



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:17 AM UTC

PDB ID : 6JXA / pdb_00006jxa
EMDB ID : EMD-9892
Title : Tel1 kinase compact monomer
Authors : Xin, J.
Deposited on : 2019-04-23
Resolution : 4.30 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

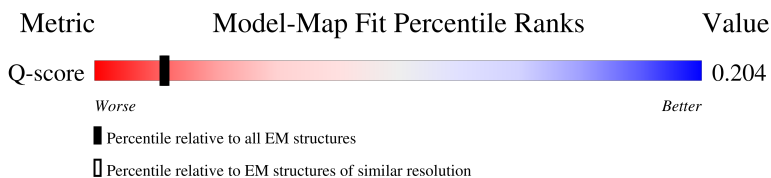
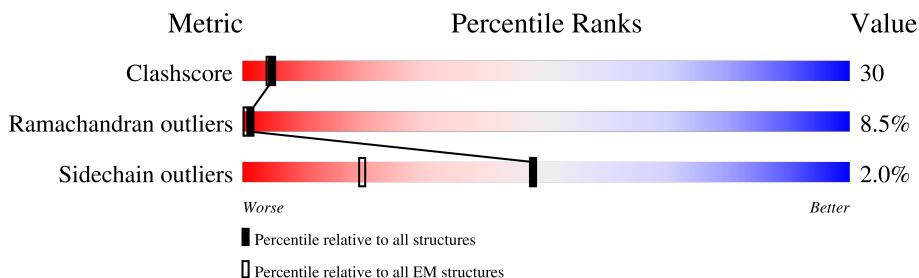
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	2787	

2 Entry composition

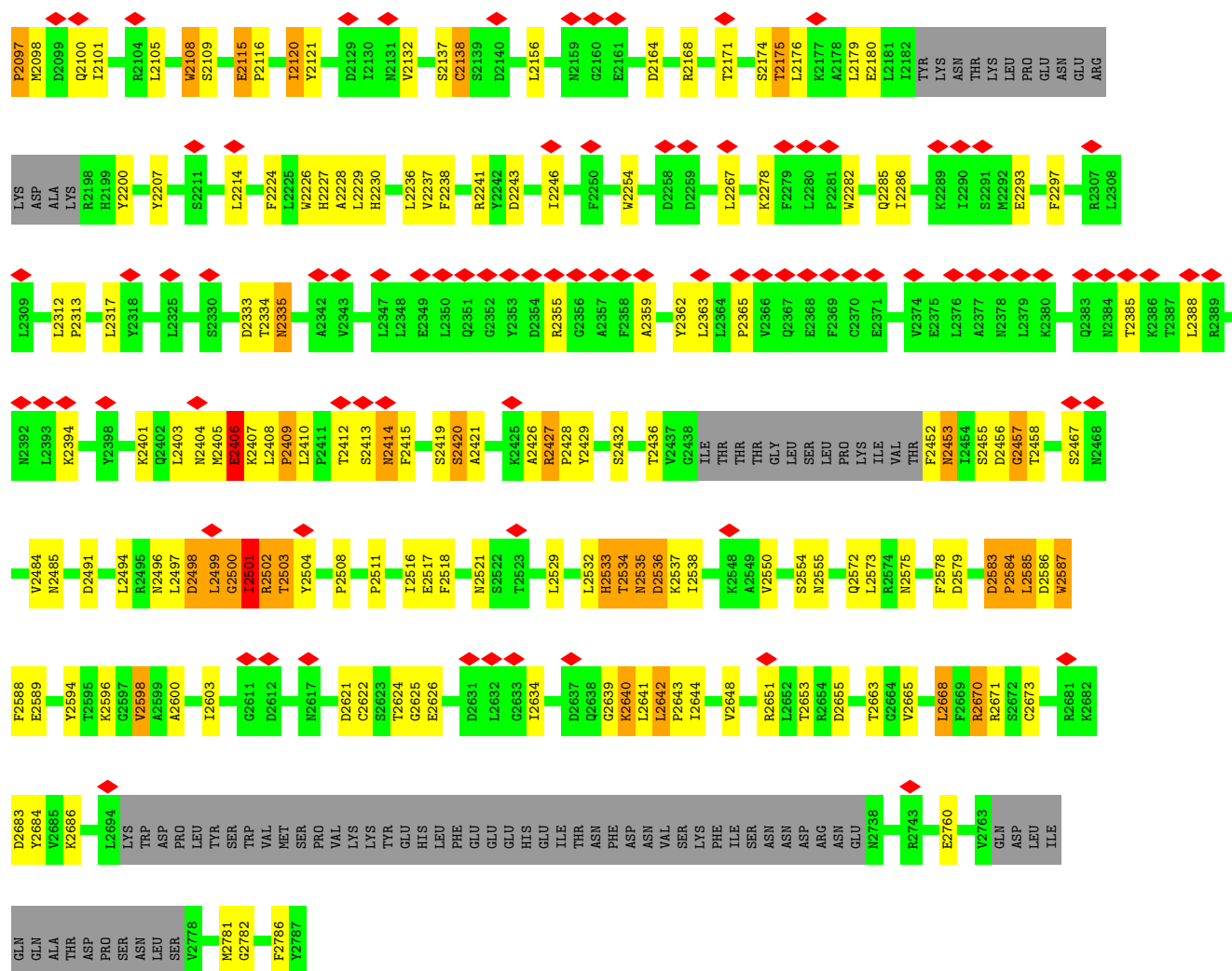
There is only 1 type of molecule in this entry. The entry contains 14100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine/threonine-protein kinase TEL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2244	14100	8748	2594	2720	38	0	0





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25708	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.02	3/14196 (0.0%)	1.29	113/19391 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1899	LEU	CB-CG	-6.91	1.39	1.53
1	A	1975	LEU	CB-CG	-6.75	1.40	1.53
1	A	1972	ARG	NE-CZ	5.34	1.39	1.33

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1691	MET	N-CA-C	-11.99	100.95	114.62
1	A	1382	ARG	N-CA-C	-11.10	98.10	108.75
1	A	1962	PHE	CA-CB-CG	-10.75	103.05	113.80
1	A	1331	ILE	N-CA-C	-10.28	100.69	111.58
1	A	22	ASN	N-CA-C	-9.21	100.84	112.90
1	A	1237	PRO	N-CA-CB	8.87	112.56	103.25
1	A	1945	THR	N-CA-C	-8.80	102.95	114.31
1	A	2097	PRO	N-CA-CB	8.80	112.49	103.25
1	A	1601	PRO	N-CA-CB	8.76	111.64	103.41
1	A	1025	PRO	N-CA-CB	8.75	111.57	103.08
1	A	1745	PHE	CA-CB-CG	8.57	122.38	113.80
1	A	1562	LEU	N-CA-C	-8.47	99.11	110.55
1	A	2648	VAL	CA-C-N	8.17	128.60	120.52
1	A	2648	VAL	C-N-CA	8.17	128.60	120.52
1	A	1706	PHE	CA-CB-CG	-8.02	105.78	113.80
1	A	287	PRO	N-CA-CB	7.91	112.03	103.33
1	A	1338	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	1737	GLN	N-CA-C	-7.40	100.76	110.53
1	A	1194	PRO	N-CA-CB	7.33	110.95	103.25
1	A	1650	PRO	N-CA-CB	7.24	110.85	103.25
1	A	1054	SER	N-CA-C	-7.23	103.37	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1785	PRO	N-CA-CB	7.13	110.74	103.25
1	A	948	PRO	N-CA-CB	7.05	110.66	103.25
1	A	1933	ALA	N-CA-C	7.03	119.02	111.36
1	A	2312	LEU	CA-C-N	7.03	127.18	119.87
1	A	2312	LEU	C-N-CA	7.03	127.18	119.87
1	A	1643	PRO	N-CA-CB	7.02	109.89	103.08
1	A	1177	PRO	N-CA-CB	7.01	111.04	103.33
1	A	40	PRO	N-CA-CB	6.92	110.61	103.00
1	A	1888	LEU	CA-C-N	6.90	127.30	119.92
1	A	1888	LEU	C-N-CA	6.90	127.30	119.92
1	A	2436	THR	CA-C-O	6.85	121.91	117.94
1	A	397	PRO	N-CA-CB	6.82	110.41	103.25
1	A	1944	GLN	N-CA-C	6.81	119.55	111.71
1	A	1329	ASN	CA-CB-CG	-6.80	105.80	112.60
1	A	321	PRO	N-CA-CB	6.63	110.72	103.30
1	A	1600	TYR	CA-C-N	6.52	126.66	119.87
1	A	1600	TYR	C-N-CA	6.52	126.66	119.87
1	A	1839	PHE	N-CA-C	6.50	120.19	107.98
1	A	1750	LEU	CA-C-N	-6.45	110.93	121.19
1	A	1750	LEU	C-N-CA	-6.45	110.93	121.19
1	A	1236	PHE	CA-C-N	6.42	127.86	119.84
1	A	1236	PHE	C-N-CA	6.42	127.86	119.84
1	A	1894	PHE	CB-CA-C	-6.40	102.18	111.91
1	A	1026	PRO	N-CA-CB	6.30	110.26	103.33
1	A	1373	LEU	N-CA-C	-6.29	104.50	111.36
1	A	1774	CYS	CA-C-N	-6.29	114.99	122.22
1	A	1774	CYS	C-N-CA	-6.29	114.99	122.22
1	A	1787	PRO	N-CA-CB	6.27	109.98	103.15
1	A	2587	TRP	N-CA-C	-6.21	104.42	111.07
1	A	2511	PRO	N-CA-CB	6.17	109.73	103.25
1	A	2334	THR	CA-C-N	6.08	133.16	121.54
1	A	2334	THR	C-N-CA	6.08	133.16	121.54
1	A	2585	LEU	N-CA-C	-6.08	104.72	111.71
1	A	2626	GLU	CA-C-N	6.06	126.08	119.90
1	A	2626	GLU	C-N-CA	6.06	126.08	119.90
1	A	383	TYR	N-CA-C	-6.06	104.49	112.24
1	A	1551	VAL	N-CA-C	-6.04	104.96	110.82
1	A	2164	ASP	N-CA-C	-5.97	104.40	111.03
1	A	1622	PRO	N-CA-CB	5.96	109.89	103.33
1	A	1885	ILE	N-CA-C	5.95	116.73	110.72
1	A	1590	PRO	N-CA-CB	5.92	109.84	103.33
1	A	2550	VAL	N-CA-C	5.91	117.85	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2508	PRO	N-CA-CB	5.91	109.77	103.39
1	A	2781	MET	N-CA-C	5.89	123.35	110.80
1	A	1431	LEU	N-CA-C	-5.89	101.58	110.24
1	A	2428	PRO	N-CA-CB	5.83	109.90	103.26
1	A	1708	VAL	N-CA-C	-5.82	104.84	110.72
1	A	2226	TRP	N-CA-C	-5.82	104.85	111.07
1	A	2335	ASN	N-CA-C	5.77	123.09	110.80
1	A	1078	ILE	CA-C-N	5.77	129.83	120.60
1	A	1078	ILE	C-N-CA	5.77	129.83	120.60
1	A	2651	ARG	N-CA-C	5.76	118.07	109.25
1	A	2285	GLN	N-CA-C	-5.75	105.37	112.90
1	A	1644	PRO	N-CA-CB	5.68	109.58	103.33
1	A	1840	TYR	N-CA-C	-5.65	105.26	111.82
1	A	493	PRO	N-CA-CB	5.62	109.19	103.00
1	A	1049	PRO	N-CA-CB	5.62	109.73	103.44
1	A	2041	VAL	N-CA-C	5.57	115.77	110.53
1	A	1916	GLN	CA-C-N	5.55	132.13	121.54
1	A	1916	GLN	C-N-CA	5.55	132.13	121.54
1	A	1703	LYS	N-CA-C	5.54	118.08	111.71
1	A	115	PRO	N-CA-CB	5.52	109.41	103.33
1	A	1387	LEU	N-CA-C	5.51	119.18	112.23
1	A	2108	TRP	CB-CA-C	-5.49	101.68	110.79
1	A	1742	ILE	N-CA-C	5.46	120.70	109.34
1	A	1243	PRO	N-CA-CB	5.44	109.53	103.44
1	A	1477	VAL	N-CA-C	5.42	120.59	108.88
1	A	2014	ALA	CA-C-N	5.42	125.03	119.56
1	A	2014	ALA	C-N-CA	5.42	125.03	119.56
1	A	2365	PRO	N-CA-CB	5.39	109.26	103.33
1	A	2214	LEU	N-CA-C	5.38	117.84	111.33
1	A	1741	LYS	N-CA-C	5.31	120.68	114.62
1	A	1815	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	2409	PRO	N-CA-C	-5.29	102.89	111.03
1	A	1877	LYS	CB-CA-C	-5.28	110.47	116.54
1	A	2246	ILE	N-CA-C	-5.27	106.00	111.58
1	A	1299	SER	CA-C-N	5.26	130.01	122.23
1	A	1299	SER	C-N-CA	5.26	130.01	122.23
1	A	1990	CYS	N-CA-C	-5.24	105.63	112.23
1	A	913	PRO	N-CA-CB	5.22	109.29	103.44
1	A	1372	ASN	CA-CB-CG	-5.17	107.42	112.60
1	A	1876	SER	N-CA-C	5.17	115.11	108.34
1	A	2579	ASP	N-CA-C	5.12	119.66	113.41
1	A	1299	SER	N-CA-C	-5.12	106.99	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2572	GLN	N-CA-C	5.09	115.77	108.74
1	A	1053	PHE	N-CA-C	5.08	116.91	107.60
1	A	2538	ILE	N-CA-C	-5.08	101.65	108.35
1	A	1912	HIS	N-CA-C	-5.06	106.79	113.17
1	A	1433	ASP	N-CA-C	-5.06	107.16	113.38
1	A	2286	ILE	N-CA-C	-5.05	105.78	110.53
1	A	1724	LEU	N-CA-C	-5.02	106.94	113.16
1	A	2436	THR	CB-CA-C	-5.02	109.85	117.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14100	0	10698	739	0
All	All	14100	0	10698	739	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 30.

