



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:10 AM UTC

PDB ID : 5VH9 / pdb_00005vh9
EMDB ID : EMD-8673
Title : Cryo-EM structure of yeast cytoplasmic dynein-1 with Lis1 and ATP
Authors : Cianfrocco, M.A.; DeSantis, M.E.; Htet, Z.M.; Tran, P.T.; Reck-Peterson, S.L.; Leschziner, A.E.
Deposited on : 2017-04-12
Resolution : 7.70 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

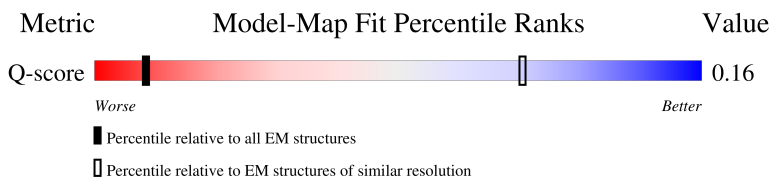
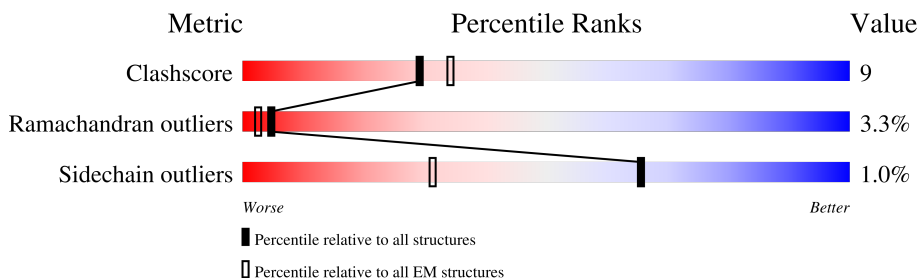
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 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	384 (7.20 - 8.20)

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	2376	
2	B	354	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41285 atoms, of which 19243 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2376	Total	C	H	N	O	S	0	0
			38423	12301	19243	3182	3607	90		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1575	PHE	LEU	conflict	UNP P36022
A	1578	SER	PHE	conflict	UNP P36022
A	1668	GLU	GLN	conflict	UNP P36022
A	1777	VAL	ILE	conflict	UNP P36022
A	1984	VAL	ILE	conflict	UNP P36022
A	2936	VAL	ILE	conflict	UNP P36022
A	3343	GLY	ALA	conflict	UNP P36022
A	3444	VAL	ILE	conflict	UNP P36022
A	3556	ARG	LYS	conflict	UNP P36022
A	3742	ASP	ASN	conflict	UNP P36022
A	3895	VAL	PHE	conflict	UNP P36022
A	4072	ASP	ASN	conflict	UNP P36022

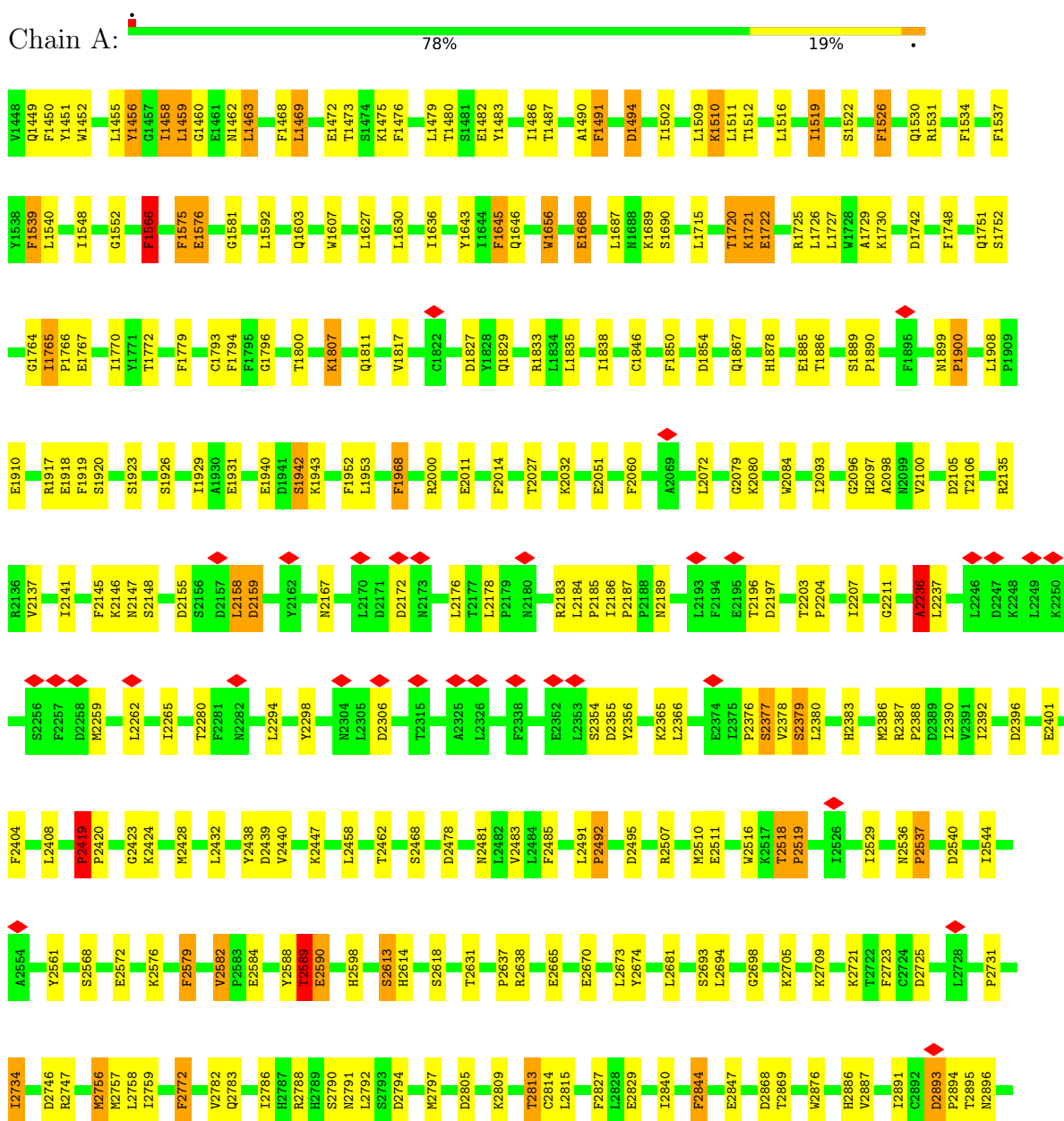
- Molecule 2 is a protein called Nuclear distribution protein PAC1.

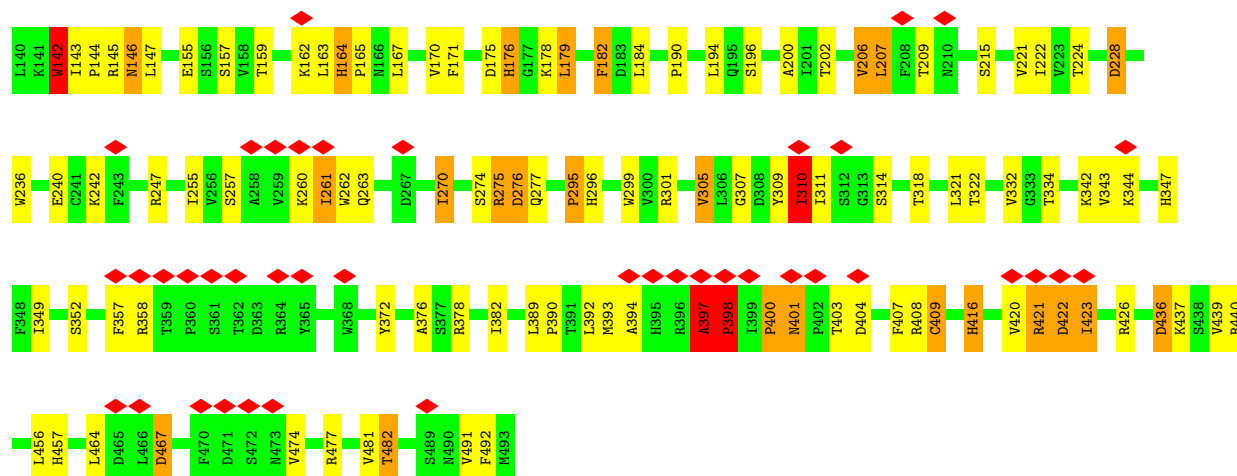
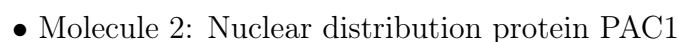
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	354	Total	C	N	O	S	0	0
			2862	1831	499	516	16		

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: Dynein heavy chain, cytoplasmic





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	82	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0119	Depositor
Map size ($\text{\AA}$)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	10/19571 (0.1%)	1.32	217/26457 (0.8%)
2	B	0.97	2/2943 (0.1%)	1.70	39/4003 (1.0%)
All	All	1.04	12/22514 (0.1%)	1.38	256/30460 (0.8%)

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
1	A	0	6
2	B	0	6
All	All	0	12

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2947	GLU	CA-C	8.02	1.63	1.52
1	A	2950	LYS	CA-C	6.61	1.59	1.53
1	A	3765	ASN	CA-C	-6.18	1.46	1.53
2	B	182	PHE	C-O	6.07	1.30	1.23
2	B	397	ALA	C-O	6.02	1.31	1.24
1	A	1459	LEU	CA-C	-5.96	1.45	1.52
1	A	1479	LEU	CA-C	-5.80	1.45	1.52
1	A	1463	LEU	CA-C	-5.76	1.45	1.52
1	A	1668	GLU	CA-C	-5.74	1.45	1.52
1	A	2948	VAL	N-CA	5.67	1.53	1.46
1	A	2946	PRO	CA-C	5.32	1.59	1.52
1	A	2951	GLU	N-CA	5.07	1.52	1.46

