



Full wwPDB EM Validation Report ⓘ

Aug 11, 2026 – 04:40 PM EDT

PDB ID : 9YQK / pdb_00009yqk
EMDB ID : EMD-73338
Title : C-terminal LRRK2 bound to C12 DARPin
Authors : Sanz-Murillo, M.; Leschziner, A.
Deposited on : 2025-10-15
Resolution : 3.60 Å(reported)
Based on initial model : 6VP7

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.dev133
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) : 2.50

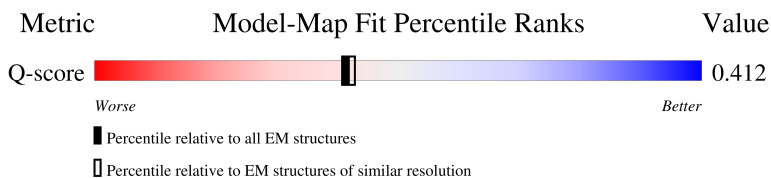
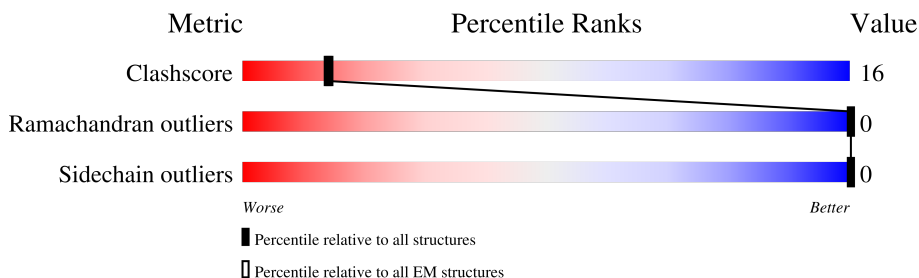
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	2527	 27% 14% 60%
2	B	131	 42% 34% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8925 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 Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1023	Total	C	N	O	S	0	0
			8174	5247	1398	1480	49		

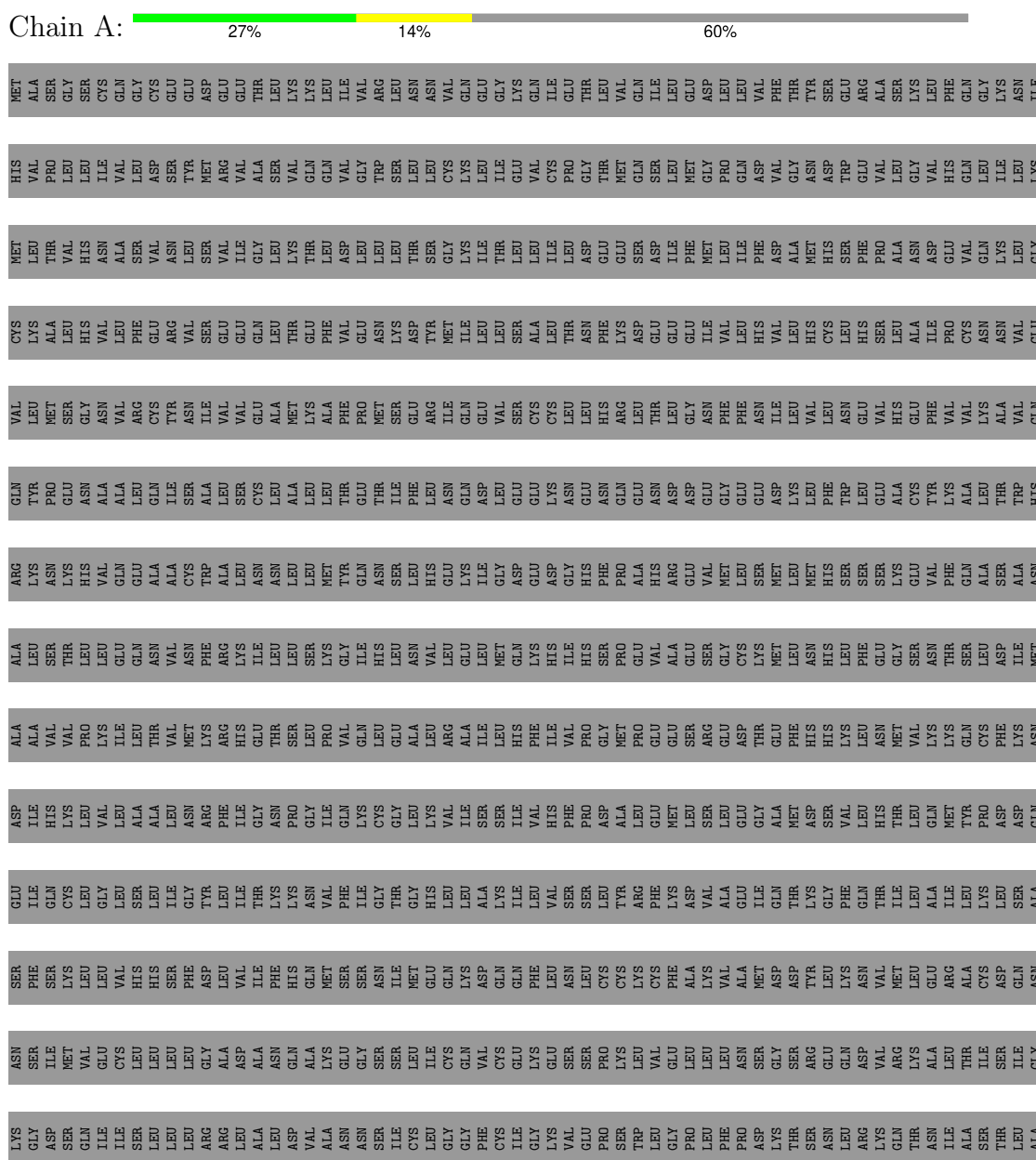
- Molecule 2 is a protein called C12 DARPin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	100	Total	C	N	O	S	0	0
			751	474	125	150	2		

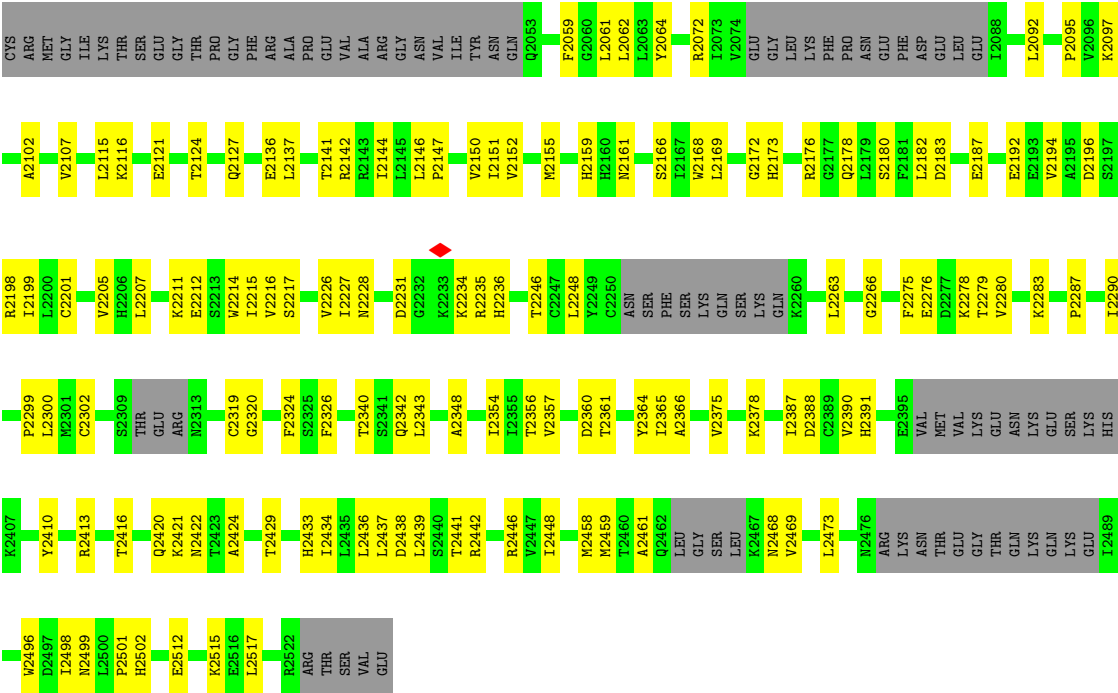
3 Residue-property plots

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.

