



## Full wwPDB EM Validation Report ⓘ

Dec 29, 2024 – 12:18 PM EST

PDB ID : 7PGR  
EMDB ID : EMD-13393  
Title : The structure of human neurofibromin isoform 2 in closed conformation  
Authors : Naschberger, A.; Baradaran, R.; Carroni, M.; Rupp, B.  
Deposited on : 2021-08-15  
Resolution : 4.00 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

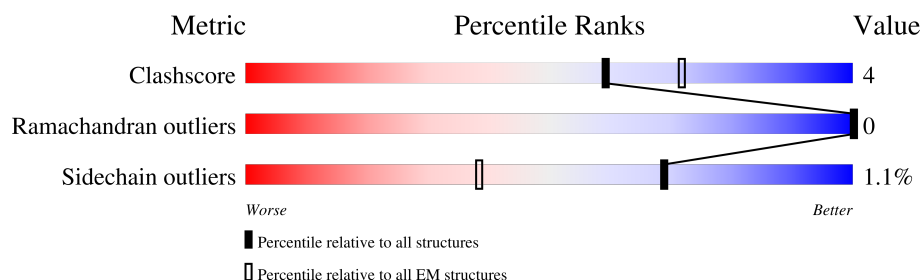
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	F	2839	<div> <div>12%</div> <div>75%</div> <div>10%</div> <div>15%</div> </div>
1	N	2839	<div> <div>16%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 77418 atoms, of which 38900 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 Neurofibromin.

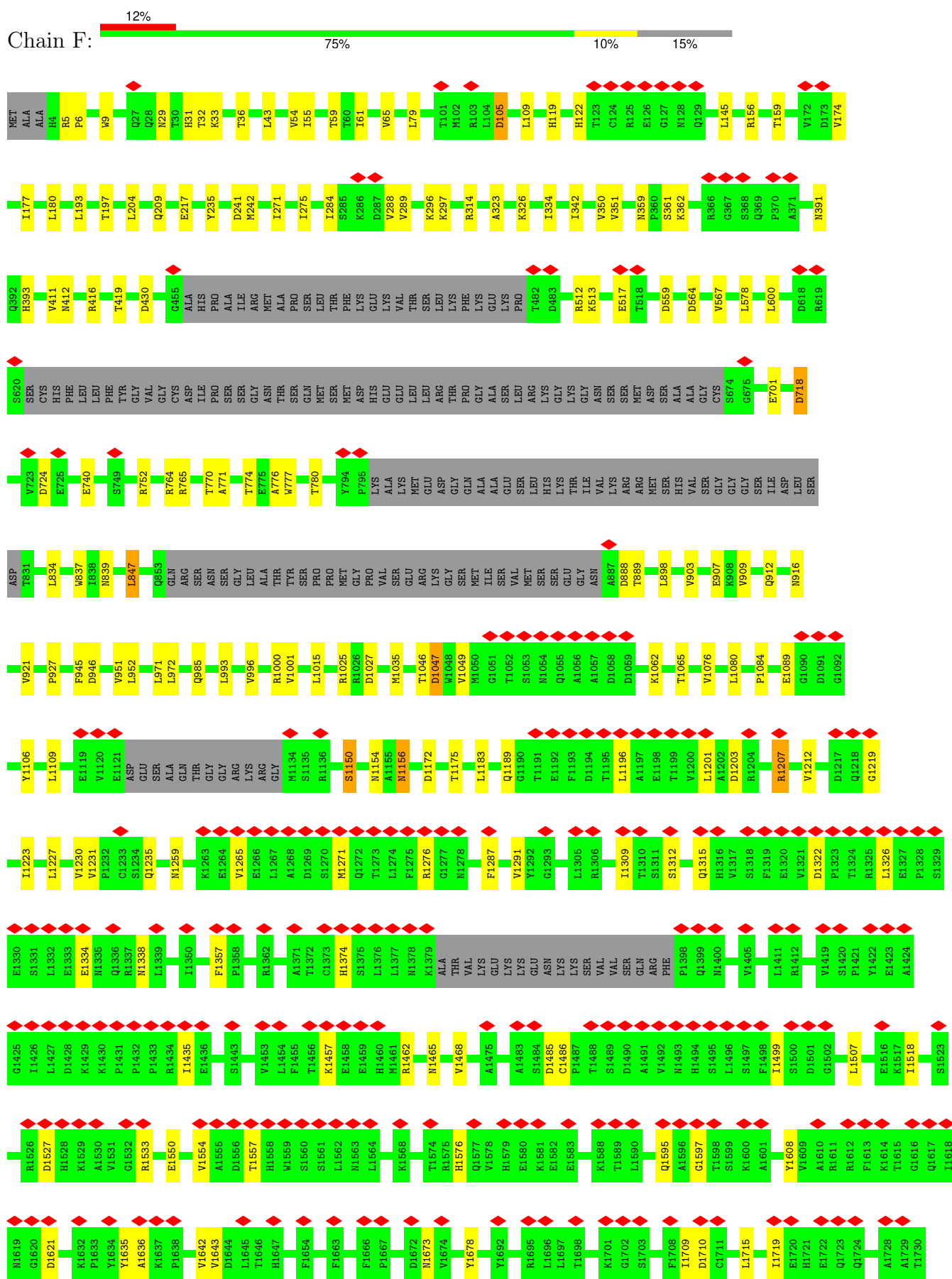
Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	2423	Total	C	H	N	O	S	0	0
			38708	12314	19450	3266	3555	123		
1	F	2423	Total	C	H	N	O	S	0	0
			38708	12314	19450	3266	3555	123		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	N	1	Total	Zn	0
			1	1	
2	F	1	Total	Zn	0
			1	1	



- Molecule 1: Neurofibromin



L1731	L1732	L1733	E1734	E1735	D1736	L1737	K1738	L1739	V1740	A1743	L1746	A1747	H1748	K1749	D1750	V1753	K1756	V1757	G1758	S1759	T1760	A1761	V1762	Q1763	A1767	E1768	R1769	T1770	K1771	I1782	Y1783	Y1784	A1785	S1786	E1787	I1788	E1789	E1790	I1791	C1792	L1793	V1794	D1795	E1796	N1797	Q1798	F1799	T1800	L1801	T1802	I1803	A1804	N1805							
Q1806	G1807	T1808	P1809	L1810	T1811	F1812	M1813	H1814	Q1815	E1816	C1817	E1818	A1819	I1820	V1821	Q1822	S1823	I1824	I1825	H1826	I1827	R1828	T1829	R1830	W1831	E1832	L1833	S1834	Q1835	P1836	D1837	S1838	I1839	P1840	Q1841	H1842	T1843	R1846	L1854	S1864	S1865	T1895	S1896	F1907	I1911	L1924	F1934	F1959	D1964											
R1968	V1971	T1980	N1984	E1985	I1992	K1995	I1996	S1999	L2000	Q2001	L2023	L2038	P2065	A2079	L2088	S2093	V2107	L2110	V2111	A2112	T2113	E2143	Q2147	S2168	K2169	S2180	Y2182	R2183	D2184	R2185	S2186	F2187	S2188	P2189	Q2190	S2191	Y2192	E2193																						
P2242	I2268	P2282	Q2288	Q2302	N2306	K2307	D2308	L2311	E2327	L2337	Q2340	H2370	N2374	V2378	N2381	F2382	N2383	T2418	N2432	S2435	H2457	R2458	LYS	SER	LEU	LEU	LEU	THR	ASP	ILE	SER	MET	GLU	ASN	ALA	VAL	PRO	MET	ASP	THR	PRO	ILE																		
HIS	HIS	GLY	ASP	PRO	SER	TYR	ARG	THR	LEU	LYS	GLU	THR	GLN	PRO	TRP	SER	LYS	PRO	GLY	TYR	LEU	ALA	ALA	THR	TYR	PRO	THR	ARG	VAL	GLY	GLN	THR	ASP	PRO	ARG	ALA	ARG	LYS	SER	MET	SER	LEU	LEU	THR	ASP	MET	GLY	GLN	PRO	GLN	ASN	PRO	MET	ASP	THR	LYS	VAL	SER	LEU	VAL
GLY	THR	ARG	LYS	SER	PHE	ASP	HIS	LEU	ILE	SER	ASP	THR	LYS	ALA	PRO	ARG	GLN	GLU	MET	GLY	SER	GLU	GLY	ILE	THR	THR	PRO	PRO	MET	ARG	ARG	VAL	ALA	GLN	THR	ASP	TYR	GLU	MET	THR	GLN	ARG	ILE	SER	PRO	HIS	PRO	GLN	HIS	LEU	ARG	LYS	VAL	SER	VAL					
SER	GLU	N2601	N2602	V2603	E2607	E2608	I2615	L2626	T2630	T2631	D2632	E2633	A2644	S2647	V2648	V2649	V2653	F2654	V2655	V2656	V2657	H2658	D2662	L2668	Q2673	D2674	P2675	N2676	L2677	N2678	P2680	I2681	V2688	E2692	E2693	L2711	L2738	I2739	L2743	P2744	G2745	ILE	ASP																	
GLU	GLU	THR	SER	GLU	SER	LEU	THR	THR	PRO	TYR	PRO	PRO	ALA	LEU	GLN	GLY	SER	ILE	THR	ASN	ILE	LYS	ILE	SER	ASN	SER	THR	LEU	ALA	THR	SER	HIS	SER	PRO	GLY	ILE	ASP	LYS	GLU	ASN	VAL	GLU	LEU	SER	PRO	THR	THR	GLY	HIS											
CYS	ASN	SER	GLY	ARG	THR	ARG	HIS	GLY	ALA	ALA	SER	GLN	VAL	GLN	LYS	GLN	ARG	ALA	GLY	SER	PHE	LYS	ARG	ASN	SER	ILE	LYS	LYS	ILE	VAL																														

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130329	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.655	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	687.98596, 687.98596, 687.98596	wwPDB
Map dimensions	470, 470, 470	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4638, 1.4638, 1.4638	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	F	0.27	0/19654	0.44	0/26645
1	N	0.27	0/19654	0.44	0/26645
All	All	0.27	0/39308	0.44	0/53290

There are no bond length outliers.

There are no bond angle outliers.

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	F	19258	19450	19458	179	0
1	N	19258	19450	19458	170	0
2	F	1	0	0	0	0
2	N	1	0	0	0	0
All	All	38518	38900	38916	342	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 4.