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	ALA	CA-C-N	-12.81	103.82	119.84
2	B	397	ALA	C-N-CA	-12.81	103.82	119.84
1	A	3653	PHE	CA-CB-CG	-10.95	102.85	113.80
1	A	3568	GLU	N-CA-C	10.86	123.11	111.28
1	A	3449	VAL	N-CA-C	10.55	123.62	109.37
1	A	2950	LYS	N-CA-C	10.27	123.92	108.31
2	B	398	PRO	N-CA-CB	-10.24	92.49	103.25
1	A	1494	ASP	N-CA-C	9.73	121.97	111.36
1	A	1534	PHE	CA-C-N	9.30	130.26	119.47
1	A	1534	PHE	C-N-CA	9.30	130.26	119.47
1	A	2582	VAL	CA-C-N	9.20	129.81	119.32
1	A	2582	VAL	C-N-CA	9.20	129.81	119.32
1	A	2203	THR	CA-C-N	9.10	128.75	119.56
1	A	2203	THR	C-N-CA	9.10	128.75	119.56
1	A	3744	LEU	N-CA-C	9.02	121.38	110.19
2	B	176	HIS	N-CA-C	9.01	121.10	111.28
1	A	3884	LEU	CA-C-N	8.99	128.75	119.76
1	A	3884	LEU	C-N-CA	8.99	128.75	119.76
1	A	2561	TYR	CA-C-N	8.98	128.92	120.03
1	A	2561	TYR	C-N-CA	8.98	128.92	120.03
1	A	3427	VAL	N-CA-C	8.89	119.71	111.45
1	A	1765	ILE	CA-C-N	8.85	128.50	119.56
1	A	1765	ILE	C-N-CA	8.85	128.50	119.56
1	A	2187	PRO	CA-C-N	8.78	129.00	119.87
1	A	2187	PRO	C-N-CA	8.78	129.00	119.87
2	B	176	HIS	CA-CB-CG	8.73	122.53	113.80
1	A	2618	SER	CA-C-N	8.70	128.34	119.56
1	A	2618	SER	C-N-CA	8.70	128.34	119.56
1	A	2178	LEU	CA-C-N	8.69	128.84	119.28
1	A	2178	LEU	C-N-CA	8.69	128.84	119.28
1	A	3359	LYS	N-CA-C	8.65	122.96	110.24
1	A	2972	PHE	CA-CB-CG	8.65	122.45	113.80
1	A	4058	SER	N-CA-C	8.61	123.20	112.87
1	A	3357	ALA	N-CA-C	8.60	124.15	107.98
1	A	3366	PHE	CA-CB-CG	-8.57	105.23	113.80
1	A	2419	PRO	CA-C-N	8.39	128.90	119.83
1	A	2419	PRO	C-N-CA	8.39	128.90	119.83
1	A	2945	VAL	CA-C-N	8.37	130.30	119.84
1	A	2945	VAL	C-N-CA	8.37	130.30	119.84
1	A	2537	PRO	CA-C-N	8.32	130.24	119.84
1	A	2537	PRO	C-N-CA	8.32	130.24	119.84
1	A	2949	ASN	CA-C-N	8.32	137.20	122.89
1	A	2949	ASN	C-N-CA	8.32	137.20	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2905	SER	CA-C-N	8.27	128.75	119.32
1	A	2905	SER	C-N-CA	8.27	128.75	119.32
1	A	3869	GLU	N-CA-C	8.21	122.59	112.58
1	A	3916	PHE	CA-CB-CG	-8.17	105.63	113.80
1	A	2681	LEU	CA-C-N	8.09	127.74	119.82
1	A	2681	LEU	C-N-CA	8.09	127.74	119.82
1	A	3500	ASP	CA-C-N	8.09	128.28	119.87
1	A	3500	ASP	C-N-CA	8.09	128.28	119.87
1	A	3745	ARG	N-CA-C	7.87	127.56	110.80
1	A	2946	PRO	N-CA-C	7.84	128.62	112.47
1	A	1796	GLY	CA-C-N	7.59	128.19	120.14
1	A	1796	GLY	C-N-CA	7.59	128.19	120.14
2	B	147	LEU	N-CA-C	-7.57	100.56	110.39
1	A	3409	ASP	N-CA-C	7.55	122.44	110.73
1	A	1458	ILE	N-CA-C	7.52	117.60	110.53
1	A	1491	PHE	N-CA-C	-7.46	103.15	111.28
1	A	1889	SER	CA-C-N	7.46	129.17	119.84
1	A	1889	SER	C-N-CA	7.46	129.17	119.84
1	A	2540	ASP	CA-C-N	7.42	127.84	119.83
1	A	2540	ASP	C-N-CA	7.42	127.84	119.83
1	A	2294	LEU	N-CA-C	-7.39	103.16	111.14
1	A	1469	LEU	CA-C-N	7.38	128.03	119.47
1	A	1469	LEU	C-N-CA	7.38	128.03	119.47
1	A	3505	ILE	CA-C-N	7.34	127.30	120.03
1	A	3505	ILE	C-N-CA	7.34	127.30	120.03
2	B	422	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	2772	PHE	CA-CB-CG	-7.24	106.56	113.80
1	A	1886	THR	CA-C-N	7.24	127.68	119.93
1	A	1886	THR	C-N-CA	7.24	127.68	119.93
1	A	3814	ILE	CA-C-N	7.22	127.19	119.76
1	A	3814	ILE	C-N-CA	7.22	127.19	119.76
1	A	3868	HIS	CA-CB-CG	-7.18	106.62	113.80
1	A	4024	VAL	CA-C-N	7.18	126.81	119.56
1	A	4024	VAL	C-N-CA	7.18	126.81	119.56
1	A	1923	SER	CA-C-N	7.16	127.33	120.31
1	A	1923	SER	C-N-CA	7.16	127.33	120.31
1	A	3675	LEU	N-CA-C	-7.15	102.90	111.69
1	A	3639	HIS	N-CA-C	7.10	119.10	111.36
1	A	1519	ILE	N-CA-C	7.08	117.18	110.53
1	A	3356	PHE	N-CA-C	-7.05	100.12	110.42
2	B	394	ALA	N-CA-CB	-7.01	100.32	110.56
1	A	3856	HIS	CA-CB-CG	-6.94	106.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1451	TYR	N-CA-C	-6.91	103.83	111.36
1	A	2159	ASP	CA-C-N	6.82	128.37	119.84
1	A	2159	ASP	C-N-CA	6.82	128.37	119.84
1	A	1748	PHE	CA-CB-CG	-6.82	106.98	113.80
1	A	2186	ILE	CA-C-N	6.81	127.39	120.38
1	A	2186	ILE	C-N-CA	6.81	127.39	120.38
2	B	142	TRP	N-CA-C	6.76	119.22	109.14
1	A	2844	PHE	CA-CB-CG	-6.76	107.04	113.80
1	A	2950	LYS	CB-CA-C	-6.76	108.77	116.54
1	A	1952	PHE	N-CA-C	-6.75	103.92	111.28
1	A	3356	PHE	CA-CB-CG	6.75	120.55	113.80
1	A	1450	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	2544	ILE	N-CA-C	6.64	114.34	108.63
1	A	2408	LEU	N-CA-C	-6.60	104.17	111.36
1	A	2027	THR	CA-C-N	6.58	126.34	119.76
1	A	2027	THR	C-N-CA	6.58	126.34	119.76
1	A	2598	HIS	CA-CB-CG	-6.52	107.28	113.80
1	A	3404	VAL	CA-C-N	6.50	127.96	119.84
1	A	3404	VAL	C-N-CA	6.50	127.96	119.84
1	A	4065	LEU	CA-C-N	6.49	127.02	120.14
1	A	4065	LEU	C-N-CA	6.49	127.02	120.14
1	A	1772	THR	CA-C-N	6.48	126.71	119.32
1	A	1772	THR	C-N-CA	6.48	126.71	119.32
1	A	2891	ILE	N-CA-C	6.48	118.04	108.45
1	A	3988	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	1800	THR	N-CA-C	-6.43	104.58	112.88
1	A	3629	PHE	CA-CB-CG	-6.43	107.37	113.80
1	A	2786	ILE	N-CA-C	6.38	117.49	108.36
1	A	1908	LEU	CA-C-N	6.33	126.28	119.76
1	A	1908	LEU	C-N-CA	6.33	126.28	119.76
1	A	2794	ASP	N-CA-C	-6.32	104.47	111.36
1	A	2827	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	2840	ILE	CA-C-N	6.28	127.69	119.84
1	A	2840	ILE	C-N-CA	6.28	127.69	119.84
1	A	3354	GLY	N-CA-C	6.28	128.06	113.18
1	A	2783	GLN	CA-C-N	6.27	126.78	120.14
1	A	2783	GLN	C-N-CA	6.27	126.78	120.14
1	A	3957	ASN	CA-CB-CG	-6.26	106.33	112.60
1	A	3415	ILE	N-CA-C	-6.25	104.66	110.53
1	A	3767	PHE	CA-CB-CG	-6.23	107.57	113.80
1	A	2579	PHE	CA-CB-CG	6.21	120.01	113.80
1	A	4015	PHE	N-CA-C	6.21	119.82	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3481	ILE	N-CA-C	-6.19	105.79	111.67
2	B	164	HIS	CA-CB-CG	6.17	119.97	113.80
1	A	3746	TYR	N-CA-C	6.16	120.52	113.19
1	A	3654	LYS	N-CA-C	-6.16	104.57	111.28
1	A	1968	PHE	CA-CB-CG	-6.15	107.65	113.80
1	A	2392	ILE	CA-C-N	6.15	126.66	120.14
1	A	2392	ILE	C-N-CA	6.15	126.66	120.14
1	A	3726	LEU	N-CA-C	6.14	118.46	108.63
1	A	2468	SER	N-CA-C	-6.14	99.81	108.96
1	A	2387	ARG	CA-C-N	6.14	127.51	119.84
1	A	2387	ARG	C-N-CA	6.14	127.51	119.84
2	B	176	HIS	O-C-N	-6.13	115.62	122.12
1	A	2887	VAL	N-CA-C	6.13	116.93	108.84
1	A	3409	ASP	CA-C-N	6.11	126.29	119.32
1	A	3409	ASP	C-N-CA	6.11	126.29	119.32
1	A	2590	GLU	CA-C-N	6.09	125.98	119.28
1	A	2590	GLU	C-N-CA	6.09	125.98	119.28
1	A	2185	PRO	CA-C-N	-6.02	116.76	123.02
1	A	2185	PRO	C-N-CA	-6.02	116.76	123.02
1	A	3352	LEU	N-CA-C	6.01	122.48	114.12
1	A	1645	PHE	CA-CB-CG	-6.00	107.81	113.80
1	A	2951	GLU	N-CA-C	5.99	123.55	110.80
2	B	182	PHE	O-C-N	-5.97	115.63	123.28
1	A	2096	GLY	N-CA-C	-5.97	104.61	114.76
1	A	2211	GLY	N-CA-C	-5.96	104.91	112.54
1	A	1766	PRO	N-CA-C	5.94	121.29	113.86
2	B	164	HIS	N-CA-C	5.94	117.37	109.83
1	A	3461	ILE	N-CA-C	5.91	118.48	111.09
1	A	4031	GLN	CA-C-N	5.90	127.22	119.84
1	A	4031	GLN	C-N-CA	5.90	127.22	119.84
1	A	2988	SER	CA-C-N	5.89	127.21	119.84
1	A	2988	SER	C-N-CA	5.89	127.21	119.84
2	B	310	ILE	N-CA-C	5.89	116.49	107.77
1	A	2236	ALA	CA-C-O	-5.87	114.88	121.81
1	A	2746	ASP	CA-CB-CG	-5.86	106.74	112.60
1	A	2756	MET	N-CA-C	5.85	118.17	108.99
1	A	3899	ASP	N-CA-C	5.84	120.80	111.81
1	A	2948	VAL	N-CA-C	5.83	121.45	109.34
1	A	3980	ILE	CA-C-N	5.82	127.12	119.84
1	A	3980	ILE	C-N-CA	5.82	127.12	119.84
1	A	1456	TYR	N-CA-C	-5.81	104.86	111.07
2	B	143	ILE	CB-CA-C	5.81	116.69	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	378	ARG	CA-C-N	5.80	128.85	120.38
2	B	378	ARG	C-N-CA	5.80	128.85	120.38
2	B	176	HIS	CA-C-N	5.78	132.10	121.70
2	B	176	HIS	C-N-CA	5.78	132.10	121.70
2	B	334	THR	N-CA-C	5.78	118.80	111.69
2	B	467	ASP	CB-CA-C	5.78	119.87	110.22
1	A	3748	TRP	N-CA-C	-5.77	104.99	111.28
2	B	207	LEU	CB-CA-C	5.76	120.36	110.86
1	A	3470	PHE	CA-CB-CG	-5.75	108.05	113.80
1	A	3449	VAL	CB-CA-C	-5.74	102.23	111.59
1	A	3516	VAL	N-CA-C	5.74	116.85	108.53
1	A	2705	LYS	N-CA-C	5.73	118.02	109.59
1	A	1566	PHE	N-CA-C	5.73	115.95	107.88
1	A	1479	LEU	N-CA-C	-5.69	104.76	110.97
1	A	3641	PHE	CA-CB-CG	-5.68	108.11	113.80
1	A	1575	PHE	CA-CB-CG	-5.68	108.12	113.80
2	B	175	ASP	CA-C-N	5.68	127.89	120.28
2	B	175	ASP	C-N-CA	5.68	127.89	120.28
1	A	2936	VAL	CA-C-N	5.68	126.94	119.84
1	A	2936	VAL	C-N-CA	5.68	126.94	119.84
1	A	2167	ASN	N-CA-C	5.64	118.15	111.33
2	B	492	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	4030	PRO	N-CA-C	-5.63	100.88	112.47
1	A	2902	MET	CA-C-N	-5.62	116.37	121.65
1	A	2902	MET	C-N-CA	-5.62	116.37	121.65
1	A	2032	LYS	N-CA-C	5.60	117.25	111.03
1	A	2485	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	3886	ALA	CA-C-N	5.60	125.06	119.24
1	A	3886	ALA	C-N-CA	5.60	125.06	119.24
2	B	436	ASP	CA-C-N	5.59	131.84	123.05
2	B	436	ASP	C-N-CA	5.59	131.84	123.05
2	B	228	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	3347	VAL	N-CA-C	-5.56	107.37	113.43
2	B	401	ASN	O-C-N	-5.55	114.94	121.32
1	A	1715	LEU	CA-C-N	5.54	127.64	120.44
1	A	1715	LEU	C-N-CA	5.54	127.64	120.44
1	A	3583	LEU	N-CA-C	-5.54	106.88	113.97
1	A	3878	HIS	N-CA-C	-5.54	101.85	110.10
1	A	1643	TYR	N-CA-C	5.51	116.90	108.42
1	A	3352	LEU	CA-C-N	-5.51	112.35	120.28
1	A	3352	LEU	C-N-CA	-5.51	112.35	120.28
1	A	2813	THR	N-CA-C	5.45	115.31	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3462	ILE	N-CA-C	5.44	116.57	108.46
2	B	314	SER	N-CA-C	5.44	116.54	108.60
1	A	3744	LEU	CA-C-N	5.44	131.93	121.54
1	A	3744	LEU	C-N-CA	5.44	131.93	121.54
1	A	1952	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	3703	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	4062	TRP	N-CA-C	-5.37	105.46	112.23
1	A	2589	THR	CA-C-N	5.33	125.75	119.83
1	A	2589	THR	C-N-CA	5.33	125.75	119.83
2	B	404	ASP	CA-CB-CG	-5.33	107.27	112.60
1	A	1539	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	2868	ASP	N-CA-C	-5.31	106.65	113.23
1	A	3755	SER	N-CA-C	-5.31	104.96	111.75
1	A	4058	SER	CA-C-O	-5.30	112.42	119.10
1	A	1656	TRP	CA-CB-CG	-5.29	103.55	113.60
1	A	3989	ILE	N-CA-C	-5.27	105.24	110.62
1	A	2419	PRO	N-CA-C	5.27	117.13	110.70
2	B	358	ARG	CA-C-N	5.25	131.15	121.70
2	B	358	ARG	C-N-CA	5.25	131.15	121.70
1	A	4054	GLU	CA-C-N	5.23	125.29	119.32
1	A	4054	GLU	C-N-CA	5.23	125.29	119.32
1	A	3611	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	2280	THR	N-CA-C	5.20	117.36	111.11
1	A	2936	VAL	N-CA-CB	-5.20	108.25	111.83
1	A	2093	ILE	CB-CA-C	-5.19	105.22	112.02
2	B	147	LEU	CB-CA-C	5.17	116.52	108.61
1	A	1752	SER	CB-CA-C	-5.16	110.60	116.54
1	A	2544	ILE	CA-C-N	5.15	126.28	119.84
1	A	2544	ILE	C-N-CA	5.15	126.28	119.84
2	B	352	SER	CA-C-N	5.15	126.28	119.84
2	B	352	SER	C-N-CA	5.15	126.28	119.84
1	A	2184	LEU	CA-C-N	5.13	126.26	119.84
1	A	2184	LEU	C-N-CA	5.13	126.26	119.84
1	A	3980	ILE	N-CA-C	5.13	113.09	107.60
1	A	2158	LEU	N-CA-C	5.12	117.58	109.24
2	B	274	SER	CA-C-N	5.11	127.63	120.28
2	B	274	SER	C-N-CA	5.11	127.63	120.28
2	B	357	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	2886	HIS	CA-CB-CG	-5.08	108.72	113.80
1	A	1526	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	1502	ILE	CA-C-N	5.05	126.15	119.84
1	A	1502	ILE	C-N-CA	5.05	126.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3900	ILE	CA-C-N	5.04	126.13	119.84
1	A	3900	ILE	C-N-CA	5.04	126.13	119.84
1	A	3597	ILE	CB-CA-C	-5.03	105.53	111.97