All (739) 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)
1:A:1939:VAL:HB	1:A:1990:CYS:CB	1.34	1.51
1:A:1939:VAL:CB	1:A:1990:CYS:HB2	1.41	1.49
1:A:1694:HIS:CE1	1:A:1730:LEU:HD13	1.46	1.49
1:A:215:LEU:CB	1:A:325:THR:HA	1.43	1.46
1:A:2603:ILE:HD11	1:A:2673:CYS:SG	1.57	1.43
1:A:1387:LEU:HD21	1:A:1416:ILE:CG2	1.47	1.41
1:A:2499:LEU:HD22	1:A:2600:ALA:CB	1.46	1.41
1:A:1750:LEU:HD23	1:A:2584:PRO:CA	1.57	1.34
1:A:165:GLU:HA	1:A:202:THR:CB	1.56	1.34
1:A:2254:TRP:CZ2	1:A:2267:LEU:HB3	1.64	1.32
1:A:1749:TYR:CD2	1:A:2585:LEU:HA	1.64	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2410:LEU:CD1	1:A:2415:PHE:HE2	1.49	1.25
1:A:1750:LEU:HB2	1:A:1754:GLU:CD	1.59	1.25
1:A:1855:ASP:O	1:A:1856:VAL:HG22	1.35	1.24
1:A:2603:ILE:CD1	1:A:2673:CYS:SG	2.23	1.24
1:A:1694:HIS:NE2	1:A:1730:LEU:HB3	1.48	1.24
1:A:1692:LEU:HD23	1:A:1730:LEU:CD2	1.68	1.23
1:A:1381:LEU:CG	1:A:1387:LEU:HG	1.68	1.23
1:A:1990:CYS:SG	1:A:1994:LEU:HD12	1.77	1.22
1:A:1808:PHE:CB	1:A:1833:ALA:HB1	1.69	1.22
1:A:1694:HIS:CE1	1:A:1730:LEU:CD1	2.23	1.21
1:A:1689:ILE:HG23	1:A:1730:LEU:CD2	1.68	1.21
1:A:2410:LEU:CD1	1:A:2415:PHE:CE2	2.23	1.21
1:A:1938:ASP:O	1:A:1939:VAL:HG22	1.43	1.19
1:A:1932:ILE:O	1:A:1935:ILE:HD13	1.38	1.18
1:A:320:LYS:HA	1:A:323:LEU:O	1.40	1.18
1:A:2501:ILE:HG12	1:A:2502:ARG:H	1.04	1.16
1:A:2583:ASP:CB	1:A:2586:ASP:HB2	1.76	1.15
1:A:52:VAL:CB	1:A:56:ALA:HB2	1.77	1.14
1:A:1387:LEU:CD2	1:A:1416:ILE:HG21	1.76	1.14
1:A:215:LEU:CB	1:A:325:THR:CA	2.26	1.14
1:A:1381:LEU:HD23	1:A:1387:LEU:CD2	1.77	1.14
1:A:1689:ILE:HG21	1:A:1730:LEU:HD11	1.26	1.14
1:A:1750:LEU:HD23	1:A:2584:PRO:HA	1.20	1.13
1:A:1751:LEU:C	1:A:1755:MET:HE2	1.71	1.13
1:A:1694:HIS:CE1	1:A:1730:LEU:HD22	1.82	1.13
1:A:1808:PHE:CB	1:A:1833:ALA:CB	2.26	1.13
1:A:1689:ILE:CG2	1:A:1730:LEU:HD21	1.78	1.13
1:A:1745:PHE:C	1:A:1746:LYS:HE2	1.73	1.12
1:A:1689:ILE:HG21	1:A:1730:LEU:CD1	1.79	1.12
1:A:1694:HIS:HE1	1:A:1730:LEU:CD2	1.60	1.12
1:A:1038:LEU:CB	1:A:1304:LYS:C	2.22	1.12
1:A:227:MET:CB	1:A:283:ASN:CB	2.27	1.12
1:A:1039:ALA:HB2	1:A:1308:ALA:CB	1.80	1.11
1:A:1752:PHE:HA	1:A:1755:MET:HE3	1.13	1.10
1:A:215:LEU:CB	1:A:326:VAL:H	1.63	1.10
1:A:296:VAL:CB	1:A:387:PHE:CB	2.29	1.09
1:A:1039:ALA:HB2	1:A:1308:ALA:HB1	1.20	1.09
1:A:2401:LYS:HB3	1:A:2404:ASN:CB	1.81	1.09
1:A:1855:ASP:O	1:A:1856:VAL:CG2	2.00	1.08
1:A:1387:LEU:CD2	1:A:1416:ILE:CG2	2.31	1.07
1:A:1387:LEU:HD23	1:A:1417:PHE:HE1	1.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1692:LEU:HD23	1:A:1730:LEU:HD23	1.34	1.07
1:A:1692:LEU:CD2	1:A:1730:LEU:HD23	1.83	1.07
1:A:215:LEU:HA	1:A:326:VAL:N	1.68	1.06
1:A:1749:TYR:HD2	1:A:2585:LEU:CA	1.68	1.06
1:A:1632:ARG:O	1:A:1703:LYS:HD2	1.56	1.06
1:A:2499:LEU:HD22	1:A:2600:ALA:HB3	1.39	1.05
1:A:165:GLU:CA	1:A:202:THR:CB	2.34	1.05
1:A:1749:TYR:CD2	1:A:2585:LEU:CA	2.40	1.05
1:A:215:LEU:CA	1:A:326:VAL:H	1.68	1.04
1:A:1387:LEU:HD23	1:A:1417:PHE:CE1	1.90	1.04
1:A:1752:PHE:HA	1:A:1755:MET:CE	1.86	1.04
1:A:1751:LEU:O	1:A:1755:MET:HG3	1.55	1.04
1:A:2058:TRP:CH2	1:A:2109:SER:HA	1.93	1.04
1:A:1381:LEU:CD2	1:A:1387:LEU:HG	1.87	1.03
1:A:1749:TYR:HD2	1:A:2585:LEU:HA	1.00	1.03
1:A:1749:TYR:CE2	1:A:2585:LEU:HD22	1.93	1.03
1:A:1757:MET:SD	1:A:2587:TRP:CZ2	2.52	1.03
1:A:1689:ILE:CG2	1:A:1730:LEU:CG	2.37	1.03
1:A:2499:LEU:HD21	1:A:2596:LYS:O	1.58	1.03
1:A:2594:TYR:O	1:A:2598:VAL:HG23	1.58	1.03
1:A:1750:LEU:HD23	1:A:2584:PRO:CB	1.87	1.02
1:A:1366:ILE:HG22	1:A:1367:GLU:H	1.25	1.02
1:A:2410:LEU:HD11	1:A:2415:PHE:CE2	1.90	1.02
1:A:944:THR:CB	1:A:949:THR:CB	2.37	1.02
1:A:1381:LEU:HD23	1:A:1387:LEU:CG	1.90	1.01
1:A:1381:LEU:HG	1:A:1387:LEU:HG	1.41	1.01
1:A:1689:ILE:HG21	1:A:1730:LEU:CG	1.91	1.01
1:A:1366:ILE:HG22	1:A:1368:PRO:CD	1.90	1.00
1:A:1744:GLU:HG2	1:A:1771:ILE:HG21	1.42	1.00
1:A:49:GLU:O	1:A:56:ALA:HB3	1.61	1.00
1:A:1381:LEU:O	1:A:1387:LEU:HD11	1.60	1.00
1:A:1689:ILE:CG2	1:A:1730:LEU:CD2	2.38	1.00
1:A:1894:PHE:CZ	1:A:1897:LYS:CB	2.44	1.00
1:A:1730:LEU:O	1:A:1734:GLU:HG3	1.58	1.00
1:A:2499:LEU:CD2	1:A:2600:ALA:CB	2.39	0.99
1:A:2410:LEU:HD13	1:A:2415:PHE:HE2	1.27	0.99
1:A:2499:LEU:HD22	1:A:2600:ALA:HB2	1.02	0.99
1:A:1694:HIS:HE1	1:A:1730:LEU:HD22	1.12	0.99
1:A:1894:PHE:CE1	1:A:1897:LYS:CB	2.45	0.99
1:A:1990:CYS:SG	1:A:1994:LEU:CD1	2.52	0.98
1:A:2058:TRP:CZ3	1:A:2108:TRP:C	2.40	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:LEU:CD2	1:A:2584:PRO:HA	1.94	0.98
1:A:2603:ILE:CG1	1:A:2673:CYS:SG	2.52	0.97
1:A:2534:THR:HG23	1:A:2535:ASN:H	1.25	0.97
1:A:1857:TYR:OH	1:A:1871:PRO:HB2	1.63	0.97
1:A:2529:LEU:O	1:A:2533:HIS:HD2	1.47	0.97
1:A:2415:PHE:HZ	1:A:2427:ARG:CB	1.77	0.96
1:A:1745:PHE:O	1:A:1746:LYS:HE2	1.65	0.96
1:A:1366:ILE:HG22	1:A:1368:PRO:HD3	1.44	0.96
1:A:1809:LEU:HG	1:A:1810:PHE:H	1.28	0.95
1:A:1751:LEU:O	1:A:1755:MET:HE2	1.65	0.95
1:A:2499:LEU:CD2	1:A:2600:ALA:HB2	1.96	0.95
1:A:1749:TYR:HB2	1:A:2584:PRO:O	1.65	0.95
1:A:1938:ASP:O	1:A:1939:VAL:CG2	2.14	0.95
1:A:215:LEU:CB	1:A:326:VAL:N	2.28	0.95
1:A:1094:CYS:CB	1:A:1136:VAL:CB	2.44	0.94
1:A:1694:HIS:CE1	1:A:1730:LEU:CG	2.49	0.94
1:A:1689:ILE:HG23	1:A:1730:LEU:HD21	0.94	0.94
1:A:2401:LYS:HB3	1:A:2404:ASN:HB2	1.47	0.94
1:A:1749:TYR:HB3	1:A:2588:PHE:HB3	1.47	0.94
1:A:1757:MET:SD	1:A:2587:TRP:CH2	2.61	0.94
1:A:2401:LYS:HD2	1:A:2404:ASN:CG	1.91	0.94
1:A:1694:HIS:HE1	1:A:1730:LEU:CG	1.81	0.93
1:A:1749:TYR:CD2	1:A:2585:LEU:CD2	2.52	0.93
1:A:1757:MET:CE	1:A:2578:PHE:HB2	1.98	0.93
1:A:215:LEU:HA	1:A:326:VAL:H	1.27	0.92
1:A:1740:LEU:C	1:A:1755:MET:SD	2.53	0.92
1:A:1938:ASP:C	1:A:1940:THR:H	1.77	0.92
1:A:1934:ALA:C	1:A:1936:PRO:HD3	1.93	0.92
1:A:1387:LEU:CD2	1:A:1417:PHE:CE1	2.53	0.92
1:A:2603:ILE:HD11	1:A:2673:CYS:HG	1.30	0.92
1:A:1381:LEU:HD23	1:A:1387:LEU:HG	1.48	0.92
1:A:2415:PHE:CZ	1:A:2427:ARG:CB	2.53	0.91
1:A:1990:CYS:HG	1:A:1994:LEU:HD12	1.30	0.91
1:A:49:GLU:CB	1:A:56:ALA:O	2.20	0.90
1:A:2501:ILE:HG12	1:A:2502:ARG:N	1.84	0.90
1:A:168:GLN:CB	1:A:202:THR:O	2.21	0.89
1:A:1689:ILE:CG2	1:A:1730:LEU:HG	2.02	0.89
1:A:1757:MET:SD	1:A:2587:TRP:HZ2	1.94	0.89
1:A:1367:GLU:H	1:A:1368:PRO:CD	1.86	0.89
1:A:1391:PHE:CD2	1:A:1417:PHE:HZ	1.91	0.89
1:A:1692:LEU:CD2	1:A:1730:LEU:CD2	2.46	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1932:ILE:O	1:A:1935:ILE:CD1	2.21	0.88
1:A:1795:ASN:O	1:A:1807:ARG:NH1	2.06	0.88
1:A:215:LEU:CA	1:A:326:VAL:N	2.32	0.88
1:A:49:GLU:O	1:A:56:ALA:CB	2.21	0.88
1:A:2499:LEU:CD2	1:A:2596:LYS:O	2.21	0.88
1:A:1381:LEU:HB3	1:A:1387:LEU:HD11	1.55	0.87
1:A:2058:TRP:HZ3	1:A:2108:TRP:CB	1.86	0.87
1:A:386:LEU:O	1:A:387:PHE:O	1.93	0.87
1:A:1694:HIS:NE2	1:A:1730:LEU:CB	2.38	0.87
1:A:2058:TRP:CH2	1:A:2109:SER:CA	2.58	0.87
1:A:1750:LEU:CD2	1:A:2584:PRO:CB	2.53	0.86
1:A:1039:ALA:CB	1:A:1308:ALA:HB1	2.05	0.86
1:A:2058:TRP:HZ3	1:A:2108:TRP:C	1.82	0.86
1:A:1749:TYR:HB2	1:A:2585:LEU:CA	2.05	0.86
1:A:2254:TRP:HZ2	1:A:2267:LEU:HB3	1.37	0.86
1:A:1694:HIS:CE1	1:A:1730:LEU:HB3	2.08	0.86
1:A:1038:LEU:CB	1:A:1304:LYS:CB	2.54	0.86
1:A:1381:LEU:HD23	1:A:1387:LEU:HD23	1.56	0.85
1:A:2254:TRP:CZ2	1:A:2267:LEU:CB	2.55	0.85
1:A:1339:LEU:O	1:A:1380:TYR:CE1	2.29	0.85
1:A:195:THR:CB	1:A:250:LYS:N	2.40	0.85
1:A:1740:LEU:HA	1:A:1755:MET:HG2	1.58	0.85
1:A:1855:ASP:C	1:A:1856:VAL:HG22	2.02	0.85
1:A:123:SER:O	1:A:124:LYS:C	2.20	0.85
1:A:1939:VAL:O	1:A:1990:CYS:HA	1.77	0.85
1:A:2603:ILE:HG12	1:A:2673:CYS:SG	2.15	0.85
1:A:2414:ASN:O	1:A:2415:PHE:CD2	2.30	0.85
1:A:1039:ALA:CB	1:A:1308:ALA:CB	2.55	0.85
1:A:1749:TYR:HE2	1:A:2585:LEU:HD22	1.42	0.85
1:A:2583:ASP:CB	1:A:2586:ASP:CB	2.55	0.84
1:A:1381:LEU:O	1:A:1387:LEU:CD1	2.25	0.84
1:A:1381:LEU:CB	1:A:1387:LEU:HG	2.07	0.84
1:A:1749:TYR:CD2	1:A:2585:LEU:HD23	2.12	0.84
1:A:1632:ARG:O	1:A:1703:LYS:CD	2.24	0.84
1:A:1939:VAL:HB	1:A:1990:CYS:CA	2.07	0.84
1:A:1207:LYS:O	1:A:1211:LEU:CB	2.25	0.84
1:A:1749:TYR:CG	1:A:2585:LEU:HA	2.11	0.84
1:A:1750:LEU:CD2	1:A:2584:PRO:CA	2.50	0.84
1:A:2407:LYS:HG2	1:A:2429:TYR:HA	1.60	0.83
1:A:1381:LEU:HB3	1:A:1387:LEU:CD1	2.08	0.83
1:A:1597:ASN:CB	1:A:1601:PRO:CB	2.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1894:PHE:CD2	1:A:1894:PHE:O	2.31	0.83
1:A:1038:LEU:CB	1:A:1304:LYS:O	2.27	0.83
1:A:227:MET:CA	1:A:283:ASN:CB	2.57	0.83
1:A:1757:MET:HE1	1:A:2578:PHE:HB2	1.59	0.83
1:A:1939:VAL:CG1	1:A:1990:CYS:HB2	2.09	0.82
1:A:215:LEU:N	1:A:325:THR:CB	2.42	0.82
1:A:2497:LEU:HG	1:A:2498:ASP:H	1.44	0.82
1:A:2668:LEU:H	1:A:2668:LEU:CD1	1.92	0.82
1:A:52:VAL:CB	1:A:56:ALA:CB	2.57	0.82
1:A:2521:ASN:CB	1:A:2622:CYS:HB3	2.10	0.81
1:A:1387:LEU:CD2	1:A:1416:ILE:HG22	2.09	0.81
1:A:894:TYR:HA	1:A:948:PRO:CB	2.10	0.81
1:A:55:LEU:O	1:A:92:ARG:CB	2.28	0.81
1:A:195:THR:CB	1:A:246:LEU:O	2.29	0.81
1:A:1387:LEU:HD22	1:A:1417:PHE:CD1	2.15	0.81
1:A:1387:LEU:HD21	1:A:1416:ILE:HG21	0.81	0.81
1:A:1957:LEU:O	1:A:1959:THR:HG23	1.81	0.81
1:A:2501:ILE:CG1	1:A:2502:ARG:H	1.89	0.80
1:A:2499:LEU:CD2	1:A:2600:ALA:HB3	2.05	0.80
1:A:2532:LEU:O	1:A:2534:THR:HG22	1.81	0.80
1:A:2414:ASN:O	1:A:2415:PHE:CG	2.35	0.79
1:A:2529:LEU:O	1:A:2533:HIS:CD2	2.35	0.79
1:A:2668:LEU:H	1:A:2668:LEU:HD13	1.48	0.79
1:A:1091:PHE:HA	1:A:1150:LYS:O	1.82	0.79
1:A:1366:ILE:HG22	1:A:1368:PRO:HD2	1.63	0.78
1:A:1955:GLU:N	1:A:1955:GLU:OE1	2.16	0.78
1:A:1749:TYR:HD2	1:A:2585:LEU:CB	1.96	0.78
1:A:2359:ALA:O	1:A:2362:TYR:CE2	2.38	0.77
1:A:594:PHE:O	1:A:595:CYS:CB	2.29	0.77
1:A:2497:LEU:HG	1:A:2498:ASP:N	2.00	0.77
1:A:227:MET:HA	1:A:283:ASN:CB	2.15	0.77
1:A:1694:HIS:CE1	1:A:1730:LEU:CB	2.68	0.77
1:A:1954:LYS:HB3	1:A:1955:GLU:OE1	1.84	0.77
1:A:1749:TYR:CB	1:A:2585:LEU:HA	2.15	0.77
1:A:1751:LEU:O	1:A:1755:MET:CE	2.33	0.77
1:A:1855:ASP:C	1:A:1857:TYR:H	1.93	0.77
1:A:2401:LYS:CB	1:A:2404:ASN:HB2	2.15	0.77
1:A:1694:HIS:HE1	1:A:1730:LEU:CD1	1.82	0.76
1:A:1749:TYR:HB2	1:A:2585:LEU:HA	1.64	0.76
1:A:1752:PHE:CA	1:A:1755:MET:HE3	2.07	0.76
1:A:172:LYS:O	1:A:209:VAL:CB	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:TYR:CE2	1:A:2585:LEU:CD2	2.69	0.76
1:A:1055:LEU:C	1:A:1057:ASP:H	1.93	0.76
1:A:165:GLU:CB	1:A:202:THR:CB	2.63	0.76
1:A:1666:LEU:C	1:A:1668:PHE:H	1.90	0.76
1:A:1391:PHE:CD2	1:A:1417:PHE:CZ	2.72	0.76
1:A:195:THR:O	1:A:246:LEU:CB	2.34	0.76
1:A:1694:HIS:CE1	1:A:1730:LEU:CD2	2.48	0.76
1:A:1750:LEU:HB2	1:A:1754:GLU:OE2	1.85	0.76
1:A:597:PHE:CB	1:A:682:ASN:CB	2.64	0.76
1:A:1381:LEU:HB3	1:A:1387:LEU:CG	2.15	0.75
1:A:1635:ILE:O	1:A:1636:HIS:O	2.05	0.75
1:A:2455:SER:C	1:A:2457:GLY:H	1.94	0.75
1:A:1194:PRO:O	1:A:1195:GLN:CB	2.35	0.75
1:A:18:ILE:O	1:A:19:LYS:CB	2.34	0.74
1:A:995:ASN:C	1:A:997:MET:H	1.94	0.74
1:A:1777:ASP:CB	1:A:1781:LEU:CB	2.66	0.74
1:A:241:SER:O	1:A:245:THR:CB	2.35	0.74
1:A:1746:LYS:HE2	1:A:1746:LYS:N	2.02	0.74
1:A:53:GLU:O	1:A:54:LEU:CB	2.34	0.74
1:A:980:THR:O	1:A:981:PHE:CB	2.36	0.74
1:A:1387:LEU:CD2	1:A:1417:PHE:HE1	1.92	0.74
1:A:1035:PHE:C	1:A:1037:SER:H	1.95	0.74
1:A:2058:TRP:HH2	1:A:2109:SER:HG	1.36	0.74
1:A:894:TYR:CB	1:A:948:PRO:CB	2.66	0.73
1:A:1731:ASP:HA	1:A:1734:GLU:CD	2.12	0.73