All (342) 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:N:1230:VAL:HG21	1:N:1518:ILE:HG22	1.44	0.96
1:F:1230:VAL:HG21	1:F:1518:ILE:HG22	1.47	0.94
1:F:2088:LEU:O	1:F:2093:SER:OG	1.90	0.90
1:N:235:TYR:OH	1:N:275:ILE:O	1.91	0.89
1:N:2088:LEU:O	1:N:2093:SER:OG	1.92	0.85
1:F:2644:ALA:O	1:F:2647:SER:OG	1.96	0.82
1:N:1035:MET:HE2	1:N:1554:VAL:HG21	1.61	0.80
1:N:1219:GLY:O	1:N:1259:ASN:ND2	2.14	0.80
1:F:235:TYR:OH	1:F:275:ILE:O	1.98	0.80
1:F:1035:MET:HE2	1:F:1554:VAL:HG21	1.64	0.79
1:N:2302:GLN:OE1	1:N:2340:GLN:NE2	2.14	0.79
1:F:1219:GLY:O	1:F:1259:ASN:ND2	2.17	0.78
1:F:1089:GLU:OE1	1:F:1089:GLU:N	2.16	0.78
1:F:1150:SER:O	1:F:1154:ASN:ND2	2.19	0.75
1:F:1709:ILE:HD13	1:F:1715:LEU:HD22	1.70	0.74
1:N:1089:GLU:N	1:N:1089:GLU:OE1	2.21	0.73
1:N:1035:MET:CE	1:N:1554:VAL:HG21	2.19	0.73
1:N:2644:ALA:O	1:N:2647:SER:OG	2.07	0.72
1:F:1334:GLU:OE2	1:F:1338:ASN:ND2	2.22	0.72
1:F:1035:MET:CE	1:F:1554:VAL:HG21	2.20	0.71
1:N:1709:ILE:HD13	1:N:1715:LEU:HD22	1.72	0.71
1:N:1334:GLU:OE2	1:N:1338:ASN:ND2	2.24	0.71
1:N:2000:LEU:HD23	1:N:2000:LEU:O	1.91	0.70
1:F:2626:LEU:O	1:F:2630:THR:OG1	2.07	0.69
1:N:31:HIS:O	1:N:32:THR:OG1	2.10	0.69
1:F:985:GLN:N	1:F:985:GLN:OE1	2.25	0.68
1:F:1832:GLU:O	1:F:1835:GLN:NE2	2.26	0.68
1:N:1832:GLU:O	1:N:1835:GLN:NE2	2.27	0.67
1:F:1156:ASN:OD1	1:F:1156:ASN:N	2.27	0.67
1:F:31:HIS:O	1:F:32:THR:OG1	2.09	0.67
1:F:1557:THR:OG1	1:F:1621:ASP:OD1	2.12	0.67
1:N:2268:ILE:HG22	1:N:2739:ILE:HD11	1.77	0.66
1:F:2000:LEU:HD23	1:F:2000:LEU:O	1.93	0.66
1:N:985:GLN:OE1	1:N:985:GLN:N	2.29	0.66
1:F:1995:LYS:O	1:F:1999:SER:OG	2.11	0.65
1:N:1150:SER:O	1:N:1154:ASN:ND2	2.29	0.64
1:N:1995:LYS:O	1:N:1999:SER:OG	2.10	0.64
1:F:1035:MET:HE2	1:F:1554:VAL:HG11	1.80	0.64
1:F:2268:ILE:HG22	1:F:2739:ILE:HD11	1.80	0.64
1:F:701:GLU:N	1:F:701:GLU:OE1	2.31	0.64
1:N:271:ILE:HD12	1:N:323:ALA:HB1	1.78	0.64
1:F:1230:VAL:CG2	1:F:1518:ILE:HG22	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1557:THR:OG1	1:N:1621:ASP:OD1	2.13	0.63
1:F:1595:GLN:NE2	1:F:1597:GLY:O	2.32	0.63
1:N:2107:VAL:O	1:N:2111:VAL:HG13	1.98	0.62
1:F:2302:GLN:OE1	1:F:2340:GLN:NE2	2.33	0.62
1:N:1595:GLN:NE2	1:N:1597:GLY:O	2.32	0.62
1:F:2658:HIS:O	1:F:2662:ASP:N	2.34	0.61
1:N:945:PHE:CE1	1:N:951:VAL:HG12	2.35	0.61
1:N:2435:SER:O	1:N:2435:SER:OG	2.14	0.61
1:N:2674:ASP:OD1	1:N:2676:ASN:N	2.33	0.60
1:F:1035:MET:CE	1:F:1554:VAL:HG11	2.31	0.60
1:N:109:LEU:HD21	1:N:145:LEU:HD21	1.84	0.59
1:N:204:LEU:O	1:N:209:GLN:NE2	2.35	0.59
1:N:1035:MET:HE2	1:N:1554:VAL:HG11	1.84	0.59
1:F:109:LEU:HD21	1:F:145:LEU:HD21	1.85	0.59
1:F:156:ARG:O	1:F:159:THR:OG1	2.19	0.59
1:F:718:ASP:N	1:F:718:ASP:OD1	2.34	0.58
1:N:1049:VAL:HG13	1:N:1049:VAL:O	2.03	0.58
1:F:912:GLN:O	1:F:916:ASN:ND2	2.37	0.58
1:F:2608:GLU:N	1:F:2608:GLU:OE1	2.31	0.58
1:N:31:HIS:ND1	1:F:2673:GLN:OE1	2.36	0.58
1:N:1035:MET:CE	1:N:1554:VAL:HG11	2.33	0.58
1:F:1049:VAL:O	1:F:1049:VAL:HG13	2.04	0.58
1:F:2674:ASP:OD1	1:F:2676:ASN:N	2.36	0.58
1:N:2626:LEU:O	1:N:2630:THR:OG1	2.10	0.58
1:F:1046:THR:O	1:F:1049:VAL:HG12	2.03	0.58
1:N:55:ILE:O	1:N:59:THR:HG23	2.03	0.57
1:F:2668:LEU:HD13	1:F:2681:ILE:HD11	1.87	0.57
1:N:996:VAL:HG12	1:N:1015:LEU:HD21	1.86	0.57
1:N:359:ASN:OD1	1:N:361:SER:OG	2.19	0.57
1:F:1172:ASP:OD2	1:F:1175:THR:N	2.33	0.57
1:N:701:GLU:N	1:N:701:GLU:OE1	2.38	0.56
1:N:1203:ASP:O	1:N:1207:ARG:NH1	2.38	0.56
1:N:1636:ALA:O	1:N:1673:ASN:ND2	2.38	0.56
1:F:271:ILE:HD12	1:F:323:ALA:HB1	1.86	0.56
1:F:2107:VAL:O	1:F:2111:VAL:HG13	2.04	0.56
1:N:1230:VAL:CG2	1:N:1518:ILE:HG22	2.26	0.56
1:N:1465:ASN:O	1:N:1468:VAL:HG22	2.05	0.56
1:F:2435:SER:O	1:F:2435:SER:OG	2.14	0.56
1:F:1636:ALA:O	1:F:1673:ASN:ND2	2.39	0.56
1:N:945:PHE:HE1	1:N:951:VAL:HG12	1.71	0.56
1:N:1957:VAL:HG22	1:N:2003:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:2607:GLU:OE1	1:N:2607:GLU:N	2.36	0.56
1:F:898:LEU:HD21	1:F:921:VAL:HG22	1.87	0.56
1:F:578:LEU:CD2	1:F:600:LEU:HD11	2.36	0.55
1:N:1715:LEU:HD11	1:N:1719:ILE:CD1	2.37	0.55
1:N:912:GLN:O	1:N:916:ASN:ND2	2.40	0.55
1:N:2110:LEU:O	1:N:2113:THR:OG1	2.24	0.55
1:N:2668:LEU:HD13	1:N:2681:ILE:HD11	1.88	0.55
1:F:204:LEU:O	1:F:209:GLN:NE2	2.40	0.55
1:F:359:ASN:OD1	1:F:361:SER:OG	2.18	0.55
1:N:1035:MET:CE	1:N:1084:PRO:HD2	2.37	0.55
1:N:1795:ASP:OD1	1:N:1796:GLU:N	2.40	0.55
1:F:996:VAL:HG12	1:F:1015:LEU:HD21	1.88	0.55
1:F:972:LEU:O	1:F:1025:ARG:NH1	2.40	0.54
1:N:2658:HIS:O	1:N:2662:ASP:N	2.40	0.54
1:F:1795:ASP:OD1	1:F:1796:GLU:N	2.40	0.54
1:N:578:LEU:CD2	1:N:600:LEU:HD11	2.37	0.54
1:N:718:ASP:OD1	1:N:718:ASP:N	2.40	0.54
1:N:1046:THR:O	1:N:1049:VAL:HG12	2.07	0.54
1:F:55:ILE:O	1:F:59:THR:HG23	2.08	0.54
1:F:1465:ASN:O	1:F:1468:VAL:HG22	2.07	0.54
1:F:945:PHE:CE1	1:F:951:VAL:HG12	2.43	0.53
1:F:2110:LEU:O	1:F:2113:THR:OG1	2.24	0.53
1:N:972:LEU:O	1:N:1025:ARG:NH1	2.41	0.53
1:F:2288:GLN:NE2	1:F:2327:GLU:OE2	2.42	0.53
1:F:1035:MET:CE	1:F:1084:PRO:HD2	2.38	0.53
1:N:1027:ASP:OD1	1:N:1027:ASP:N	2.42	0.53
1:N:1980:THR:O	1:N:1984:ASN:ND2	2.36	0.53
1:F:1642:VAL:HG22	1:F:1678:TYR:HB2	1.90	0.53
1:F:1710:ASP:OD2	1:F:1769:ARG:NH2	2.36	0.53
1:F:1203:ASP:O	1:F:1207:ARG:NH1	2.41	0.53
1:N:1864:SER:OG	1:N:1865:SER:N	2.42	0.53
1:F:1715:LEU:HD11	1:F:1719:ILE:CD1	2.38	0.53
1:N:1642:VAL:HG22	1:N:1678:TYR:HB2	1.90	0.52
1:F:740:GLU:OE2	1:F:765:ARG:NH2	2.42	0.52
1:F:1027:ASP:OD1	1:F:1027:ASP:N	2.42	0.52
1:F:2374:MET:O	1:F:2378:VAL:HG12	2.09	0.52
1:F:1828:ARG:NE	1:F:1832:GLU:OE2	2.43	0.52
1:F:2653:VAL:O	1:F:2656:VAL:HG22	2.09	0.52
1:F:2143:GLU:OE2	1:F:2147:GLN:NE2	2.41	0.52
1:N:1001:VAL:O	1:N:1001:VAL:HG12	2.09	0.52
1:F:109:LEU:CD2	1:F:145:LEU:HD21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:898:LEU:HD21	1:N:921:VAL:HG22	1.91	0.52
1:F:724:ASP:OD1	1:F:724:ASP:N	2.43	0.52
1:N:724:ASP:OD1	1:N:724:ASP:N	2.43	0.51
1:F:903:VAL:HG22	1:F:903:VAL:O	2.11	0.51
1:N:391:ASN:OD1	1:N:393:HIS:N	2.43	0.51
1:F:996:VAL:O	1:F:1000:ARG:N	2.41	0.51
1:F:1499:ILE:HD12	1:F:1499:ILE:H	1.76	0.51
1:N:776:ALA:O	1:N:780:THR:HG22	2.11	0.51
1:N:903:VAL:O	1:N:903:VAL:HG22	2.10	0.51
1:N:1265:VAL:HG13	1:N:1271:MET:HB3	1.93	0.51
1:F:1759:SER:O	1:F:1830:ARG:NH2	2.41	0.51
1:F:2001:GLY:HA3	1:F:2038:LEU:HD12	1.92	0.51
1:N:430:ASP:N	1:N:430:ASP:OD1	2.43	0.51
1:N:996:VAL:O	1:N:1000:ARG:N	2.36	0.51
1:F:391:ASN:OD1	1:F:393:HIS:N	2.41	0.51
1:F:1001:VAL:HG12	1:F:1001:VAL:O	2.10	0.51
1:N:109:LEU:CD2	1:N:145:LEU:HD21	2.40	0.51
1:N:1759:SER:O	1:N:1830:ARG:NH2	2.44	0.51
1:N:1499:ILE:HD12	1:N:1499:ILE:H	1.76	0.51
1:N:2306:ASN:ND2	1:N:2308:ASP:OD1	2.44	0.51
1:F:241:ASP:OD1	1:F:242:MET:N	2.44	0.51
1:F:2306:ASN:ND2	1:F:2308:ASP:OD1	2.44	0.51
1:N:1047:ASP:N	1:N:1047:ASP:OD1	2.43	0.51
1:N:1715:LEU:HD11	1:N:1719:ILE:HD12	1.93	0.51
1:N:1062:LYS:O	1:N:1065:THR:HG22	2.11	0.50
1:N:1828:ARG:NE	1:N:1832:GLU:OE2	2.44	0.50
1:N:1895:THR:HG22	1:N:1896:SER:N	2.26	0.50
1:N:2143:GLU:OE2	1:N:2147:GLN:NE2	2.41	0.50
1:N:2654:PHE:N	1:N:2655:PRO:HD2	2.25	0.50
1:F:1709:ILE:CD1	1:F:1715:LEU:HD22	2.41	0.50
1:F:764:ARG:HD3	1:F:927:PRO:HD3	1.92	0.50
1:F:1265:VAL:HG13	1:F:1271:MET:HB3	1.93	0.50
1:F:1895:THR:HG22	1:F:1896:SER:N	2.27	0.50
1:N:33:LYS:HA	1:N:36:THR:HG22	1.93	0.50
1:N:1235:GLN:OE1	1:N:1235:GLN:N	2.43	0.50
1:N:1709:ILE:HD11	1:N:1715:LEU:HD13	1.93	0.50
1:F:770:THR:HG22	1:F:771:ALA:N	2.27	0.50
1:F:2654:PHE:N	1:F:2655:PRO:HD2	2.26	0.50
1:F:2607:GLU:OE1	1:F:2607:GLU:N	2.41	0.49
1:N:777:TRP:HD1	1:N:847:LEU:HD23	1.77	0.49
1:N:1709:ILE:CD1	1:N:1715:LEU:HD22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1047:ASP:N	1:F:1047:ASP:OD1	2.45	0.49
1:F:2065:PRO:HB3	1:F:2242:PRO:HD2	1.95	0.49
1:N:2657:VAL:HG12	1:N:2657:VAL:O	2.13	0.49
1:N:740:GLU:OE2	1:N:765:ARG:NH2	2.45	0.49
1:N:1076:VAL:HG12	1:N:1080:LEU:HD12	1.95	0.49
1:F:1287:PHE:O	1:F:1291:VAL:HG12	2.13	0.49
1:N:2288:GLN:NE2	1:N:2327:GLU:OE2	2.46	0.49
1:F:1715:LEU:HD11	1:F:1719:ILE:HD12	1.93	0.49
1:F:2738:LEU:C	1:F:2738:LEU:HD23	2.33	0.49