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2236	ALA	Mainchain,Peptide
1	A	2976	PHE	Mainchain,Peptide
1	A	4058	SER	Mainchain,Peptide
2	B	182	PHE	Peptide
2	B	347	HIS	Sidechain
2	B	372	TYR	Sidechain
2	B	397	ALA	Peptide
2	B	416	HIS	Peptide
2	B	421	ARG	Sidechain

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	19180	19243	19240	342	0
2	B	2862	0	2820	69	0
All	All	22042	19243	22060	411	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 9.

All (411) 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:B:311:ILE:HG21	2:B:343:VAL:HG21	1.56	0.86
1:A:3642:TYR:O	1:A:3642:TYR:CD2	2.28	0.86
1:A:3710:ILE:HG22	1:A:3710:ILE:O	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2638:ARG:O	1:A:2638:ARG:NH1	2.08	0.85
1:A:3028:VAL:HG12	1:A:3028:VAL:O	1.76	0.84
2:B:305:VAL:HG12	2:B:310:ILE:HD11	1.62	0.82
1:A:3526:GLU:OE1	1:A:3526:GLU:N	2.14	0.81
1:A:1689:LYS:O	1:A:1689:LYS:HD3	1.82	0.80
1:A:1720:THR:HG23	1:A:1720:THR:O	1.82	0.78
1:A:1486:ILE:HG22	1:A:1486:ILE:O	1.85	0.76
1:A:1689:LYS:HD3	1:A:1689:LYS:C	2.12	0.74
1:A:3318:GLN:N	1:A:3318:GLN:OE1	2.21	0.73
2:B:262:TRP:CH2	2:B:310:ILE:HD13	2.24	0.72
1:A:3606:GLU:OE1	1:A:3606:GLU:N	2.20	0.71
1:A:2638:ARG:O	1:A:2638:ARG:HD3	1.89	0.71
1:A:1854:ASP:C	1:A:1854:ASP:OD1	2.35	0.69
1:A:1931:GLU:OE1	1:A:1931:GLU:HA	1.92	0.69
1:A:2792:LEU:C	1:A:2792:LEU:HD12	2.18	0.69
2:B:170:VAL:HG21	2:B:184:LEU:CD1	2.22	0.69
1:A:3997:LYS:O	1:A:3997:LYS:HG3	1.92	0.68
1:A:1486:ILE:O	1:A:1486:ILE:CG2	2.41	0.67
1:A:3691:ASP:OD1	1:A:3691:ASP:C	2.36	0.67
2:B:194:LEU:HD21	2:B:242:LYS:HB2	1.78	0.66
1:A:2386:MET:SD	1:A:2386:MET:C	2.78	0.66
1:A:2259:MET:O	1:A:2259:MET:HG3	1.96	0.66
2:B:163:LEU:HA	2:B:170:VAL:HG22	1.78	0.66
2:B:382:ILE:HG23	2:B:423:ILE:HD11	1.78	0.66
1:A:2159:ASP:OD1	1:A:2159:ASP:O	2.14	0.65
2:B:456:LEU:HD21	2:B:482:THR:HG21	1.79	0.65
1:A:2952:LEU:HG	1:A:2952:LEU:O	1.95	0.65
1:A:3028:VAL:O	1:A:3028:VAL:CG1	2.45	0.64
1:A:3313:PHE:CD1	1:A:3313:PHE:C	2.77	0.63
1:A:4038:GLU:OE1	1:A:4038:GLU:N	2.30	0.63
1:A:2665:GLU:OE1	1:A:2665:GLU:N	2.28	0.62
1:A:3437:VAL:HG12	1:A:3437:VAL:O	1.98	0.62
2:B:305:VAL:CG1	2:B:310:ILE:HD11	2.29	0.62
2:B:342:LYS:HB3	2:B:376:ALA:HB3	1.82	0.62
2:B:159:THR:HG21	2:B:202:THR:HA	1.82	0.62
1:A:3749:ASP:C	1:A:3749:ASP:OD1	2.42	0.61
1:A:3354:GLY:O	1:A:3356:PHE:N	2.34	0.61
1:A:1452:TRP:HA	1:A:1452:TRP:CE3	2.35	0.61
1:A:3526:GLU:H	1:A:3526:GLU:CD	2.01	0.61
2:B:179:LEU:HD11	2:B:224:THR:HG21	1.81	0.61
1:A:3679:TYR:OH	1:A:3765:ASN:O	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2051:GLU:H	1:A:2051:GLU:CD	2.09	0.60
2:B:261:ILE:HD11	2:B:270:ILE:HD13	1.83	0.59
1:A:1968:PHE:CD1	1:A:1968:PHE:O	2.55	0.59
1:A:1931:GLU:OE1	1:A:1931:GLU:CA	2.48	0.59
1:A:2298:TYR:N	1:A:2298:TYR:HD1	1.99	0.59
2:B:170:VAL:HG21	2:B:184:LEU:HD11	1.84	0.59
1:A:3710:ILE:O	1:A:3710:ILE:CG2	2.48	0.58
1:A:2638:ARG:O	1:A:2638:ARG:CD	2.51	0.58
1:A:1516:LEU:C	1:A:1516:LEU:HD23	2.28	0.58
2:B:207:LEU:HD21	2:B:222:ILE:HD11	1.86	0.57
1:A:1953:LEU:C	1:A:1953:LEU:HD23	2.29	0.57
1:A:3331:GLU:OE1	1:A:3331:GLU:N	2.38	0.57
1:A:4019:ASP:C	1:A:4019:ASP:OD1	2.45	0.57
1:A:4068:GLU:OE1	1:A:4068:GLU:N	2.30	0.57
2:B:393:MET:HG2	2:B:400:PRO:CG	2.34	0.57
1:A:2298:TYR:N	1:A:2298:TYR:CD1	2.70	0.56
1:A:2694:LEU:C	1:A:2694:LEU:HD23	2.30	0.56
1:A:1452:TRP:O	1:A:1456:TYR:N	2.39	0.56
1:A:3696:MET:HE3	1:A:3696:MET:O	2.06	0.56
2:B:393:MET:HG2	2:B:400:PRO:HG2	1.88	0.56
1:A:3911:TRP:NE1	1:A:3933:SER:OG	2.39	0.55
1:A:1480:THR:HA	1:A:1483:TYR:HB3	1.87	0.55
1:A:3715:TYR:N	1:A:3715:TYR:CD1	2.74	0.55
2:B:184:LEU:HD22	2:B:491:VAL:HG22	1.89	0.55
1:A:1917:ARG:NE	1:A:1917:ARG:HA	2.22	0.55
1:A:2396:ASP:N	1:A:2396:ASP:OD1	2.36	0.55
1:A:1482:GLU:OE1	1:A:1482:GLU:HA	2.06	0.55
1:A:2386:MET:SD	1:A:2386:MET:O	2.65	0.55
1:A:1566:PHE:C	1:A:1566:PHE:CD1	2.84	0.55
1:A:2734:ILE:HG22	1:A:2734:ILE:O	2.06	0.55
1:A:2943:PHE:CD1	1:A:2943:PHE:N	2.74	0.54
1:A:2158:LEU:C	1:A:2158:LEU:HD23	2.31	0.54
1:A:2366:LEU:HG	1:A:2366:LEU:O	2.07	0.54
1:A:1566:PHE:C	1:A:1566:PHE:HD1	2.15	0.54
1:A:2588:TYR:CD1	1:A:2588:TYR:C	2.85	0.54
1:A:3655:ARG:HA	1:A:3659:LYS:HB2	1.90	0.54
1:A:1899:ASN:O	1:A:1900:PRO:C	2.51	0.54
2:B:206:VAL:HG12	2:B:206:VAL:O	2.08	0.54
1:A:2447:LYS:HA	1:A:2492:PRO:HA	1.90	0.54
1:A:2792:LEU:HD12	1:A:2792:LEU:O	2.08	0.53
1:A:2969:LEU:HA	1:A:2972:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3820:GLU:OE1	1:A:3820:GLU:N	2.31	0.53
2:B:310:ILE:HG22	2:B:322:THR:HB	1.89	0.53
1:A:2507:ARG:O	1:A:2511:GLU:N	2.41	0.53
2:B:209:THR:HG21	2:B:215:SER:CB	2.39	0.53
1:A:1449:GLN:CD	1:A:1449:GLN:O	2.52	0.53
1:A:2584:GLU:OE1	1:A:2584:GLU:N	2.32	0.53
1:A:2949:ASN:C	1:A:3354:GLY:HA3	2.34	0.52
1:A:3306:TRP:HA	1:A:3306:TRP:CE3	2.44	0.52
1:A:1689:LYS:C	1:A:1689:LYS:CD	2.81	0.52
1:A:2758:LEU:C	1:A:2758:LEU:HD23	2.35	0.52
1:A:2815:LEU:HD23	1:A:2815:LEU:C	2.35	0.52
1:A:2900:SER:OG	1:A:2902:MET:O	2.28	0.52
1:A:2631:THR:OG1	1:A:2747:ARG:NH2	2.41	0.52
1:A:2390:ILE:C	1:A:2390:ILE:HD12	2.35	0.52
1:A:2813:THR:OG1	1:A:2814:CYS:N	2.43	0.52
2:B:179:LEU:CD1	2:B:224:THR:HG21	2.39	0.52
1:A:1462:ASN:C	1:A:1462:ASN:OD1	2.52	0.52
1:A:1918:GLU:OE1	1:A:1918:GLU:N	2.32	0.52
1:A:2693:SER:OG	1:A:2709:LYS:NZ	2.43	0.51
2:B:209:THR:HG21	2:B:215:SER:HB2	1.92	0.51
2:B:407:PHE:CD1	2:B:409:CYS:HB3	2.45	0.51
1:A:2673:LEU:C	1:A:2673:LEU:HD23	2.35	0.51
1:A:3967:TYR:CD1	1:A:3967:TYR:O	2.63	0.51
2:B:456:LEU:CD2	2:B:482:THR:HG21	2.39	0.51
1:A:1968:PHE:N	1:A:1968:PHE:CD2	2.79	0.51
1:A:2014:PHE:C	1:A:2014:PHE:CD1	2.88	0.51
2:B:456:LEU:HD21	2:B:482:THR:CG2	2.40	0.51
1:A:1807:LYS:HB2	1:A:1807:LYS:NZ	2.24	0.51
1:A:2947:GLU:HB2	1:A:3354:GLY:O	2.10	0.51
1:A:3345:MET:HA	1:A:3348:ILE:HB	1.93	0.51
1:A:2518:THR:N	1:A:2519:PRO:CD	2.74	0.51
1:A:3020:GLY:CA	1:A:3563:GLU:HA	2.41	0.51
1:A:2797:MET:SD	1:A:2797:MET:C	2.94	0.50
2:B:163:LEU:HD12	2:B:170:VAL:CG2	2.41	0.50
1:A:2915:ASN:OD1	1:A:2915:ASN:C	2.54	0.50
1:A:2428:MET:SD	1:A:2428:MET:C	2.95	0.50
1:A:1486:ILE:O	1:A:1490:ALA:HB3	2.12	0.50
1:A:3394:MET:SD	1:A:3516:VAL:HG13	2.52	0.50
1:A:2976:PHE:CG	1:A:2976:PHE:O	2.62	0.49
1:A:4062:TRP:HA	1:A:4062:TRP:CE3	2.47	0.49
1:A:1449:GLN:O	1:A:1449:GLN:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3299:LEU:HD11	1:A:3591:LYS:HB2	1.93	0.49
1:A:4035:GLN:O	1:A:4035:GLN:HG2	2.13	0.49
1:A:2638:ARG:O	1:A:2638:ARG:CG	2.60	0.49
1:A:3751:VAL:HG12	1:A:3751:VAL:O	2.13	0.49