1:A:1744:GLU:CG	1:A:1771:ILE:HG21	2.18	0.73
1:A:2174:SER:O	1:A:2176:LEU:N	2.21	0.73
1:A:1751:LEU:O	1:A:1755:MET:CG	2.35	0.73
1:A:967:HIS:O	1:A:970:ILE:N	2.21	0.73
1:A:1391:PHE:CE2	1:A:1417:PHE:CZ	2.77	0.73
1:A:1757:MET:SD	1:A:2587:TRP:HH2	2.12	0.73
1:A:223:THR:CB	1:A:280:GLU:O	2.37	0.72
1:A:1666:LEU:O	1:A:1668:PHE:N	2.21	0.72
1:A:1689:ILE:HD13	1:A:1730:LEU:HD11	1.71	0.72
1:A:1757:MET:HE2	1:A:2578:PHE:HB2	1.69	0.72
1:A:2534:THR:HG23	1:A:2535:ASN:N	2.03	0.72
1:A:768:ILE:O	1:A:769:VAL:C	2.33	0.72
1:A:254:SER:O	1:A:257:LEU:CB	2.37	0.72
1:A:1752:PHE:CA	1:A:1755:MET:CE	2.65	0.72
1:A:1210:LEU:C	1:A:1212:MET:H	1.97	0.72
1:A:2362:TYR:CD1	1:A:2363:LEU:N	2.58	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:TYR:CA	1:A:948:PRO:CB	2.67	0.72
1:A:1749:TYR:CD2	1:A:2585:LEU:CB	2.71	0.72
1:A:1749:TYR:CB	1:A:2584:PRO:O	2.36	0.72
1:A:50:ALA:O	1:A:52:VAL:N	2.23	0.72
1:A:382:ASN:CB	1:A:385:LEU:H	2.02	0.72
1:A:1752:PHE:O	1:A:1755:MET:HB2	1.90	0.72
1:A:1366:ILE:HG22	1:A:1367:GLU:N	2.03	0.71
1:A:2452:PHE:O	1:A:2453:ASN:O	2.08	0.71
1:A:1745:PHE:C	1:A:1746:LYS:CE	2.60	0.71
1:A:2516:ILE:C	1:A:2518:PHE:H	1.99	0.71
1:A:2401:LYS:HB3	1:A:2404:ASN:HB3	1.73	0.71
1:A:1673:TYR:HD1	1:A:1676:LYS:HD2	1.55	0.71
1:A:1745:PHE:CD2	1:A:1746:LYS:CD	2.74	0.70
1:A:1296:GLU:OE2	1:A:1550:GLU:HB3	1.92	0.70
1:A:1809:LEU:O	1:A:1812:ASN:CG	2.34	0.70
1:A:214:ARG:CB	1:A:325:THR:CB	2.69	0.70
1:A:1749:TYR:CD2	1:A:2585:LEU:HD22	2.24	0.70
1:A:1391:PHE:HD2	1:A:1417:PHE:HZ	1.37	0.70
1:A:1938:ASP:C	1:A:1940:THR:N	2.45	0.70
1:A:995:ASN:O	1:A:997:MET:N	2.23	0.70
1:A:1750:LEU:HB2	1:A:1754:GLU:CG	2.22	0.70
1:A:1857:TYR:OH	1:A:1871:PRO:CB	2.39	0.70
1:A:1746:LYS:O	1:A:1747:PHE:CG	2.45	0.70
1:A:2455:SER:O	1:A:2457:GLY:N	2.25	0.69
1:A:1809:LEU:O	1:A:1812:ASN:ND2	2.25	0.69
1:A:1366:ILE:CG2	1:A:1368:PRO:CD	2.68	0.69
1:A:1367:GLU:H	1:A:1368:PRO:HD2	1.55	0.69
1:A:1607:GLY:HA2	1:A:1668:PHE:CB	2.22	0.69
1:A:1635:ILE:O	1:A:1636:HIS:C	2.36	0.69
1:A:889:LEU:O	1:A:890:LEU:CB	2.41	0.69
1:A:1694:HIS:ND1	1:A:1730:LEU:HD13	2.06	0.69
1:A:2058:TRP:CZ3	1:A:2108:TRP:O	2.46	0.69
1:A:386:LEU:O	1:A:387:PHE:C	2.36	0.68
1:A:1387:LEU:HD22	1:A:1417:PHE:HD1	1.58	0.68
1:A:1749:TYR:HD2	1:A:2585:LEU:CD2	2.00	0.68
1:A:1036:TYR:O	1:A:1038:LEU:N	2.26	0.68
1:A:1095:LYS:O	1:A:1154:ASP:CB	2.42	0.68
1:A:1749:TYR:HD2	1:A:2585:LEU:HD23	1.58	0.68
1:A:1757:MET:HE1	1:A:2578:PHE:CB	2.24	0.68
1:A:161:ASP:CB	1:A:198:ILE:CB	2.71	0.68
1:A:1391:PHE:CE2	1:A:1417:PHE:HZ	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1812:ASN:C	1:A:1812:ASN:OD1	2.35	0.68
1:A:49:GLU:C	1:A:56:ALA:O	2.37	0.68
1:A:1633:SER:O	1:A:1635:ILE:N	2.26	0.68
1:A:2670:ARG:O	1:A:2671:ARG:C	2.35	0.68
1:A:1038:LEU:HA	1:A:1305:LEU:CA	2.24	0.68
1:A:967:HIS:O	1:A:969:SER:N	2.28	0.67
1:A:1757:MET:HE1	1:A:2578:PHE:CA	2.24	0.67
1:A:1036:TYR:O	1:A:1304:LYS:CB	2.41	0.67
1:A:1807:ARG:O	1:A:1809:LEU:HD23	1.95	0.67
1:A:215:LEU:CB	1:A:325:THR:C	2.67	0.67
1:A:1391:PHE:HD2	1:A:1417:PHE:CZ	2.12	0.67
1:A:215:LEU:H	1:A:325:THR:CB	2.07	0.67
1:A:1689:ILE:CG2	1:A:1730:LEU:HD11	2.16	0.67
1:A:1807:ARG:C	1:A:1809:LEU:HD23	2.20	0.66
1:A:1529:PRO:HG2	1:A:1533:TYR:HE2	1.59	0.66
1:A:1606:PHE:O	1:A:1607:GLY:O	2.14	0.66
1:A:1730:LEU:C	1:A:1734:GLU:HG3	2.21	0.66
1:A:1750:LEU:CG	1:A:2584:PRO:HA	2.25	0.66
1:A:1366:ILE:CG2	1:A:1368:PRO:HD2	2.26	0.66
1:A:941:ASN:O	1:A:942:SER:CB	2.43	0.66
1:A:66:LEU:O	1:A:67:ARG:C	2.39	0.66
1:A:1752:PHE:N	1:A:1755:MET:HE2	2.08	0.66
1:A:2410:LEU:HD12	1:A:2415:PHE:CE2	2.27	0.66
1:A:1809:LEU:CG	1:A:1810:PHE:H	2.04	0.65
1:A:598:ILE:O	1:A:601:LEU:N	2.29	0.65
1:A:1529:PRO:O	1:A:1533:TYR:CD2	2.48	0.65
1:A:50:ALA:C	1:A:52:VAL:N	2.53	0.65
1:A:1750:LEU:O	1:A:1751:LEU:C	2.33	0.65
1:A:50:ALA:C	1:A:52:VAL:H	2.05	0.65
1:A:1367:GLU:N	1:A:1368:PRO:CD	2.58	0.65
1:A:1740:LEU:HA	1:A:1755:MET:CG	2.26	0.65
1:A:546:GLU:CB	1:A:595:CYS:CB	2.75	0.65
1:A:2058:TRP:CZ3	1:A:2109:SER:N	2.65	0.65
1:A:1751:LEU:C	1:A:1755:MET:CE	2.62	0.64
1:A:14:SER:O	1:A:15:SER:C	2.40	0.64
1:A:2058:TRP:HH2	1:A:2109:SER:OG	1.79	0.64
1:A:1039:ALA:CB	1:A:1308:ALA:HB2	2.27	0.64
1:A:1857:TYR:HH	1:A:1871:PRO:HB2	1.61	0.64
1:A:1596:LEU:O	1:A:1597:ASN:C	2.41	0.64
1:A:1749:TYR:HB2	1:A:2585:LEU:C	2.21	0.64
1:A:2497:LEU:CG	1:A:2498:ASP:H	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1561:TYR:CD2	1:A:1565:TYR:HE2	2.15	0.64
1:A:884:VAL:O	1:A:885:LEU:C	2.41	0.64
1:A:1809:LEU:HG	1:A:1810:PHE:N	2.05	0.64
1:A:1934:ALA:O	1:A:1936:PRO:HD3	1.97	0.64
1:A:1296:GLU:OE2	1:A:1550:GLU:CB	2.45	0.64
1:A:57:SER:O	1:A:60:THR:N	2.30	0.64
1:A:2313:PRO:HG3	1:A:2362:TYR:CE1	2.33	0.64
1:A:1561:TYR:CD2	1:A:1565:TYR:CE2	2.86	0.63
1:A:1749:TYR:HB3	1:A:2588:PHE:CB	2.27	0.63
1:A:2500:GLY:O	1:A:2501:ILE:O	2.16	0.63
1:A:1750:LEU:HD12	1:A:1751:LEU:N	2.12	0.63
1:A:1598:ALA:O	1:A:1601:PRO:N	2.32	0.63
1:A:1666:LEU:C	1:A:1668:PHE:N	2.55	0.63
1:A:1939:VAL:CB	1:A:1990:CYS:CB	2.28	0.63
1:A:1598:ALA:O	1:A:1600:TYR:N	2.31	0.63
1:A:242:VAL:C	1:A:244:ASP:H	2.06	0.63
1:A:1750:LEU:CB	1:A:1754:GLU:CD	2.54	0.63
1:A:1750:LEU:HB3	1:A:2584:PRO:HA	1.81	0.63
1:A:888:LYS:CB	1:A:892:ASN:H	2.11	0.62
1:A:1605:ASN:C	1:A:1607:GLY:H	2.06	0.62
1:A:1038:LEU:HA	1:A:1305:LEU:HA	1.81	0.62
1:A:2485:ASN:HB2	1:A:2501:ILE:O	1.99	0.62
1:A:1210:LEU:C	1:A:1212:MET:N	2.53	0.62
1:A:2058:TRP:CZ3	1:A:2108:TRP:CB	2.76	0.62
1:A:260:GLY:O	1:A:263:SER:N	2.33	0.62
1:A:1745:PHE:CD2	1:A:1746:LYS:HE3	2.35	0.61
1:A:1035:PHE:O	1:A:1037:SER:N	2.32	0.61
1:A:1529:PRO:HG2	1:A:1533:TYR:CE2	2.33	0.61
1:A:1661:LEU:O	1:A:1665:ASP:CB	2.48	0.61
1:A:1204:TYR:HA	1:A:1595:VAL:O	2.00	0.61
1:A:1807:ARG:HG3	1:A:1807:ARG:HH11	1.64	0.61
1:A:1807:ARG:N	1:A:1809:LEU:HD23	2.15	0.61
1:A:1938:ASP:C	1:A:1939:VAL:HG22	2.22	0.61
1:A:1812:ASN:OD1	1:A:1813:ALA:N	2.33	0.61
1:A:22:ASN:O	1:A:25:LEU:N	2.34	0.61
1:A:200:GLN:O	1:A:203:ARG:N	2.31	0.61
1:A:1529:PRO:O	1:A:1533:TYR:HD2	1.84	0.61
1:A:1807:ARG:HH11	1:A:1807:ARG:CG	2.14	0.61
1:A:1808:PHE:CB	1:A:1833:ALA:HB3	2.28	0.61
1:A:1748:GLY:C	1:A:1750:LEU:H	2.09	0.61
1:A:1628:SER:CB	1:A:1701:LYS:CG	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1757:MET:SD	1:A:2578:PHE:HD1	2.24	0.60
1:A:1954:LYS:CB	1:A:1955:GLU:OE1	2.49	0.60
1:A:1387:LEU:CD2	1:A:1417:PHE:CD1	2.78	0.60
1:A:1958:ASN:C	1:A:1959:THR:HG23	2.26	0.60
1:A:1495:ARG:NH1	1:A:1958:ASN:OD1	2.34	0.60
1:A:981:PHE:C	1:A:983:LYS:H	2.08	0.60
1:A:1938:ASP:O	1:A:1940:THR:N	2.33	0.60
1:A:308:TYR:C	1:A:310:GLU:H	2.10	0.60
1:A:1367:GLU:H	1:A:1368:PRO:HD3	1.64	0.60
1:A:371:LEU:O	1:A:395:ASP:CB	2.50	0.60
1:A:1628:SER:CB	1:A:1701:LYS:HG2	2.30	0.60
1:A:1746:LYS:HE2	1:A:1746:LYS:CA	2.31	0.60
1:A:1561:TYR:O	1:A:1565:TYR:HD2	1.85	0.60
1:A:1630:PHE:C	1:A:1632:ARG:H	2.10	0.60
1:A:1680:ASN:O	1:A:1684:ARG:HG2	2.02	0.60
1:A:257:LEU:C	1:A:259:ILE:H	2.09	0.60
1:A:1627:LEU:C	1:A:1629:LYS:H	2.10	0.60
1:A:1750:LEU:HD12	1:A:1750:LEU:C	2.27	0.60
1:A:1855:ASP:HA	1:A:1857:TYR:HD2	1.67	0.59
1:A:1054:SER:O	1:A:1055:LEU:CB	2.50	0.59
1:A:967:HIS:O	1:A:968:GLY:C	2.46	0.59
1:A:1781:LEU:O	1:A:1782:ALA:C	2.45	0.59
1:A:1939:VAL:HB	1:A:1990:CYS:HB2	0.62	0.59
1:A:2171:THR:O	1:A:2175:THR:N	2.35	0.59
1:A:2254:TRP:CH2	1:A:2267:LEU:HB3	2.33	0.59
1:A:2455:SER:C	1:A:2457:GLY:N	2.60	0.59
1:A:1053:PHE:C	1:A:1055:LEU:H	2.10	0.59
1:A:2254:TRP:CZ3	1:A:2297:PHE:CD1	2.90	0.59
1:A:387:PHE:O	1:A:389:ARG:N	2.28	0.59
1:A:1781:LEU:HA	1:A:2668:LEU:HB3	1.84	0.59
1:A:1692:LEU:HD23	1:A:1730:LEU:HD22	1.76	0.59
1:A:995:ASN:C	1:A:997:MET:N	2.61	0.58
1:A:946:VAL:C	1:A:948:PRO:N	2.59	0.58
1:A:1780:PHE:O	1:A:1781:LEU:C	2.45	0.58
1:A:1757:MET:CE	1:A:2578:PHE:CB	2.79	0.58
1:A:1056:GLU:O	1:A:1059:MET:N	2.37	0.58
1:A:2313:PRO:CG	1:A:2362:TYR:CE1	2.86	0.58
1:A:49:GLU:O	1:A:56:ALA:O	2.21	0.58
1:A:195:THR:O	1:A:246:LEU:CA	2.52	0.58
1:A:1749:TYR:C	1:A:2584:PRO:O	2.47	0.58
1:A:1853:SER:C	1:A:1855:ASP:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:O	1:A:322:GLN:N	2.34	0.58
1:A:2401:LYS:CA	1:A:2404:ASN:HB2	2.34	0.57
1:A:1339:LEU:O	1:A:1380:TYR:CD1	2.57	0.57
1:A:2497:LEU:CG	1:A:2498:ASP:N	2.68	0.57
1:A:946:VAL:O	1:A:948:PRO:N	2.37	0.57
1:A:943:PHE:O	1:A:944:THR:C	2.48	0.57
1:A:1744:GLU:OE2	1:A:1771:ILE:HG23	2.05	0.57
1:A:1750:LEU:HD13	1:A:1754:GLU:OE1	2.05	0.57
1:A:2415:PHE:CZ	1:A:2427:ARG:N	2.69	0.57
1:A:1387:LEU:HD22	1:A:1416:ILE:HG22	1.85	0.57
1:A:195:THR:CB	1:A:250:LYS:CA	2.82	0.56
1:A:1035:PHE:C	1:A:1037:SER:N	2.58	0.56
1:A:296:VAL:CA	1:A:387:PHE:CB	2.83	0.56
1:A:2359:ALA:O	1:A:2362:TYR:CD2	2.58	0.56
1:A:2401:LYS:HB3	1:A:2404:ASN:CG	2.30	0.56
1:A:2668:LEU:HD13	1:A:2668:LEU:N	2.14	0.56
1:A:1745:PHE:CD2	1:A:1746:LYS:HD3	2.40	0.56
1:A:1750:LEU:CB	1:A:1754:GLU:OE2	2.52	0.56
1:A:1757:MET:CG	1:A:2663:THR:OG1	2.53	0.56
1:A:227:MET:HA	1:A:283:ASN:C	2.30	0.56
1:A:1055:LEU:C	1:A:1057:ASP:N	2.61	0.56
1:A:1391:PHE:HE2	1:A:1417:PHE:CZ	2.24	0.56
1:A:1958:ASN:O	1:A:1959:THR:CG2	2.53	0.56
1:A:2484:VAL:HG12	1:A:2500:GLY:O	2.06	0.56
1:A:1205:HIS:O	1:A:1209:ARG:CB	2.53	0.56
1:A:1855:ASP:O	1:A:1857:TYR:CD2	2.58	0.56
1:A:1855:ASP:HB3	1:A:1879:LYS:CD	2.35	0.56
1:A:1855:ASP:C	1:A:1857:TYR:N	2.62	0.56
1:A:1344:ILE:CB	1:A:1380:TYR:OH	2.54	0.56
1:A:1689:ILE:HG22	1:A:1730:LEU:HG	1.87	0.56
1:A:1932:ILE:C	1:A:1935:ILE:HD13	2.26	0.55
1:A:52:VAL:C	1:A:54:LEU:H	2.15	0.55
1:A:1777:ASP:O	1:A:2668:LEU:HB2	2.06	0.55
1:A:2420:SER:OG	1:A:2421:ALA:N	2.38	0.55
1:A:1780:PHE:CB	1:A:2668:LEU:HA	2.37	0.55
1:A:2362:TYR:CG	1:A:2363:LEU:N	2.74	0.55
1:A:2058:TRP:CH2	1:A:2109:SER:N	2.75	0.55
1:A:2313:PRO:CB	1:A:2362:TYR:CE1	2.89	0.55
1:A:2410:LEU:HD13	1:A:2415:PHE:CE2	2.19	0.55
1:A:195:THR:O	1:A:246:LEU:C	2.50	0.55
1:A:240:PHE:O	1:A:242:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2536:ASP:O	1:A:2537:LYS:C	2.48	0.55
1:A:1632:ARG:C	1:A:1703:LYS:HD2	2.31	0.55
1:A:1807:ARG:C	1:A:1809:LEU:H	2.15	0.55
1:A:2668:LEU:CD1	1:A:2668:LEU:N	2.63	0.55
1:A:57:SER:O	1:A:58:GLU:C	2.50	0.54
1:A:1038:LEU:CB	1:A:1304:LYS:CA	2.84	0.54
1:A:1608:MET:C	1:A:1610:SER:N	2.64	0.54
1:A:825:TYR:O	1:A:826:LEU:C	2.50	0.54
1:A:1894:PHE:HE2	1:A:1898:SER:HB3	1.71	0.54
1:A:1746:LYS:CE	1:A:1746:LYS:CA	2.86	0.54
1:A:1743:LYS:CB	1:A:1751:LEU:CB	2.86	0.54
1:A:1746:LYS:O	1:A:1747:PHE:CD2	2.60	0.54
1:A:888:LYS:CB	1:A:892:ASN:N	2.70	0.53
1:A:1495:ARG:NH2	1:A:1958:ASN:OD1	2.40	0.53
1:A:1598:ALA:O	1:A:1599:ILE:C	2.51	0.53
1:A:1598:ALA:C	1:A:1600:TYR:N	2.67	0.53
1:A:1750:LEU:CB	1:A:2584:PRO:HA	2.37	0.53
1:A:1381:LEU:CD2	1:A:1387:LEU:CG	2.60	0.53
1:A:1381:LEU:CB	1:A:1387:LEU:CD1	2.83	0.53
1:A:1635:ILE:C	1:A:1636:HIS:O	2.49	0.53
1:A:1692:LEU:HD23	1:A:1730:LEU:HD21	1.83	0.53
1:A:1855:ASP:HA	1:A:1857:TYR:CD2	2.42	0.53
1:A:767:GLU:O	1:A:768:ILE:CB	2.56	0.53
1:A:2081:ILE:C	1:A:2083:GLU:H	2.15	0.53
1:A:2401:LYS:HD2	1:A:2404:ASN:ND2	2.24	0.53
1:A:2414:ASN:C	1:A:2415:PHE:CD2	2.87	0.53
1:A:1745:PHE:HD2	1:A:1746:LYS:CD	2.22	0.53
1:A:1853:SER:OG	1:A:1856:VAL:HG13	2.09	0.53
