG:HG3	2.56	0.41
2:E:381:LEU:O	2:E:385:GLN:NE2	2.54	0.41
4:D:258:LEU:HD22	4:D:286:LYS:HG3	2.03	0.41
4:D:307:ASP:HB2	4:D:311:LYS:NZ	2.36	0.41
7:c:50:TYR:O	7:c:54:VAL:HG13	2.21	0.41
9:i:-73:DA:H1'	9:i:-72:DT:H5'	2.03	0.41
1:A:778:LEU:HD11	3:B:171:ILE:HD11	2.03	0.41
1:A:809:LYS:O	1:A:813:GLU:HG3	2.21	0.41
1:A:1016:TYR:HB3	1:A:1065:LEU:HD13	2.03	0.41
1:A:1150:HIS:O	1:A:1154:ILE:HG13	2.21	0.41
1:A:1279:SER:O	1:A:1283:GLN:HG2	2.21	0.41
2:E:182:ARG:HD3	3:B:128:MET:HE1	2.03	0.41
2:E:307:LYS:HA	2:E:310:ILE:HG22	2.02	0.41
3:B:128:MET:HB3	3:B:128:MET:HE2	1.47	0.41
9:i:-28:DG:H2''	9:i:-27:DC:C6	2.56	0.41
1:A:867:ILE:O	1:A:871:TYR:HB2	2.21	0.41
1:A:877:PHE:O	1:A:880:ILE:HG22	2.21	0.41
1:A:1271:LYS:HB2	1:A:1271:LYS:HE2	1.87	0.41
2:E:277:THR:CG2	2:E:306:CYS:SG	3.09	0.41
2:F:342:ASN:O	2:F:346:HIS:HB2	2.20	0.41
2:E:415:LEU:O	2:E:423:THR:HB	2.21	0.40
4:C:285:LEU:HA	4:C:285:LEU:HD23	1.80	0.40
4:D:299:TYR:CE1	2:F:351:PHE:HD1	2.39	0.40
2:F:305:GLU:O	2:F:309:LYS:HG2	2.21	0.40
5:e:65:LEU:HB3	5:e:66:PRO:HD3	2.03	0.40
9:i:-51:DT:C2	9:i:-50:DA:N7	2.88	0.40
1:A:912:TRP:CH2	2:E:111:THR:HG23	2.57	0.40
4:D:363:LEU:O	4:D:366:LEU:HB3	2.22	0.40
7:g:40:SER:OG	8:h:89:ILE:HG13	2.22	0.40
1:A:1286:TYR:O	1:A:1290:VAL:HG12	2.21	0.40
2:E:572:SER:HA	2:E:575:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:283:ALA:O	4:D:287:LEU:HD22	2.21	0.40
9:i:-20:DA:H2''	9:i:-19:DA:OP2	2.21	0.40
9:i:55:DT:H2''	9:i:56:DC:C6	2.57	0.40
10:j:-60:DT:H2''	10:j:-59:DG:C8	2.56	0.40
1:A:810:ILE:HD11	1:A:919:LEU:HG	2.04	0.40
1:A:868:ARG:HD2	1:A:873:LYS:NZ	2.36	0.40
2:E:107:LYS:HB2	2:E:107:LYS:NZ	2.35	0.40
2:E:501:LYS:HA	2:E:501:LYS:HD2	1.90	0.40
3:B:103:LYS:HD2	3:B:104:PHE:CE1	2.57	0.40
4:C:255:GLU:HB2	4:C:323:ILE:HG12	2.02	0.40
4:D:313:SER:HA	4:D:316:ASP:HB2	2.04	0.40
7:g:58:LEU:HD13	8:h:69:ILE:HD13	2.03	0.40
9:i:54:DA:H2'	9:i:55:DT:H71	2.03	0.40
1:A:876:GLY:O	1:A:879:ILE:HG22	2.22	0.40
9:i:-14:DC:H2''	9:i:-13:DA:C8	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/1536 (39%)	568 (95%)	27 (4%)	3 (0%)	24	59
2	E	343/684 (50%)	293 (85%)	41 (12%)	9 (3%)	4	28
2	F	152/684 (22%)	146 (96%)	6 (4%)	0	100	100
3	B	383/433 (88%)	365 (95%)	16 (4%)	2 (0%)	24	59
4	C	181/401 (45%)	168 (93%)	12 (7%)	1 (1%)	21	55
4	D	183/401 (46%)	172 (94%)	11 (6%)	0	100	100
4	G	63/401 (16%)	62 (98%)	1 (2%)	0	100	100
5	a	95/136 (70%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	100/136 (74%)	96 (96%)	4 (4%)	0	100	100
6	b	80/103 (78%)	77 (96%)	1 (1%)	2 (2%)	4	29
6	f	80/103 (78%)	77 (96%)	2 (2%)	1 (1%)	9	40
7	c	104/130 (80%)	101 (97%)	3 (3%)	0	100	100
7	g	106/130 (82%)	104 (98%)	2 (2%)	0	100	100
8	d	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
8	h	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
11	H	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2655/5535 (48%)	2507 (94%)	130 (5%)	18 (1%)	20	53

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	171	LEU
2	E	174	ASN
2	E	470	SER
4	C	241	LYS
6	b	25	ASN
1	A	873	LYS
1	A	1200	GLY
2	E	125	ARG
2	E	390	SER
2	E	517	ASN
6	b	24	ASP
1	A	1233	ASN
2	E	471	PRO
3	B	136	ARG
2	E	492	TRP
6	f	24	ASP
2	E	453	PRO
3	B	107	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	560/1391 (40%)	511 (91%)	49 (9%)	9	32
2	E	332/653 (51%)	287 (86%)	45 (14%)	3	18
2	F	148/653 (23%)	134 (90%)	14 (10%)	8	29
3	B	326/367 (89%)	304 (93%)	22 (7%)	15	41
4	C	172/359 (48%)	162 (94%)	10 (6%)	18	44
4	D	174/359 (48%)	158 (91%)	16 (9%)	8	30
4	G	56/359 (16%)	56 (100%)	0	100	100
5	a	85/111 (77%)	83 (98%)	2 (2%)	43	63
5	e	90/111 (81%)	86 (96%)	4 (4%)	25	49
6	b	67/79 (85%)	60 (90%)	7 (10%)	7	26
6	f	67/79 (85%)	58 (87%)	9 (13%)	4	19
7	c	83/100 (83%)	76 (92%)	7 (8%)	10	33
7	g	84/100 (84%)	80 (95%)	4 (5%)	23	48
8	d	81/105 (77%)	74 (91%)	7 (9%)	10	33
8	h	81/105 (77%)	77 (95%)	4 (5%)	22	47
11	H	1/1 (100%)	0	1 (100%)	0	0
All	All	2407/4932 (49%)	2206 (92%)	201 (8%)	12	33