1:A:1509:LEU:O	1:A:1510:LYS:C	2.55	0.49
2:B:342:LYS:HG3	2:B:423:ILE:HG22	1.94	0.49
1:A:2379:SER:OG	1:A:2380:LEU:N	2.46	0.49
1:A:2439:ASP:N	1:A:2481:ASN:O	2.46	0.49
1:A:3302:GLU:H	1:A:3302:GLU:CD	2.21	0.49
1:A:4062:TRP:HA	1:A:4062:TRP:HE3	1.76	0.49
2:B:260:LYS:CE	2:B:263:GLN:HE22	2.24	0.49
1:A:1793:CYS:HB2	1:A:1918:GLU:HA	1.95	0.49
1:A:2262:LEU:HA	1:A:2265:ILE:HB	1.95	0.48
1:A:3369:TYR:N	1:A:3369:TYR:CD1	2.79	0.48
1:A:1607:TRP:CD1	1:A:1607:TRP:C	2.89	0.48
1:A:1687:LEU:C	1:A:1687:LEU:HD23	2.38	0.48
1:A:3876:THR:OG1	1:A:3877:CYS:N	2.37	0.48
1:A:2491:LEU:N	1:A:2492:PRO:CD	2.76	0.48
1:A:2674:TYR:CD2	1:A:2674:TYR:C	2.90	0.48
1:A:3016:PHE:CD1	1:A:3016:PHE:N	2.78	0.48
2:B:382:ILE:CG2	2:B:423:ILE:HD11	2.44	0.48
1:A:1459:LEU:O	1:A:1463:LEU:N	2.44	0.48
1:A:2782:VAL:HB	1:A:2815:LEU:HA	1.96	0.48
2:B:260:LYS:HE2	2:B:263:GLN:HE22	1.77	0.48
2:B:342:LYS:CG	2:B:423:ILE:HG22	2.43	0.48
1:A:2483:VAL:O	1:A:2483:VAL:HG12	2.12	0.48
1:A:2916:TRP:O	1:A:2916:TRP:CE3	2.67	0.48
1:A:3642:TYR:O	1:A:3642:TYR:CG	2.61	0.48
2:B:165:PRO:HG3	2:B:207:LEU:O	2.13	0.48
1:A:2440:VAL:HA	1:A:2483:VAL:O	2.14	0.48
1:A:3772:TRP:O	1:A:3773:ASN:C	2.57	0.48
1:A:2952:LEU:HB2	1:A:3355:LYS:HB2	1.96	0.48
1:A:3795:ASP:C	1:A:3795:ASP:OD1	2.54	0.48
1:A:1449:GLN:OE1	1:A:1449:GLN:C	2.57	0.48
1:A:2432:LEU:C	1:A:2432:LEU:HD23	2.39	0.48
1:A:3344:ASP:C	1:A:3344:ASP:OD1	2.56	0.48
1:A:3635:PHE:HB2	1:A:3642:TYR:CE1	2.49	0.48
1:A:1522:SER:O	1:A:1526:PHE:N	2.46	0.47
1:A:1720:THR:O	1:A:1722:GLU:N	2.46	0.47
1:A:3427:VAL:HB	1:A:3446:PHE:HB2	1.96	0.47
1:A:3757:ILE:HG12	1:A:3757:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4022:GLN:HA	1:A:4030:PRO:HA	1.96	0.47
1:A:1918:GLU:HB3	1:A:3997:LYS:HB2	1.96	0.47
1:A:2354:SER:OG	1:A:2355:ASP:N	2.46	0.47
1:A:2147:ASN:CG	1:A:2147:ASN:O	2.56	0.47
1:A:3487:ASP:C	1:A:3487:ASP:OD1	2.56	0.47
1:A:1899:ASN:OD1	1:A:1899:ASN:C	2.57	0.47
1:A:2984:VAL:O	1:A:2984:VAL:HG22	2.14	0.47
1:A:3642:TYR:O	1:A:3642:TYR:HD2	1.91	0.47
1:A:1646:GLN:HB2	1:A:1764:GLY:O	2.14	0.47
1:A:1829:GLN:OE1	1:A:1829:GLN:HA	2.13	0.47
1:A:3967:TYR:CD1	1:A:3967:TYR:C	2.88	0.47
1:A:1539:PHE:CD1	1:A:1539:PHE:N	2.82	0.47
1:A:2141:ILE:O	1:A:2145:PHE:N	2.48	0.47
1:A:1767:GLU:HB2	1:A:1811:GLN:OE1	2.14	0.47
1:A:2098:ALA:O	1:A:2148:SER:OG	2.33	0.47
1:A:2516:TRP:CD1	1:A:2516:TRP:C	2.92	0.47
1:A:2847:GLU:OE1	1:A:2847:GLU:N	2.36	0.47
2:B:422:ASP:HB3	2:B:464:LEU:HD23	1.97	0.47
2:B:457:HIS:CE1	2:B:482:THR:HG22	2.49	0.47
1:A:1910:GLU:C	1:A:1910:GLU:CD	2.82	0.47
1:A:2423:GLY:O	1:A:2424:LYS:C	2.58	0.47
1:A:3303:LYS:HD2	1:A:3303:LYS:C	2.40	0.47
1:A:4051:ASN:OD1	1:A:4051:ASN:C	2.57	0.47
2:B:305:VAL:HG12	2:B:310:ILE:CD1	2.41	0.47
1:A:2895:THR:OG1	1:A:2896:ASN:N	2.47	0.47
1:A:3024:LEU:HD21	1:A:3303:LYS:HA	1.96	0.47
2:B:467:ASP:OD1	2:B:477:ARG:HD2	2.14	0.47
1:A:1468:PHE:O	1:A:1469:LEU:C	2.57	0.46
1:A:3355:LYS:O	1:A:3356:PHE:C	2.58	0.46
1:A:1540:LEU:O	1:A:1833:ARG:NH1	2.48	0.46
1:A:1807:LYS:NZ	1:A:1807:LYS:CB	2.78	0.46
1:A:2401:GLU:HA	1:A:2404:PHE:HB3	1.97	0.46
1:A:3348:ILE:O	1:A:3352:LEU:N	2.48	0.46
2:B:206:VAL:CG2	2:B:261:ILE:HD13	2.46	0.46
2:B:311:ILE:CG2	2:B:343:VAL:HG21	2.37	0.46
1:A:1483:TYR:HA	1:A:1486:ILE:HB	1.98	0.46
1:A:2772:PHE:CD2	1:A:2772:PHE:C	2.92	0.46
1:A:1459:LEU:O	1:A:1460:GLY:C	2.59	0.46
1:A:2084:TRP:HA	1:A:2084:TRP:CE3	2.50	0.46
1:A:4086:GLU:C	1:A:4086:GLU:CD	2.83	0.46
1:A:2945:VAL:O	1:A:3357:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3020:GLY:HA3	1:A:3563:GLU:HA	1.97	0.46
1:A:3450:VAL:O	1:A:3492:PHE:HA	2.16	0.46
1:A:3722:MET:SD	1:A:4079:LYS:HG2	2.56	0.46
1:A:2572:GLU:O	1:A:2576:LYS:N	2.49	0.46
1:A:2495:ASP:OD1	1:A:2495:ASP:C	2.59	0.46
2:B:162:LYS:CG	2:B:207:LEU:HD12	2.45	0.46
1:A:1581:GLY:HA2	1:A:1592:LEU:HG	1.99	0.46
1:A:2137:VAL:HA	1:A:2141:ILE:HB	1.97	0.46
1:A:2259:MET:O	1:A:2259:MET:CG	2.64	0.46
1:A:2419:PRO:HA	1:A:2420:PRO:HD3	1.84	0.46
2:B:155:GLU:OE1	2:B:176:HIS:CE1	2.68	0.46
2:B:332:VAL:HB	2:B:392:LEU:HD22	1.97	0.46
1:A:1721:LYS:O	1:A:1725:ARG:N	2.49	0.45
1:A:3839:ILE:HG23	1:A:3839:ILE:O	2.17	0.45
1:A:1726:LEU:O	1:A:1730:LYS:HG2	2.16	0.45
1:A:2844:PHE:CD1	1:A:2844:PHE:C	2.94	0.45
1:A:2950:LYS:HB2	1:A:3352:LEU:HA	1.97	0.45
1:A:2377:SER:OG	1:A:2378:VAL:N	2.48	0.45
2:B:142:TRP:HB2	2:B:426:ARG:HH11	1.80	0.45
2:B:163:LEU:HD12	2:B:170:VAL:HG22	1.98	0.45
1:A:1455:LEU:HA	1:A:1458:ILE:HB	1.98	0.45
1:A:2298:TYR:HD1	1:A:2298:TYR:H	1.63	0.45
1:A:3345:MET:O	1:A:3346:LEU:C	2.60	0.45
1:A:3500:ASP:OD1	1:A:3500:ASP:C	2.59	0.45
1:A:3792:ARG:O	1:A:3792:ARG:HG3	2.16	0.45
1:A:1656:TRP:CE3	1:A:1656:TRP:HA	2.51	0.45
1:A:2951:GLU:HB3	1:A:3352:LEU:O	2.17	0.45
1:A:3301:PHE:CD2	1:A:3301:PHE:C	2.94	0.45
2:B:167:LEU:HD13	2:B:240:GLU:HG2	1.99	0.45
1:A:1770:ILE:HG21	1:A:1929:ILE:HA	1.99	0.45
1:A:2097:HIS:HB3	1:A:2148:SER:HA	1.99	0.45
1:A:1475:LYS:HB3	1:A:1519:ILE:HD11	1.98	0.45
1:A:2458:LEU:O	1:A:2462:THR:N	2.49	0.45
1:A:2447:LYS:N	1:A:2829:GLU:OE1	2.50	0.45
1:A:2893:ASP:N	1:A:2894:PRO:CD	2.80	0.45
1:A:2670:GLU:C	1:A:2670:GLU:CD	2.84	0.44
1:A:3784:ASN:OD1	1:A:3784:ASN:C	2.59	0.44
2:B:309:TYR:HB3	2:B:321:LEU:HD11	1.99	0.44
1:A:2105:ASP:C	1:A:2105:ASP:OD1	2.60	0.44
1:A:2135:ARG:CZ	1:A:2135:ARG:HB3	2.47	0.44
1:A:3302:GLU:OE1	1:A:3302:GLU:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3428:LEU:C	1:A:3428:LEU:HD23	2.42	0.44
1:A:2439:ASP:OD1	1:A:2439:ASP:C	2.59	0.44
1:A:2759:ILE:O	1:A:2917:MET:N	2.51	0.44
1:A:3412:SER:HB3	1:A:3415:ILE:HD12	1.99	0.44
2:B:206:VAL:HG22	2:B:261:ILE:HD13	1.98	0.44
1:A:2159:ASP:OD1	1:A:2159:ASP:C	2.60	0.44
1:A:3731:ASP:HA	1:A:3753:THR:HA	1.99	0.44
1:A:2365:LYS:O	1:A:2366:LEU:HB3	2.18	0.44
2:B:389:LEU:HB2	2:B:408:ARG:HG2	2.00	0.44
1:A:3685:GLN:OE1	1:A:3685:GLN:HA	2.17	0.44
1:A:1794:PHE:HA	1:A:1919:PHE:HB2	2.00	0.44
1:A:2947:GLU:HB2	1:A:3356:PHE:HB2	2.00	0.44
1:A:2950:LYS:O	1:A:3355:LYS:N	2.50	0.44
1:A:3930:PHE:CE2	1:A:4038:GLU:HA	2.53	0.44
1:A:3967:TYR:O	1:A:3967:TYR:HD1	1.99	0.44
1:A:3631:MET:SD	1:A:4091:GLU:HB2	2.57	0.44
1:A:2723:PHE:HB2	1:A:2772:PHE:CE1	2.53	0.43
1:A:2961:ILE:HD13	1:A:2961:ILE:HA	1.72	0.43
1:A:3731:ASP:HB2	1:A:3755:SER:HB2	2.00	0.43
1:A:3846:MET:HE2	1:A:3846:MET:HA	2.00	0.43
1:A:1548:ILE:O	1:A:1552:GLY:N	2.51	0.43
1:A:1726:LEU:O	1:A:1727:LEU:C	2.60	0.43
1:A:2756:MET:CG	1:A:2757:MET:N	2.81	0.43
1:A:3997:LYS:O	1:A:3997:LYS:CG	2.58	0.43