1:A:1895:ALA:O	1:A:1899:LEU:HB2	2.08	0.53
1:A:2407:LYS:HG2	1:A:2429:TYR:CA	2.37	0.53
1:A:1524:ARG:O	1:A:1525:HIS:C	2.52	0.53
1:A:1760:ILE:HG23	1:A:1760:ILE:O	2.09	0.53
1:A:2243:ASP:N	1:A:2243:ASP:OD1	2.37	0.53
1:A:1935:ILE:N	1:A:1936:PRO:HD3	2.25	0.52
1:A:1814:ASP:HA	1:A:1817:ALA:CB	2.39	0.52
1:A:2453:ASN:CB	1:A:2458:THR:N	2.73	0.52
1:A:172:LYS:HA	1:A:209:VAL:CB	2.39	0.52
1:A:2405:MET:O	1:A:2407:LYS:N	2.42	0.52
1:A:99:CYS:C	1:A:101:ARG:N	2.65	0.52
1:A:1367:GLU:N	1:A:1368:PRO:HD2	2.24	0.52
1:A:1807:ARG:N	1:A:1809:LEU:CD2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:HA	1:A:340:LYS:CB	2.40	0.52
1:A:984:CYS:O	1:A:985:LEU:CB	2.58	0.52
1:A:22:ASN:O	1:A:23:ASN:C	2.53	0.52
1:A:1810:PHE:O	1:A:1811:ASN:C	2.53	0.52
1:A:1813:ALA:O	1:A:1817:ALA:HB2	2.10	0.52
1:A:2412:THR:OG1	1:A:2413:SER:N	2.43	0.52
1:A:49:GLU:CA	1:A:56:ALA:O	2.58	0.52
1:A:1020:LYS:C	1:A:1022:LEU:H	2.17	0.52
1:A:1206:LYS:O	1:A:1210:LEU:N	2.42	0.52
1:A:1746:LYS:HE2	1:A:1746:LYS:HA	1.91	0.52
1:A:2406:GLU:O	1:A:2432:SER:CB	2.58	0.52
1:A:1749:TYR:CD2	1:A:2585:LEU:HB3	2.43	0.51
1:A:1093:TYR:CB	1:A:1155:MET:CB	2.89	0.51
1:A:195:THR:CB	1:A:250:LYS:H	2.20	0.51
1:A:1195:GLN:O	1:A:1196:ILE:C	2.53	0.51
1:A:1941:SER:O	1:A:1942:PHE:C	2.54	0.51
1:A:2583:ASP:O	1:A:2586:ASP:N	2.22	0.51
1:A:964:ASP:O	1:A:965:LEU:C	2.54	0.51
1:A:1332:ILE:O	1:A:1334:ARG:N	2.44	0.51
1:A:1745:PHE:CD2	1:A:1746:LYS:CE	2.93	0.51
1:A:1810:PHE:O	1:A:1812:ASN:N	2.44	0.51
1:A:49:GLU:CB	1:A:57:SER:HA	2.41	0.51
1:A:1746:LYS:N	1:A:1746:LYS:CD	2.73	0.51
1:A:1454:ARG:O	1:A:1455:PRO:C	2.54	0.51
1:A:1746:LYS:C	1:A:1747:PHE:CG	2.89	0.51
1:A:2243:ASP:OD2	1:A:2278:LYS:NZ	2.42	0.51
1:A:1210:LEU:O	1:A:1212:MET:N	2.44	0.50
1:A:1939:VAL:CA	1:A:1990:CYS:HB2	2.33	0.50
1:A:1807:ARG:NH1	1:A:1807:ARG:CG	2.73	0.50
1:A:1958:ASN:C	1:A:1959:THR:CG2	2.84	0.50
1:A:1749:TYR:HB2	1:A:2584:PRO:C	2.34	0.50
1:A:1746:LYS:C	1:A:1747:PHE:CD2	2.89	0.50
1:A:195:THR:CB	1:A:250:LYS:CB	2.89	0.50
1:A:1251:VAL:O	1:A:1252:SER:C	2.54	0.50
1:A:1441:ASP:N	1:A:1441:ASP:OD1	2.43	0.50
1:A:1814:ASP:HA	1:A:1817:ALA:HB3	1.94	0.49
1:A:1746:LYS:N	1:A:1746:LYS:HD2	2.26	0.49
1:A:2668:LEU:C	1:A:2668:LEU:HD22	2.37	0.49
1:A:1038:LEU:HA	1:A:1305:LEU:N	2.27	0.49
1:A:1746:LYS:N	1:A:1746:LYS:CE	2.73	0.49
1:A:1955:GLU:OE2	1:A:2241:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2254:TRP:NE1	1:A:2267:LEU:HD22	2.28	0.49
1:A:598:ILE:O	1:A:599:SER:C	2.55	0.49
1:A:887:GLU:O	1:A:889:LEU:N	2.46	0.49
1:A:279:SER:C	1:A:281:LEU:N	2.69	0.49
1:A:308:TYR:C	1:A:310:GLU:N	2.66	0.49
1:A:387:PHE:C	1:A:389:ARG:H	2.20	0.49
1:A:1855:ASP:O	1:A:1857:TYR:N	2.45	0.49
1:A:2176:LEU:O	1:A:2180:GLU:N	2.44	0.49
1:A:2500:GLY:O	1:A:2501:ILE:C	2.54	0.49
1:A:215:LEU:CA	1:A:325:THR:CA	2.89	0.49
1:A:2516:ILE:C	1:A:2518:PHE:N	2.66	0.49
1:A:1038:LEU:CB	1:A:1305:LEU:N	2.75	0.49
1:A:1561:TYR:HA	1:A:1565:TYR:CE2	2.48	0.49
1:A:1750:LEU:HD23	1:A:2584:PRO:N	2.23	0.49
1:A:1894:PHE:O	1:A:1894:PHE:CG	2.58	0.49
1:A:2502:ARG:O	1:A:2503:THR:OG1	2.29	0.49
1:A:50:ALA:O	1:A:51:LEU:C	2.56	0.49
1:A:1746:LYS:CE	1:A:1746:LYS:HA	2.43	0.49
1:A:981:PHE:O	1:A:983:LYS:N	2.43	0.48
1:A:1066:HIS:O	1:A:1070:PHE:N	2.46	0.48
1:A:1040:MET:O	1:A:1043:LEU:N	2.41	0.48
1:A:967:HIS:C	1:A:969:SER:N	2.70	0.48
1:A:1561:TYR:HD2	1:A:1565:TYR:CE2	2.29	0.48
1:A:1608:MET:CB	1:A:1611:PHE:H	2.27	0.48
1:A:1019:ILE:O	1:A:1021:SER:N	2.46	0.48
1:A:1628:SER:CB	1:A:1701:LYS:HD2	2.43	0.48
1:A:1954:LYS:HG2	1:A:1955:GLU:OE2	2.14	0.48
1:A:100:GLU:O	1:A:101:ARG:CB	2.61	0.48
1:A:397:PRO:O	1:A:398:SER:C	2.57	0.48
1:A:1607:GLY:HA3	1:A:1666:LEU:HA	1.96	0.48
1:A:1695:VAL:HG22	1:A:1734:GLU:HG2	1.96	0.48
1:A:1853:SER:C	1:A:1855:ASP:N	2.72	0.48
1:A:2401:LYS:HD2	1:A:2404:ASN:OD1	2.11	0.48
1:A:1769:GLN:HE22	1:A:1782:ALA:HB3	1.78	0.48
1:A:2668:LEU:H	1:A:2668:LEU:HD12	1.78	0.48
1:A:269:ASP:O	1:A:443:PHE:CB	2.62	0.47
1:A:1633:SER:C	1:A:1635:ILE:H	2.21	0.47
1:A:2521:ASN:O	1:A:2621:ASP:HA	2.14	0.47
1:A:1022:LEU:O	1:A:1025:PRO:N	2.47	0.47
1:A:2683:ASP:HB3	1:A:2686:LYS:HB3	1.96	0.47
1:A:1757:MET:HG2	1:A:2663:THR:OG1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:CYS:C	1:A:101:ARG:H	2.21	0.47
1:A:387:PHE:C	1:A:389:ARG:N	2.72	0.47
1:A:1627:LEU:C	1:A:1629:LYS:N	2.72	0.47
1:A:1633:SER:C	1:A:1635:ILE:N	2.73	0.47
1:A:1041:SER:O	1:A:1042:MET:C	2.54	0.47
1:A:2254:TRP:CE2	1:A:2267:LEU:HD13	2.50	0.47
1:A:2494:LEU:HA	1:A:2497:LEU:HB3	1.95	0.47
1:A:981:PHE:C	1:A:983:LYS:N	2.73	0.47
1:A:1807:ARG:CA	1:A:1809:LEU:HD23	2.45	0.47
1:A:1953:ASP:HA	1:A:1956:ARG:CB	2.44	0.47
1:A:1955:GLU:N	1:A:1955:GLU:CD	2.73	0.47
1:A:2410:LEU:HD12	1:A:2415:PHE:CD2	2.50	0.47
1:A:1855:ASP:HB3	1:A:1879:LYS:HD3	1.96	0.47
1:A:1430:GLU:O	1:A:1431:LEU:C	2.56	0.47
1:A:2060:SER:OG	1:A:2061:ARG:N	2.46	0.47
1:A:87:ILE:O	1:A:88:SER:C	2.53	0.47
1:A:319:TYR:O	1:A:322:GLN:C	2.58	0.47
1:A:887:GLU:C	1:A:889:LEU:N	2.73	0.47
1:A:1778:GLY:O	1:A:2671:ARG:CB	2.63	0.47
1:A:1990:CYS:SG	1:A:1994:LEU:HD11	2.52	0.47
1:A:201:VAL:C	1:A:203:ARG:H	2.23	0.46
1:A:2413:SER:O	1:A:2504:TYR:OH	2.23	0.46
1:A:2516:ILE:O	1:A:2517:GLU:CB	2.64	0.46
1:A:397:PRO:O	1:A:398:SER:O	2.32	0.46
1:A:1033:SER:C	1:A:1035:PHE:H	2.24	0.46
1:A:1056:GLU:O	1:A:1057:ASP:C	2.58	0.46
1:A:1483:SER:OG	1:A:1484:LYS:N	2.47	0.46
1:A:1053:PHE:C	1:A:1055:LEU:N	2.73	0.46
1:A:1606:PHE:C	1:A:1607:GLY:O	2.58	0.46
1:A:1207:LYS:O	1:A:1211:LEU:N	2.43	0.46
1:A:2554:SER:OG	1:A:2555:ASN:N	2.46	0.46
1:A:1630:PHE:C	1:A:1632:ARG:N	2.73	0.46
1:A:1705:LEU:HD22	1:A:1746:LYS:HG2	1.96	0.46
1:A:2082:SER:C	1:A:2084:SER:N	2.70	0.46
1:A:201:VAL:C	1:A:203:ARG:N	2.72	0.46
1:A:211:ASP:HA	1:A:214:ARG:CB	2.46	0.46
1:A:257:LEU:C	1:A:259:ILE:N	2.73	0.46
1:A:887:GLU:C	1:A:889:LEU:H	2.24	0.46
1:A:1807:ARG:C	1:A:1809:LEU:N	2.73	0.46
1:A:1939:VAL:C	1:A:1990:CYS:HA	2.39	0.45
1:A:2401:LYS:CG	1:A:2404:ASN:ND2	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:TRP:CZ3	1:A:2109:SER:HA	2.48	0.45
1:A:2499:LEU:O	1:A:2501:ILE:N	2.43	0.45
1:A:940:ASP:C	1:A:942:SER:N	2.72	0.45
1:A:1807:ARG:O	1:A:1809:LEU:N	2.50	0.45
1:A:1855:ASP:O	1:A:1856:VAL:HG23	2.03	0.45
1:A:1855:ASP:N	1:A:1855:ASP:OD1	2.48	0.45
1:A:2254:TRP:CH2	1:A:2267:LEU:CB	2.97	0.45
1:A:1392:GLN:HG3	1:A:1417:PHE:HE2	1.82	0.45
1:A:1781:LEU:CA	1:A:2668:LEU:HB3	2.46	0.45
1:A:1810:PHE:O	1:A:1813:ALA:N	2.20	0.45
1:A:2624:THR:OG1	1:A:2625:GLY:N	2.49	0.45
1:A:52:VAL:C	1:A:54:LEU:N	2.75	0.45
1:A:1750:LEU:HD21	1:A:2584:PRO:CB	2.43	0.45
1:A:2100:GLN:O	1:A:2101:ILE:C	2.58	0.45
1:A:1741:LYS:N	1:A:1755:MET:SD	2.90	0.45
1:A:2137:SER:O	1:A:2138:CYS:HB3	2.17	0.44
1:A:1330:PHE:CE1	1:A:1333:ILE:HG21	2.53	0.44
1:A:1608:MET:C	1:A:1610:SER:H	2.24	0.44
1:A:2236:LEU:O	1:A:2238:PHE:N	2.51	0.44
1:A:87:ILE:O	1:A:90:VAL:N	2.50	0.44
1:A:1935:ILE:N	1:A:1936:PRO:CD	2.80	0.44
1:A:2534:THR:CG2	1:A:2535:ASN:H	2.04	0.44
1:A:57:SER:O	1:A:59:HIS:N	2.50	0.44
1:A:1013:SER:C	1:A:1015:ILE:N	2.74	0.44
1:A:1381:LEU:HD23	1:A:1387:LEU:HD21	1.86	0.44
1:A:212:PHE:C	1:A:214:ARG:N	2.73	0.44
1:A:2051:PHE:CG	1:A:2105:LEU:HD22	2.52	0.44
1:A:2639:GLY:O	1:A:2640:LYS:CB	2.65	0.44
1:A:1980:SER:O	1:A:1984:LEU:N	2.51	0.44
1:A:2227:HIS:O	1:A:2228:ALA:C	2.58	0.44
1:A:2408:LEU:O	1:A:2409:PRO:C	2.59	0.44
1:A:2414:ASN:C	1:A:2415:PHE:CG	2.93	0.44
1:A:1561:TYR:HA	1:A:1565:TYR:CD2	2.53	0.44
1:A:195:THR:O	1:A:246:LEU:O	2.36	0.43
1:A:1628:SER:CB	1:A:1701:LYS:CD	2.96	0.43
1:A:2401:LYS:HB3	1:A:2404:ASN:ND2	2.32	0.43
1:A:2641:LEU:O	1:A:2642:LEU:HB2	2.18	0.43
1:A:242:VAL:C	1:A:244:ASP:N	2.73	0.43
1:A:1606:PHE:O	1:A:1607:GLY:C	2.60	0.43
1:A:2229:LEU:O	1:A:2230:HIS:C	2.60	0.43
1:A:2081:ILE:C	1:A:2083:GLU:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2585:LEU:O	1:A:2589:GLU:HG2	2.18	0.43
1:A:2501:ILE:O	1:A:2502:ARG:CB	2.67	0.43
1:A:19:LYS:O	1:A:20:GLU:CB	2.65	0.43
1:A:2499:LEU:HD23	1:A:2596:LYS:O	2.10	0.43
1:A:2653:THR:O	1:A:2655:ASP:N	2.51	0.43
1:A:581:TRP:O	1:A:582:ASN:C	2.62	0.43
1:A:1366:ILE:CG2	1:A:1368:PRO:HD3	2.31	0.43
1:A:1706:PHE:CD2	1:A:1706:PHE:C	2.90	0.43
1:A:759:VAL:O	1:A:760:LEU:C	2.62	0.43
1:A:1958:ASN:O	1:A:1959:THR:HG23	2.17	0.43
1:A:2120:ILE:HG13	1:A:2121:TYR:H	1.84	0.43
1:A:1178:LEU:O	1:A:1182:SER:N	2.52	0.43
1:A:1374:PHE:O	1:A:1375:CYS:C	2.60	0.43
1:A:1954:LYS:C	1:A:1955:GLU:OE1	2.61	0.43
1:A:1381:LEU:CB	1:A:1387:LEU:CG	2.77	0.43
1:A:1899:LEU:HD11	1:A:1930:ILE:HA	2.00	0.43
1:A:2224:PHE:CD1	1:A:2224:PHE:C	2.97	0.43
1:A:1740:LEU:CA	1:A:1755:MET:SD	3.06	0.42
1:A:1744:GLU:CG	1:A:1771:ILE:CG2	2.94	0.42
1:A:1635:ILE:O	1:A:1638:ILE:N	2.52	0.42
1:A:2082:SER:O	1:A:2084:SER:N	2.52	0.42
1:A:2086:LEU:O	1:A:2087:TYR:O	2.37	0.42
1:A:1605:ASN:C	1:A:1607:GLY:N	2.73	0.42
1:A:1608:MET:O	1:A:1610:SER:N	2.52	0.42
1:A:1381:LEU:C	1:A:1387:LEU:HD11	2.39	0.42
1:A:2491:ASP:C	1:A:2491:ASP:OD1	2.62	0.42
1:A:1750:LEU:HB2	1:A:1754:GLU:HG3	2.00	0.42
1:A:2532:LEU:O	1:A:2533:HIS:C	2.61	0.42
1:A:1039:ALA:H	1:A:1308:ALA:HB2	1.85	0.42
1:A:1598:ALA:C	1:A:1600:TYR:H	2.28	0.42
1:A:1809:LEU:CG	1:A:1810:PHE:N	2.73	0.42
1:A:2419:SER:O	1:A:2420:SER:HB3	2.20	0.42
1:A:1885:ILE:HG12	1:A:1975:LEU:HD21	2.01	0.42
1:A:966:SER:C	1:A:968:GLY:H	2.27	0.41
1:A:1204:TYR:HA	1:A:1595:VAL:CB	2.51	0.41
1:A:1748:GLY:C	1:A:1750:LEU:N	2.72	0.41
1:A:1757:MET:HG3	1:A:2663:THR:OG1	2.19	0.41
1:A:1958:ASN:O	1:A:1959:THR:HG22	2.21	0.41
1:A:2529:LEU:C	1:A:2533:HIS:HD2	2.22	0.41
1:A:1855:ASP:HB3	1:A:1879:LYS:HD2	2.00	0.41
1:A:2179:LEU:O	1:A:2200:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:TYR:CA	1:A:2584:PRO:O	2.68	0.41
1:A:2137:SER:O	1:A:2138:CYS:CB	2.67	0.41
1:A:1528:GLN:NE2	1:A:1576:PHE:O	2.54	0.41
1:A:1954:LYS:HG2	1:A:1955:GLU:CD	2.46	0.41
1:A:1092:GLU:O	1:A:1093:TYR:CB	2.67	0.41
1:A:2039:PRO:O	1:A:2040:SER:HB3	2.20	0.41
1:A:2362:TYR:CD1	1:A:2362:TYR:C	2.97	0.41
1:A:320:LYS:C	1:A:322:GLN:N	2.77	0.41
1:A:1955:GLU:C	1:A:1957:LEU:H	2.29	0.41
1:A:260:GLY:O	1:A:261:CYS:C	2.63	0.41
1:A:2058:TRP:CZ2	1:A:2109:SER:HA	2.49	0.41
1:A:2500:GLY:C	1:A:2501:ILE:O	2.63	0.41
1:A:1853:SER:OG	1:A:1856:VAL:CG1	2.69	0.41
1:A:1990:CYS:HG	1:A:1994:LEU:CD1	2.15	0.41
1:A:2415:PHE:CD1	1:A:2426:ALA:HA	2.56	0.41
1:A:2521:ASN:CB	1:A:2622:CYS:CB	2.93	0.41
1:A:2642:LEU:CB	1:A:2643:PRO:CD	2.99	0.41
1:A:2168:ARG:CB	1:A:2207:TYR:HE1	2.34	0.41
1:A:279:SER:C	1:A:281:LEU:H	2.27	0.40
1:A:2115:GLU:CB	1:A:2116:PRO:CD	2.98	0.40
1:A:2313:PRO:HG3	1:A:2362:TYR:CZ	2.55	0.40
1:A:1673:TYR:CD1	1:A:1676:LYS:HD2	2.45	0.40
1:A:1757:MET:HE1	1:A:2578:PHE:N	2.36	0.40
1:A:1775:ILE:O	1:A:1776:ASN:HB2	2.20	0.40
1:A:2313:PRO:CB	1:A:2362:TYR:HE1	2.33	0.40
1:A:210:ILE:C	1:A:212:PHE:N	2.78	0.40
1:A:2415:PHE:CE1	1:A:2427:ARG:N	2.89	0.40
1:A:1055:LEU:O	1:A:1057:ASP:N	2.54	0.40
1:A:1565:TYR:OH	1:A:1597:ASN:O	2.39	0.40
1:A:2168:ARG:CB	1:A:2207:TYR:CE1	3.05	0.40
1:A:2401:LYS:CD	1:A:2404:ASN:CG	2.79	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	2174/2787 (78%)	1724 (79%)	266 (12%)	184 (8%)	0 9