1:N:1462:ARG:O	1:N:1465:ASN:ND2	2.46	0.48
1:N:1322:ASP:O	1:N:1326:LEU:N	2.46	0.48
1:F:1227:LEU:O	1:F:1231:VAL:HG23	2.13	0.48
1:N:145:LEU:C	1:N:145:LEU:HD23	2.34	0.48
1:N:742:ALA:O	1:N:745:SER:OG	2.26	0.48
1:N:1287:PHE:O	1:N:1291:VAL:HG12	2.13	0.48
1:F:145:LEU:C	1:F:145:LEU:HD23	2.34	0.48
1:F:1709:ILE:HD11	1:F:1715:LEU:HD13	1.94	0.48
1:N:1805:ASN:O	1:N:1805:ASN:ND2	2.46	0.48
1:F:1322:ASP:O	1:F:1326:LEU:N	2.46	0.48
1:N:1931:ILE:HG21	1:N:1977:LYS:HB3	1.96	0.48
1:F:1907:PHE:CZ	1:F:1911:ILE:HD11	2.48	0.48
1:F:1106:TYR:O	1:F:1109:LEU:N	2.47	0.48
1:N:2411:ARG:NH1	1:F:1527:ASP:OD2	2.46	0.48
1:N:1845:ILE:HG13	1:N:1845:ILE:O	2.14	0.48
1:N:2673:GLN:OE1	1:F:31:HIS:ND1	2.47	0.48
1:N:2374:MET:O	1:N:2378:VAL:HG12	2.13	0.47
1:F:1805:ASN:ND2	1:F:1805:ASN:O	2.46	0.47
1:F:1980:THR:O	1:F:1984:ASN:ND2	2.41	0.47
1:N:2653:VAL:O	1:N:2656:VAL:HG22	2.14	0.47
1:F:1864:SER:OG	1:F:1865:SER:N	2.45	0.47
1:F:1062:LYS:O	1:F:1065:THR:HG22	2.14	0.47
1:N:1608:TYR:HD2	1:N:1643:VAL:HG23	1.79	0.47
1:F:1462:ARG:O	1:F:1465:ASN:ND2	2.48	0.47
1:N:1662:TRP:O	1:N:1671:TYR:OH	2.30	0.47
1:F:1992:ILE:HG23	1:F:1996:ILE:HD12	1.97	0.46
1:F:2615:ILE:HG22	1:F:2615:ILE:O	2.15	0.46
1:N:1992:ILE:HG23	1:N:1996:ILE:HD12	1.96	0.46
1:F:2657:VAL:HG12	1:F:2657:VAL:O	2.15	0.46
1:N:5:ARG:O	1:N:8:GLU:N	2.49	0.46
1:N:156:ARG:O	1:N:159:THR:OG1	2.32	0.46
1:N:993:LEU:O	1:N:996:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1227:LEU:O	1:N:1231:VAL:HG23	2.16	0.46
1:N:2395:LEU:HD22	1:N:2626:LEU:HD21	1.97	0.46
1:N:2653:VAL:HG12	1:N:2698:TYR:CD2	2.51	0.46
1:F:1235:GLN:OE1	1:F:1235:GLN:N	2.47	0.46
1:F:174:VAL:O	1:F:177:ILE:N	2.48	0.46
1:N:241:ASP:OD1	1:N:242:MET:N	2.48	0.46
1:N:752:ARG:NH1	1:N:839:ASN:OD1	2.49	0.46
1:N:2738:LEU:C	1:N:2738:LEU:HD23	2.36	0.46
1:F:1183:LEU:HD21	1:F:1854:LEU:HD22	1.98	0.46
1:F:564:ASP:OD1	1:F:564:ASP:N	2.49	0.46
1:N:6:PRO:HB3	1:F:2688:VAL:HG11	1.98	0.45
1:N:1968:ARG:O	1:N:1971:VAL:HG22	2.15	0.45
1:F:193:LEU:O	1:F:197:THR:HG22	2.16	0.45
1:F:909:VAL:HG22	1:F:909:VAL:O	2.16	0.45
1:N:1710:ASP:OD2	1:N:1769:ARG:NH2	2.40	0.45
1:N:411:VAL:HG23	1:N:412:ASN:N	2.32	0.45
1:N:1212:VAL:HA	1:N:1223:ILE:HG21	1.97	0.45
1:F:2648:VAL:HG23	1:F:2649:VAL:N	2.32	0.45
1:F:1309:ILE:HD13	1:F:1435:ILE:HG21	1.97	0.45
1:N:888:ASP:O	1:N:889:THR:HG23	2.17	0.45
1:N:1309:ILE:HD13	1:N:1435:ILE:HG21	1.99	0.45
1:N:2023:LEU:HD13	1:N:2079:ALA:HB1	1.98	0.45
1:F:888:ASP:O	1:F:889:THR:HG23	2.16	0.45
1:F:1076:VAL:HG12	1:F:1080:LEU:HD12	1.99	0.45
1:N:1035:MET:HE2	1:N:1554:VAL:CG2	2.39	0.44
1:N:907:GLU:OE1	1:N:907:GLU:N	2.42	0.44
1:N:1289:PHE:O	1:N:1293:GLY:N	2.43	0.44
1:N:2608:GLU:OE1	1:N:2608:GLU:N	2.43	0.44
1:F:43:LEU:HD11	1:F:54:VAL:HG13	1.99	0.44
1:N:404:SER:O	1:N:407:HIS:N	2.50	0.44
1:N:564:ASP:N	1:N:564:ASP:OD1	2.50	0.44
1:N:1064:LEU:O	1:N:1067:ASP:N	2.51	0.44
1:F:79:LEU:O	1:F:79:LEU:HD23	2.18	0.44
1:N:770:THR:HG22	1:N:771:ALA:N	2.32	0.44
1:F:411:VAL:HG23	1:F:412:ASN:N	2.32	0.44
1:F:2674:ASP:OD1	1:F:2677:LEU:N	2.46	0.44
1:F:776:ALA:O	1:F:780:THR:HG22	2.17	0.44
1:F:1035:MET:HE2	1:F:1554:VAL:CG2	2.42	0.44
1:N:512:ARG:O	1:N:513:LYS:HB2	2.17	0.44
1:F:1968:ARG:O	1:F:1971:VAL:HG22	2.18	0.44
1:F:359:ASN:OD1	1:F:362:LYS:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:2655:PRO:HA	1:N:2658:HIS:CE1	2.53	0.43
1:F:5:ARG:N	1:F:6:PRO:HD2	2.33	0.43
1:F:145:LEU:HD23	1:F:145:LEU:O	2.18	0.43
1:N:284:ILE:HD11	1:N:296:LYS:HB3	1.99	0.43
1:N:334:ILE:HD12	1:N:342:ILE:HG21	2.00	0.43
1:N:909:VAL:HG22	1:N:909:VAL:O	2.18	0.43
1:F:512:ARG:O	1:F:513:LYS:HB2	2.18	0.43
1:F:907:GLU:OE1	1:F:907:GLU:N	2.43	0.43
1:F:2023:LEU:HD13	1:F:2079:ALA:HB1	1.99	0.43
1:F:33:LYS:HA	1:F:36:THR:HG22	2.00	0.43
1:F:284:ILE:HD11	1:F:296:LYS:HB3	2.00	0.43
1:F:350:VAL:HG13	1:F:351:VAL:N	2.34	0.43
1:F:945:PHE:HE1	1:F:951:VAL:HG12	1.82	0.43
1:F:2655:PRO:HA	1:F:2658:HIS:CE1	2.53	0.43
1:F:2337:LEU:HD12	1:F:2337:LEU:O	2.19	0.43
1:N:5:ARG:N	1:N:6:PRO:HD2	2.34	0.43
1:N:2679:ASN:HB2	1:N:2680:PRO:HD3	2.00	0.43
1:N:2636:GLN:OE1	1:N:2664:LYS:NZ	2.37	0.43
1:F:430:ASP:OD1	1:F:430:ASP:N	2.51	0.43
1:F:2711:LEU:O	1:F:2711:LEU:HD23	2.19	0.43
1:N:61:ILE:O	1:N:65:VAL:HG23	2.19	0.42
1:F:1312:SER:O	1:F:1315:GLN:NE2	2.50	0.42
1:N:1803:ILE:HG22	1:N:1804:ALA:N	2.34	0.42
1:N:372:ASP:OD2	1:N:375:LEU:HB2	2.20	0.42
1:F:770:THR:O	1:F:774:THR:HG22	2.19	0.42
1:F:2168:SER:O	1:F:2169:LYS:HB2	2.19	0.42
1:N:2711:LEU:O	1:N:2711:LEU:HD23	2.19	0.42
1:F:1608:TYR:HD2	1:F:1643:VAL:HG23	1.85	0.42
1:N:359:ASN:OD1	1:N:362:LYS:N	2.42	0.42
1:N:2692:GLU:HG2	1:N:2693:GLU:H	1.85	0.42
1:F:1803:ILE:HG22	1:F:1804:ALA:N	2.34	0.42
1:N:2688:VAL:HG11	1:F:6:PRO:HB3	2.02	0.42
1:F:2738:LEU:HD23	1:F:2738:LEU:O	2.19	0.42
1:F:1934:PHE:CE1	1:F:1985:GLU:OE2	2.73	0.42
1:F:2632:ASP:OD1	1:F:2633:GLU:N	2.53	0.42
1:N:971:LEU:C	1:N:971:LEU:HD23	2.40	0.42
1:N:1162:MET:HA	1:N:1845:ILE:HD11	2.01	0.42
1:F:1485:ASP:OD1	1:F:1486:CYS:N	2.53	0.42
1:N:2059:ASP:OD1	1:N:2059:ASP:O	2.38	0.42
1:F:993:LEU:O	1:F:996:VAL:HG22	2.20	0.42
1:N:350:VAL:HG13	1:N:351:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:2311:LEU:HD11	1:N:2743:LEU:HD21	2.02	0.41
1:N:2627:VAL:HG13	1:N:2639:LEU:HD13	2.01	0.41
1:N:2648:VAL:HG23	1:N:2649:VAL:N	2.35	0.41
1:F:752:ARG:NH1	1:F:839:ASN:OD1	2.53	0.41
1:F:2418:THR:HG22	1:F:2418:THR:O	2.20	0.41
1:N:79:LEU:HD23	1:N:79:LEU:O	2.20	0.41
1:N:174:VAL:O	1:N:177:ILE:N	2.53	0.41
1:F:2381:ASN:OD1	1:F:2383:ASN:N	2.54	0.41
1:N:288:VAL:HG13	1:N:293:ASN:O	2.20	0.41
1:F:61:ILE:O	1:F:65:VAL:HG23	2.21	0.41
1:F:334:ILE:HD12	1:F:342:ILE:HG21	2.02	0.41
1:F:971:LEU:HD23	1:F:971:LEU:C	2.40	0.41
1:F:105:ASP:OD1	1:F:105:ASP:N	2.53	0.41
1:F:217:GLU:OE2	1:F:326:LYS:NZ	2.40	0.41
1:F:1788:ILE:HG22	1:F:1791:ILE:HD11	2.02	0.41
1:F:2311:LEU:HD11	1:F:2743:LEU:HD21	2.03	0.41
1:N:31:HIS:O	1:N:34:VAL:HG12	2.21	0.41
1:N:1850:VAL:N	1:N:1851:PRO:CD	2.84	0.41
1:F:416:ARG:HA	1:F:419:THR:HG22	2.02	0.41
1:F:1172:ASP:OD2	1:F:1175:THR:OG1	2.25	0.41
1:N:2673:GLN:NE2	1:F:29:ASN:OD1	2.53	0.41
1:F:1212:VAL:HA	1:F:1223:ILE:HG21	2.02	0.41
1:F:1924:LEU:HD11	1:F:1959:PHE:CD2	2.56	0.41
1:N:1146:VAL:O	1:N:1150:SER:OG	2.37	0.41
1:N:1788:ILE:HG22	1:N:1791:ILE:HD11	2.01	0.41
1:N:2668:LEU:HD13	1:N:2681:ILE:CD1	2.51	0.41
1:N:2688:VAL:HG21	1:F:9:TRP:HZ3	1.85	0.41
1:F:2679:ASN:HB2	1:F:2680:PRO:HD3	2.02	0.41
1:N:764:ARG:HD3	1:N:927:PRO:HD3	2.02	0.41
1:N:1465:ASN:OD1	1:N:1466:ASP:N	2.53	0.41
1:N:1485:ASP:OD1	1:N:1486:CYS:N	2.53	0.41
1:F:288:VAL:HG12	1:F:289:VAL:O	2.21	0.41
1:F:777:TRP:HD1	1:F:847:LEU:HD23	1.86	0.41
1:F:834:LEU:O	1:F:837:TRP:N	2.54	0.41
1:F:567:VAL:HG12	1:F:567:VAL:O	2.21	0.41
1:F:1259:ASN:OD1	1:F:1259:ASN:N	2.54	0.41
1:F:2692:GLU:HG2	1:F:2693:GLU:H	1.86	0.41
1:N:517:GLU:N	1:N:517:GLU:OE1	2.54	0.40
1:F:1212:VAL:HG21	1:F:1507:LEU:HD21	2.03	0.40
1:N:145:LEU:HD23	1:N:145:LEU:O	2.21	0.40
1:F:2603:VAL:O	1:F:2603:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2615:ILE:O	1:F:2615:ILE:CG2	2.69	0.40
1:N:726:VAL:HG23	1:N:727:SER:N	2.36	0.40
1:F:1189:GLN:NE2	1:F:1550:GLU:OE2	2.55	0.40
1:N:2029:GLU:HG2	1:N:2182:TYR:HB2	2.03	0.40
1:F:180:LEU:HD23	1:F:193:LEU:HD23	2.02	0.40
1:F:517:GLU:N	1:F:517:GLU:OE1	2.54	0.40
1:F:946:ASP:HB3	1:F:952:LEU:HD11	2.02	0.40
1:N:288:VAL:HG12	1:N:289:VAL:O	2.22	0.40
1:N:567:VAL:HG12	1:N:567:VAL:O	2.22	0.40
1:N:1556:ASP:O	1:N:1619:ASN:ND2	2.55	0.40
1:N:2168:SER:O	1:N:2169:LYS:HB2	2.22	0.40
1:F:2001:GLY:CA	1:F:2038:LEU:HD12	2.51	0.40
1:F:2668:LEU:HD13	1:F:2681:ILE:CD1	2.50	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	F	2407/2839 (85%)	2370 (98%)	37 (2%)	0	100	100
1	N	2407/2839 (85%)	2376 (99%)	31 (1%)	0	100	100
All	All	4814/5678 (85%)	4746 (99%)	68 (1%)	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	F	2170/2531 (86%)	2145 (99%)	25 (1%)	67	78
1	N	2170/2531 (86%)	2147 (99%)	23 (1%)	70	80
All	All	4340/5062 (86%)	4292 (99%)	48 (1%)	69	80