1:A:2952:LEU:O	1:A:2952:LEU:CG	2.66	0.43
2:B:393:MET:CG	2:B:400:PRO:HG2	2.48	0.43
1:A:1850:PHE:CD2	1:A:1850:PHE:C	2.92	0.43
1:A:3302:GLU:CD	1:A:3302:GLU:N	2.76	0.43
1:A:3448:SER:O	1:A:3492:PHE:HB3	2.19	0.43
1:A:3534:LEU:C	1:A:3534:LEU:HD23	2.44	0.43
1:A:3720:LEU:HG	1:A:3725:VAL:HB	2.01	0.43
1:A:3722:MET:SD	1:A:4079:LYS:HA	2.58	0.43
1:A:2306:ASP:C	1:A:2306:ASP:OD1	2.60	0.43
1:A:2529:ILE:N	1:A:2529:ILE:HD12	2.33	0.43
1:A:3409:ASP:HB3	1:A:3412:SER:HA	1.99	0.43
1:A:3683:TYR:OH	1:A:3766:GLU:O	2.31	0.43
1:A:1627:LEU:C	1:A:1627:LEU:HD12	2.44	0.43
1:A:1827:ASP:C	1:A:1827:ASP:OD1	2.60	0.43
1:A:2478:ASP:C	1:A:2478:ASP:OD1	2.60	0.43
1:A:2588:TYR:O	1:A:2589:THR:C	2.61	0.43
1:A:1494:ASP:OD1	1:A:1494:ASP:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2189:ASN:C	1:A:2189:ASN:OD1	2.61	0.43
1:A:2844:PHE:CD1	1:A:2844:PHE:O	2.71	0.43
1:A:3635:PHE:CD1	1:A:3635:PHE:N	2.86	0.43
1:A:3851:VAL:HA	1:A:3854:TYR:HB3	2.00	0.43
2:B:222:ILE:CG1	2:B:242:LYS:HE3	2.48	0.43
1:A:1575:PHE:O	1:A:1576:GLU:C	2.62	0.43
1:A:2196:THR:OG1	1:A:2197:ASP:N	2.51	0.43
1:A:1726:LEU:HA	1:A:1729:ALA:HB3	2.01	0.43
1:A:3000:VAL:O	1:A:3003:VAL:HG12	2.19	0.43
1:A:3696:MET:SD	1:A:3760:LEU:HB3	2.59	0.43
1:A:1817:VAL:HG21	1:A:1846:CYS:SG	2.58	0.42
1:A:1878:HIS:HB3	1:A:1885:GLU:HB3	2.01	0.42
1:A:1940:GLU:OE1	1:A:1940:GLU:N	2.30	0.42
1:A:2060:PHE:CD2	1:A:2060:PHE:C	2.97	0.42
1:A:2948:VAL:C	1:A:3354:GLY:HA2	2.44	0.42
1:A:2976:PHE:CE2	1:A:3333:TYR:HB2	2.54	0.42
1:A:4027:VAL:O	1:A:4028:ARG:HB2	2.19	0.42
2:B:206:VAL:HG21	2:B:221:VAL:HG12	2.00	0.42
1:A:1668:GLU:OE1	1:A:1668:GLU:HA	2.20	0.42
1:A:2977:TYR:CD2	1:A:3337:LEU:HD22	2.54	0.42
1:A:3470:PHE:CD2	1:A:3470:PHE:C	2.96	0.42
1:A:1742:ASP:OD1	1:A:1742:ASP:C	2.62	0.42
1:A:2924:THR:O	1:A:2927:GLN:HB3	2.19	0.42
1:A:3467:SER:OG	1:A:3468:ARG:N	2.51	0.42
1:A:3344:ASP:OD1	1:A:3345:MET:N	2.52	0.42
2:B:376:ALA:HB1	2:B:420:VAL:HB	2.02	0.42
1:A:1765:ILE:O	1:A:1765:ILE:HG13	2.19	0.42
1:A:2145:PHE:HB3	1:A:2148:SER:HB2	2.01	0.42
1:A:2876:TRP:N	1:A:2876:TRP:CD1	2.88	0.42
1:A:4060:SER:O	1:A:4064:GLN:N	2.52	0.42
1:A:1530:GLN:HA	1:A:1530:GLN:NE2	2.35	0.42
1:A:1835:LEU:HA	1:A:1838:ILE:HB	2.02	0.42
1:A:2204:PRO:HA	1:A:2207:ILE:HB	2.02	0.42
2:B:167:LEU:HD12	2:B:236:TRP:CZ2	2.55	0.42
1:A:1487:THR:O	1:A:1491:PHE:N	2.53	0.42
1:A:1751:GLN:C	1:A:1751:GLN:CD	2.88	0.42
1:A:2072:LEU:C	1:A:2072:LEU:HD23	2.45	0.42
1:A:3352:LEU:O	1:A:3353:LEU:C	2.62	0.42
1:A:3451:ILE:O	1:A:3453:GLN:N	2.53	0.42
1:A:3893:ASP:C	1:A:3893:ASP:OD1	2.60	0.42
2:B:145:ARG:HG3	2:B:146:ASN:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1720:THR:O	1:A:1720:THR:CG2	2.53	0.42
1:A:1779:PHE:N	1:A:1779:PHE:CD1	2.85	0.42
1:A:1942:SER:OG	1:A:1943:LYS:N	2.53	0.42
1:A:2155:ASP:OD1	1:A:2155:ASP:C	2.63	0.42
1:A:2176:LEU:O	1:A:2183:ARG:HA	2.20	0.42
1:A:2790:SER:OG	1:A:2791:ASN:N	2.51	0.42
1:A:3332:THR:HG22	1:A:3333:TYR:CD1	2.54	0.42
1:A:3765:ASN:O	1:A:3766:GLU:C	2.62	0.42
2:B:171:PHE:CE2	2:B:242:LYS:NZ	2.85	0.42
1:A:1449:GLN:HA	1:A:1452:TRP:HB2	2.02	0.41
1:A:2383:HIS:CD2	1:A:2383:HIS:C	2.96	0.41
1:A:4085:THR:O	1:A:4086:GLU:C	2.63	0.41
1:A:2000:ARG:NE	1:A:2000:ARG:HA	2.35	0.41
1:A:2146:LYS:HA	1:A:2146:LYS:HD3	1.89	0.41
1:A:2576:LYS:HA	1:A:2579:PHE:CE2	2.54	0.41
1:A:3339:GLU:H	1:A:3339:GLU:CD	2.29	0.41
1:A:3854:TYR:HA	1:A:3857:LYS:HB3	2.02	0.41
2:B:176:HIS:CG	2:B:178:LYS:HG3	2.56	0.41
2:B:275:ARG:HG2	2:B:299:TRP:CD2	2.55	0.41
1:A:1867:GLN:OE1	1:A:1867:GLN:HA	2.20	0.41
1:A:1899:ASN:HB2	1:A:1900:PRO:CD	2.50	0.41
1:A:2084:TRP:HA	1:A:2084:TRP:HE3	1.85	0.41
1:A:2236:ALA:HB1	1:A:2237:LEU:HB2	2.02	0.41
1:A:2568:SER:O	1:A:2572:GLU:HB3	2.20	0.41
1:A:2721:LYS:HA	1:A:2721:LYS:HD2	1.84	0.41
1:A:3658:ILE:O	1:A:3664:THR:OG1	2.38	0.41
2:B:295:PRO:HG2	2:B:296:HIS:ND1	2.35	0.41
1:A:1807:LYS:HB2	1:A:1807:LYS:HZ2	1.83	0.41
1:A:3415:ILE:HG12	1:A:3454:ASP:HB3	2.03	0.41
2:B:221:VAL:O	2:B:222:ILE:HD13	2.20	0.41
2:B:456:LEU:HD23	2:B:456:LEU:C	2.45	0.41
1:A:1469:LEU:O	1:A:1472:GLU:N	2.53	0.41
1:A:2491:LEU:N	1:A:2492:PRO:HD2	2.35	0.41
1:A:2725:ASP:O	1:A:2725:ASP:CG	2.60	0.41
1:A:3661:SER:OG	1:A:3662:ARG:N	2.52	0.41
1:A:3815:PRO:HA	1:A:3842:GLN:HB2	2.01	0.41
2:B:262:TRP:CH2	2:B:310:ILE:CD1	2.98	0.41
1:A:3747:LEU:HD23	1:A:3747:LEU:HA	1.83	0.41
1:A:3759:ALA:HA	1:A:3762:TRP:CD2	2.56	0.41
1:A:1645:PHE:O	1:A:1645:PHE:CG	2.70	0.41
1:A:2589:THR:OG1	1:A:2590:GLU:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2956:GLU:O	1:A:2957:PRO:C	2.62	0.41
2:B:170:VAL:HG21	2:B:184:LEU:HD12	2.00	0.41
1:A:1630:LEU:HD21	1:A:1636:ILE:HA	2.03	0.41
1:A:2613:SER:OG	1:A:2614:HIS:N	2.54	0.41
1:A:2936:VAL:HB	1:A:2937:PRO:HD2	2.03	0.41
1:A:3310:THR:HA	1:A:3313:PHE:CE2	2.55	0.41
1:A:3427:VAL:HG13	1:A:3450:VAL:HB	2.03	0.41
2:B:164:HIS:HA	2:B:165:PRO:HD3	1.95	0.41
2:B:206:VAL:HG22	2:B:261:ILE:CD1	2.50	0.41
2:B:407:PHE:CE1	2:B:409:CYS:HB3	2.56	0.41
1:A:2510:MET:SD	1:A:2511:GLU:N	2.94	0.41
1:A:2579:PHE:CD1	1:A:2579:PHE:C	2.98	0.41
1:A:3920:ILE:O	1:A:3920:ILE:HG23	2.21	0.41
1:A:4057:ASP:C	1:A:4059:LEU:HA	2.46	0.41
2:B:184:LEU:HD22	2:B:491:VAL:CG2	2.50	0.41
2:B:439:VAL:CG2	2:B:456:LEU:HD13	2.51	0.41
1:A:1473:THR:HA	1:A:1476:PHE:CD1	2.56	0.40
1:A:2438:TYR:CD2	1:A:2481:ASN:HB2	2.55	0.40
1:A:2536:ASN:HB2	1:A:2537:PRO:HD2	2.03	0.40
1:A:3401:GLN:HG3	1:A:3403:ALA:O	2.21	0.40
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	2.04	0.40
1:A:2100:VAL:O	1:A:2100:VAL:HG12	2.20	0.40
1:A:2638:ARG:HD3	1:A:2638:ARG:N	2.37	0.40
1:A:2805:ASP:HA	1:A:2809:LYS:HB3	2.04	0.40
1:A:3774:ILE:HD12	1:A:3774:ILE:HA	1.95	0.40
1:A:4091:GLU:O	1:A:4092:MET:HB2	2.20	0.40
2:B:295:PRO:HG2	2:B:296:HIS:H	1.86	0.40
1:A:2582:VAL:HG23	1:A:2582:VAL:O	2.22	0.40
1:A:3366:PHE:CD2	1:A:3369:TYR:HB2	2.57	0.40
1:A:3882:ASP:C	1:A:3882:ASP:OD1	2.63	0.40
1:A:1482:GLU:HG3	1:A:1511:LEU:HB2	2.04	0.40
1:A:2079:GLY:O	1:A:2080:LYS:C	2.64	0.40
1:A:2950:LYS:HB2	1:A:3351:ARG:O	2.22	0.40
1:A:3523:GLU:OE1	1:A:3523:GLU:N	2.45	0.40
1:A:1468:PHE:O	1:A:1473:THR:OG1	2.35	0.40
1:A:1779:PHE:N	1:A:1779:PHE:HD1	2.20	0.40
1:A:2366:LEU:O	1:A:2366:LEU:CG	2.70	0.40
1:A:3989:ILE:O	1:A:3993:VAL:HB	2.21	0.40
2:B:343:VAL:HG22	2:B:344:LYS:N	2.37	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	2374/2376 (100%)	2097 (88%)	209 (9%)	68 (3%)	3	23
2	B	352/354 (99%)	300 (85%)	31 (9%)	21 (6%)	1	13
All	All	2726/2730 (100%)	2397 (88%)	240 (9%)	89 (3%)	5	21

