



## Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 01:57 am BST

PDB ID : 9QB8 / pdb\_00009qb8  
EMDB ID : EMD-52990  
Title : Lymphostatin - Conformation II - pH 8 Hepes  
Authors : Bottcher, B.; Schneider, R.; Griessmann, M.; Ramussen, T.  
Deposited on : 2025-02-28  
Resolution : 3.40 Å(reported)  
Based on initial model : 9euw

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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

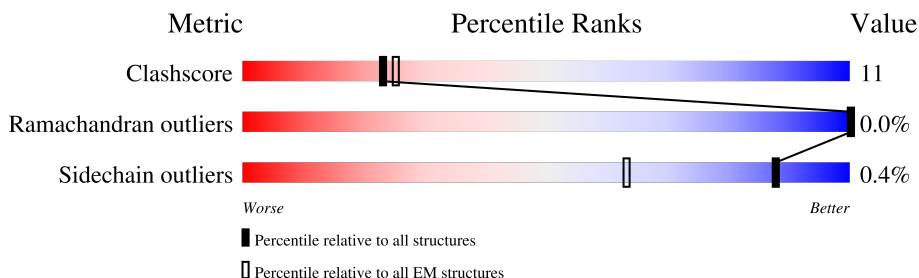
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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	A	3223	<p>65% 21% 13%</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22339 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 Lymphostatin.

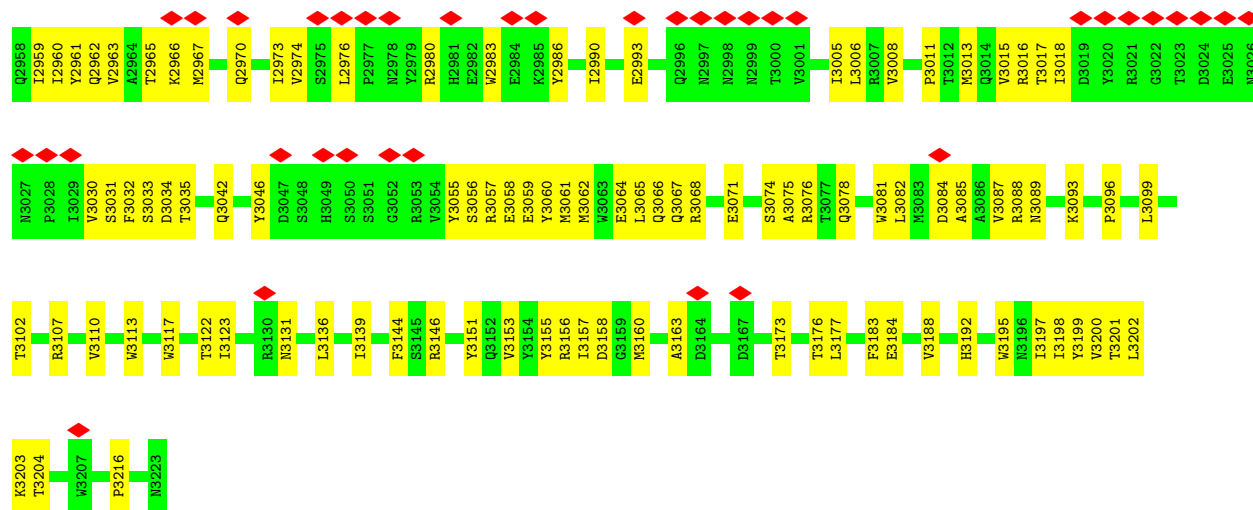
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2803	22338	14119	3874	4269	76	0	0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mn	0
			1	1	