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	665	GLU
1	A	676	ILE
1	A	679	LYS
1	A	702	LEU
1	A	724	VAL
1	A	763	THR
1	A	767	CYS
1	A	783	VAL
1	A	802	GLN
1	A	807	LEU
1	A	816	GLU
1	A	828	ILE
1	A	830	CYS
1	A	831	LEU
1	A	837	LYS

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Mol	Chain	Res	Type
1	A	839	GLU
1	A	841	MET
1	A	857	HIS
1	A	871	TYR
1	A	872	ASP
1	A	874	GLU
1	A	878	GLU
1	A	879	ILE
1	A	883	LEU
1	A	889	VAL
1	A	911	GLU
1	A	912	TRP
1	A	919	LEU
1	A	920	GLU
1	A	921	GLN
1	A	931	LEU
1	A	934	THR
1	A	961	ASN
1	A	997	THR
1	A	1008	GLU
1	A	1018	ILE
1	A	1069	LEU
1	A	1076	LYS
1	A	1121	VAL
1	A	1141	ASN
1	A	1153	THR
1	A	1176	SER
1	A	1182	LYS
1	A	1243	ASP
1	A	1310	LEU
1	A	1313	SER
1	A	1320	ASP
1	A	1337	TYR
1	A	1339	THR
2	E	105	ASP
2	E	107	LYS
2	E	108	VAL
2	E	110	VAL
2	E	111	THR
2	E	113	LEU
2	E	114	PRO
2	E	115	LEU

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Mol	Chain	Res	Type
2	E	123	ILE
2	E	125	ARG
2	E	126	GLU
2	E	175	MET
2	E	177	GLU
2	E	178	GLU
2	E	179	SER
2	E	180	ASN
2	E	181	ILE
2	E	185	ILE
2	E	187	TRP
2	E	298	LYS
2	E	315	SER
2	E	332	ASN
2	E	357	ILE
2	E	375	GLU
2	E	379	ILE
2	E	384	ARG
2	E	386	LEU
2	E	387	PHE
2	E	388	ASN
2	E	390	SER
2	E	391	TYR
2	E	395	ILE
2	E	398	LEU
2	E	409	SER
2	E	413	LYS
2	E	437	ILE
2	E	452	VAL
2	E	491	VAL
2	E	492	TRP
2	E	494	LYS
2	E	510	GLN
2	E	516	ASN
2	E	543	ASP
2	E	555	ILE
2	E	567	PHE
3	B	2	VAL
3	B	14	LYS
3	B	40	MET
3	B	41	LYS
3	B	42	PRO

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Mol	Chain	Res	Type
3	B	81	GLU
3	B	90	THR
3	B	108	ASP
3	B	136	ARG
3	B	141	VAL
3	B	163	LEU
3	B	176	TYR
3	B	193	VAL
3	B	207	SER
3	B	218	THR
3	B	240	ASP
3	B	259	MET
3	B	267	VAL
3	B	293	ASN
3	B	318	VAL
3	B	358	SER
3	B	385	TYR
4	C	235	ASP
4	C	246	CYS
4	C	287	LEU
4	C	310	LEU
4	C	321	VAL
4	C	323	ILE
4	C	337	VAL
4	C	348	ASP
4	C	350	GLN
4	C	361	ASP
4	D	217	THR
4	D	248	LEU
4	D	254	VAL
4	D	274	SER
4	D	287	LEU
4	D	293	LEU
4	D	296	MET
4	D	304	LEU
4	D	321	VAL
4	D	325	ILE
4	D	331	LEU
4	D	337	VAL
4	D	345	THR
4	D	349	LEU
4	D	363	LEU

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Mol	Chain	Res	Type
4	D	377	LYS
2	F	256	ASP
2	F	264	SER
2	F	276	ASP
2	F	285	LEU
2	F	291	ILE
2	F	304	ASN
2	F	312	ILE
2	F	332	ASN
2	F	346	HIS
2	F	349	LYS
2	F	353	LEU
2	F	371	GLN
2	F	564	ARG
2	F	573	LEU
5	a	59	GLU
5	a	86	SER
6	b	21	VAL
6	b	50	ILE
6	b	52	GLU
6	b	54	THR
6	b	74	GLU
6	b	79	LYS
6	b	80	THR
7	c	13	LYS
7	c	15	LYS
7	c	19	SER
7	c	71	ARG
7	c	90	ASP
7	c	108	LEU
7	c	118	LYS
8	d	30	LYS
8	d	31	ARG
8	d	33	ARG
8	d	71	GLU
8	d	78	SER
8	d	87	SER
8	d	123	SER
5	e	2	ARG
5	e	37	LYS
5	e	61	LEU
5	e	87	SER

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Mol	Chain	Res	Type
6	f	21	VAL
6	f	22	LEU
6	f	23	ARG
6	f	50	ILE
6	f	52	GLU
6	f	54	THR
6	f	74	GLU
6	f	79	LYS
6	f	80	THR
7	g	11	ARG
7	g	13	LYS
7	g	15	LYS
7	g	64	GLU
8	h	30	LYS
8	h	31	ARG
8	h	63	ASN
8	h	106	LEU
11	H	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	663	ASN
1	A	690	ASN
1	A	722	ASN
1	A	779	ASN
1	A	798	HIS
1	A	802	GLN
1	A	824	ASN
1	A	1038	GLN
1	A	1075	GLN
1	A	1165	ASN
1	A	1216	ASN
1	A	1233	ASN
1	A	1234	ASN
1	A	1254	HIS
2	E	130	ASN
2	E	180	ASN
2	E	259	ASN
2	E	330	ASN
2	E	376	ASN
2	E	388	ASN

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Mol	Chain	Res	Type
2	E	448	HIS
2	E	495	GLN
2	E	516	ASN
2	E	517	ASN
2	E	519	ASN
2	E	541	GLN
3	B	76	GLN
3	B	164	ASN
3	B	188	HIS
3	B	330	ASN
3	B	341	ASN
4	C	267	GLN
4	C	393	GLN
4	D	277	GLN
4	D	295	ASN
4	D	350	GLN
4	D	358	GLN
4	D	389	ASN
2	F	259	ASN
2	F	294	ASN
2	F	347	ASN
2	F	371	GLN
2	F	568	GLN
5	a	39	HIS
6	b	75	HIS
7	c	38	ASN
7	c	104	GLN
7	c	112	GLN
5	e	5	GLN
5	e	39	HIS
5	e	76	GLN
5	e	113	HIS
5	e	125	GLN
6	f	25	ASN
7	g	31	HIS
7	g	38	ASN
8	h	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

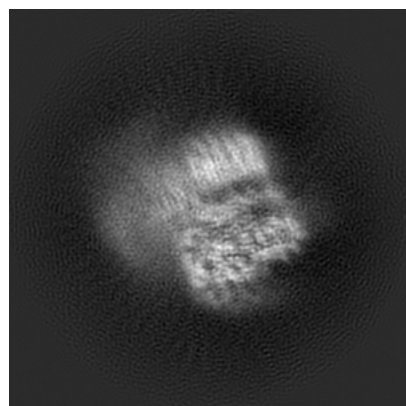
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37365. These allow visual inspection of the internal detail of the map and identification of artifacts.