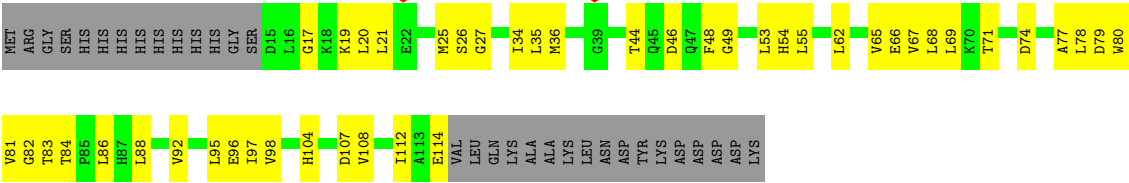
- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2



L1932	I1933	P1846	GLN	E1753	GLU	TTR	LEU	R1501	E1400	PHE	PRO	LEU	TLE	LYS	ASN	SER	ARG
I1934	R1847	P1846	GLN	K1502	F1401		GLN	K1502	F1401	LEU	PRO	ASP	SER	CYS	ALA	SER	MET
L1935	L1848	D1756	L1592	I1503	Y1402		GLN	I1503	Y1402	GLN	GLU	MET	LEU	PRO	THR	LEU	VAL
L1936	L1849	H1757	D1594	I1505	S1593		ARG	I1505	S1593	ARG	GLY	SER	SER	LEU	THR	GLN	VAL
A1937	I1850	H1758	L1595	F1511	H1405		LEU	H1405	H1405	LEU	CYS	ASN	GLU	LYS	PHE	LYS	TYR
A1938	P1851	L1763	L1596	F1511	P1406		LYS	F1511	P1406	LYS	LEU	ASP	ASN	GLN	PRO	GLN	LYS
G1939	I1855	K1764	Y1597	L1597			ALA	L1597		LYS	GLU	ILE	PHE	PHE	GLN	MET	SER
I1940			W1598	I1598			VAL	I1598		VAL	ASN	GLN	LEU	GLN	GLN	ASN	ARG
M1944	L1859	P1768	K1601	ASP	Q1411		ASP	ASP	Q1411	P1331	SER	PRO	CYS	TYR	VAL	VAL	ASP
L1945	I1860	I1680	W1602	GLN	R1412		GLN	GLN	R1412	M1335	LEU	GLY	GLU	ASN	THR	GLY	GLU
V1946	R1693	I1692	L1603	LEU	L1413		VAL	VAL	L1413	K1336	VAL	PRO	VAL	LEU	LEU	GLY	GLY
M1947	A1862	L1694	VAL	VAL	L1414		GLY	GLY	L1414	L1337	ASP	PRO	LYS	GLN	LEU	GLY	GLY
E1948	D1863	Y1695	II606	GLY	A1417		GLN	GLY	A1417	M1338	VAL	ALA	VAL	LEU	LYS	GLU	THR
L1949	L1864	E1696	Q1609	GLN	Y1418		LEU	LEU	Y1418	I1339	TYR	TRP	SER	GLU	LEU	TYR	ALA
P1895	P1865	M1697	L1611	ILE	Y1419		ILE	ILE	Y1419	V1340	ASN	LYS	PHE	VAL	THR	ARG	SER
R1866	W1791	P1701	T1612	PRO	A1430		GLU	GLU	A1430	L1351	LEU	LEU	ALA	PRO	GLY	GLY	ASP
M1869	P1792	F1792	W1613	D1525	M1430		LEU	LEU	M1430	M1355	ASN	ASN	ARG	ASN	ASP	ALA	SER
L1870	P1793	F1793	LYS	L1530	M1431		VAL	L1530	M1431	LYS	ARG	LEU	MET	LEU	GLY	GLY	VAL
L1875	L1795	W1705	VAL	E1531	P1432		GLY	E1531	P1432	THR	SER	GLU	PHE	GLN	GLN	ASN	GLY
E1876	L1796	R1707	GLY	II534	F1436		CYS	II534	F1436	LYS	PRO	LEU	LEU	VAL	VAL	CYS	PHE
F1877	ASP	I1709	CYS	R1538	R1441		PRO	R1538	R1441	LYS	ASN	LEU	ALA	GLY	GLY	SER	GLU
E1878	ILE	M1710	LYS	R1538	S1445		LYS	R1538	S1445	ASP	GLY	HIS	MET	GLY	VAL	ASN	VAL
F1883	CYS	R1711	HIS	P1542			PRO	P1542		GLY	LYS	ASN	PHE	LEU	PHE	GLN	SER
L1884	GLY	L1712	PRO	II543	L1454		GLY	II543	L1454	MET	LEU	GLN	LEU	GLN	PRO	ARG	LYS
L1885	GLY	E1714	GLY	E1544	D1455		ILE	E1544	D1455	GLN	SER	ILE	PRO	ILE	ASN	PHE	ASP
G1888	GLU	I1715	ILE	F1545			ILE	F1545		ALA	LYS	ILE	PRO	ILE	TYR	SER	GLU
G1891	L1807	Y1718	ILE	II548	D1458		ASP	II548	D1458	THR	ASP	ASP	THR	ILE	GLY	GLY	PHE
S1892	L1808	MET	S1627	D1548	R1462		LEU	D1548	R1462	W1369	LEU	LEU	ILE	ASN	MET	PHE	ASP
V1893	K1809	LEU	R1628	R1550			LEU	R1550		G1370	SER	SER	LEU	LYS	SER	GLY	GLY
Y1894	K1810	SER	R1629	K1551	K1468		GLY	K1551	K1468	I1371	PRO	LEU	LEU	ILE	PRO	ILE	PRO
R1895	V1811	GLY	E1632	R1552	I1469		ARG	R1552	I1469	D1372	ASP	GLU	LEU	GLY	ALA	PHE	ASP
Y1898	A1812	ARG	E1632	L1553	T1470		GLU	L1553	T1470	V1373	LEU	ALA	SER	ASP	ASP	SER	SER
E1899	L1813	GLU	K1637	L1554	Y1471		ALA	L1554	Y1471	I1378	LEU	TYR	GLN	ILE	ASN	HIS	GLY
	Y1814	ALA	K1638		E1472		LEU		E1472	GLN	HIS	LEU	ASN	CYS	LEU	MET	GLY
V1905	K1824	LEU	R1728	N1560			LEU	N1560		ILE	TRP	TRP	LYS	ASP	ASP	ASP	ASP
K1906	I1825		R1728	Q1561	E1472		LEU	Q1561	E1472	ARG	LEU	TRP	LYS	ASP	VAL	LEU	SER
I1907	L1826	SER	R1731	L1562	L1473		ASN	L1562	L1473	ILE	ASN	SER	PHE	PRO	VAL	LEU	SER
F1908	L1827	GLY	M1731	Q1563	L1474		PHE	Q1563	L1474	ASP	PHE	ARG	SER	LEU	VAL	PHE	VAL
N1909	L1830	ARG	Y1732	E1566	N1475		ASP	E1566	N1475	LYS	ASP	VAL	CYS	ARG	ARG	LYS	LYS
K1910	L1831	ALA	M1646	N1567	F1479		LEU	N1567	F1479	ARG	LEU	PHE	ILE	LEU	VAL	ARG	ALA
R1915	K1832	R1733	S1647	E1568	A1481		GLU	E1568	A1481	LYS	HIS	GLY	GLY	LYS	ASP	GLY	GLN
	E1836	Y1734	Q1648	P1570	D1484		ASP	P1570	D1484	ASP	ILE	LEU	ALA	LEU	ILE	ARG	SER
R1918	E1836	R1735	Y1649	L1569	Y1485		GLY	L1569	Y1485	L1388	GLY	HIS	PRO	LYS	GLY	GLY	ASP
L1921	G1837	Y1739	F1656	P1570			CYS	P1570		V1392	LEU	LEU	ILE	LEU	PRO	ILE	ASP
Y2018	D1838	L1740	Q1657	L1576	Y1485		LYS	L1576		W1393	HIS	LEU	ASN	LEU	VAL	SER	LEU
	L1839	N1741	L1660	L1582	N1489		LYS	L1582	N1489	A1396	ASN	LYS	ASN	ASN	VAL	SER	ASP
GLY	L1924	W1742	L1661	L1587	A1490		ASP	L1587	A1490	G1397	LEU	LEU	PRO	LEU	LEU	GLY	GLY
ILE		A1746	P1661	D1587			ILE	D1587		R1398	LEU	LYS	HIS	LEU	ASP	ASP	ASP
ALA	H1928	Y1747	TLE	PRO			GLY	PRO		E1399	ILE	LYS	ARG	ASN	PRO	SER	SER
L1929	H1929		GLY	ALA			GLU	ALA			GLU	GLU	THR	LEU	THR	GLY	GLY
TYR			GLU								ARG	ILE	SER	HIS	VAL	ARG	ARG
CYS																	



• Molecule 2: C12 DARPin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	392016	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	36000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	89.698	Depositor
Minimum map value	-71.407	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.930	Depositor
Recommended contour level	5.14	Depositor
Map size ($\text{\AA}$)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	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	0.19	0/8329	0.44	2/11254 (0.0%)
2	B	0.17	0/761	0.47	0/1036
All	All	0.19	0/9090	0.45	2/12290 (0.0%)

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	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1928	HIS	CA-C-N	5.17	127.19	120.26
1	A	1928	HIS	C-N-CA	5.17	127.19	120.26

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1928	HIS	Peptide
1	A	1929	HIS	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8174	0	8315	251	0
2	B	751	0	745	33	0
All	All	8925	0	9060	279	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 16.