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1721	LYS
1	A	1722	GLU
1	A	1920	SER
1	A	1942	SER
1	A	2376	PRO
1	A	2589	THR
1	A	2613	SER
1	A	2986	PRO
1	A	3354	GLY
1	A	3355	LYS
1	A	3387	ASN
1	A	3430	SER
1	A	3445	ARG
1	A	3727	SER
1	A	4028	ARG
1	A	4030	PRO
2	B	196	SER
2	B	206	VAL
2	B	295	PRO
2	B	349	ILE
2	B	397	ALA
2	B	398	PRO
2	B	401	ASN
2	B	474	VAL
1	A	1510	LYS

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Mol	Chain	Res	Type
1	A	1576	GLU
1	A	1690	SER
1	A	1720	THR
1	A	2106	THR
1	A	2172	ASP
1	A	2377	SER
1	A	2637	PRO
1	A	3773	ASN
1	A	3871	PHE
1	A	3922	GLY
1	A	4089	LEU
2	B	144	PRO
2	B	146	ASN
2	B	255	ILE
2	B	307	GLY
2	B	409	CYS
1	A	1603	GLN
1	A	1926	SER
1	A	2419	PRO
1	A	2731	PRO
1	A	2788	ARG
1	A	2904	SER
1	A	2979	LYS
1	A	3339	GLU
1	A	3592	LYS
1	A	3717	GLU
1	A	3745	ARG
2	B	200	ALA
2	B	277	GLN
2	B	400	PRO
2	B	423	ILE
1	A	1900	PRO
1	A	2379	SER
1	A	2869	THR
1	A	2951	GLU
1	A	2957	PRO
1	A	3332	THR
1	A	3400	SER
1	A	3734	PRO
2	B	157	SER
1	A	2011	GLU
1	A	2356	TYR

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Mol	Chain	Res	Type
1	A	2519	PRO
1	A	3022	GLU
1	A	3460	PRO
1	A	3901	PRO
1	A	4045	LEU
2	B	190	PRO
2	B	276	ASP
1	A	3507	ILE
1	A	3680	GLN
1	A	3710	ILE
1	A	3732	GLY
1	A	2734	ILE
1	A	2893	ASP
2	B	390	PRO
1	A	1890	PRO
1	A	3490	GLY
1	A	2388	PRO
1	A	2698	GLY
1	A	3996	GLY
1	A	2492	PRO
1	A	3028	VAL
1	A	2518	THR

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	2162/2162 (100%)	2159 (100%)	3 (0%)	88	89
2	B	327/327 (100%)	305 (93%)	22 (7%)	15	36
All	All	2489/2489 (100%)	2464 (99%)	25 (1%)	65	78

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1512	THR

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Mol	Chain	Res	Type
1	A	1566	PHE
1	A	1807	LYS
2	B	142	TRP
2	B	179	LEU
2	B	228	ASP
2	B	247	ARG
2	B	257	SER
2	B	261	ILE
2	B	270	ILE
2	B	275	ARG
2	B	276	ASP
2	B	301	ARG
2	B	305	VAL
2	B	310	ILE
2	B	318	THR
2	B	398	PRO
2	B	403	THR
2	B	416	HIS
2	B	421	ARG
2	B	436	ASP
2	B	437	LYS
2	B	440	ARG
2	B	481	VAL
2	B	482	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1504	ASN
1	A	1709	ASN
1	A	1717	ASN
1	A	2097	HIS
1	A	4087	GLN
2	B	176	HIS
2	B	232	HIS
2	B	254	HIS
2	B	263	GLN
2	B	266	ASN
2	B	457	HIS
2	B	490	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

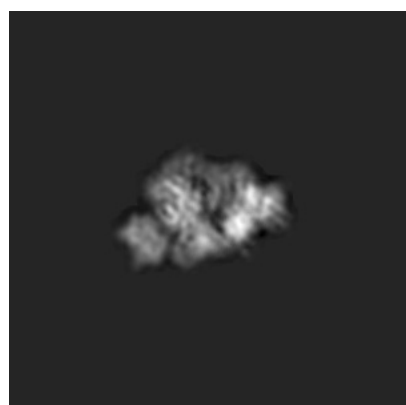
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8673. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