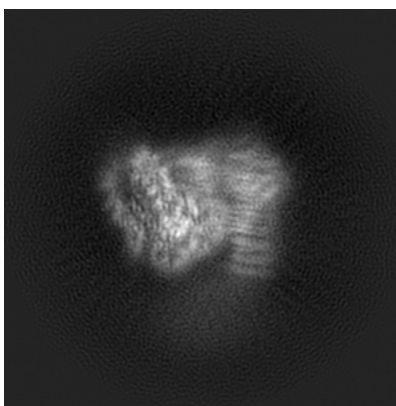
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

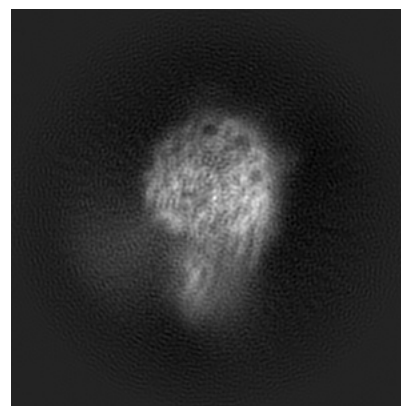
6.1.1 Primary map



X

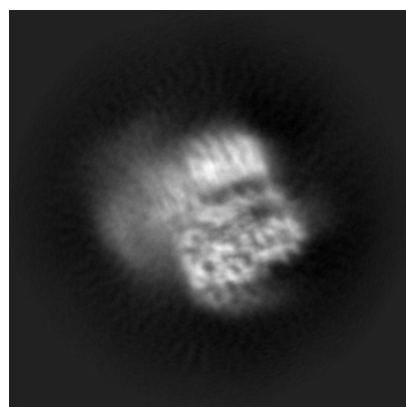


Y

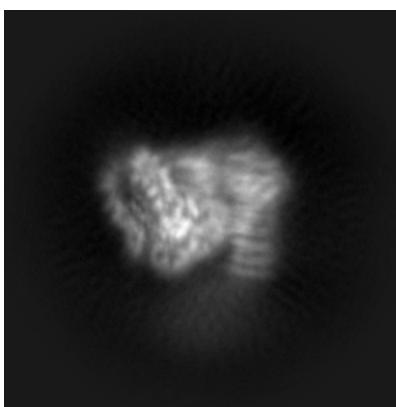


Z

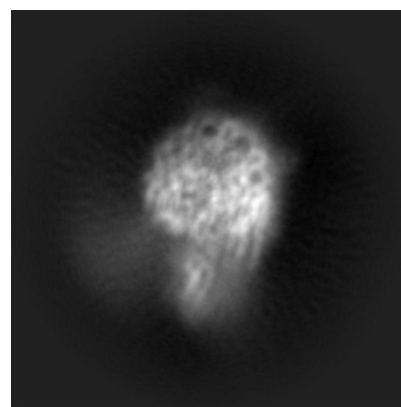
6.1.2 Raw map



X



Y

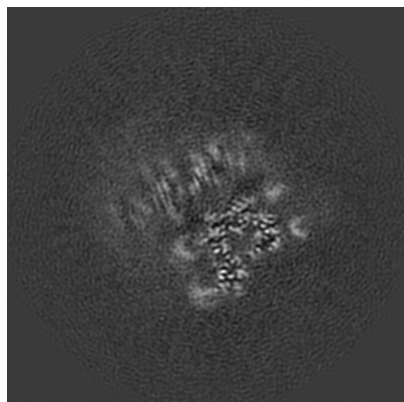


Z

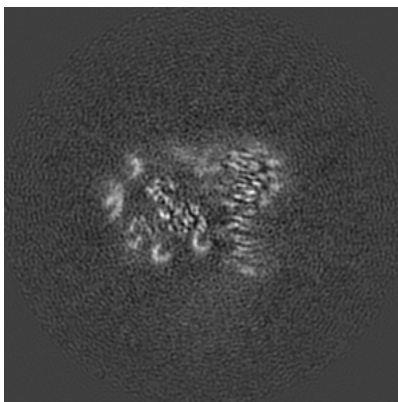
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