All (279) 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:1468:LYS:NZ	1:A:1472:GLU:OE1	2.13	0.82
1:A:2375:VAL:HG21	1:A:2442:ARG:HH22	1.42	0.82
2:B:20:LEU:HD23	2:B:44:THR:HG21	1.65	0.79
1:A:1400:GLU:OE1	1:A:1657:GLN:NE2	2.14	0.79
1:A:1733:TYR:HB3	1:A:1738:ILE:HG22	1.64	0.79
1:A:1935:LEU:HD11	1:A:1945:LEU:HD22	1.63	0.79
1:A:1592:LEU:HD21	1:A:1648:GLN:HB3	1.66	0.77
1:A:1419:TYR:HB3	1:A:1431:MET:HE1	1.69	0.74
2:B:74:ASP:HB3	2:B:77:ALA:HB2	1.70	0.74
1:A:1396:ALA:HB3	1:A:1398:ARG:HH21	1.52	0.74
1:A:1933:ILE:HD11	1:A:2001:LEU:HD12	1.68	0.73
1:A:2092:LEU:HD21	1:A:2115:LEU:HD23	1.70	0.73
1:A:2155:MET:HE1	1:A:2473:LEU:HB2	1.72	0.72
1:A:1602:TRP:O	1:A:1606:ILE:HG13	1.91	0.71
1:A:1863:ASP:OD2	1:A:1918:ARG:NH2	2.21	0.70
1:A:1771:ARG:HH22	1:A:1866:ARG:HG2	1.57	0.70
1:A:1888:GLY:O	1:A:1910:LYS:NZ	2.22	0.69
1:A:1883:PHE:HE2	1:A:1895:ARG:HD3	1.57	0.69
1:A:1712:LEU:HD22	1:A:1738:ILE:HD11	1.75	0.69
1:A:1660:LEU:O	1:A:1668:LEU:N	2.26	0.68
1:A:2136:GLU:OE2	1:A:2446:ARG:NH2	2.26	0.68
1:A:1639:ARG:NH1	1:A:1640:LYS:O	2.26	0.68
2:B:53:LEU:HD22	2:B:68:LEU:HD13	1.74	0.68
1:A:1705:TRP:O	1:A:1709:ILE:HG12	1.93	0.68
1:A:1660:LEU:HD13	1:A:1710:ASN:HB3	1.75	0.67
1:A:2194:VAL:HG11	1:A:2227:ILE:HD11	1.77	0.67
2:B:25:MET:HG2	2:B:55:LEU:HD23	1.76	0.67
1:A:1405:HIS:HA	1:A:1441:ARG:NH1	2.10	0.67
1:A:1371:ILE:HD11	1:A:1402:TYR:HE2	1.60	0.66
1:A:1404:THR:O	1:A:1441:ARG:NH1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1673:LEU:HB2	1:A:1735:ARG:HB3	1.78	0.66
1:A:2207:LEU:O	1:A:2211:LYS:N	2.29	0.65
1:A:2212:GLU:OE2	1:A:2228:ASN:ND2	2.30	0.65
2:B:54:HIS:NE2	2:B:83:THR:O	2.28	0.65
1:A:1552:ARG:HD2	1:A:1552:ARG:O	1.97	0.65
1:A:2299:PRO:O	1:A:2320:GLY:N	2.27	0.65
1:A:1924:LEU:HD21	1:A:1947:MET:HE1	1.78	0.64
1:A:2107:VAL:HG23	1:A:2137:LEU:HD11	1.78	0.64
2:B:36:MET:HE3	2:B:71:THR:HG21	1.79	0.64
1:A:1337:LEU:HD23	1:A:1392:VAL:HG12	1.80	0.64
1:A:1531:GLU:HG3	1:A:1576:LEU:HD11	1.80	0.64
1:A:1827:LEU:HD12	1:A:1859:LEU:HD21	1.81	0.63
1:A:1405:HIS:CE1	1:A:1656:PHE:HA	2.34	0.63
1:A:2360:ASP:OD1	1:A:2361:THR:N	2.30	0.62
1:A:2287:PRO:HG2	1:A:2290:ILE:HD11	1.81	0.62
1:A:1543:ILE:HG13	1:A:1545:PHE:H	1.63	0.61
1:A:1870:LEU:HB3	1:A:1937:ALA:HB1	1.83	0.60
1:A:1569:LEU:HD23	1:A:1570:PRO:HD3	1.83	0.59
1:A:1756:ASP:O	1:A:1758:HIS:ND1	2.34	0.59
1:A:2442:ARG:HD2	2:B:48:PHE:CE1	2.37	0.59
1:A:1629:ARG:HH21	1:A:1632:GLU:HG3	1.67	0.59
1:A:1470:THR:HG23	1:A:1474:LEU:HD12	1.84	0.59
1:A:2152:VAL:HG13	1:A:2473:LEU:HD21	1.84	0.59
1:A:2246:THR:OG1	1:A:2300:LEU:O	2.21	0.59
1:A:2410:TYR:O	1:A:2413:ARG:NH1	2.36	0.58
1:A:1657:GLN:HB2	1:A:1707:ARG:HH12	1.68	0.58
2:B:69:LEU:HD23	2:B:104:HIS:CG	2.39	0.58
1:A:1489:ASN:OD1	1:A:1490:ALA:N	2.36	0.58
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.86	0.58
1:A:1530:LEU:HD11	1:A:1561:GLN:HE21	1.68	0.57
1:A:1405:HIS:O	1:A:1441:ARG:NH2	2.32	0.57
1:A:2227:ILE:HG12	1:A:2235:ARG:HG2	1.85	0.57
1:A:2429:THR:OG1	1:A:2433:HIS:HB2	2.05	0.57
1:A:2512:GLU:OE1	1:A:2515:LYS:NZ	2.33	0.57
1:A:1921:LEU:HD21	1:A:1945:LEU:HD21	1.86	0.56
1:A:2061:LEU:HD12	1:A:2072:ARG:CZ	2.35	0.56
1:A:2266:GLY:HA3	1:A:2300:LEU:HD22	1.87	0.56
1:A:2300:LEU:HA	1:A:2319:CYS:HA	1.86	0.56
1:A:1746:ALA:HA	1:A:1768:PRO:HG2	1.87	0.56
1:A:1934:SER:OG	1:A:1948:GLU:OE1	2.19	0.56
1:A:2391:HIS:NE2	2:B:81:VAL:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2342:GLN:HE22	1:A:2348:ALA:HA	1.70	0.56
1:A:1791:TRP:HD1	1:A:1791:TRP:O	1.88	0.56
1:A:1878:GLU:OE1	1:A:1878:GLU:N	2.38	0.56
1:A:2166:SER:HA	1:A:2183:ASP:HA	1.88	0.56
1:A:2172:GLY:O	1:A:2198:ARG:NH1	2.39	0.56
1:A:1405:HIS:CE1	1:A:1406:PRO:HG3	2.41	0.55
1:A:1371:ILE:HD11	1:A:1402:TYR:CE2	2.39	0.55
1:A:1909:ASN:OD1	1:A:1910:LYS:N	2.40	0.55
1:A:1810:LYS:NZ	1:A:1811:TRP:O	2.40	0.54
1:A:1739:TYR:CE2	1:A:1741:ASN:HB2	2.43	0.54
1:A:1924:LEU:HD23	1:A:1935:LEU:HD13	1.89	0.54
1:A:2375:VAL:HG21	1:A:2442:ARG:NH2	2.19	0.54
1:A:2216:VAL:HG13	1:A:2248:LEU:HD23	1.89	0.54
1:A:2231:ASP:OD2	1:A:2234:LYS:NZ	2.40	0.54
1:A:2420:GLN:HE21	1:A:2424:ALA:HB3	1.72	0.54
1:A:2468:ASN:HB2	1:A:2498:ILE:HG21	1.89	0.54
1:A:1459:GLU:HG2	1:A:1462:ARG:HH21	1.73	0.53
1:A:2159:HIS:ND1	1:A:2161:ASN:OD1	2.38	0.53
1:A:2416:THR:OG1	1:A:2458:MET:HE3	2.07	0.53
1:A:2228:ASN:OD1	1:A:2231:ASP:N	2.38	0.53
1:A:2448:ILE:HG21	1:A:2496:TRP:CH2	2.43	0.53
1:A:1885:LEU:HD11	1:A:1895:ARG:HD2	1.91	0.53
1:A:1895:ARG:NH2	1:A:1949:LEU:O	2.42	0.53
1:A:1560:ASN:HB3	1:A:1563:GLN:HB2	1.91	0.52
1:A:1861:LEU:HG	1:A:1940:ILE:HD13	1.91	0.52
1:A:2420:GLN:NE2	1:A:2501:PRO:HG2	2.24	0.52
1:A:1594:ASP:OD1	1:A:1595:LEU:N	2.42	0.52
1:A:1713:LEU:HD22	1:A:1731:ARG:HD3	1.91	0.52
1:A:2141:THR:HG22	1:A:2142:ARG:HG2	1.90	0.52
1:A:1405:HIS:HA	1:A:1441:ARG:HH12	1.74	0.52
1:A:1551:LYS:HD3	1:A:1551:LYS:O	2.09	0.52
1:A:1875:LEU:HD13	1:A:1898:TYR:HD2	1.75	0.52
1:A:1401:PHE:HZ	1:A:1611:LEU:HD13	1.75	0.51
1:A:2302:CYS:SG	1:A:2357:VAL:N	2.83	0.51
1:A:2207:LEU:O	1:A:2211:LYS:CA	2.58	0.51
1:A:1791:TRP:C	1:A:1793:PRO:HD3	2.36	0.51
1:A:2176:ARG:HH21	1:A:2196:ASP:HA	1.76	0.51
1:A:1469:ILE:HG23	1:A:1473:LEU:HD12	1.92	0.51
1:A:1484:ASP:OD1	1:A:1485:TYR:N	2.44	0.51
1:A:1530:LEU:HD11	1:A:1561:GLN:HG3	1.93	0.51
1:A:1807:LEU:HG	1:A:1808:LEU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1814:TYR:HB2	1:A:1855:ILE:HD12	1.92	0.50
1:A:2152:VAL:HG21	1:A:2169:LEU:HD23	1.93	0.50
1:A:1863:ASP:OD1	1:A:1864:LEU:N	2.44	0.50
1:A:1531:GLU:O	1:A:1534:ILE:HG12	2.11	0.50
2:B:62:LEU:HD13	2:B:97:ILE:HD13	1.93	0.50
1:A:1335:MET:HE1	1:A:1414:LEU:HD11	1.94	0.49
1:A:1538:ARG:HD2	1:A:1598:VAL:HG21	1.94	0.49
1:A:1606:ILE:HG21	1:A:1641:PHE:HE1	1.76	0.49
1:A:1709:ILE:O	1:A:1713:LEU:HG	2.12	0.49
2:B:86:LEU:HD11	2:B:98:VAL:HG13	1.94	0.49
1:A:1339:ILE:HD12	1:A:1351:LEU:HD12	1.94	0.49
1:A:1534:ILE:O	1:A:1538:ARG:HG2	2.13	0.49
1:A:2391:HIS:CD2	2:B:82:GLY:HA3	2.48	0.49
1:A:1469:ILE:O	1:A:1473:LEU:HB2	2.13	0.49
2:B:79:ASP:OD1	2:B:80:TRP:N	2.45	0.49
1:A:1982:LEU:HD21	1:A:1995:LEU:HD22	1.93	0.49
1:A:2236:HIS:HB2	1:A:2283:LYS:HD3	1.94	0.49
1:A:1693:ARG:HB3	1:A:1810:LYS:NZ	2.28	0.49
1:A:2438:ASP:HB3	1:A:2441:THR:O	2.13	0.48
1:A:2421:LYS:HG3	1:A:2422:ASN:ND2	2.28	0.48
1:A:2124:THR:HG23	1:A:2127:GLN:H	1.78	0.48
2:B:34:ILE:HG13	2:B:35:LEU:HD12	1.96	0.48
1:A:2207:LEU:O	1:A:2211:LYS:HA	2.13	0.48
1:A:2343:LEU:HD21	2:B:95:LEU:HD22	1.94	0.48
1:A:1693:ARG:HB3	1:A:1810:LYS:HZ3	1.78	0.48
1:A:2354:ILE:HD11	1:A:2365:ILE:HG23	1.95	0.48
2:B:21:LEU:HD11	2:B:46:ASP:HB3	1.94	0.48
1:A:1336:LYS:HE2	1:A:1409:MET:HE1	1.96	0.48
1:A:1693:ARG:HH21	1:A:1810:LYS:HE3	1.78	0.48
2:B:78:LEU:HD11	2:B:82:GLY:HA2	1.96	0.48
1:A:2276:GLU:HG3	1:A:2278:LYS:H	1.78	0.48
1:A:1609:GLN:O	1:A:1612:THR:OG1	2.23	0.48
1:A:1840:LEU:O	1:A:1848:LEU:HB2	2.14	0.48