All (184) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	19	LYS
1	A	90	VAL
1	A	95	VAL
1	A	196	VAL
1	A	199	PHE
1	A	210	ILE
1	A	241	SER
1	A	274	PHE
1	A	279	SER
1	A	387	PHE
1	A	389	ARG
1	A	397	PRO
1	A	595	CYS
1	A	753	ILE
1	A	768	ILE
1	A	769	VAL
1	A	942	SER
1	A	947	ALA
1	A	964	ASP
1	A	966	SER
1	A	981	PHE
1	A	996	ILE
1	A	1001	SER
1	A	1002	SER
1	A	1020	LYS
1	A	1036	TYR
1	A	1037	SER
1	A	1055	LEU
1	A	1071	ILE
1	A	1194	PRO
1	A	1195	GLN
1	A	1237	PRO
1	A	1367	GLU
1	A	1420	ILE

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Mol	Chain	Res	Type
1	A	1577	ARG
1	A	1580	ILE
1	A	1610	SER
1	A	1634	LEU
1	A	1636	HIS
1	A	1667	PHE
1	A	1785	PRO
1	A	1786	VAL
1	A	1809	LEU
1	A	1856	VAL
1	A	1917	THR
1	A	1939	VAL
1	A	1988	VAL
1	A	2040	SER
1	A	2096	VAL
1	A	2097	PRO
1	A	2115	GLU
1	A	2175	THR
1	A	2237	VAL
1	A	2335	ASN
1	A	2420	SER
1	A	2453	ASN
1	A	2456	ASP
1	A	2467	SER
1	A	2501	ILE
1	A	2502	ARG
1	A	2535	ASN
1	A	2575	ASN
1	A	2584	PRO
1	A	2640	LYS
1	A	2642	LEU
1	A	51	LEU
1	A	54	LEU
1	A	208	THR
1	A	212	PHE
1	A	243	ILE
1	A	275	ASP
1	A	278	SER
1	A	323	LEU
1	A	326	VAL
1	A	367	THR
1	A	369	SER