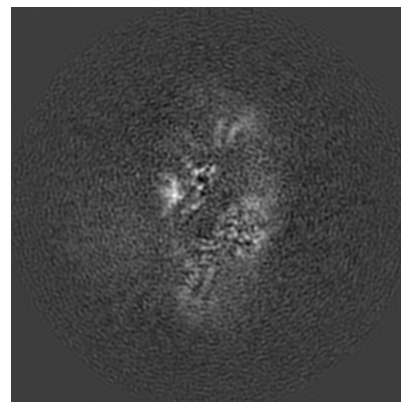
6.2.1 Primary map



X Index: 140

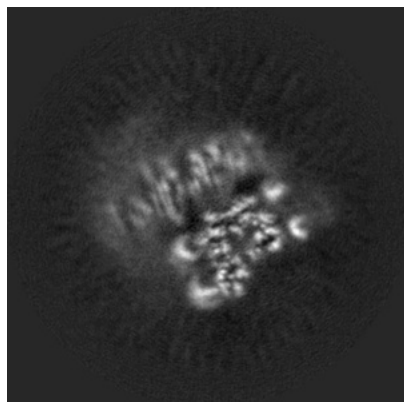


Y Index: 140

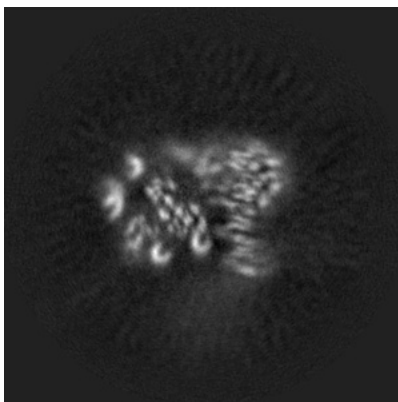


Z Index: 140

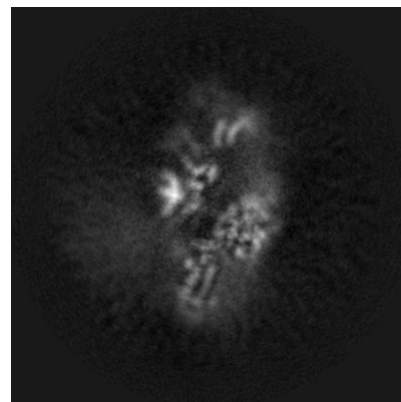
6.2.2 Raw map



X Index: 140



Y Index: 140

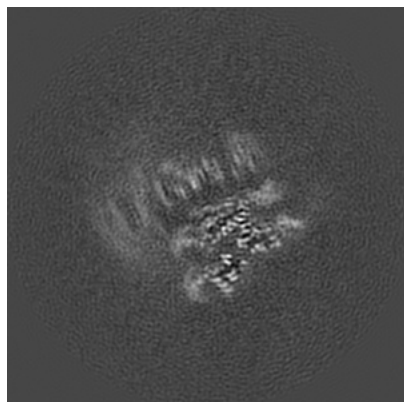


Z Index: 140

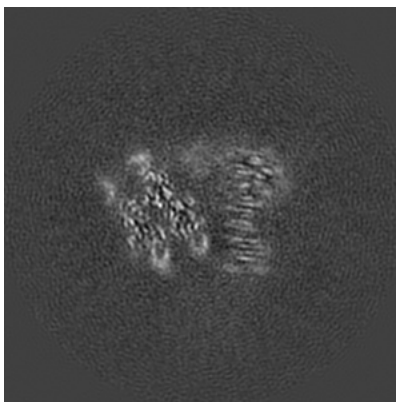
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

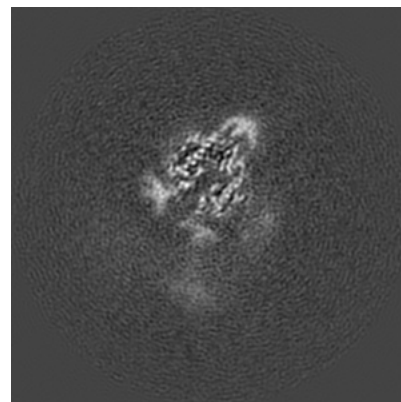
6.3.1 Primary map



X Index: 130

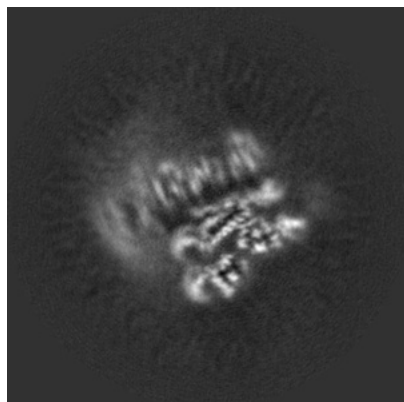


Y Index: 147

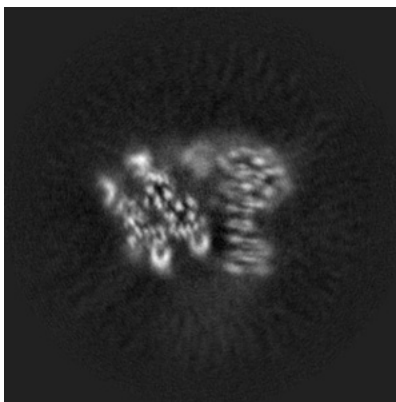


Z Index: 113

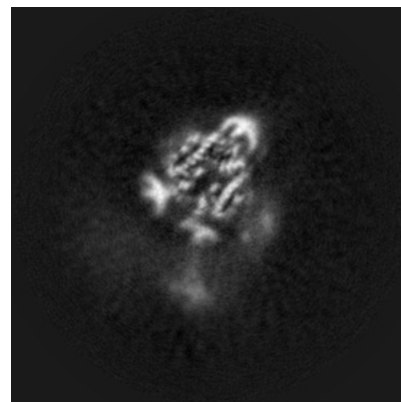
6.3.2 Raw map



X Index: 131



Y Index: 146

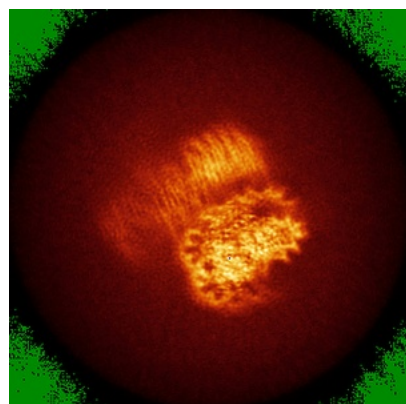


Z Index: 113

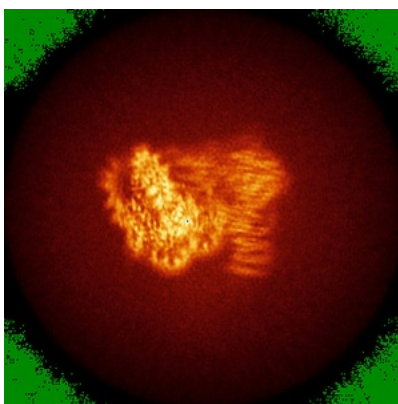
The images above show the largest variance slices of the map in three orthogonal directions.