1:A:1641:PHE:HD2	1:A:1642:PRO:HD2	1.79	0.47
1:A:1497:LEU:HB3	1:A:1501:ARG:HH22	1.80	0.47
1:A:1795:LEU:H	1:A:1795:LEU:HD23	1.79	0.47
1:A:1410:THR:O	1:A:1445:SER:OG	2.33	0.47
1:A:2146:LEU:HD21	1:A:2182:LEU:HD22	1.95	0.47
1:A:2340:THR:HB	2:B:92:VAL:HA	1.95	0.47
1:A:1968:ARG:HH21	1:A:2102:ALA:HB3	1.79	0.47
2:B:95:LEU:H	2:B:95:LEU:HD23	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.95	0.47
1:A:1430:ALA:O	1:A:1433:PRO:HD2	2.15	0.47
1:A:2422:ASN:HA	1:A:2439:LEU:HD12	1.96	0.47
1:A:1811:TRP:CE3	1:A:1824:LYS:HB3	2.49	0.47
1:A:2387:ILE:HD11	1:A:2442:ARG:CZ	2.45	0.47
2:B:84:THR:C	2:B:86:LEU:H	2.23	0.47
1:A:2420:GLN:HE22	1:A:2501:PRO:HG2	1.80	0.46
1:A:1401:PHE:CE1	1:A:1611:LEU:HD22	2.51	0.46
2:B:46:ASP:OD1	2:B:49:GLY:N	2.48	0.46
1:A:1836:GLU:HG3	1:A:1838:ASP:H	1.80	0.46
1:A:2199:ILE:HD11	1:A:2217:SER:HB3	1.96	0.46
2:B:17:GLY:O	2:B:21:LEU:HG	2.15	0.46
1:A:1753:GLU:OE2	1:A:1764:LYS:HD2	2.16	0.46
1:A:1832:LYS:HB2	1:A:1832:LYS:HE3	1.80	0.46
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	1.98	0.46
1:A:2064:TYR:CE1	1:A:2095:PRO:HG3	2.50	0.46
1:A:2214:TRP:CE3	1:A:2226:VAL:HG12	2.51	0.46
1:A:1404:THR:OG1	1:A:1405:HIS:N	2.50	0.45
1:A:1628:ARG:O	1:A:1632:GLU:HG2	2.15	0.45
1:A:1436:PHE:CD2	1:A:1701:PRO:HB3	2.51	0.45
1:A:1775:ILE:HA	1:A:1863:ASP:HB2	1.98	0.45
1:A:1786:SER:OG	1:A:1915:ARG:NH2	2.49	0.45
1:A:2438:ASP:OD1	1:A:2439:LEU:N	2.49	0.45
1:A:1603:LEU:HA	1:A:1606:ILE:HD12	1.99	0.45
1:A:1791:TRP:O	1:A:1791:TRP:CD1	2.68	0.45
1:A:1810:LYS:HG3	1:A:1827:LEU:HD23	1.98	0.45
1:A:1810:LYS:O	1:A:1826:LEU:HD12	2.17	0.45
1:A:1966:LEU:HD13	1:A:1970:LEU:HD23	1.99	0.45
1:A:2178:GLN:HB2	1:A:2192:GLU:O	2.16	0.45
2:B:62:LEU:HD11	2:B:96:GLU:HB3	1.99	0.45
1:A:1695:TYR:HD2	1:A:1808:LEU:HD11	1.82	0.45
1:A:1712:LEU:HD23	1:A:1712:LEU:O	2.17	0.45
1:A:2361:THR:O	1:A:2378:LYS:NZ	2.45	0.45
1:A:2364:TYR:CD2	1:A:2375:VAL:HG22	2.51	0.45
1:A:1877:PHE:HE2	1:A:1907:ILE:HD13	1.82	0.44
1:A:2201:CYS:SG	1:A:2248:LEU:HD13	2.58	0.44
1:A:1891:GLY:HA2	1:A:1910:LYS:HE2	1.98	0.44
1:A:2155:MET:HE3	1:A:2459:MET:HE1	1.99	0.44
1:A:1955:LEU:HD13	1:A:2002:LEU:HD11	1.99	0.44
2:B:88:LEU:O	2:B:92:VAL:HG12	2.17	0.44
2:B:92:VAL:HG13	2:B:92:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1814:TYR:HE1	1:A:1825:ILE:HB	1.82	0.44
2:B:26:SER:OG	2:B:27:GLY:N	2.51	0.44
1:A:1747:TYR:CD1	1:A:1768:PRO:HG3	2.53	0.44
1:A:1962:ASP:OD1	1:A:1962:ASP:N	2.51	0.44
1:A:1697:MET:HE1	1:A:1704:PHE:CE2	2.53	0.44
1:A:2151:ILE:HG12	1:A:2173:HIS:HB3	1.99	0.44
1:A:1340:VAL:O	1:A:1417:ALA:HA	2.18	0.43
1:A:1715:ILE:O	1:A:1742:TRP:HZ2	2.01	0.43
1:A:1898:TYR:HD1	1:A:1899:GLU:OE1	2.01	0.43
1:A:1455:ASP:OD1	1:A:1455:ASP:N	2.50	0.43
1:A:1606:ILE:HD13	1:A:1641:PHE:CE1	2.53	0.43
1:A:1864:LEU:HD11	1:A:1869:MET:SD	2.58	0.43
1:A:2097:LYS:HA	1:A:2097:LYS:HE2	2.00	0.43
1:A:2168:TRP:CE3	1:A:2215:ILE:HD13	2.53	0.43
1:A:2276:GLU:HG2	1:A:2279:THR:HG23	2.00	0.43
2:B:19:LYS:HA	2:B:19:LYS:HE2	1.99	0.43
1:A:1747:TYR:O	1:A:1768:PRO:HD3	2.18	0.43
1:A:1839:LEU:HD22	1:A:1851:PRO:HA	2.01	0.43
1:A:2356:THR:HG22	1:A:2366:ALA:HB3	2.00	0.43
2:B:65:VAL:HG21	2:B:97:ILE:HD12	2.00	0.43
1:A:1603:LEU:HD13	1:A:1606:ILE:HD12	1.99	0.43
1:A:1979:ALA:HB2	1:A:2059:PHE:CZ	2.53	0.43
1:A:1677:ARG:HH21	1:A:1680:ILE:HD13	1.84	0.43
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	2.00	0.43
2:B:62:LEU:O	2:B:66:GLU:HG3	2.19	0.43
1:A:1741:ASN:ND2	1:A:1747:TYR:HB3	2.34	0.43
1:A:1968:ARG:NH2	1:A:2102:ALA:HB3	2.34	0.43
1:A:2169:LEU:HB2	1:A:2180:SER:HB2	2.01	0.43
2:B:107:ASP:OD1	2:B:108:VAL:N	2.51	0.43
1:A:1458:ASP:O	1:A:1462:ARG:HG3	2.18	0.43
1:A:1470:THR:HA	1:A:1474:LEU:HG	1.99	0.43
1:A:1646:MET:HA	1:A:1649:TYR:CD2	2.53	0.43
1:A:1945:LEU:HD23	1:A:1945:LEU:HA	1.81	0.43
1:A:1933:ILE:HD12	1:A:2016:ALA:HA	2.00	0.43
1:A:2176:ARG:HE	1:A:2196:ASP:HA	1.82	0.43
1:A:2324:PHE:HE2	1:A:2326:PHE:HE2	1.67	0.43
1:A:1405:HIS:NE2	1:A:1656:PHE:HA	2.34	0.42
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.85	0.42
1:A:1538:ARG:NH2	1:A:1548:ILE:HD13	2.34	0.42
1:A:1610:ILE:HD12	1:A:1610:ILE:H	1.84	0.42
1:A:2064:TYR:HE1	1:A:2095:PRO:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1841:VAL:HA	1:A:1848:LEU:HB2	2.01	0.42
1:A:1978:VAL:HG11	1:A:2062:LEU:CD2	2.50	0.42
1:A:2147:PRO:O	1:A:2150:VAL:HG12	2.20	0.42
2:B:66:GLU:OE2	2:B:67:VAL:HG13	2.20	0.42
1:A:1550:ARG:HB2	1:A:1594:ASP:HB2	2.01	0.42
1:A:1893:VAL:HG12	1:A:1906:LYS:HA	2.02	0.41
1:A:1582:LEU:HB2	1:A:1597:PHE:O	2.21	0.41
1:A:1677:ARG:HE	1:A:1680:ILE:HD13	1.85	0.41
1:A:1692:ILE:HG21	1:A:1764:LYS:HE2	2.02	0.41
1:A:1973:ARG:HB3	1:A:2012:ILE:HD12	2.02	0.41
1:A:2388:ASP:OD1	1:A:2390:VAL:HG22	2.20	0.41
2:B:112:ILE:O	2:B:114:GLU:HG3	2.20	0.41
1:A:1939:GLY:HA3	1:A:1944:MET:HG2	2.02	0.41
1:A:2263:LEU:HD23	1:A:2275:PHE:HD2	1.84	0.41
1:A:1830:LEU:HD12	1:A:1830:LEU:HA	1.93	0.41
1:A:2116:LYS:HG3	1:A:2121:GLU:OE1	2.20	0.41
1:A:2144:ILE:HD12	1:A:2187:GLU:OE1	2.20	0.41
1:A:2436:LEU:O	1:A:2437:LEU:HD22	2.20	0.41
2:B:62:LEU:HD21	2:B:96:GLU:HB2	2.01	0.41
1:A:1479:PHE:O	1:A:1481:ALA:N	2.47	0.41
1:A:1501:ARG:O	1:A:1505:ILE:HG12	2.21	0.41
1:A:1548:ILE:HD12	1:A:1554:LEU:HD12	2.01	0.41
1:A:2388:ASP:HB3	1:A:2391:HIS:CE1	2.55	0.41
1:A:1431:MET:HE3	1:A:1431:MET:HB2	1.93	0.41
1:A:1932:LEU:HD23	1:A:1932:LEU:HA	1.82	0.41
1:A:1371:ILE:H	1:A:1601:LYS:HG3	1.85	0.41
1:A:1373:VAL:HG22	1:A:1393:TRP:CD1	2.56	0.41
1:A:2205:VAL:HG21	1:A:2280:VAL:HG11	2.02	0.41
1:A:1569:LEU:CD2	1:A:1570:PRO:HD3	2.49	0.41
1:A:1847:ARG:HD3	1:A:1849:THR:H	1.85	0.41
1:A:2517:LEU:HD23	1:A:2517:LEU:HA	1.94	0.41
1:A:1500:LEU:HA	1:A:1503:THR:HG22	2.02	0.41
1:A:1606:ILE:O	1:A:1609:GLN:HB2	2.21	0.40
1:A:2152:VAL:HG21	1:A:2169:LEU:HB3	2.02	0.40
1:A:2434:ILE:HG22	1:A:2434:ILE:O	2.21	0.40
1:A:2461:ALA:HB3	1:A:2469:VAL:HG23	2.03	0.40
1:A:1692:ILE:CG2	1:A:1813:LEU:HD12	2.50	0.40
1:A:1472:GLU:O	1:A:1472:GLU:HG2	2.21	0.40
1:A:1739:TYR:HE2	1:A:1747:TYR:HB2	1.85	0.40
1:A:2003:PHE:CE2	1:A:2014:LYS:HE3	2.57	0.40
1:A:2499:ASN:OD1	1:A:2502:HIS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1335:MET:HG2	1:A:1412:ARG:HG3	2.04	0.40
1:A:1814:TYR:CB	1:A:1855:ILE:HD12	2.51	0.40
1:A:1992:TYR:CE2	1:A:1995:LEU:HD13	2.57	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	987/2527 (39%)	908 (92%)	79 (8%)	0	100	100
2	B	98/131 (75%)	90 (92%)	8 (8%)	0	100	100
All	All	1085/2658 (41%)	998 (92%)	87 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	912/2281 (40%)	912 (100%)	0	100	100
2	B	79/106 (74%)	79 (100%)	0	100	100
All	All	991/2387 (42%)	991 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1352	GLN
1	A	1437	ASN
1	A	1561	GLN
1	A	1741	ASN
1	A	1879	GLN
1	A	1919	GLN
1	A	2420	GLN
1	A	2476	ASN
2	B	38	ASN
2	B	104	HIS