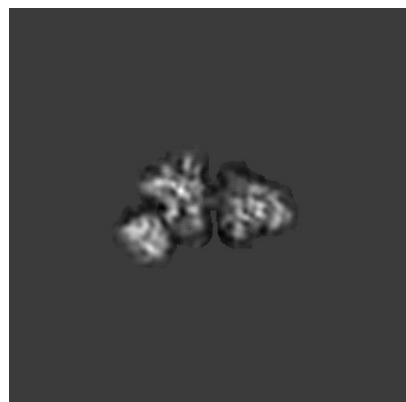


Z

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

6.2 Central slices [i](#)

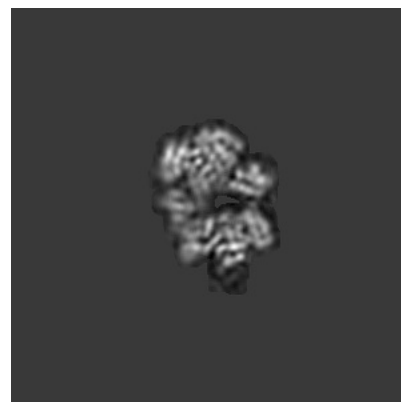
6.2.1 Primary map



X Index: 162



Y Index: 162



Z Index: 162

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

6.3 Largest variance slices [i](#)

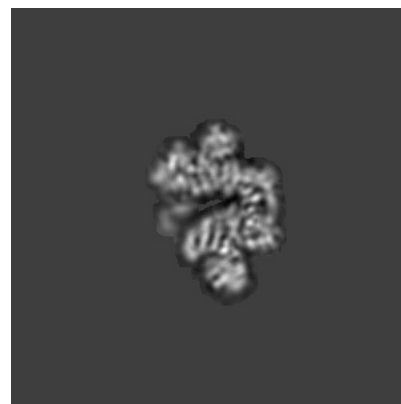
6.3.1 Primary map



X Index: 177



Y Index: 186

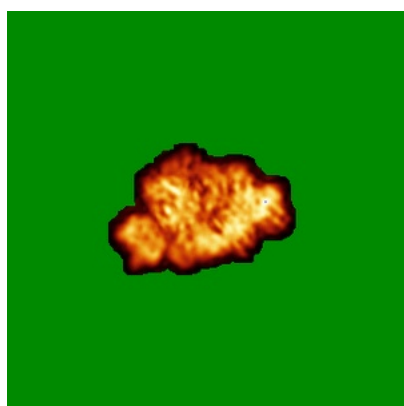


Z Index: 153

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

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

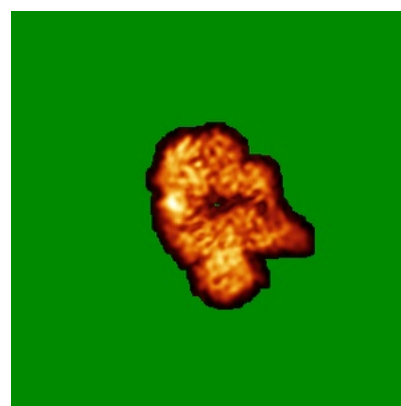
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0119. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

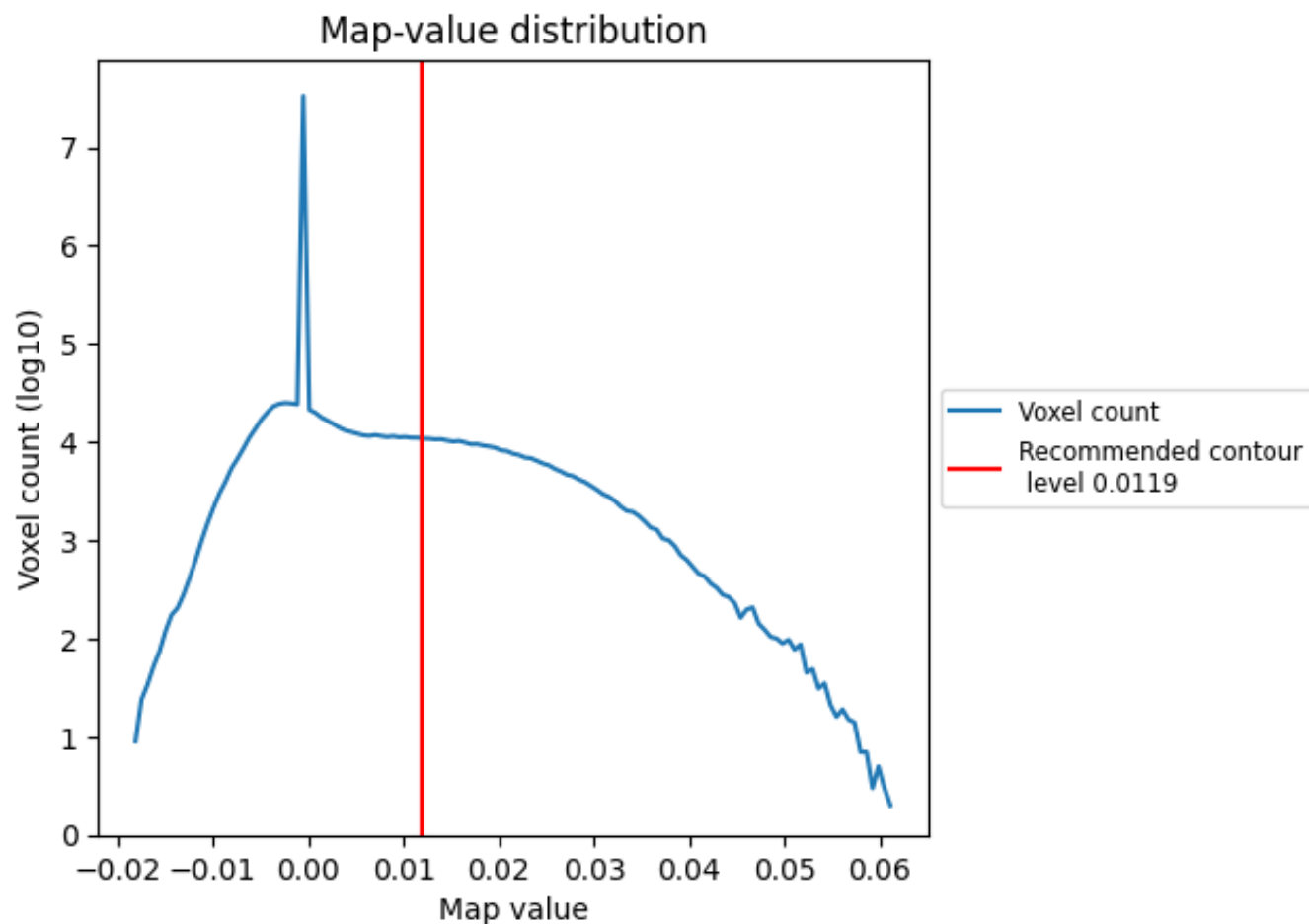
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

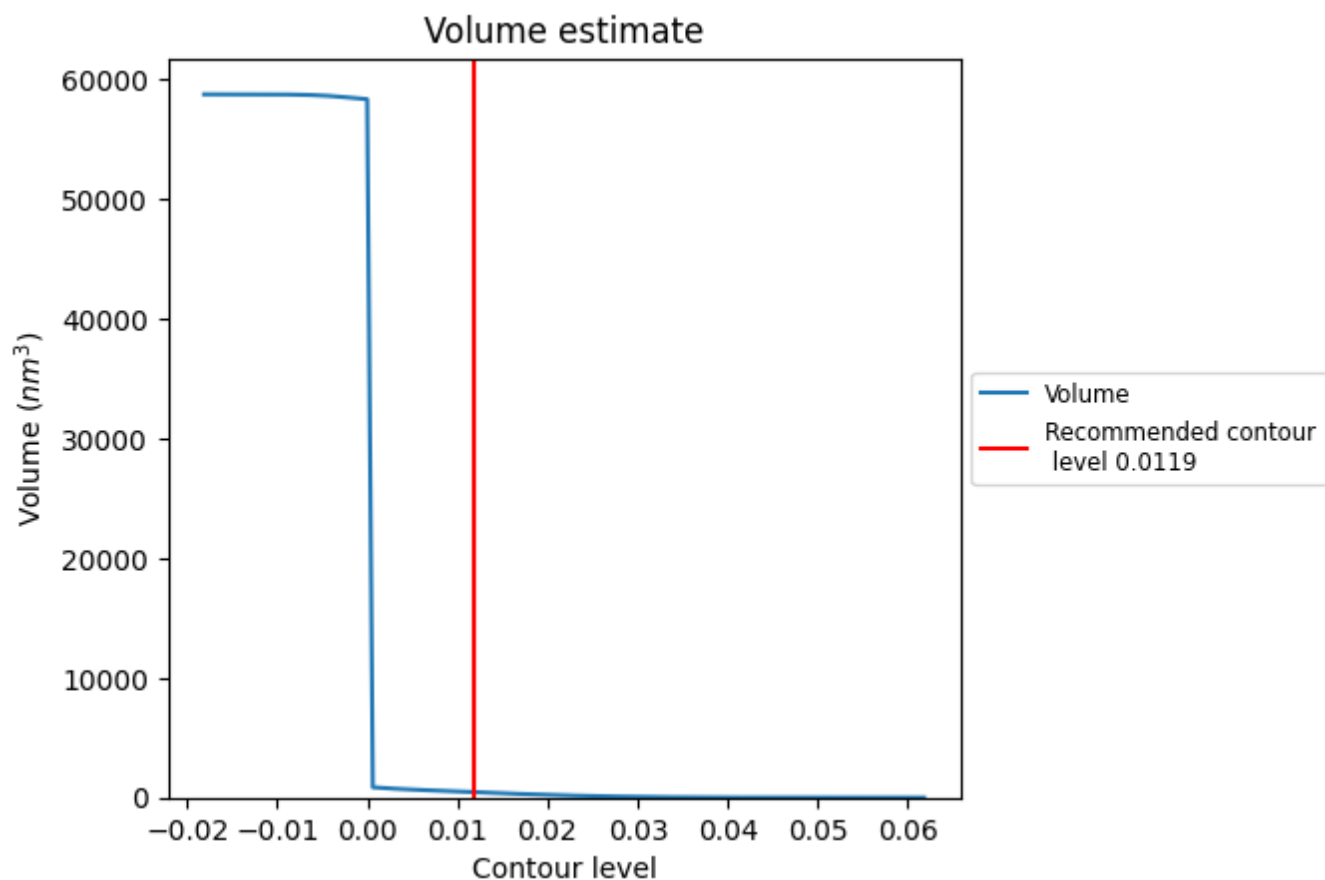
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