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	105	ASP
1	N	119	HIS
1	N	297	LYS
1	N	314	ARG
1	N	430	ASP
1	N	718	ASP
1	N	847	LEU
1	N	1047	ASP
1	N	1150	SER
1	N	1196	LEU
1	N	1201	LEU
1	N	1207	ARG
1	N	1276	ARG
1	N	1357	PHE
1	N	1374	HIS
1	N	1457	LYS
1	N	1533	ARG
1	N	1576	HIS
1	N	1635	TYR
1	N	1802	THR
1	N	1828	ARG
1	N	1844	LYS
1	N	2432	ASN
1	F	105	ASP
1	F	119	HIS
1	F	122	HIS
1	F	297	LYS
1	F	314	ARG
1	F	559	ASP
1	F	718	ASP
1	F	847	LEU
1	F	1047	ASP
1	F	1150	SER

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Mol	Chain	Res	Type
1	F	1156	ASN
1	F	1196	LEU
1	F	1201	LEU
1	F	1207	ARG
1	F	1276	ARG
1	F	1357	PHE
1	F	1374	HIS
1	F	1457	LYS
1	F	1533	ARG
1	F	1576	HIS
1	F	1635	TYR
1	F	1802	THR
1	F	1828	ARG
1	F	1846	ARG
1	F	2432	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	20	GLN
1	N	400	GLN
1	N	435	HIS
1	N	535	GLN
1	N	554	GLN
1	N	1054	ASN
1	N	1055	GLN
1	N	1856	ASN
1	N	1943	HIS
1	N	2425	ASN
1	N	2432	ASN
1	N	2658	HIS
1	F	20	GLN
1	F	400	GLN
1	F	435	HIS
1	F	554	GLN
1	F	1055	GLN
1	F	1943	HIS
1	F	2099	HIS
1	F	2425	ASN
1	F	2432	ASN
1	F	2658	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [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-13393. These allow visual inspection of the internal detail of the map and identification of artifacts.