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

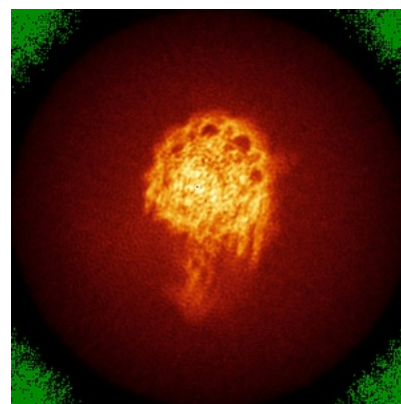
6.4.1 Primary map



X

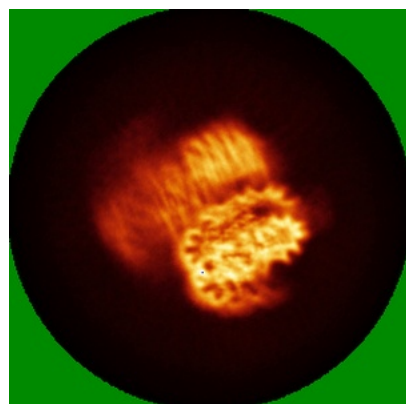


Y

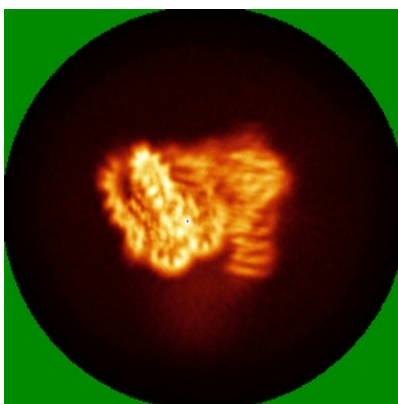


Z

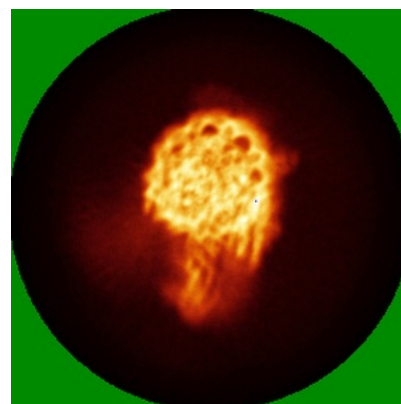
6.4.2 Raw map



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.

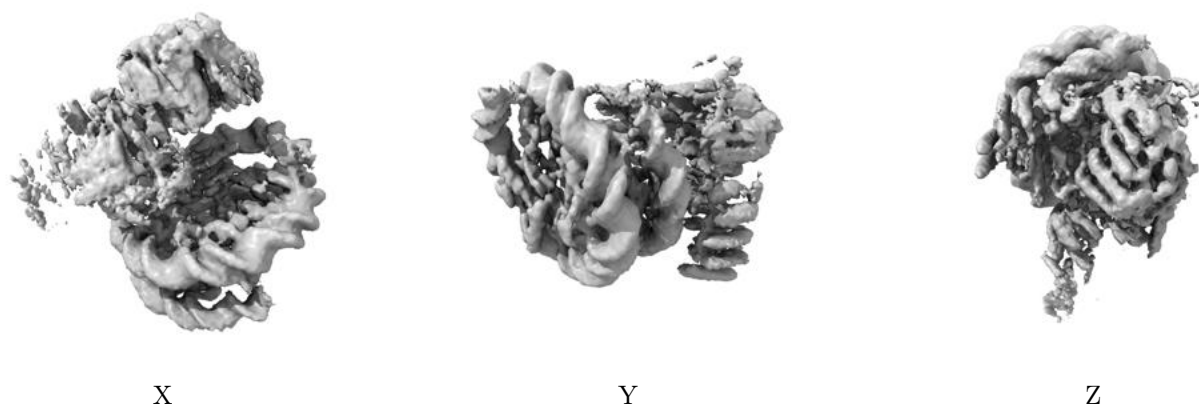
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

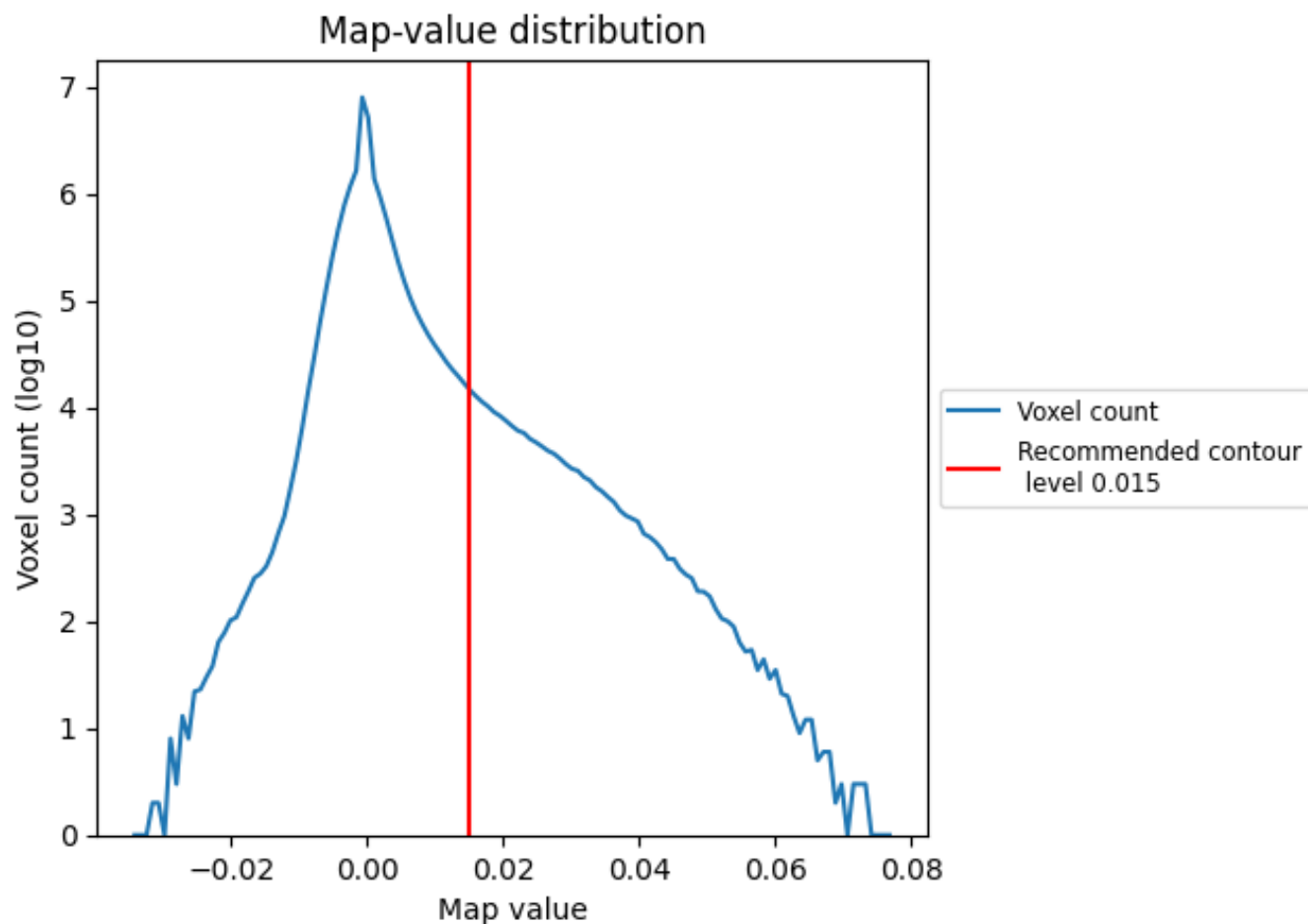
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