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Mol	Chain	Res	Type
1	A	384	SER
1	A	398	SER
1	A	399	ILE
1	A	596	ASN
1	A	771	ASP
1	A	773	ILE
1	A	885	LEU
1	A	887	GLU
1	A	890	LEU
1	A	968	GLY
1	A	982	ILE
1	A	985	LEU
1	A	1040	MET
1	A	1192	ILE
1	A	1284	PHE
1	A	1333	ILE
1	A	1338	PHE
1	A	1343	GLN
1	A	1476	HIS
1	A	1480	GLU
1	A	1599	ILE
1	A	1607	GLY
1	A	1630	PHE
1	A	1699	GLU
1	A	1811	ASN
1	A	1957	LEU
1	A	2087	TYR
1	A	2098	MET
1	A	2120	ILE
1	A	2132	VAL
1	A	2138	CYS
1	A	2282	TRP
1	A	2293	GLU
1	A	2406	GLU
1	A	2457	GLY
1	A	2496	ASN
1	A	2533	HIS
1	A	2665	VAL
1	A	2684	TYR
1	A	2782	GLY
1	A	2786	PHE
1	A	15	SER

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Mol	Chain	Res	Type
1	A	175	MET
1	A	214	ARG
1	A	385	LEU
1	A	888	LYS
1	A	963	HIS
1	A	999	SER
1	A	1041	SER
1	A	1093	TYR
1	A	1421	VAL
1	A	1455	PRO
1	A	1780	PHE
1	A	1808	PHE
1	A	1938	ASP
1	A	2317	LEU
1	A	2355	ARG
1	A	2385	THR
1	A	2534	THR
1	A	2644	ILE
1	A	2760	GLU
1	A	58	GLU
1	A	239	CYS
1	A	258	THR
1	A	886	GLY
1	A	983	LYS
1	A	1019	ILE
1	A	1056	GLU
1	A	1203	LYS
1	A	1325	SER
1	A	1571	GLU
1	A	1612	ILE
1	A	1776	ASN
1	A	1781	LEU
1	A	1789	SER
1	A	2333	ASP
1	A	2394	LYS
1	A	2503	THR
1	A	2536	ASP
1	A	2573	LEU
1	A	325	THR
1	A	1332	ILE
1	A	1366	ILE
1	A	1749	TYR

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Mol	Chain	Res	Type
1	A	1765	ILE
1	A	1942	PHE
1	A	2083	GLU
1	A	2156	LEU
1	A	240	PHE
1	A	257	LEU
1	A	1193	LEU
1	A	1211	LEU
1	A	1525	HIS
1	A	1747	PHE
1	A	1874	VAL
1	A	2089	ASP
1	A	2388	LEU
1	A	1388	SER
1	A	2583	ASP
1	A	396	ILE
1	A	198	ILE
1	A	1635	ILE
1	A	2085	ILE
1	A	2427	ARG
1	A	2500	GLY
1	A	2634	ILE
1	A	948	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	881/2569 (34%)	863 (98%)	18 (2%)	48 66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1367	GLU
1	A	1746	LYS
1	A	1807	ARG

Continued on next page...

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Mol	Chain	Res	Type
1	A	1816	ASP
1	A	1855	ASP
1	A	1935	ILE
1	A	1940	THR
1	A	1955	GLU
1	A	1990	CYS
1	A	2403	LEU
1	A	2406	GLU
1	A	2414	ASN
1	A	2498	ASP
1	A	2499	LEU
1	A	2501	ILE
1	A	2598	VAL
1	A	2668	LEU
1	A	2670	ARG

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

Mol	Chain	Res	Type
1	A	1500	GLN
1	A	1528	GLN
1	A	1694	HIS
1	A	1764	ASN
1	A	1769	GLN
1	A	1973	HIS
1	A	2001	GLN
1	A	2004	ASN
1	A	2227	HIS
1	A	2265	GLN
1	A	2404	ASN
1	A	2414	ASN
1	A	2533	HIS

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 [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.