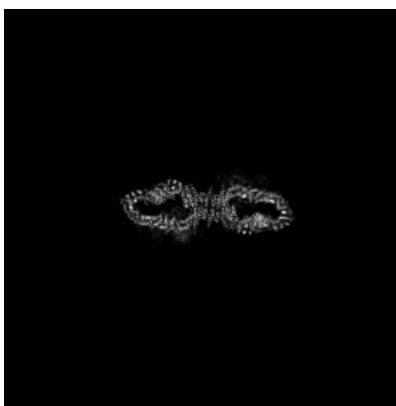
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

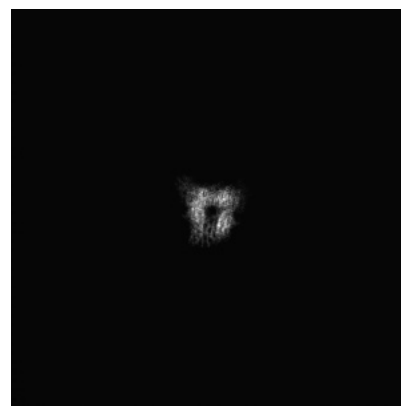
#### 6.1.1 Primary map



X

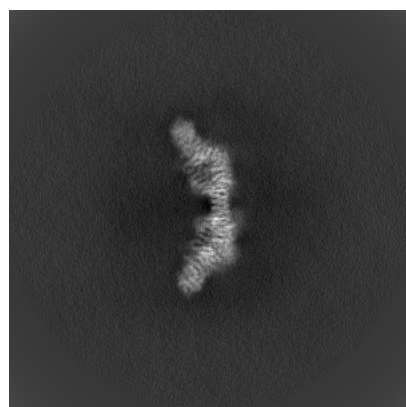


Y

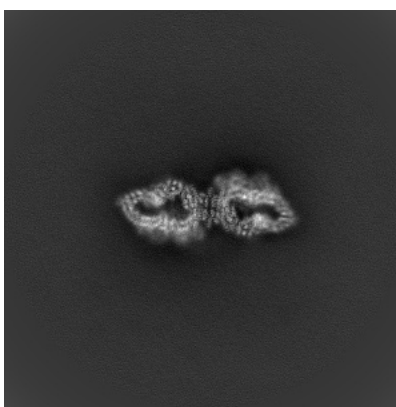


Z

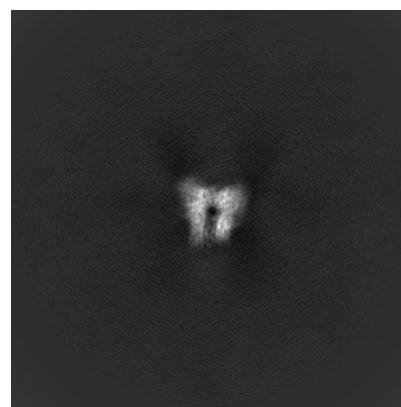
#### 6.1.2 Raw map



X



Y



Z

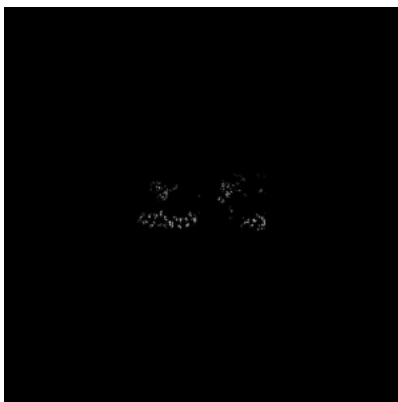
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