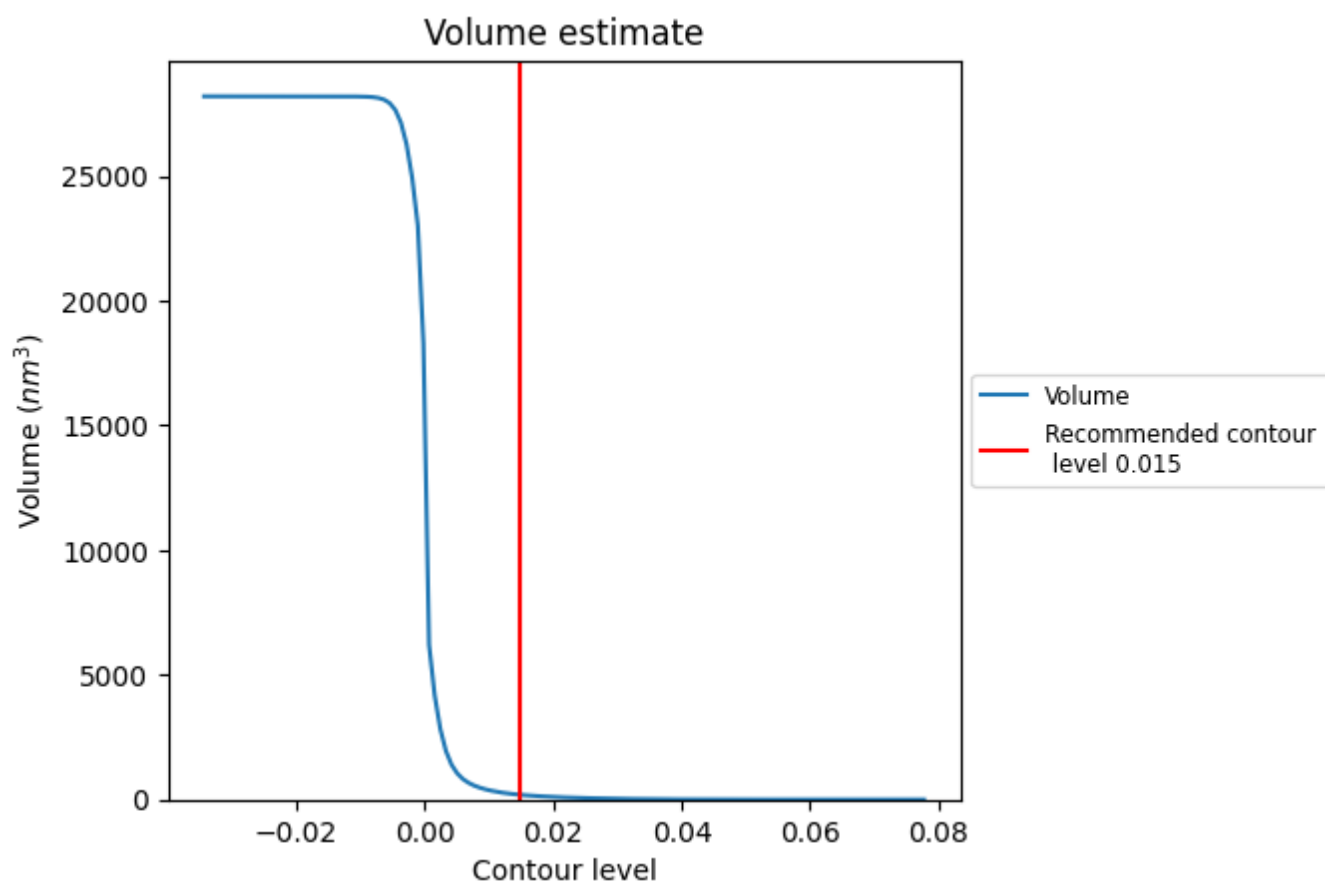
This section contains the results of statistical analysis of the map.

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.

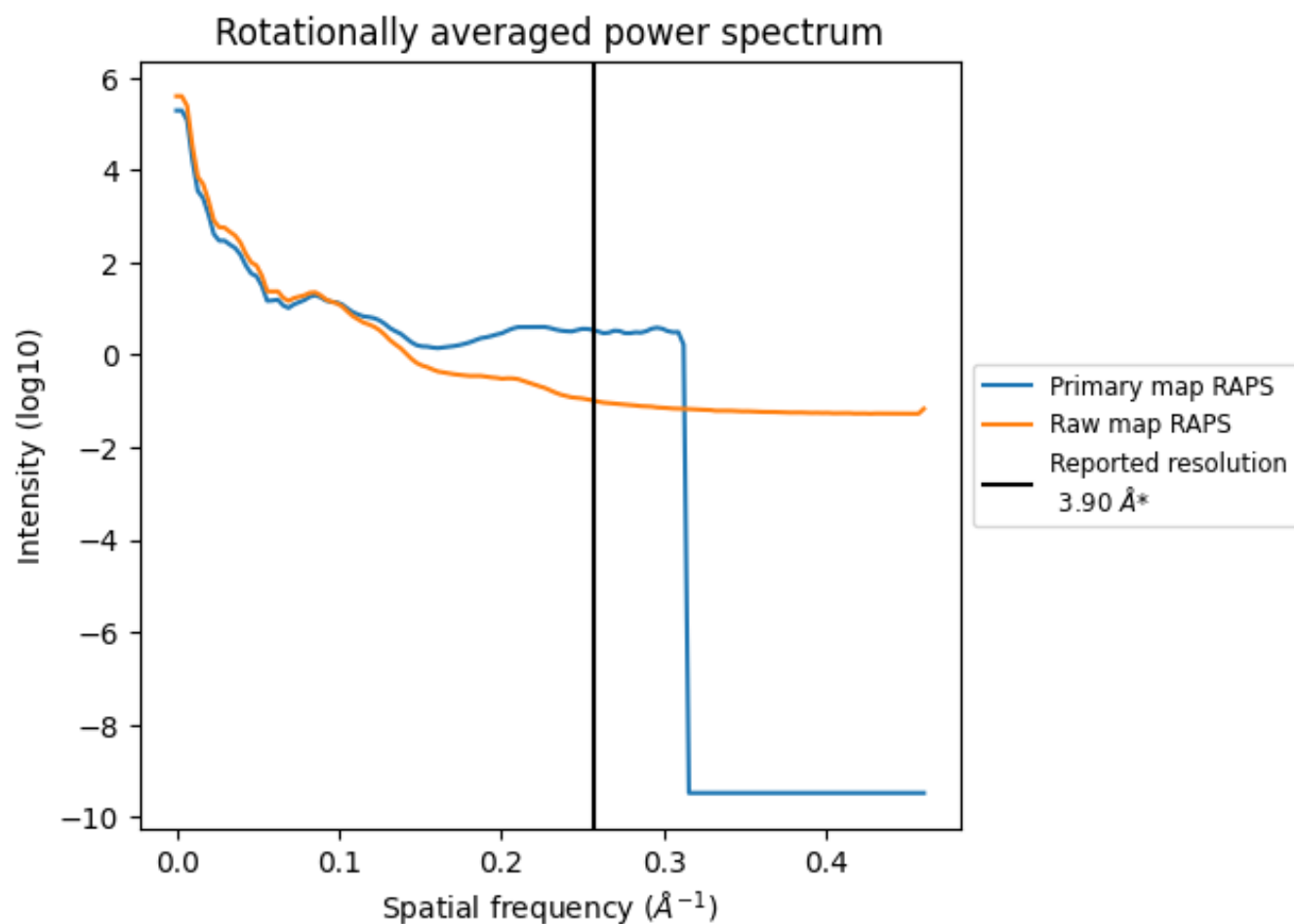
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm³; this corresponds to an approximate mass of 171 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 ⓘ