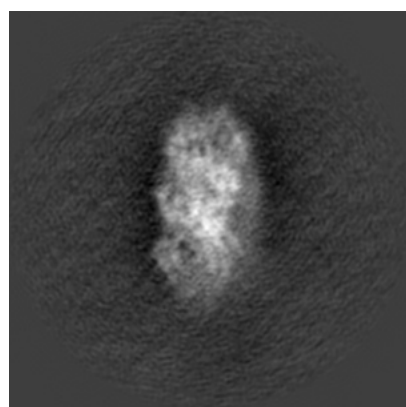
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9892. These allow visual inspection of the internal detail of the map and identification of artifacts.

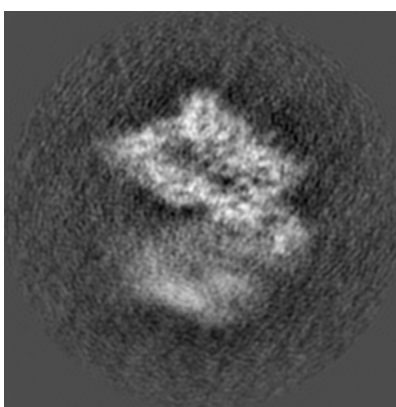
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

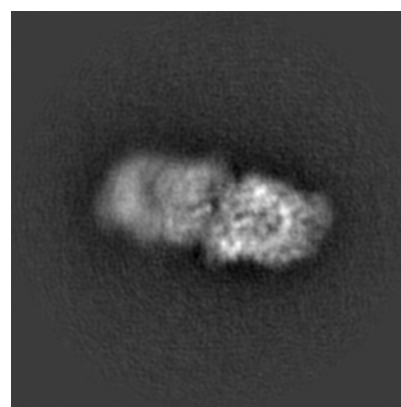
6.1.1 Primary map



X



Y

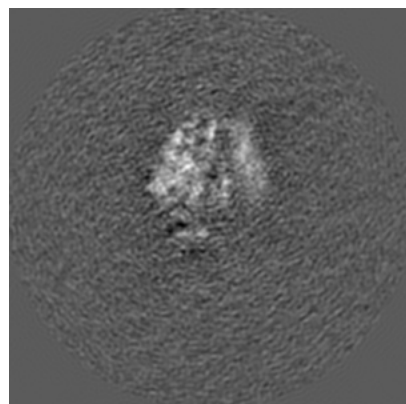


Z

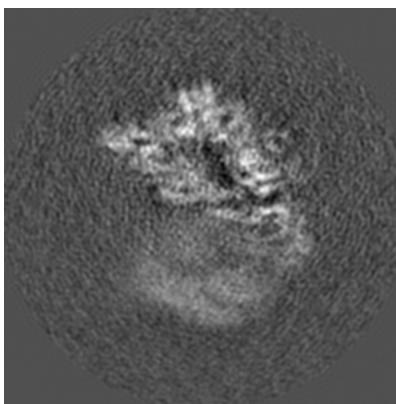
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

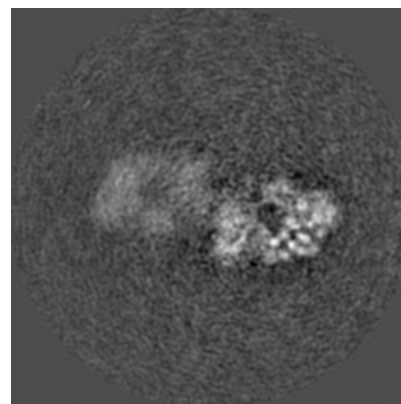
6.2.1 Primary map



X Index: 128



Y Index: 128

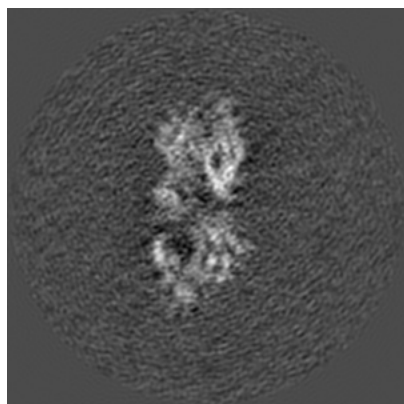


Z Index: 128

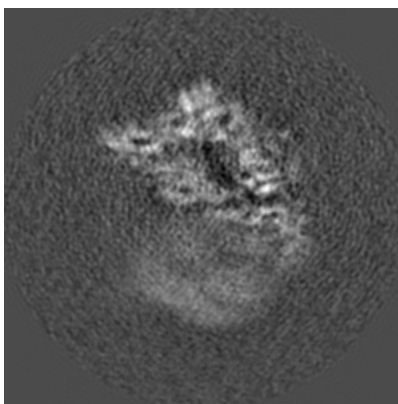
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

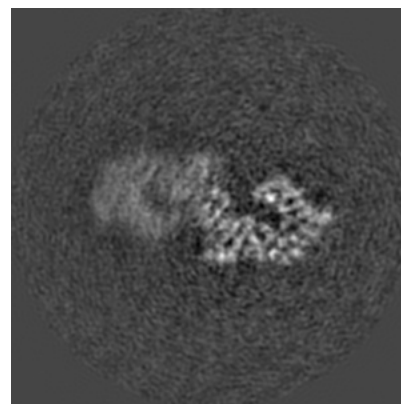
6.3.1 Primary map



X Index: 158



Y Index: 127

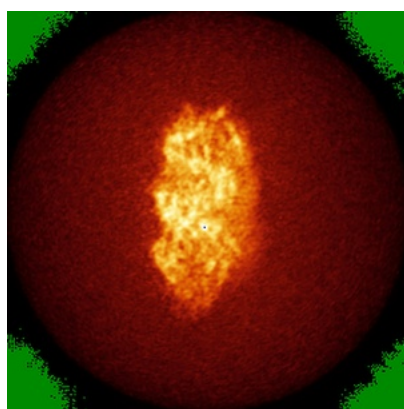


Z Index: 137

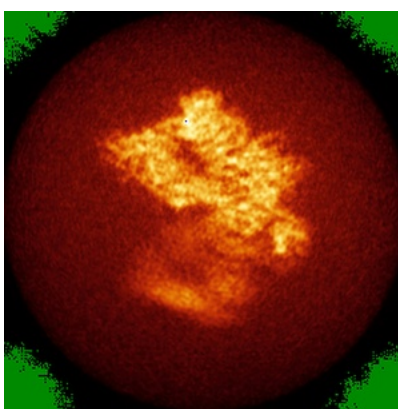
The images above show the largest variance slices of the map in three orthogonal directions.

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

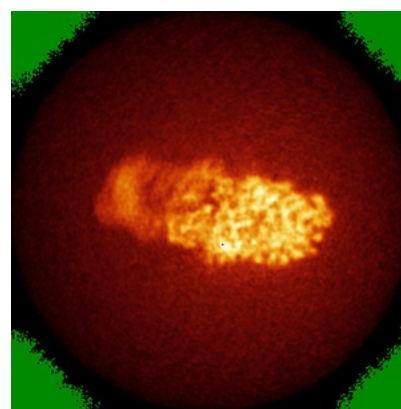
6.4.1 Primary map



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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

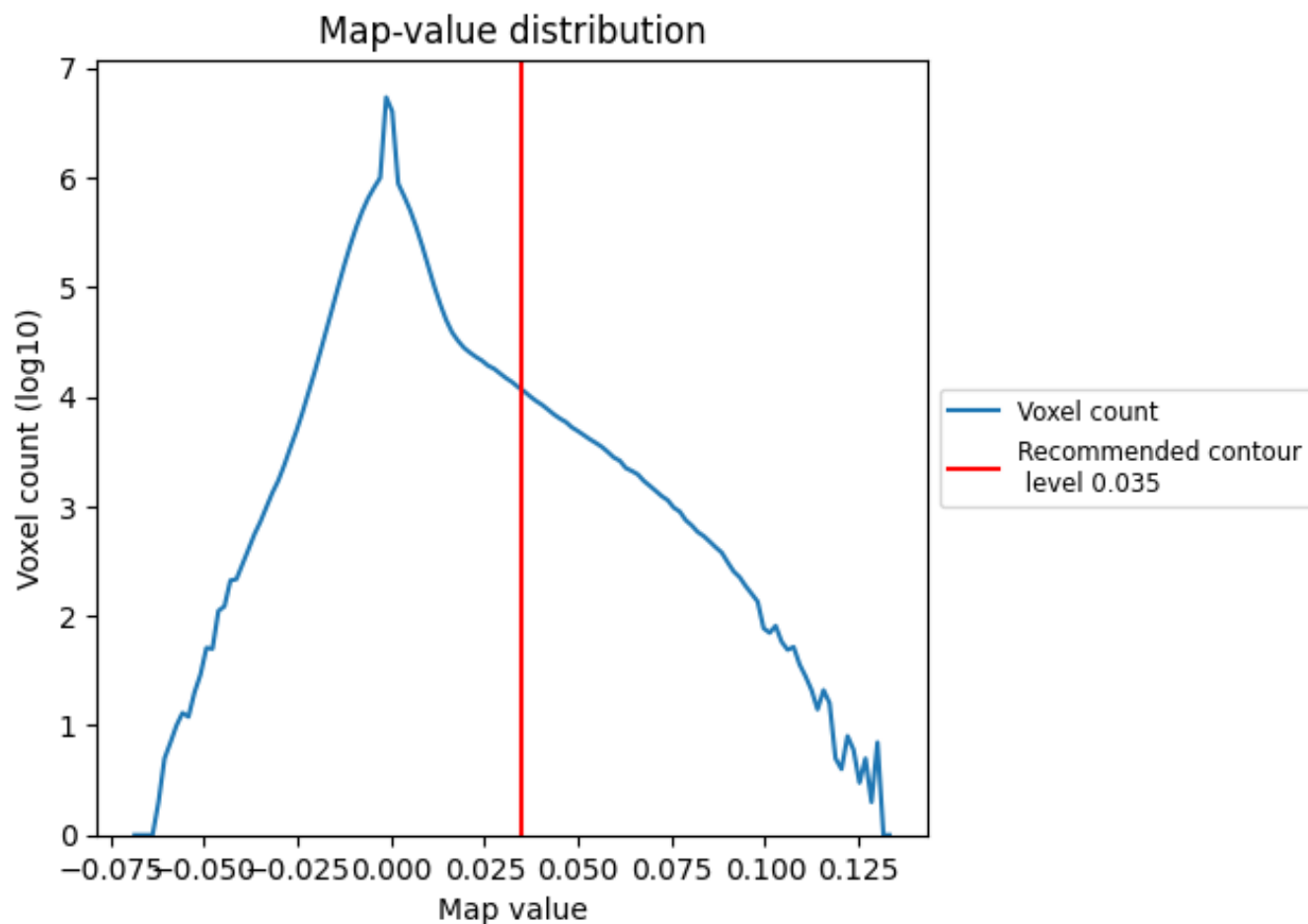
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

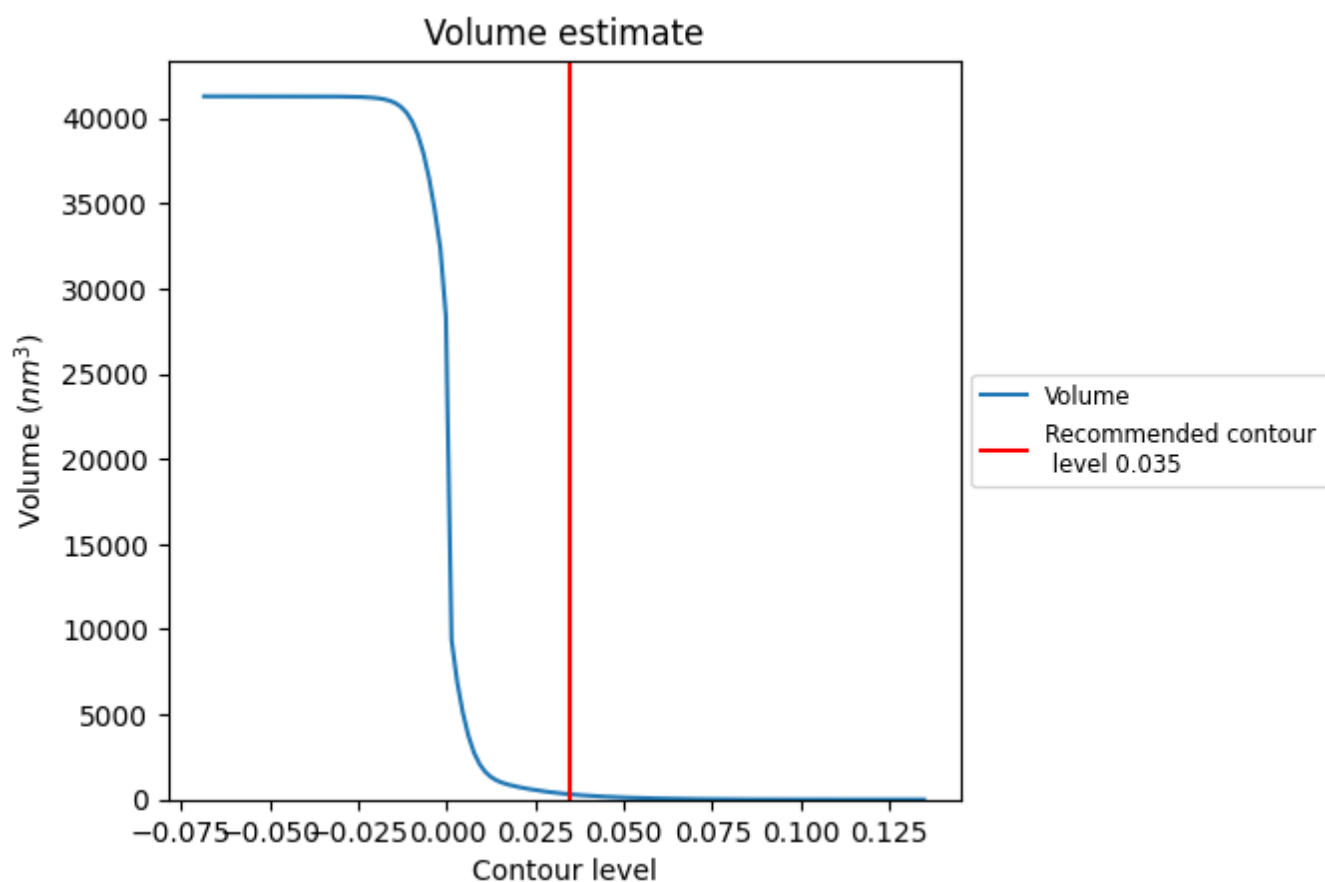
This section contains the results of statistical analysis of the map.