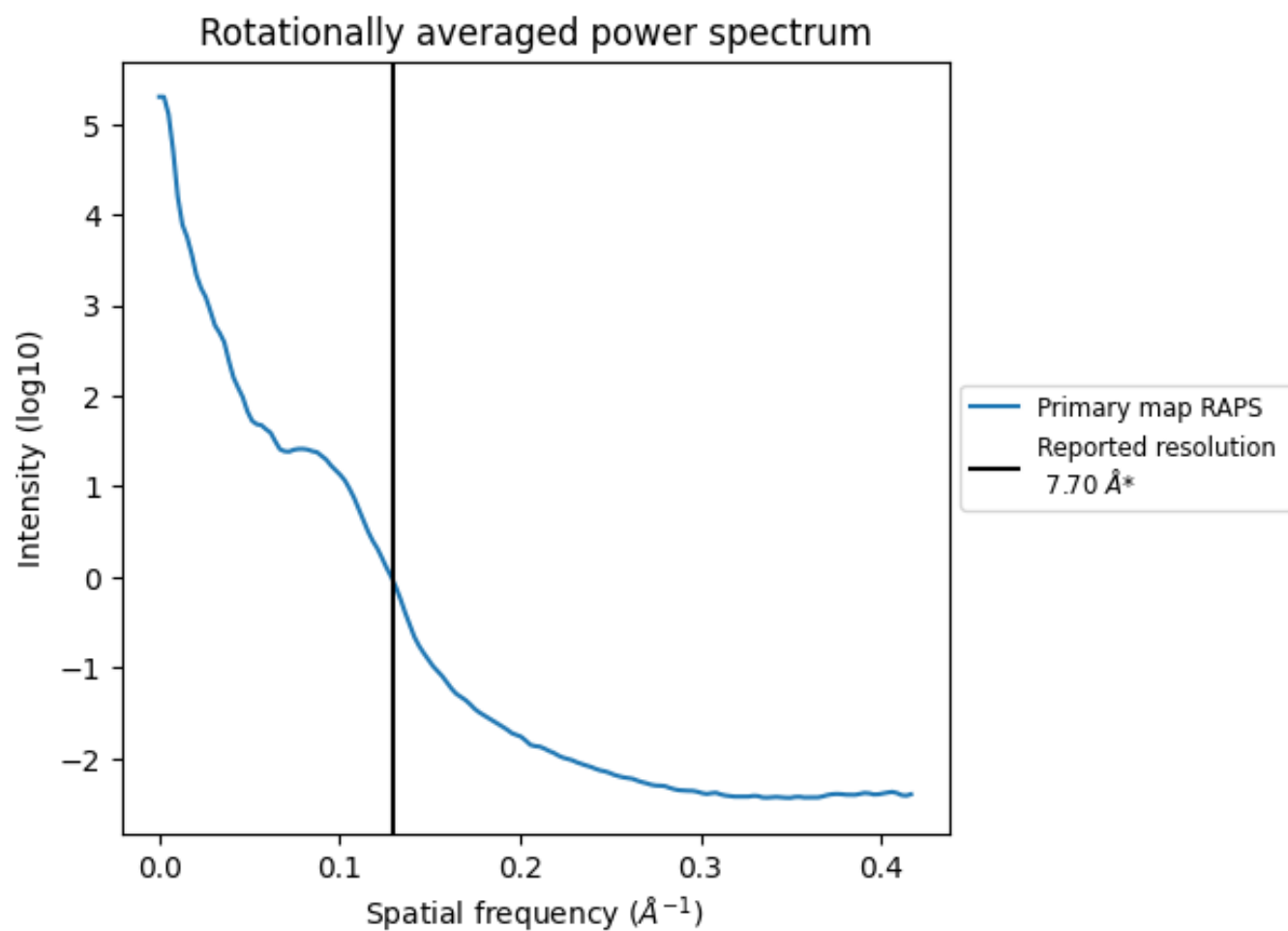
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 448 nm^3 ; this corresponds to an approximate mass of 405 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 0.130 Å⁻¹

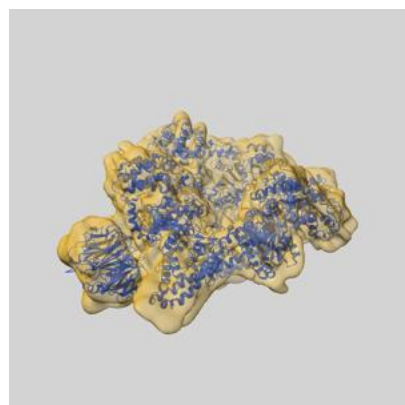
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

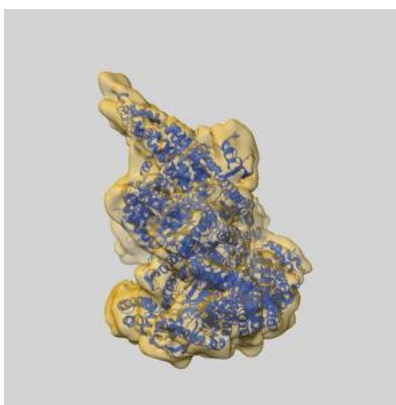
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8673 and PDB model 5VH9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

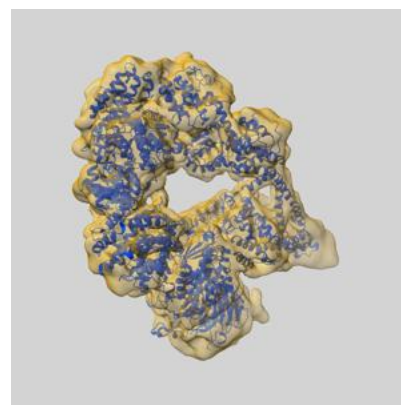
9.1 Map-model overlay [i](#)



X



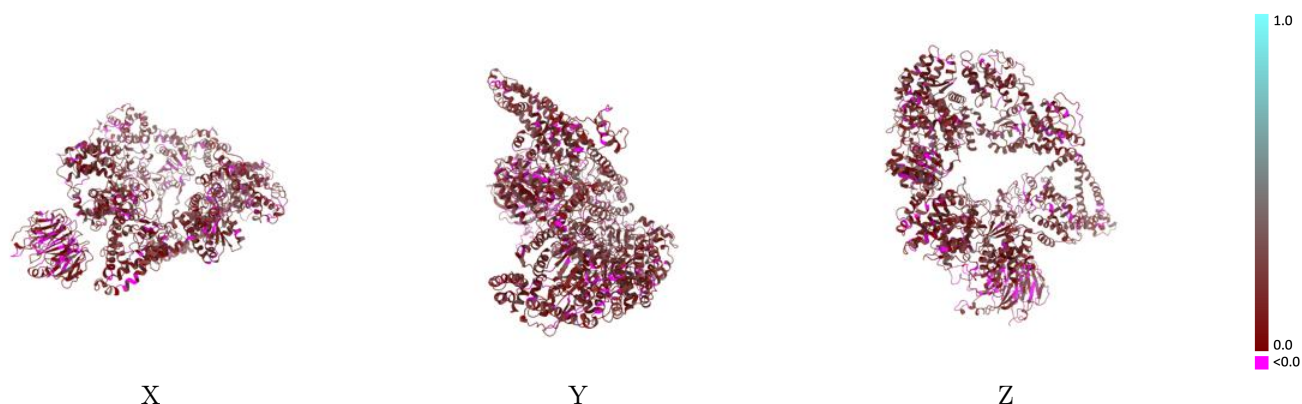
Y



Z

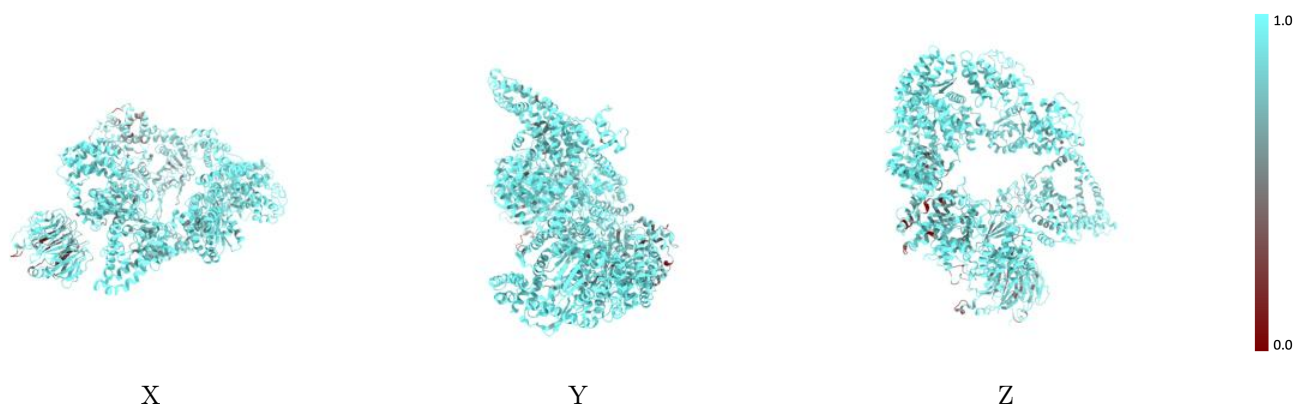
The images above show the 3D surface view of the map at the recommended contour level 0.0119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



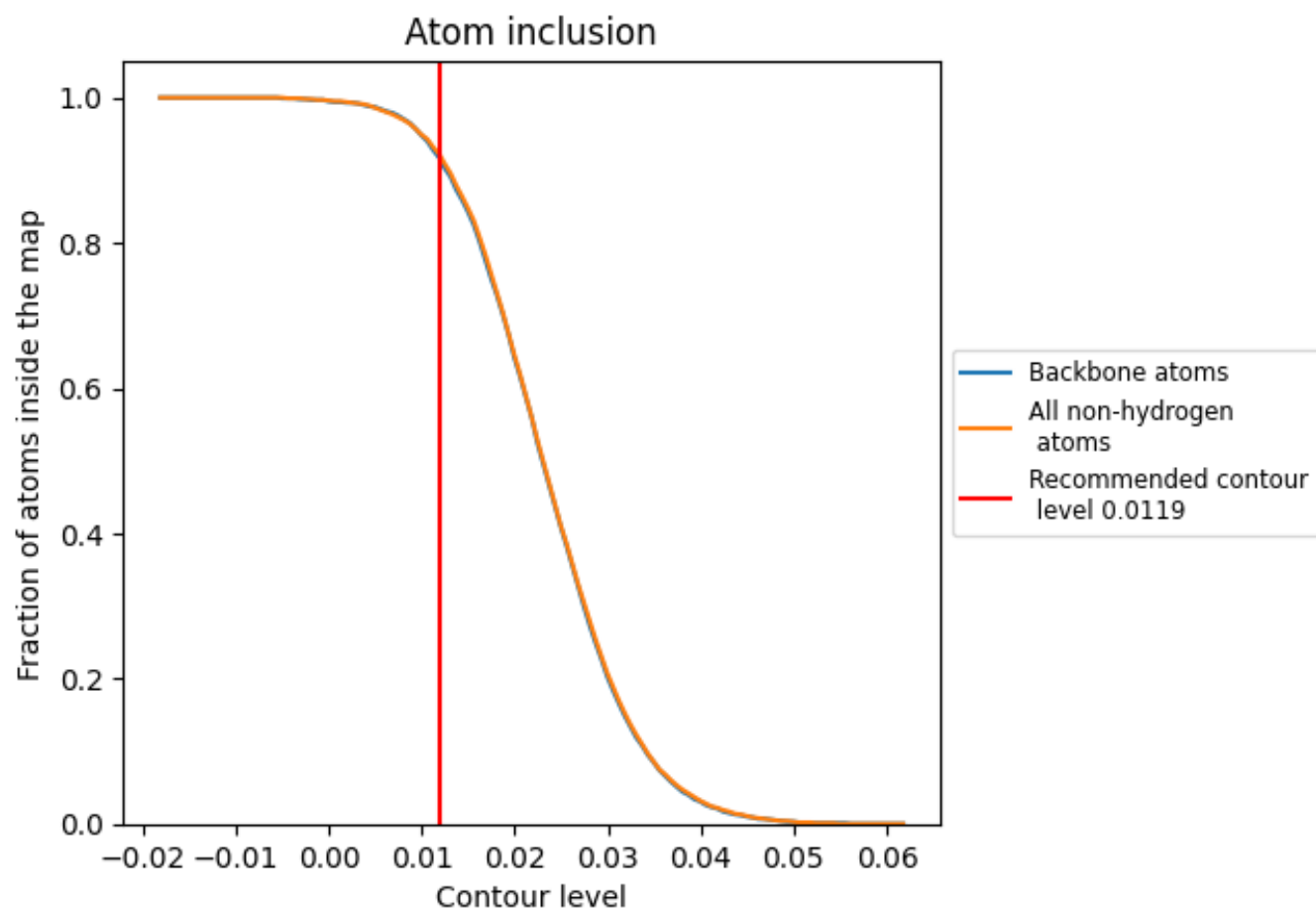
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0119).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9220	0.1600
A	0.9370	0.1710
B	0.8330	0.0870