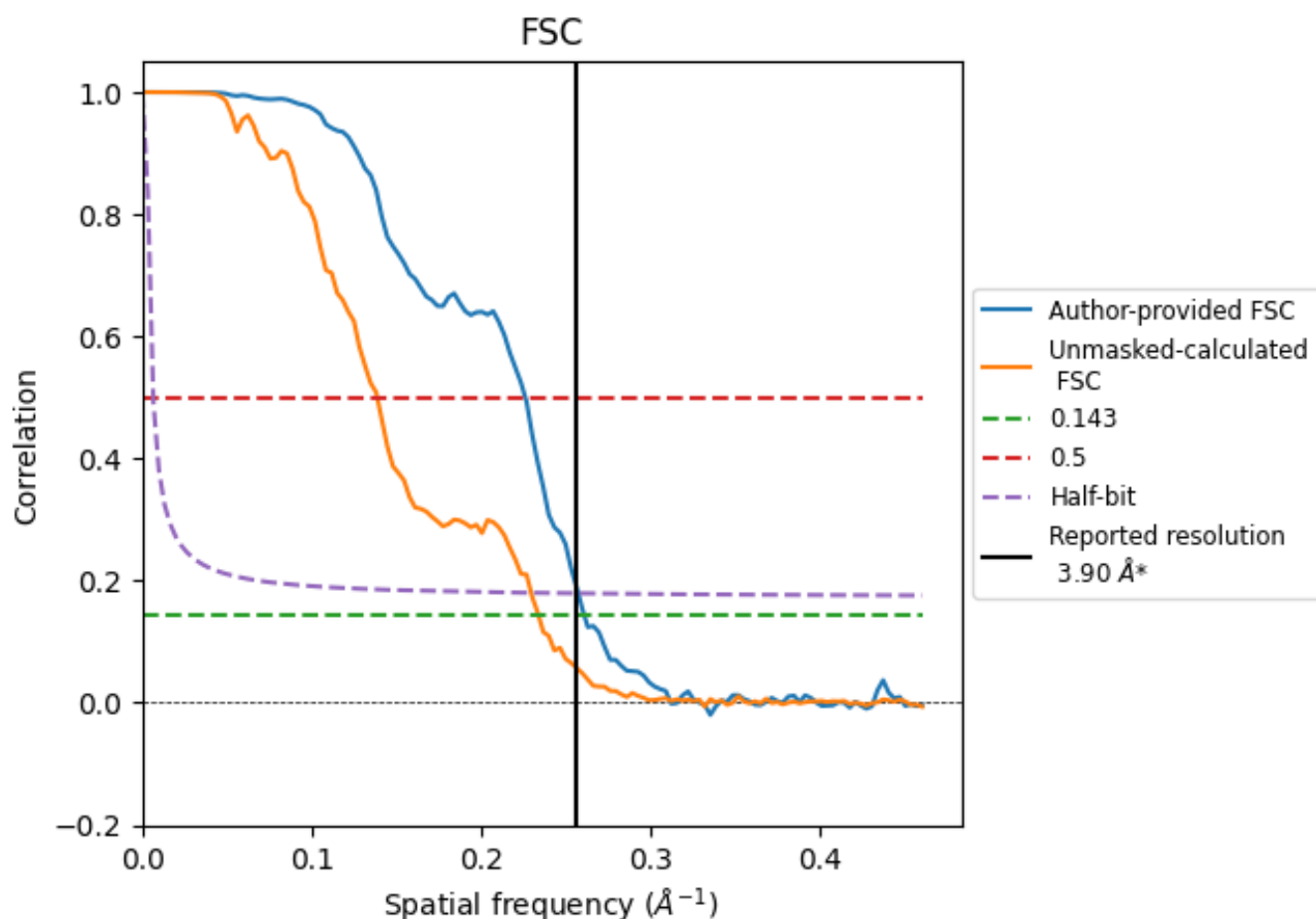


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

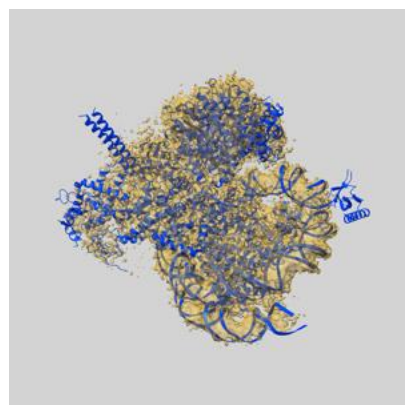
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.84	4.42	3.89
Unmasked-calculated*	4.28	7.22	4.36

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

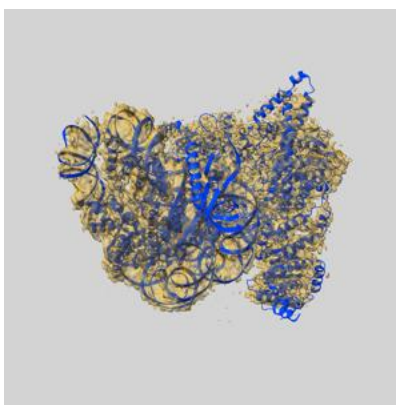
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37365 and PDB model 8W9D. Per-residue inclusion information can be found in section [3](#) on page [7](#).