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.

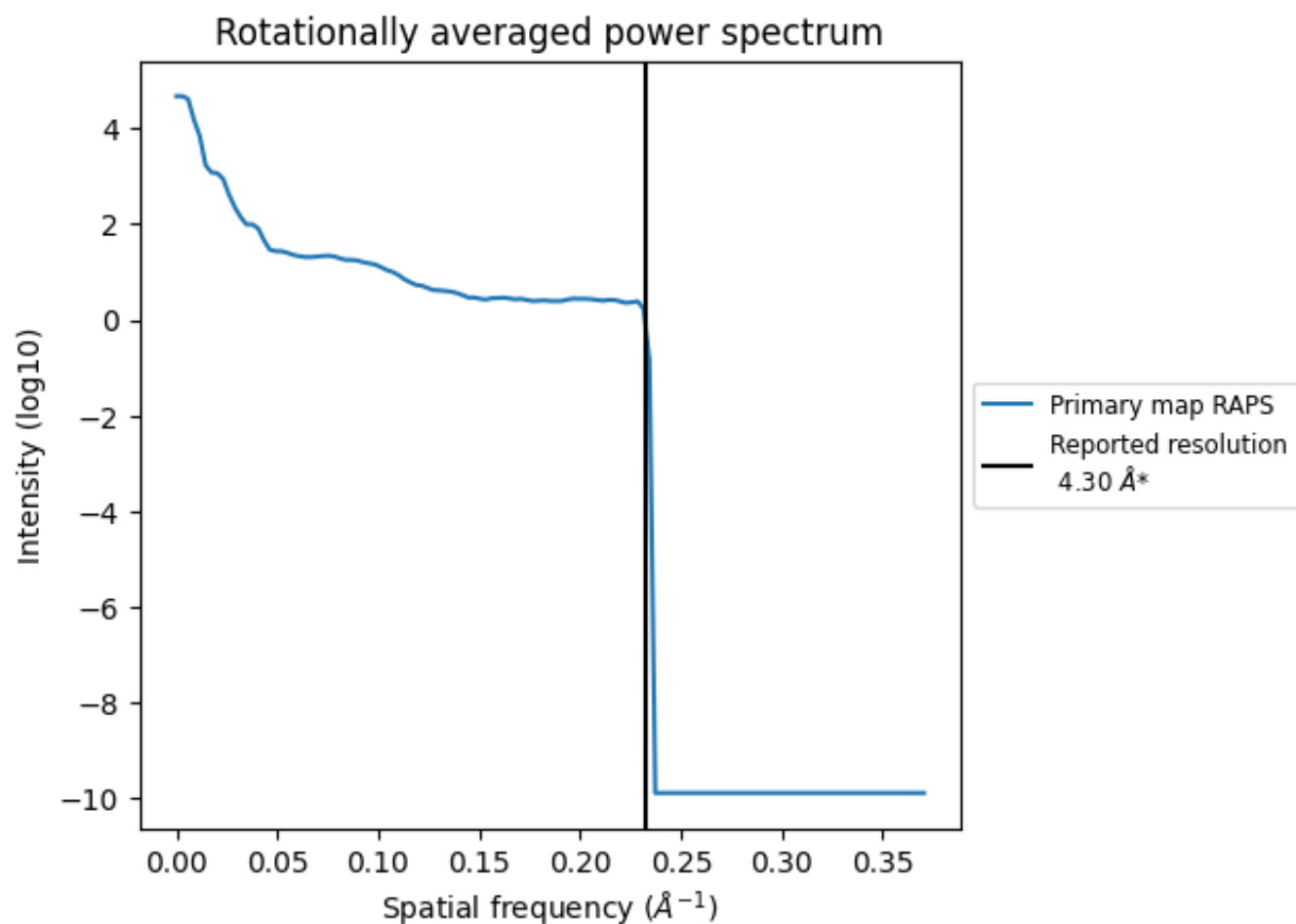
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; this corresponds to an approximate mass of 277 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 0.233 $\text{\AA}^{-1}$

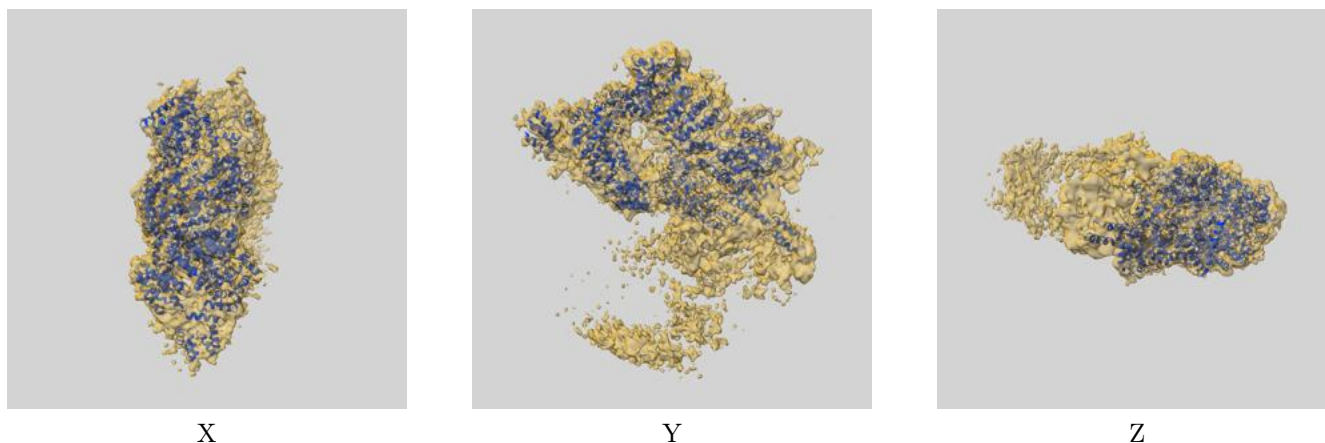
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

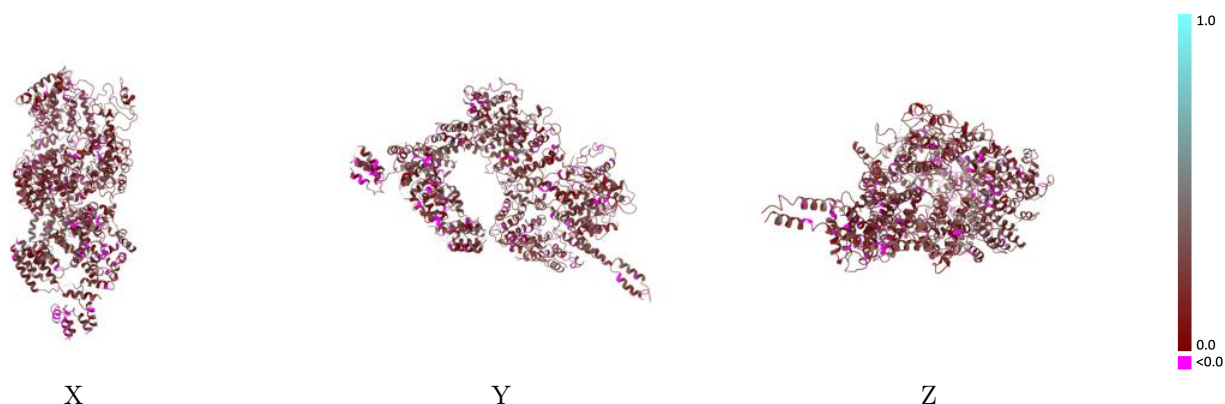
This section contains information regarding the fit between EMDB map EMD-9892 and PDB model 6JXA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



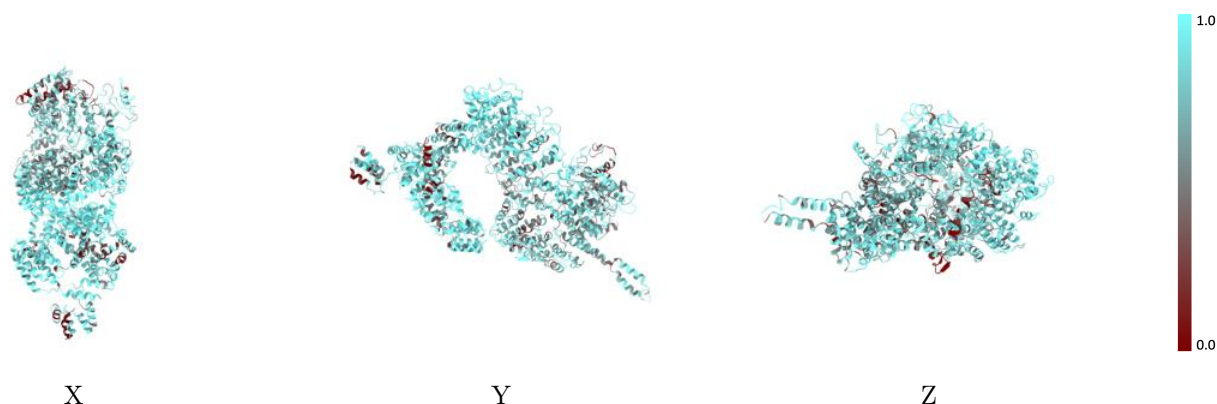
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



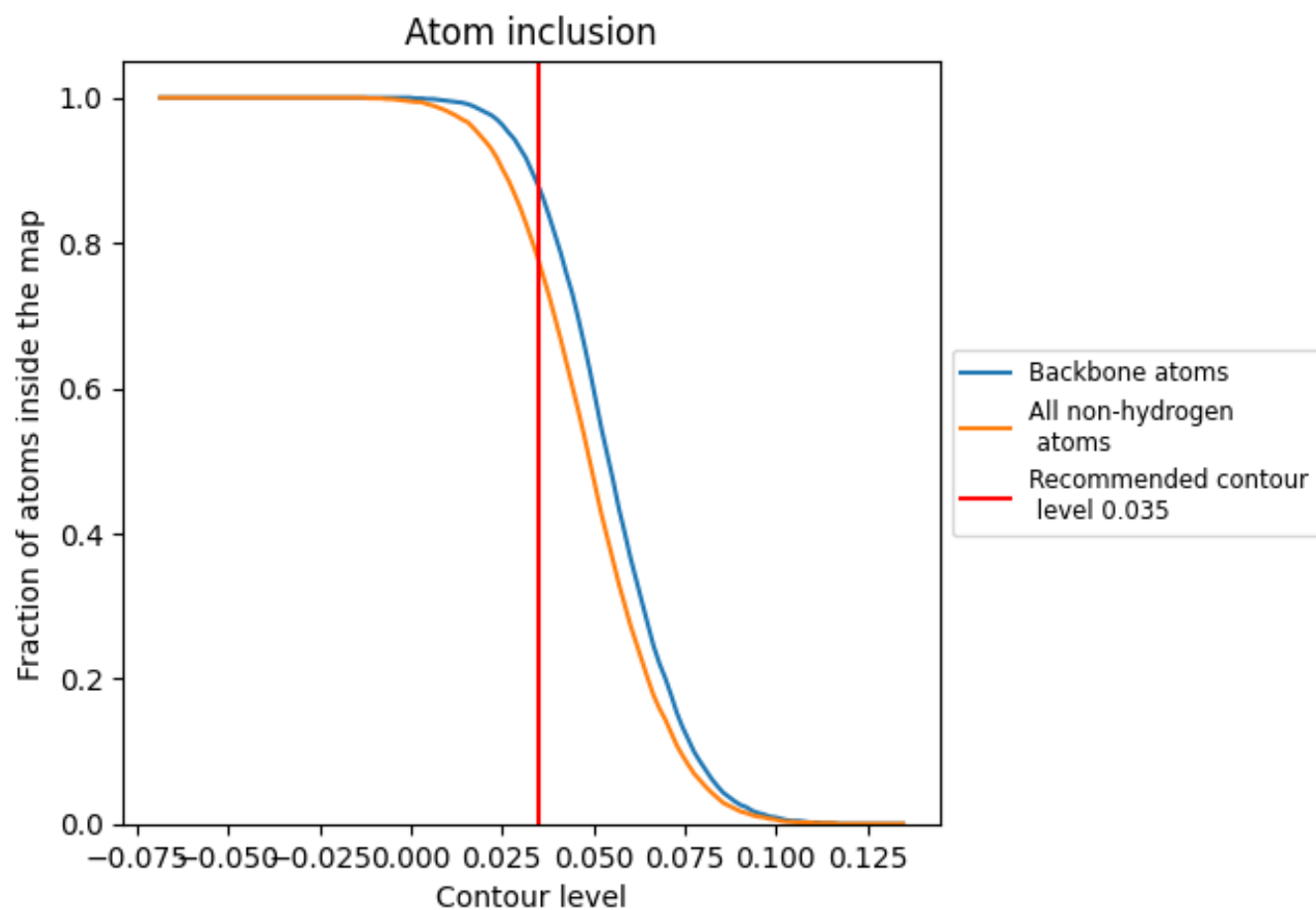
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.2040
A	0.7760	0.2040