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.

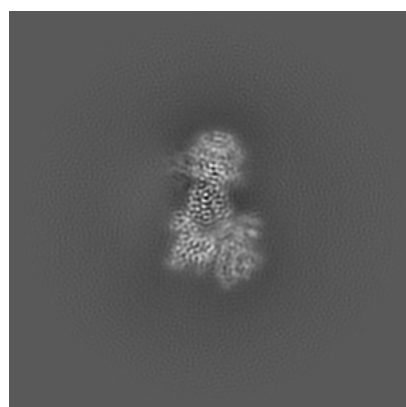
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73338. These allow visual inspection of the internal detail of the map and identification of artifacts.

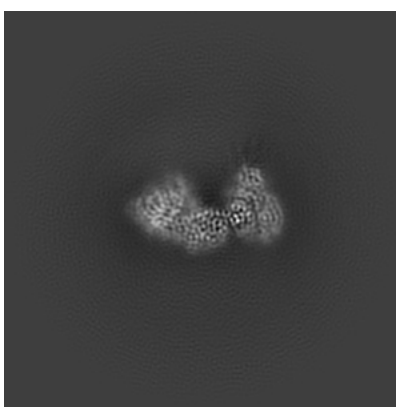
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

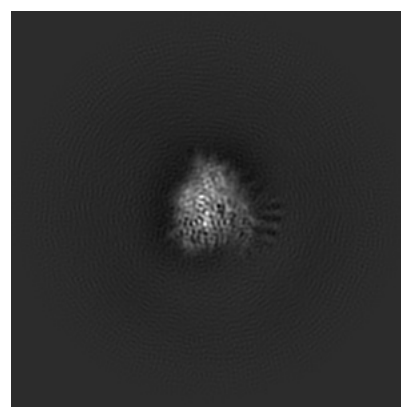
6.1.1 Primary map



X



Y

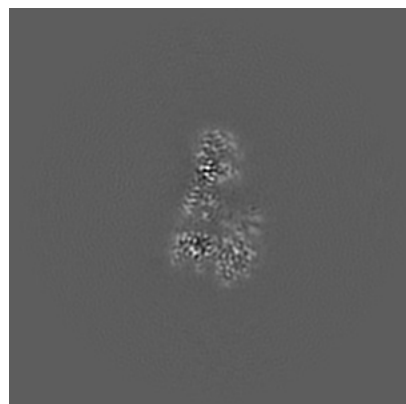


Z

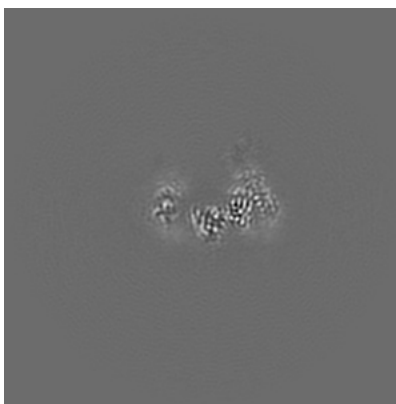
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