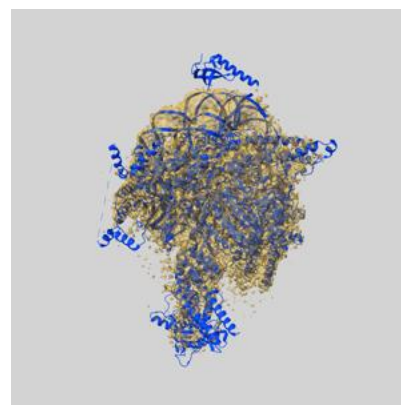
9.1 Map-model overlay [i](#)



X



Y



Z

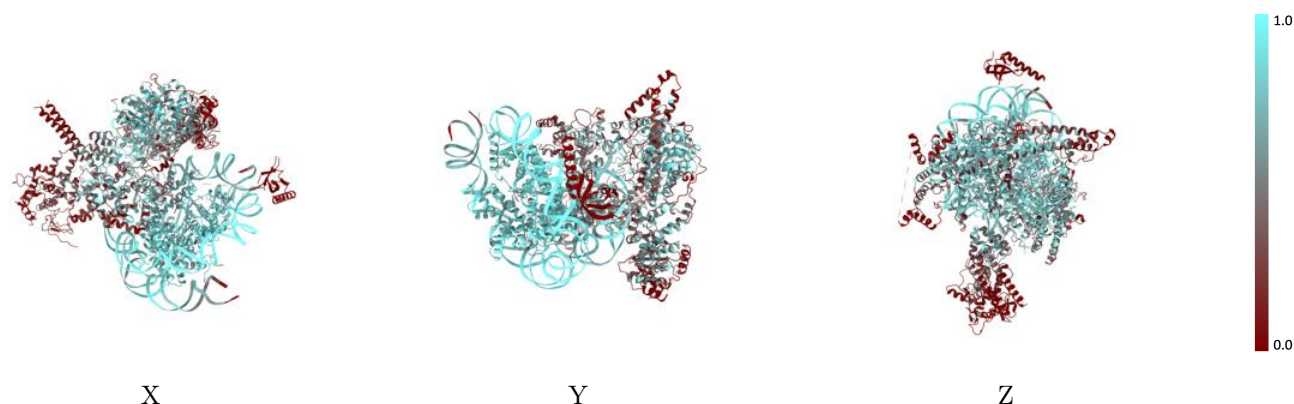
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



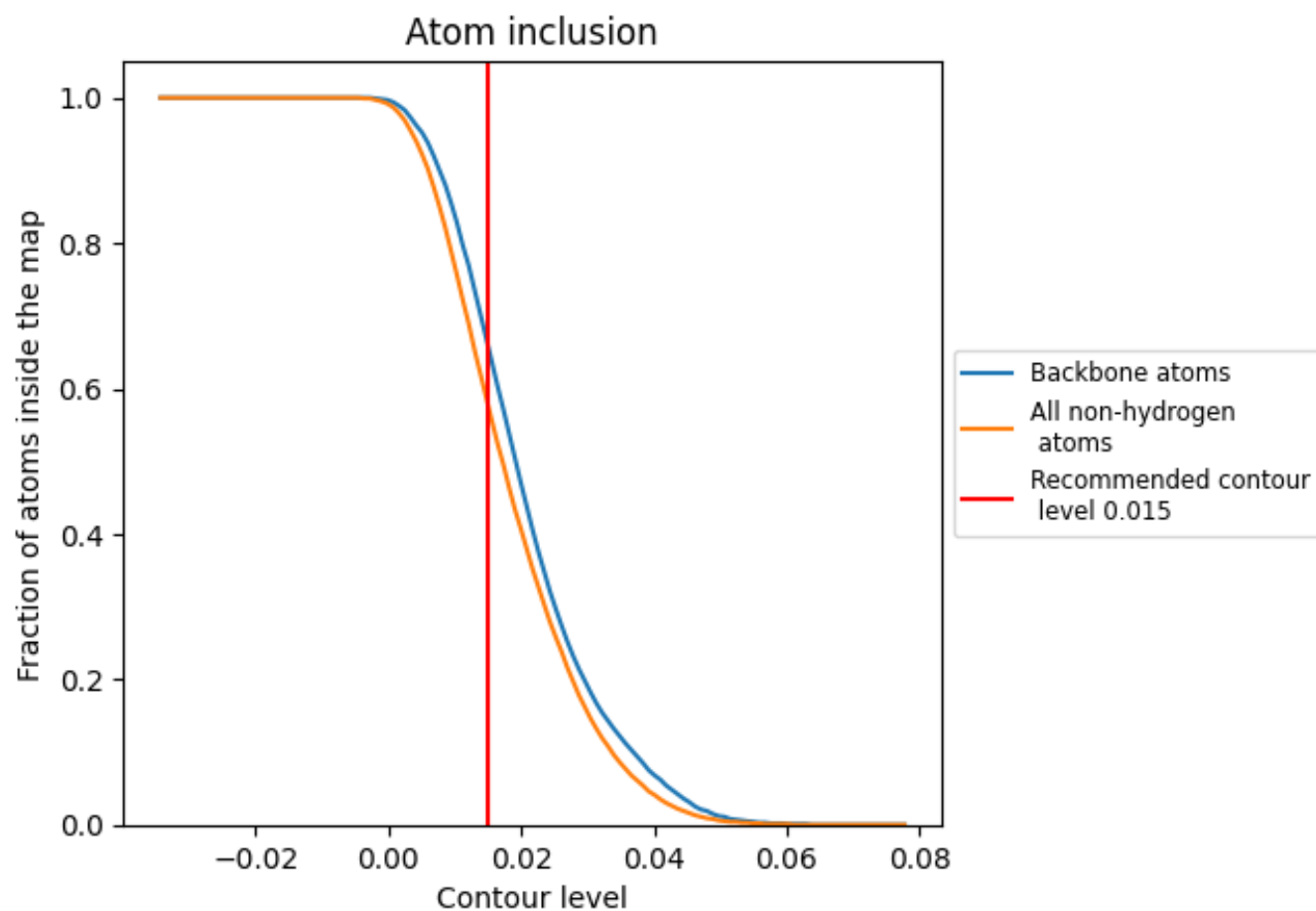
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 58% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.2630
A	 0.3950	 0.1890
B	 0.6660	 0.2830
C	 0.5420	 0.2350
D	 0.1440	 0.1220
E	 0.3520	 0.1680
F	 0.1270	 0.0710
G	 0.0000	 -0.0020
H	 0.1380	 0.1700
a	 0.8130	 0.4420
b	 0.8260	 0.4720
c	 0.7540	 0.4290
d	 0.7310	 0.4020
e	 0.7920	 0.4370
f	 0.8690	 0.4680
g	 0.8090	 0.4530
h	 0.8180	 0.4470
i	 0.8300	 0.2880
j	 0.8530	 0.2860