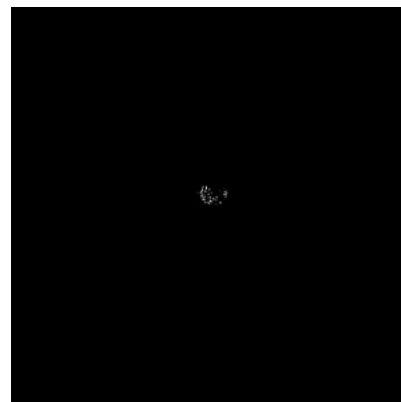
### 6.2.1 Primary map



X Index: 235

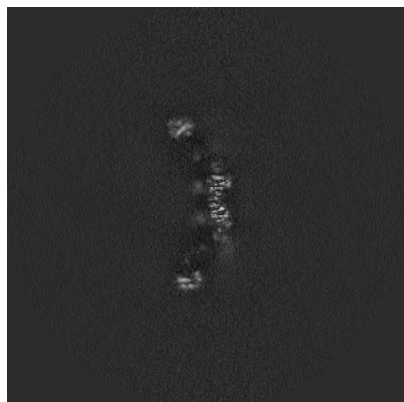


Y Index: 235

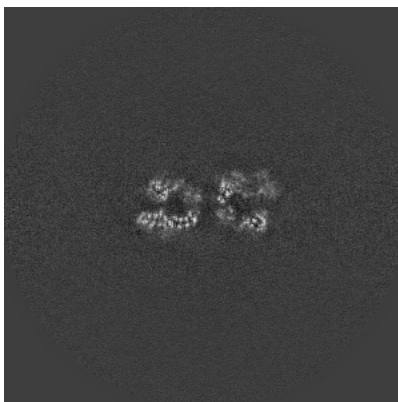


Z Index: 235

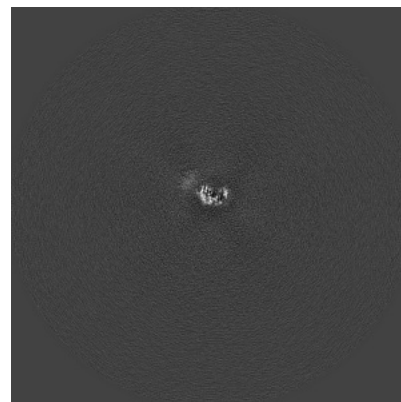
### 6.2.2 Raw map



X Index: 200



Y Index: 200

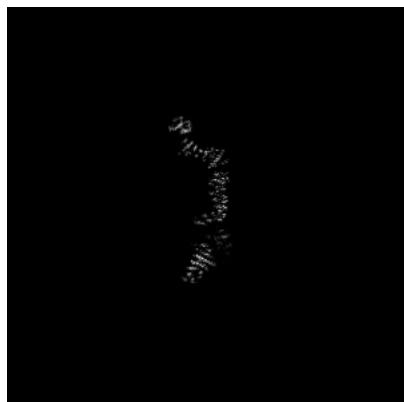


Z Index: 200

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

## 6.3 Largest variance slices [i](#)

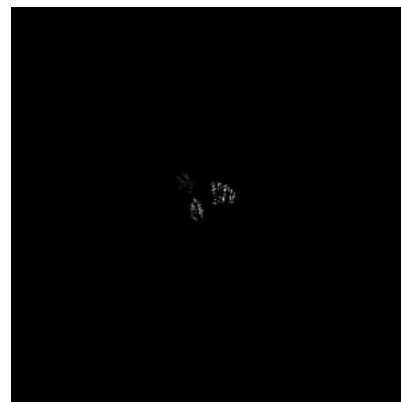
### 6.3.1 Primary map



X Index: 224

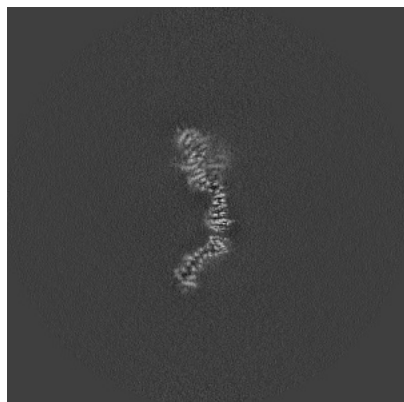


Y Index: 246

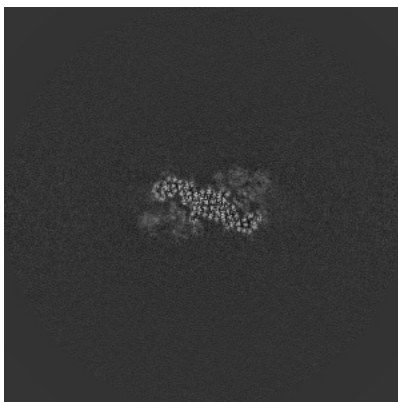


Z Index: 215

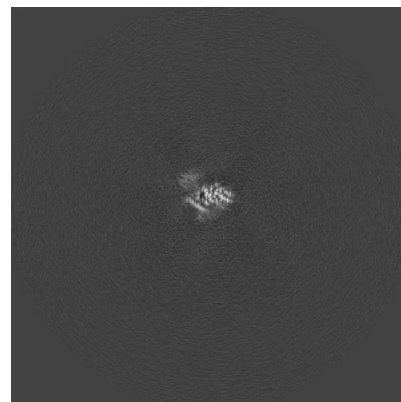
### 6.3.2 Raw map



X Index: 213



Y Index: 209



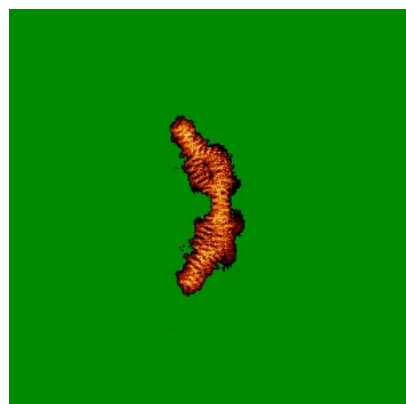
Z Index: 191

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

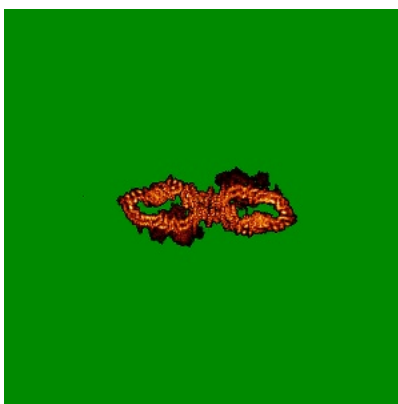


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

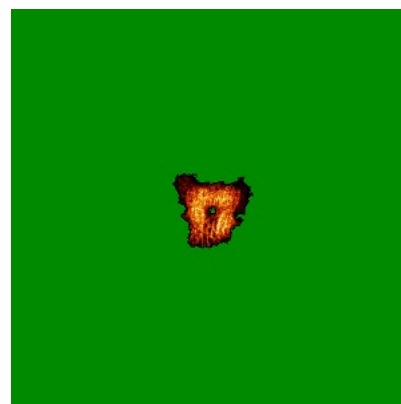
### 6.4.1 Primary map



X

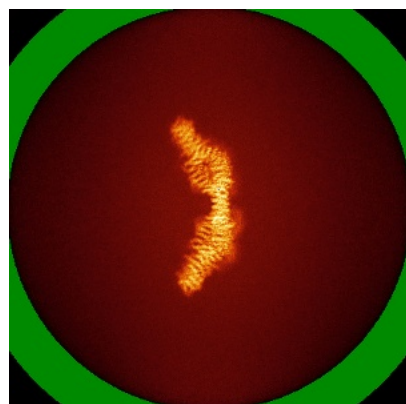


Y

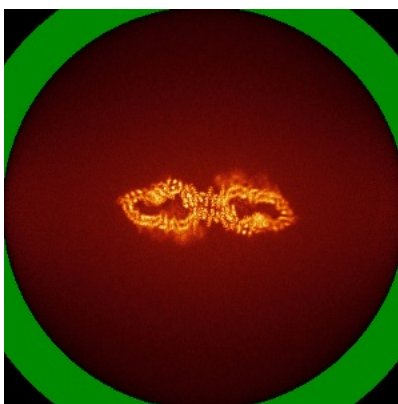


Z

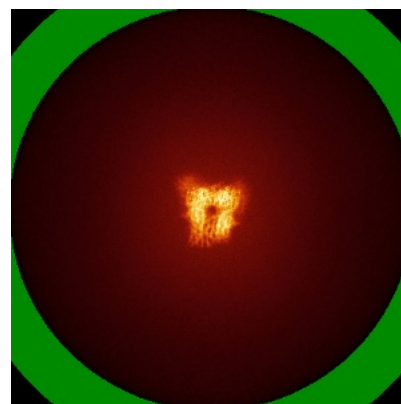
### 6.4.2 Raw map



X



Y

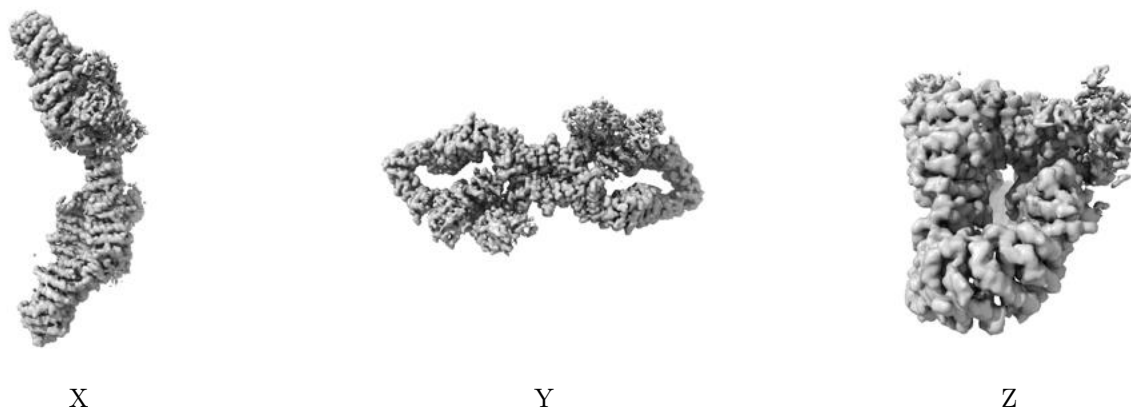


Z

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

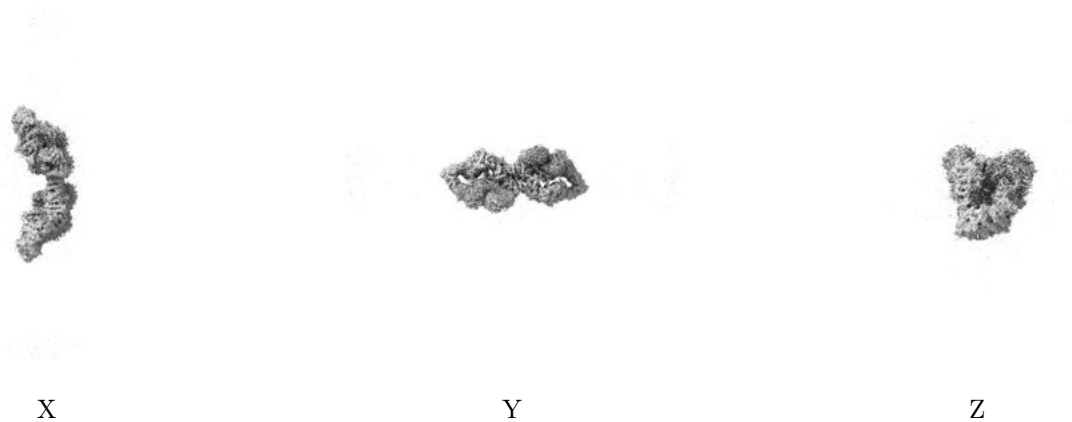
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

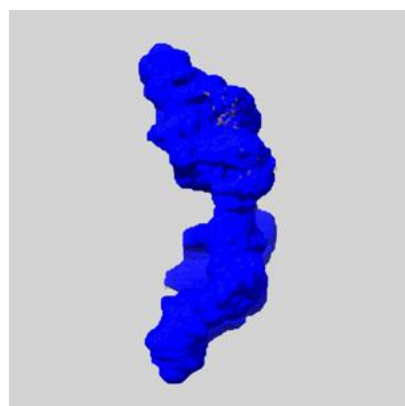
## 6.6 Mask visualisation [i](#)

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

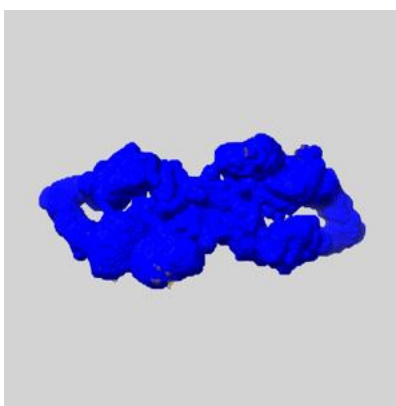
A mask typically either:

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

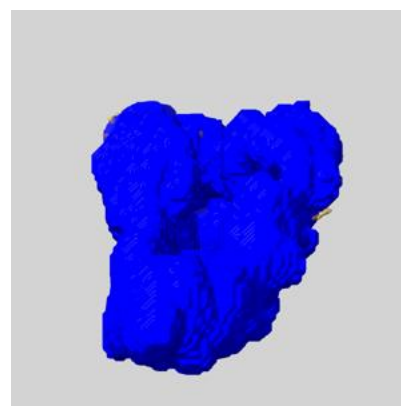
### 6.6.1 emd\_13393\_msk\_1.map [i](#)