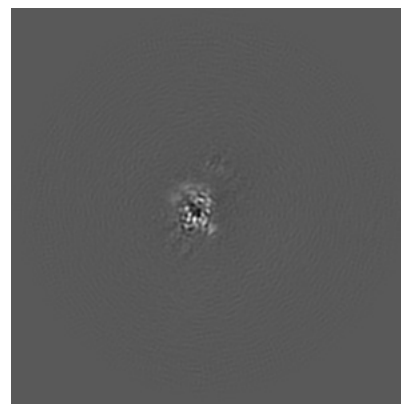
6.2.1 Primary map



X Index: 144



Y Index: 144

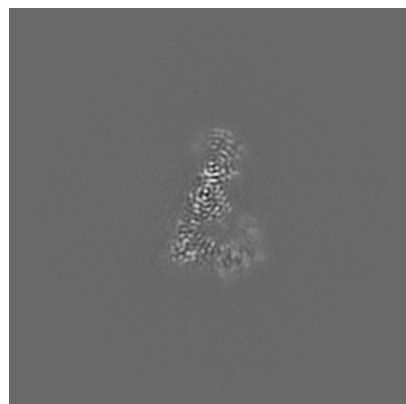


Z Index: 144

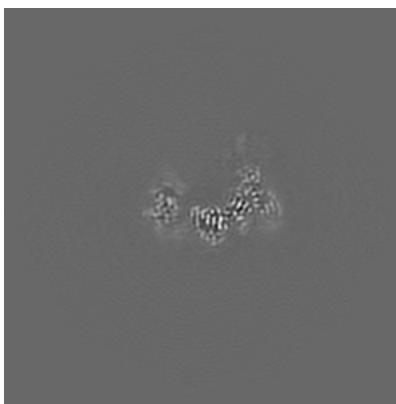
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

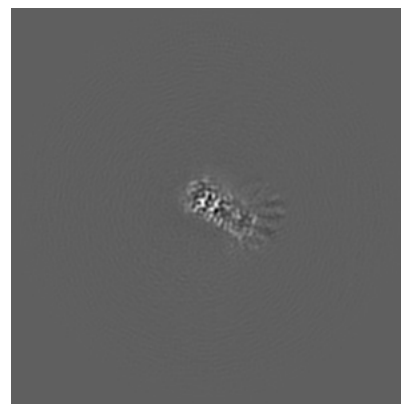
6.3.1 Primary map



X Index: 136



Y Index: 141

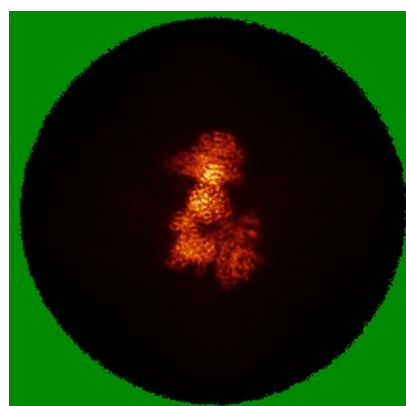


Z Index: 172

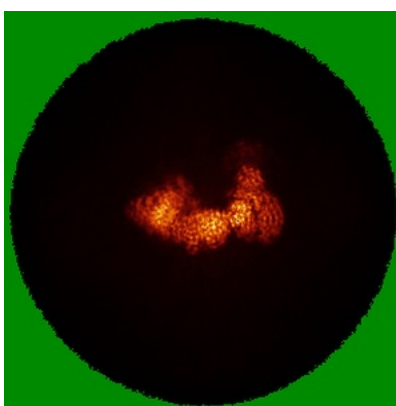
The images above show the largest variance slices of the map in three orthogonal directions.

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

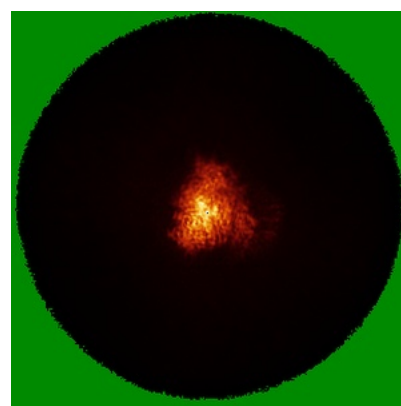
6.4.1 Primary map



X



Y

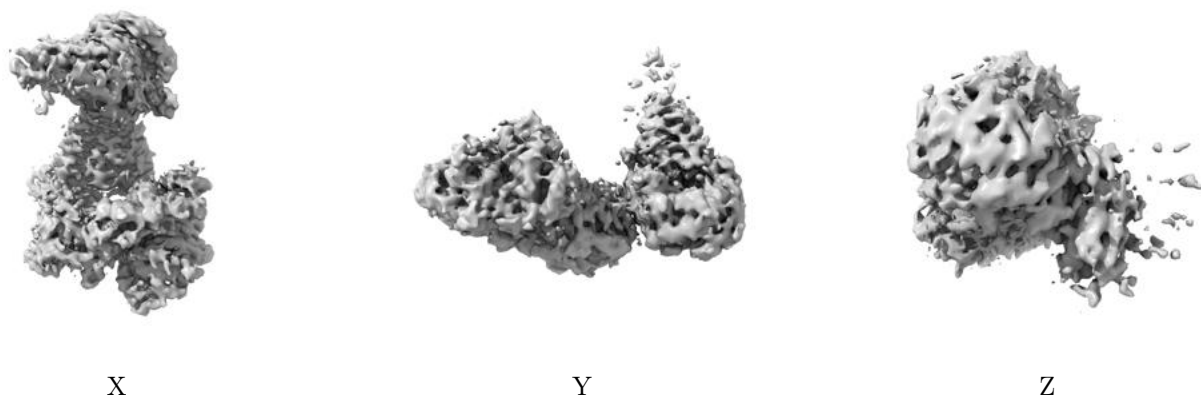


Z

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

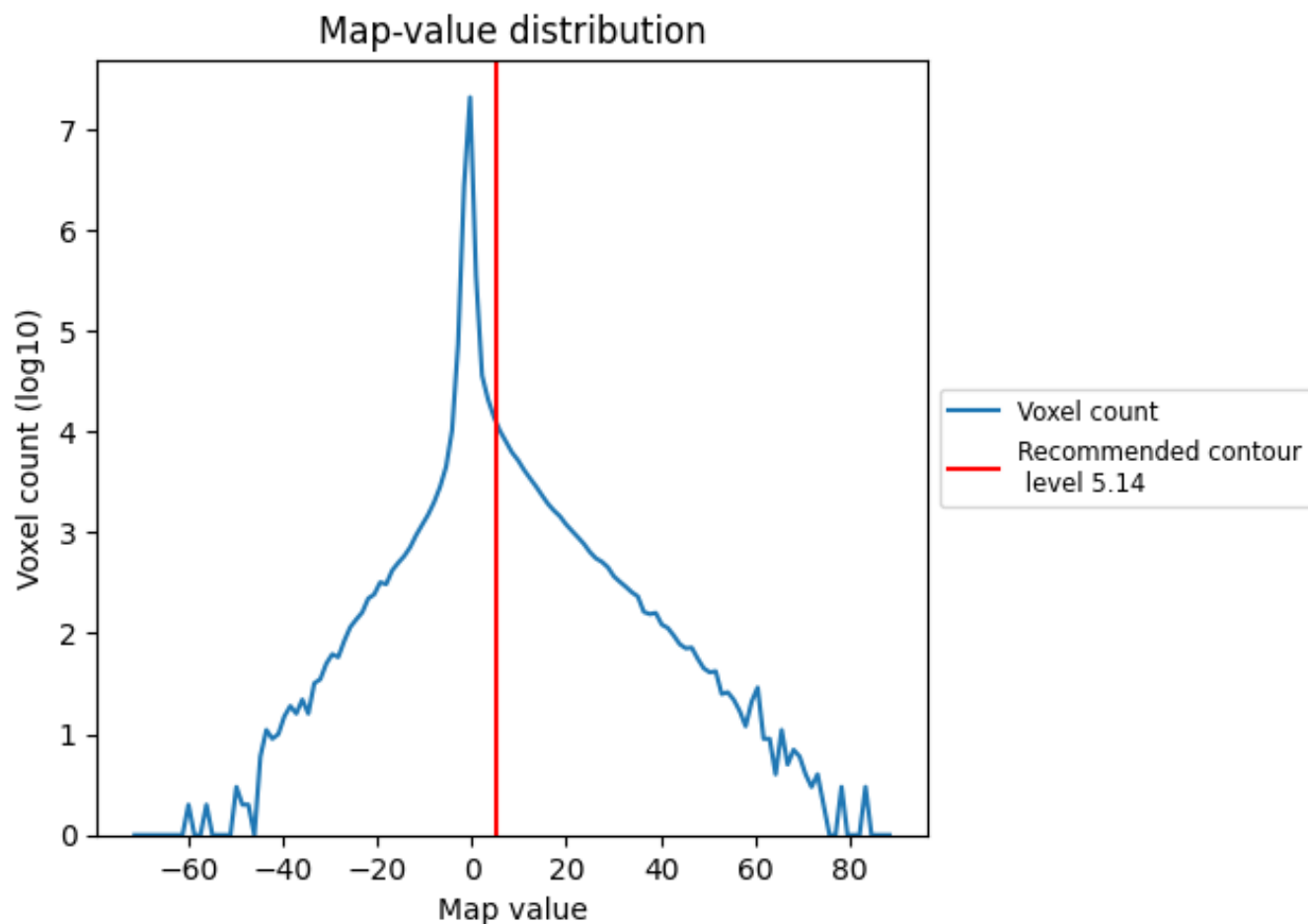
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

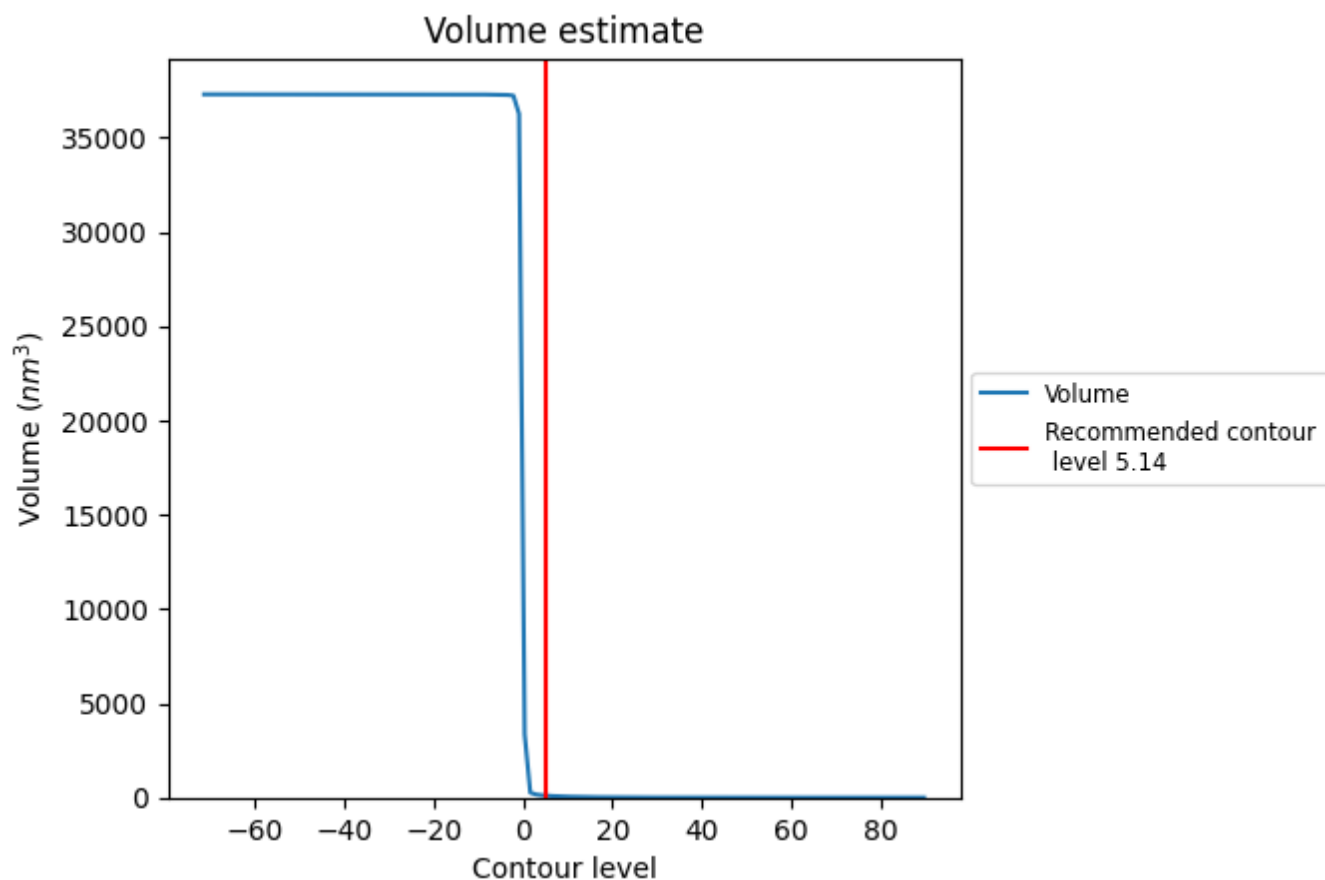
This section contains the results of statistical analysis of the map.

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.

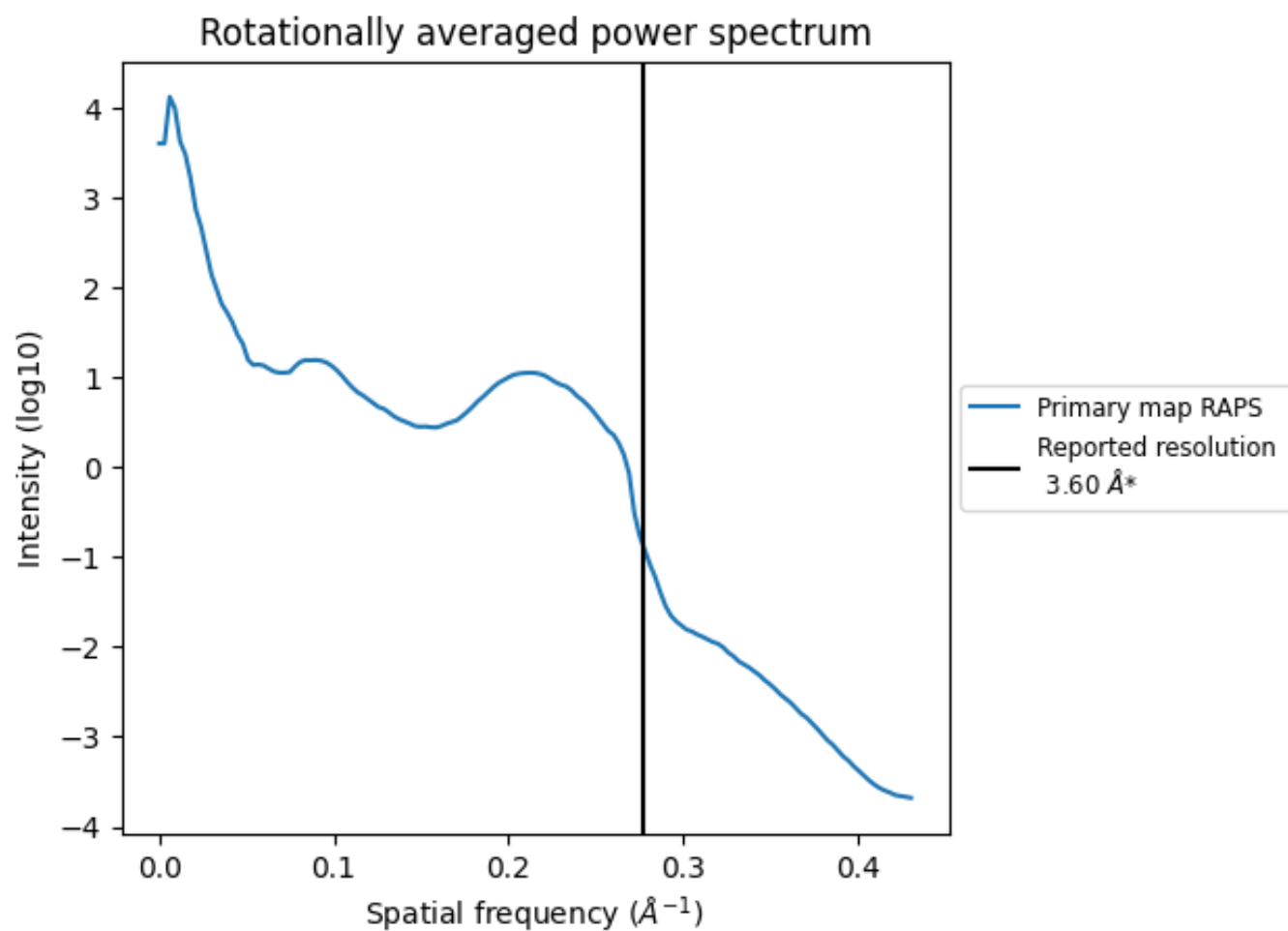
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm^3 ; this corresponds to an approximate mass of 92 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 0.278 Å⁻¹