X



Y

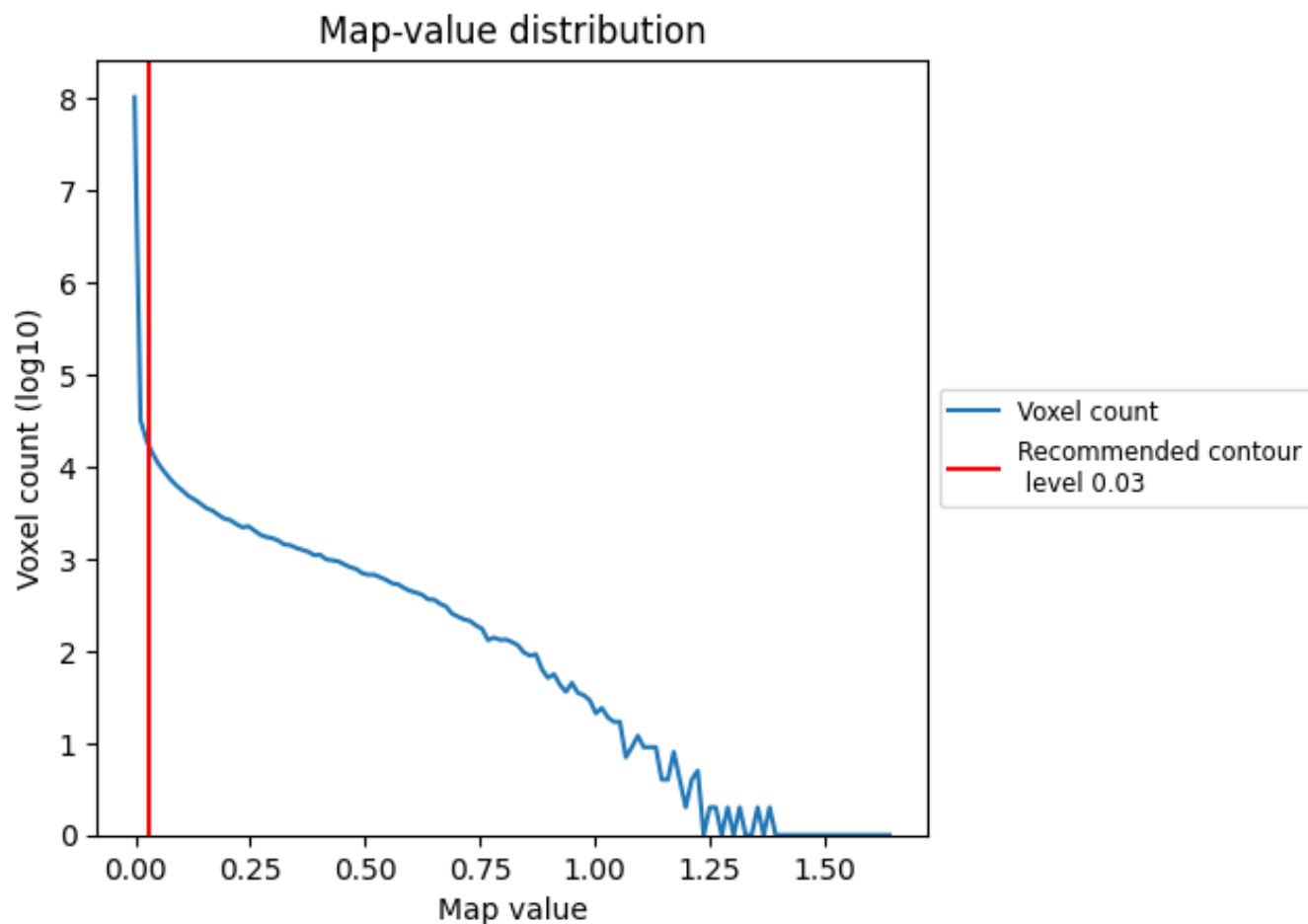


Z

## 7 Map analysis [i](#)

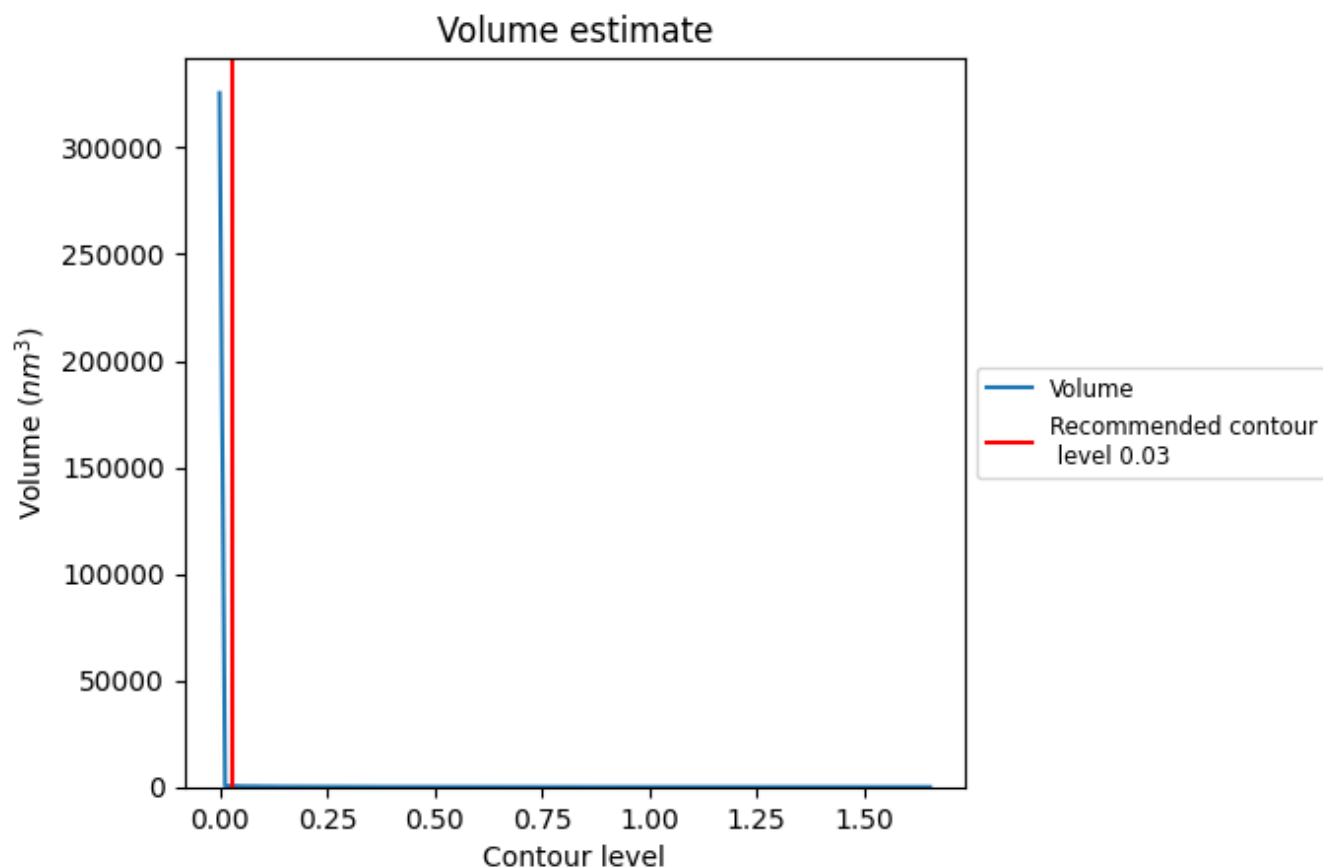
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

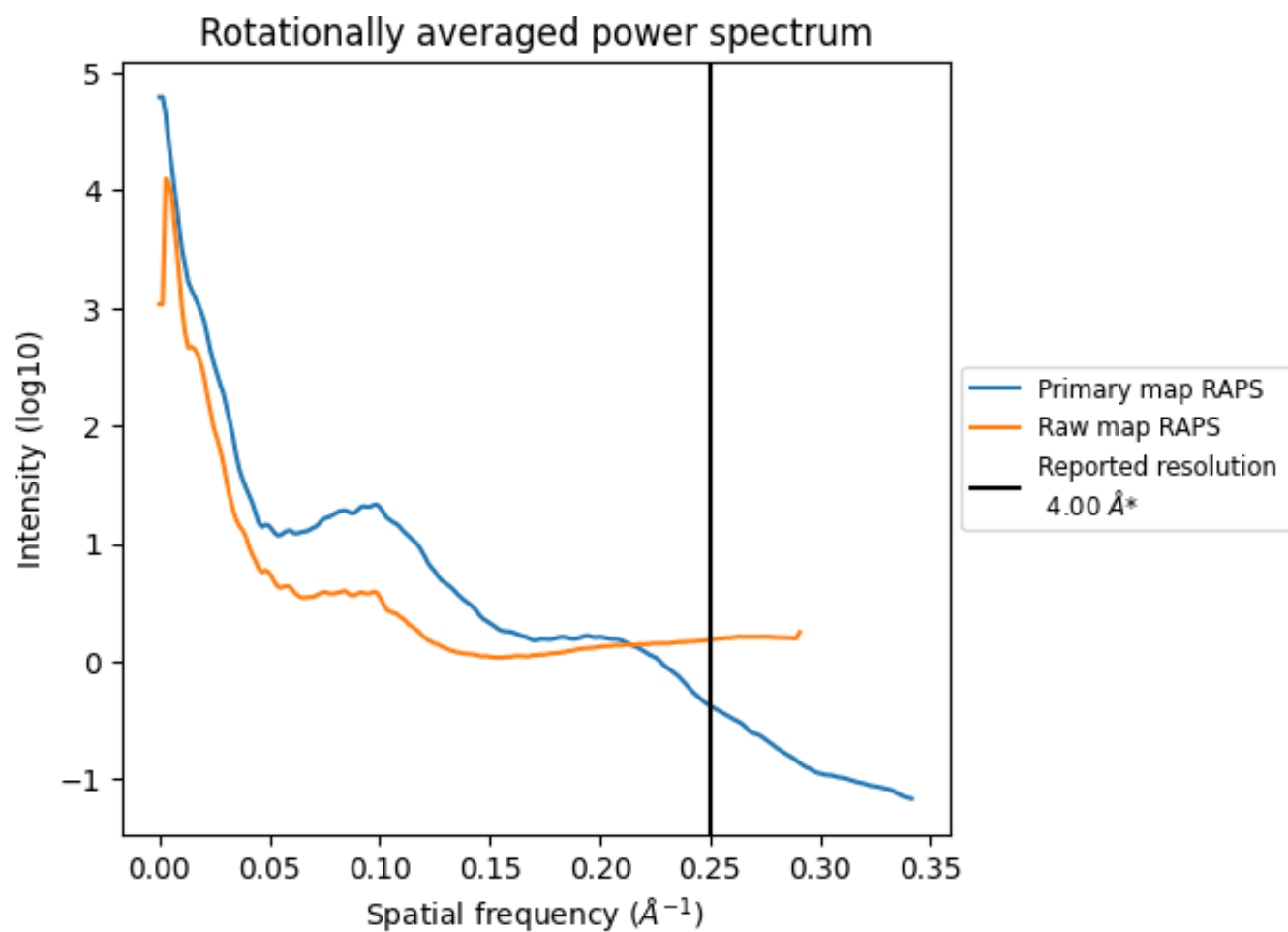
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm<sup>3</sup>; this corresponds to an approximate mass of 375 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 ⓘ

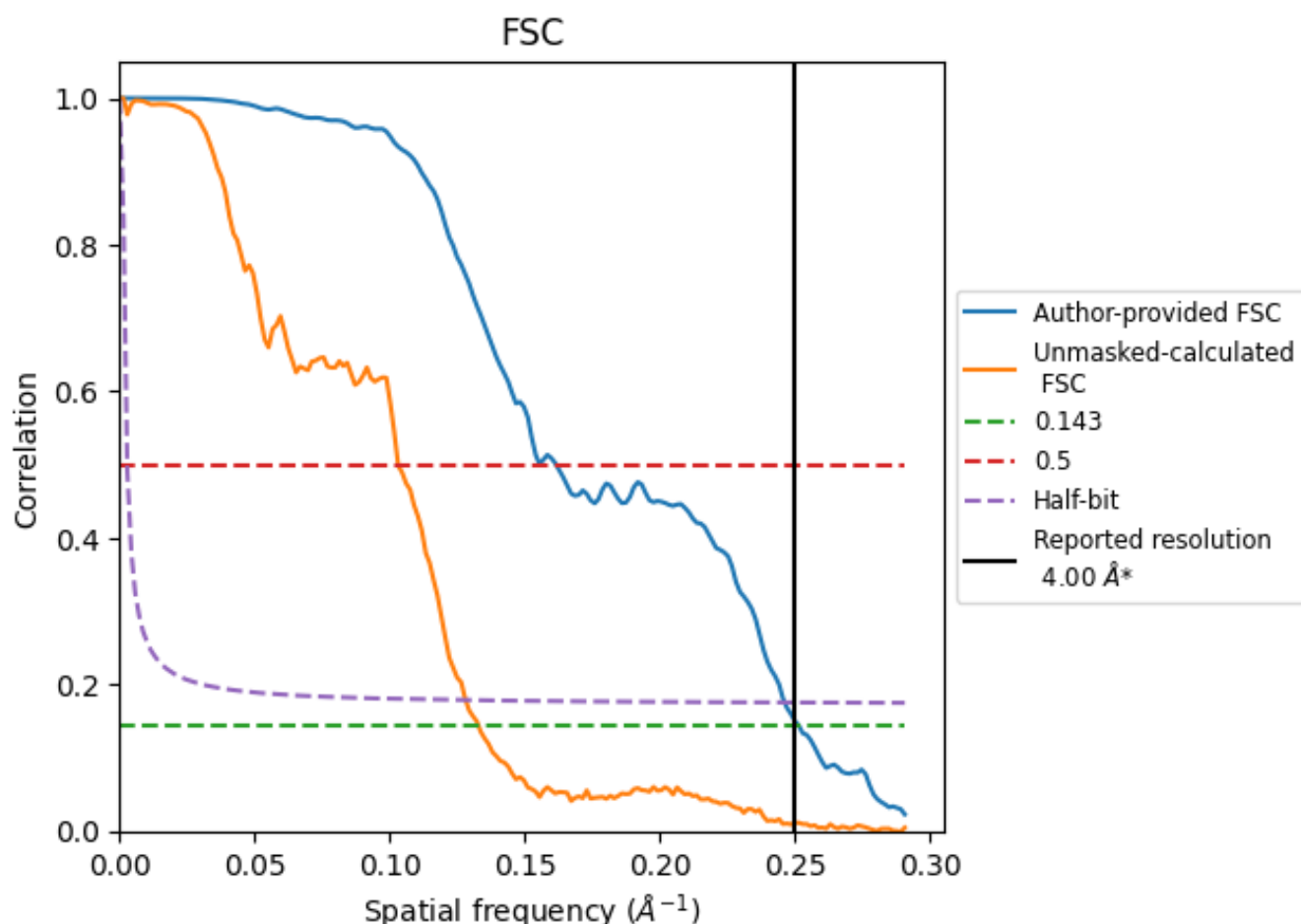


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	6.19	4.06
Unmasked-calculated*	7.52	9.70	7.80