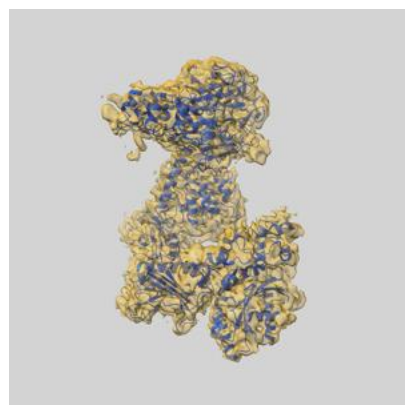
8 Fourier-Shell correlation ⓘ

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

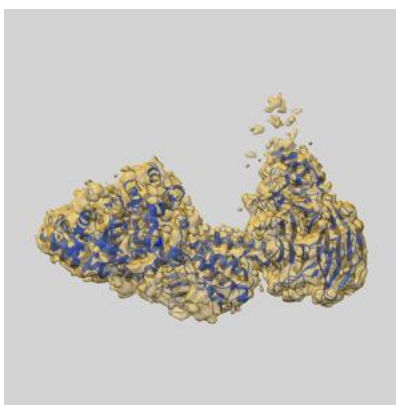
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73338 and PDB model 9YQK. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

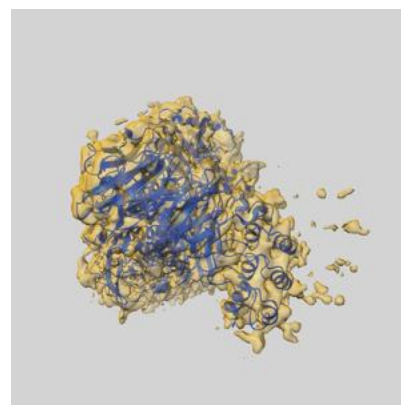
9.1 Map-model overlay [i](#)



X



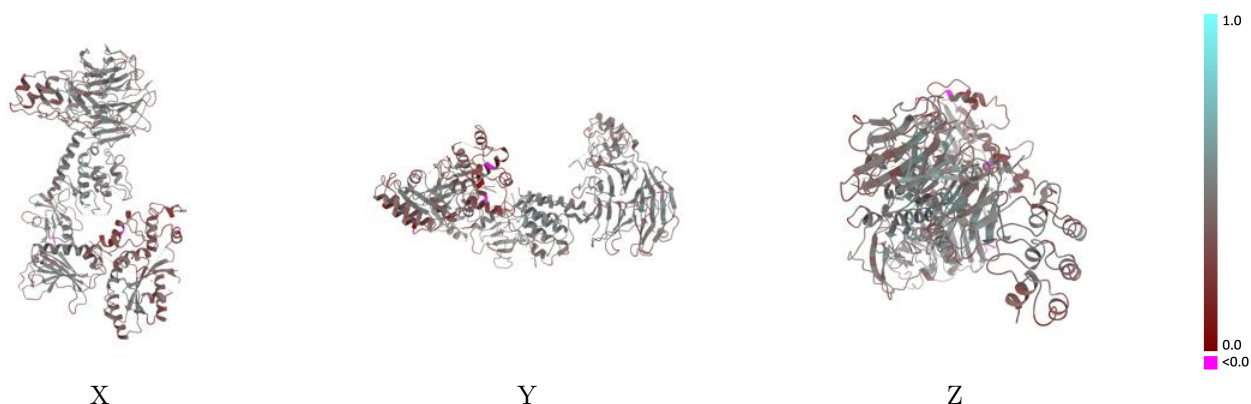
Y



Z

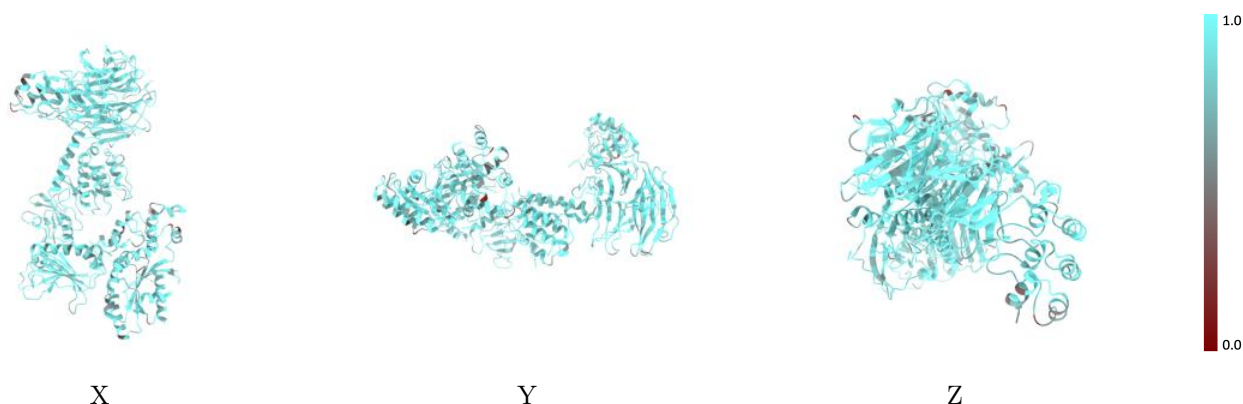
The images above show the 3D surface view of the map at the recommended contour level 5.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



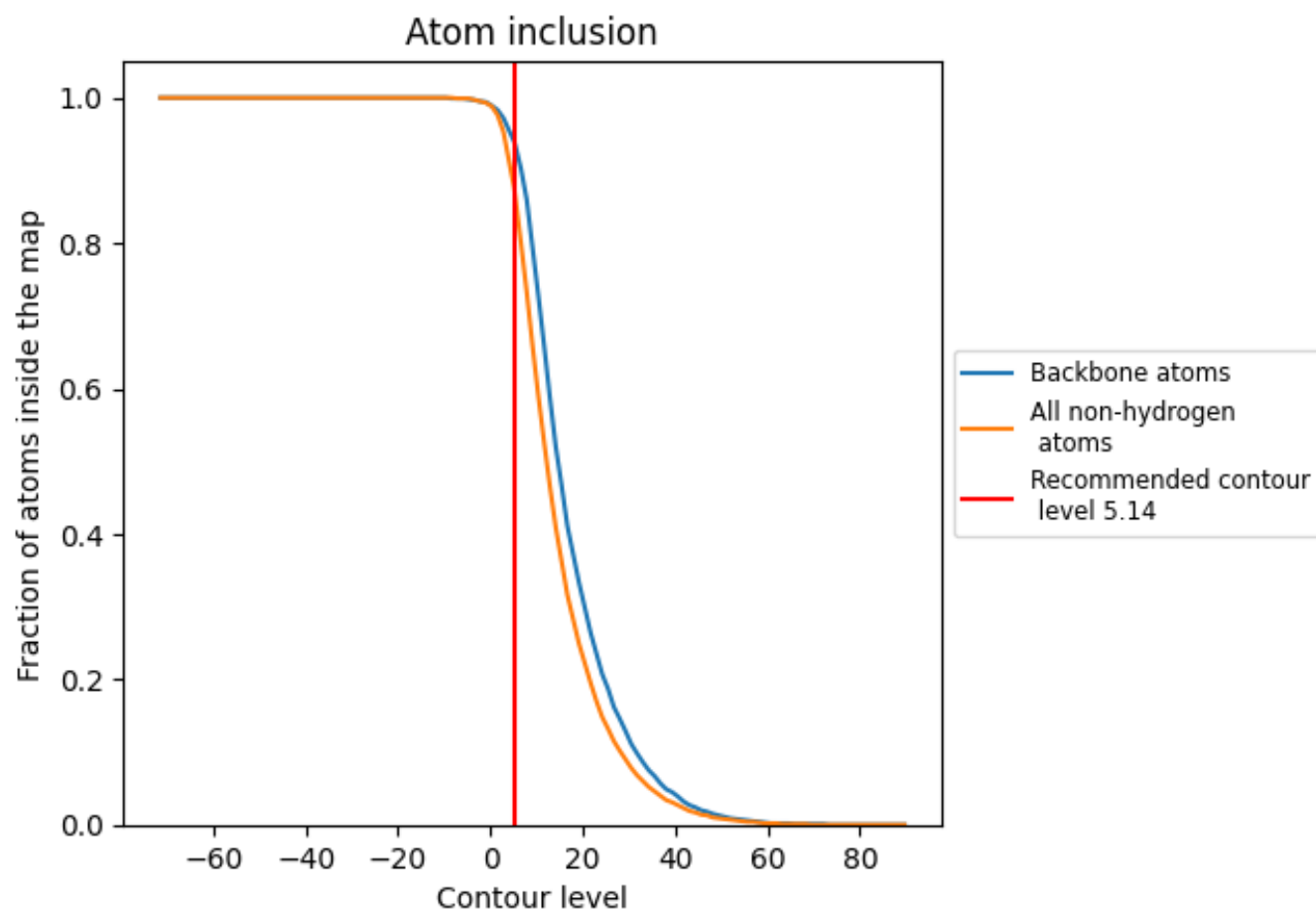
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (5.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.4120
A	0.8820	0.4150
B	0.8260	0.3800