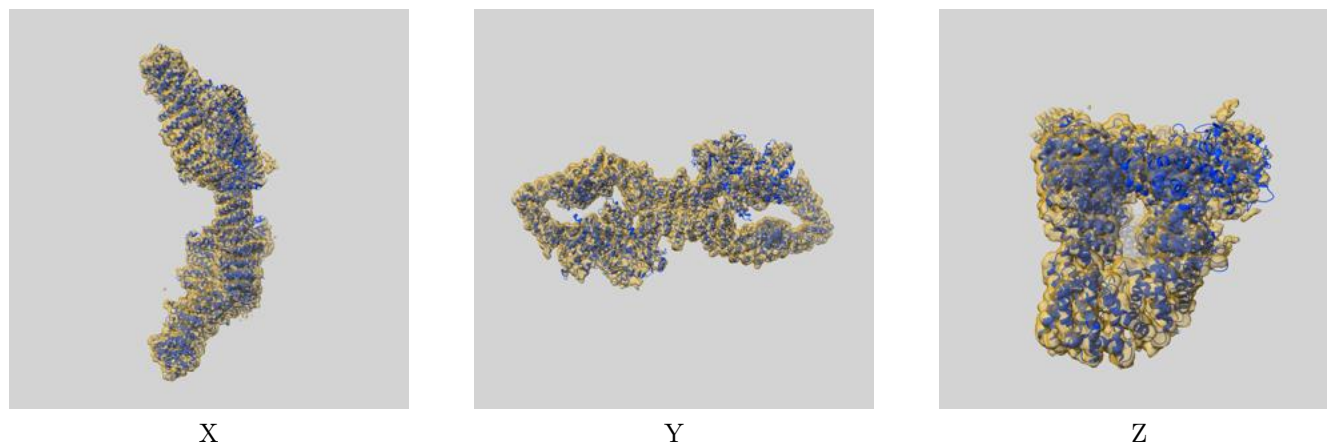
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.52 differs from the reported value 4.0 by more than 10 %



## 9 Map-model fit [i](#)

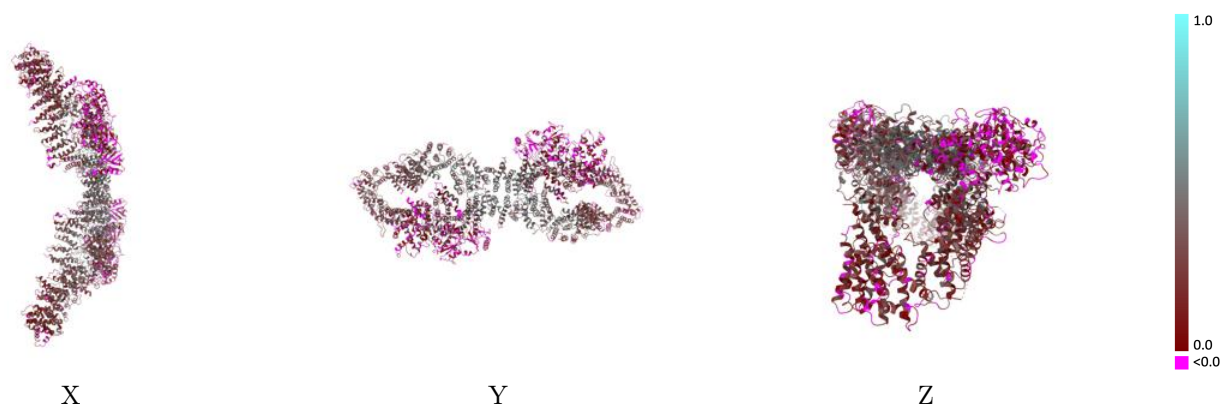
This section contains information regarding the fit between EMDB map EMD-13393 and PDB model 7PGR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

### 9.1 Map-model overlay [i](#)



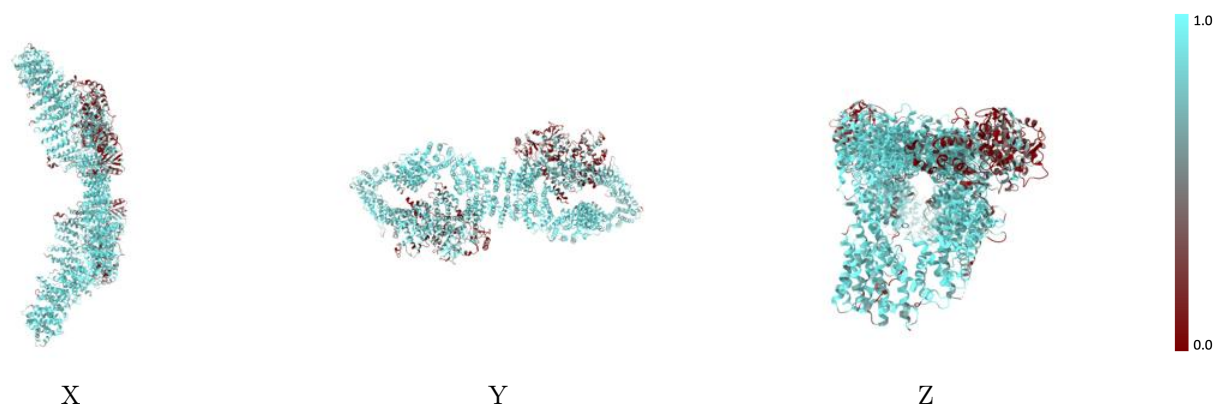
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



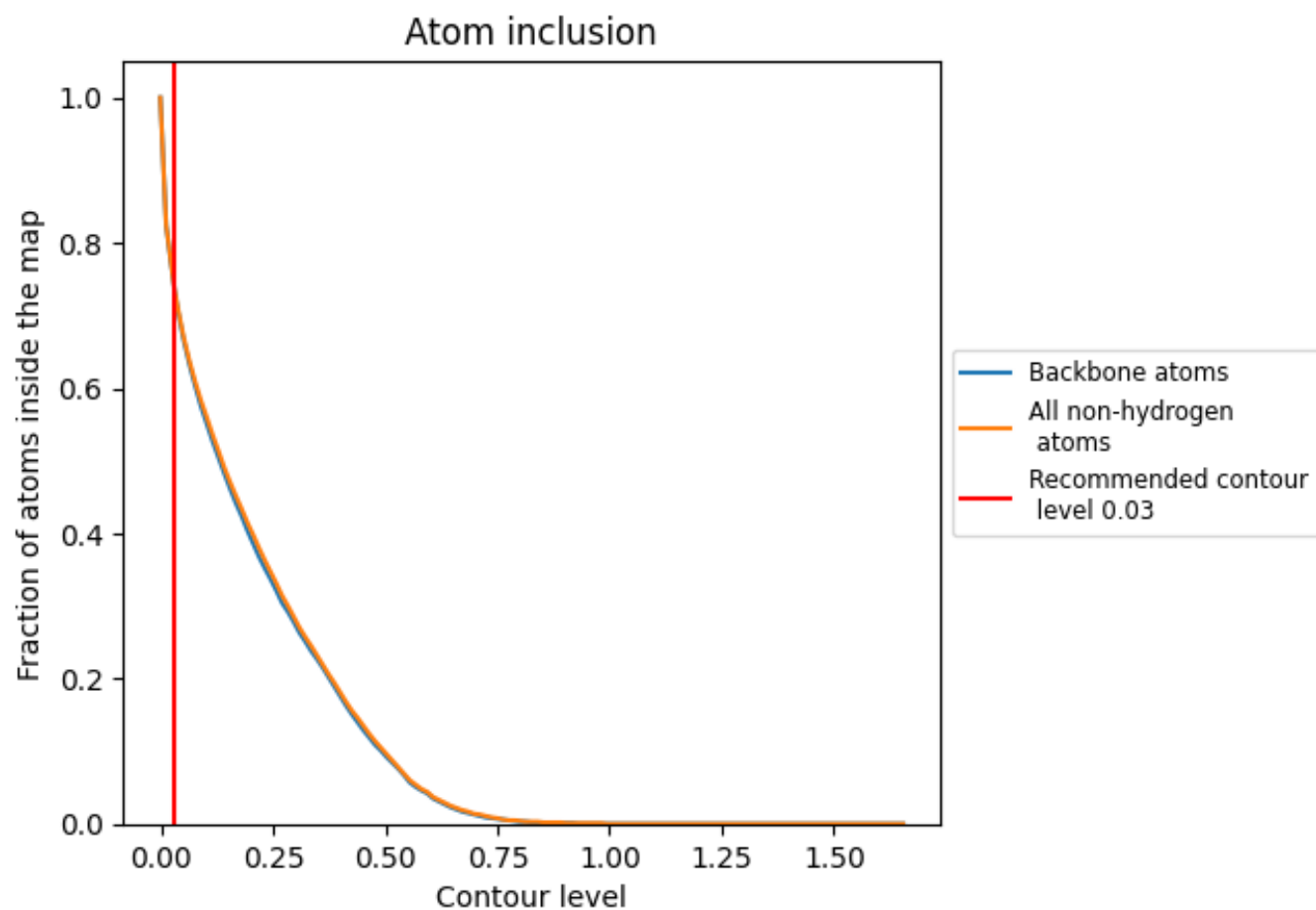
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7350	<div></div> 0.2320
F	<div></div> 0.7670	<div></div> 0.2400
N	<div></div> 0.7230	<div></div> 0.2230