GLY	ALA	E2823	V2654	L2555	A2461	N2303	I2115	G1861	L1654	F1403	P1248	SER	GLY	LEU
MET	V2824	E2759	S2657	L2556	I2462	T2304	V2119	I1862	I1685	F1414	E1251	ASN	ILE	GLU
LYS	M2825	A2760	L2557	E2557	L2463	T2305	G2120	M1863	T1686	T1414	T1687	THR	THR	THR
LYS	D2826	P2761	L2558	S2559	D2464	Q2307	Y2121	F1865	L1699	S1427	P1256	GLU	THR	PHE
THR	T2827	L2762	E2665	P2560	R2465	L2310	N2137	L1867	T1709	F1454	L1257	LYS	THR	THR
ASP	T2828	L2763	N2666	V2561	W2469	L2311	W2140	G1868	T1713	R1479	N1262	ASP	THR	THR
GLY	D2829	L2765	V2674	L2562	V2477	T2312	P2141	M1869	T1716	R1480	N1263	HIS	GLY	GLY
PRO	R2830	E2766	E2675	E2563	R2478	L2313	R2142	S1870	L1716	M1481	L1264	ASN	ASN	ASN
SER	E2831	E2767	G2676	E2564	F2479	V2314	Y2159	V1871	Q1736	L1485	G1273	ARG	PHE	PHE
VAL	E2832	R2768	K2682	L2573	S2487	A2317	Y2166	G1873	Q1736	L1485	G1273	LEU	LEU	LEU
GLU	L2833	R2770	L2574	L2575	Y2488	K2320	N2186	V1874	I1740	L1488	K1274	ASP	ASP	ASP
ASP	E2834	S2774	W2687	T2576	Y2488	D2329	I2169	H1885	I1741	Q1489	V1279	LYS	LYS	GLY
ASP	K2835	D2775	K2688	L2577	A2577	R2343	R2191	ASP	K1742	S1497	V1280	ILE	ILE	ILE
ASP	E2836	A2689	E2690	T2578	Q2494	S2343	R2191	THR	T1746	E1501	S1282	ALA	ALA	ALA
ASP	L2837	G2691	E2692	Y2581	L2495	L2358	T2202	LEU	R1754	K1517	V1281	VAL	VAL	VAL
ASP	R2838	F2779	V2692	L2585	V2496	N2347	N2198	SER	R1754	K1517	V1281	LYS	LYS	LYS
ASP	P2839	L2780	V2695	T2590	R2502	N2348	S2199	THR	K1517	K1517	V1281	ASN	ASN	ASN
ASP	T2840	L2781	V2695	T2590	Y2503	Q2200	Q2200	LEU	M1760	M1528	V1281	MET	MET	MET
ASP	L2841	L2782	I2699	L2594	S2504	T2358	C2201	ALA	M1760	M1528	V1281	ASN	ASN	ASN
ASP	T2842	L2783	I2699	P2595	E2505	L2364	T2202	ILE	T1784	M1537	V1281	SER	SER	SER
ASP	G2843	M2784	L2702	L2602	R2508	L2364	V2212	ASN	Q1772	M1537	V1281	HIS	HIS	HIS
ASP	D2844	L2785	F2714	Q2603	A2509	H2371	L2213	ALA	Q1772	Y1545	V1281	GLY	GLY	GLY
ASP	T2845	H2786	V2720	P2604	R2512	K2384	L2215	M1897	L1775	Y1545	V1281	LEU	LEU	LEU
ASP	H2846	Q2787	L2721	Q2605	H2513	L2392	P2223	D1898	F1797	T1547	V1281	THR	THR	THR
ASP	R2847	G2788	L2721	D2606	H2513	L2392	P2223	I1899	Q1798	R1573	V1281	PHE	PHE	PHE
ASP	M2848	M2789	P2730	V2613	T2516	L2392	P2223	K1917	Q1798	R1573	V1281	GLY	GLY	GLY
ASP	P2849	V2790	L2731	L2614	A2517	Y2394	T2226	R1917	Q1798	R1573	V1281	LYS	LYS	LYS
ASP	T2849	L2791	K2732	R2615	G2522	N2399	E2227	R1943	R1802	Y1577	V1281	ILE	ILE	ILE
ASP	M2850	L2792	L2733	R2615	G2522	N2399	E2227	R1943	R1802	Y1577	V1281	LYS	LYS	LYS
ASP	A2851	D2793	T2734	P2618	S2524	L2400	I2230	R1957	L1808	Y1592	V1281	GLN	GLN	GLN
ASP	T2852	R2794	T2734	D2619	R2525	P2404	K2236	V1963	E1811	Y1592	V1281	ASN	ASN	ASN
ASP	Y2853	R2795	S2735	M2620	Y2525	P2404	K2236	V1963	E1811	Y1592	V1281	THR	THR	THR
ASP	H2854	L2796	A2736	Q2625	I2527	K2409	L2239	L1968	L1815	P1607	V1327	THR	THR	THR
ASP	L2855	L2797	Q2737	L2626	M2529	N2411	V2250	T1968	A1816	P1607	V1327	GLN	GLN	GLN
ASP	H2856	R2798	E2738	F2627	Q2540	H2412	V2250	Y1974	R1822	K1612	V1327	ASP	ASP	ASP
ASP	L2857	R2800	Q2739	T2632	P2531	G2424	T2268	L1978	F1823	F1613	V1327	LEU	LEU	LEU
ASP	M2858	L2801	Q2740	T2633	V2532	M2425	T2268	L1978	F1823	F1613	V1327	THR	THR	THR
ASP	L2859	F2802	L2741	T2634	T2533	T2426	L2269	T1984	M1824	I1614	V1327	LYS	LYS	LYS
ASP	A2860	R2805	E2744	R2637	Q2535	T2436	S2270	F1998	R1828	Q1625	V1327	GLN	GLN	GLN
ASP	A2861	E2806	Q2745	L2638	I2536	L2436	E2276	V2036	T1832	E1626	V1327	LEU	LEU	LEU
ASP	D2862	Q2807	Q2746	E2639	T2539	L2442	E2276	Q2045	L1833	L1631	V1327	GLN	GLN	GLN
ASP	T2863	L2808	Q2747	N2640	Q2540	R2447	T2281	Q2045	H1834	E1645	V1327	ILE	ILE	ILE
ASP	G2809	G2809	Q2748	M2642	L2543	N2456	V2291	K2080	T1835	G1376	V1327	LYS	LYS	LYS
ASP	R2814	E2750	Q2749	M2642	L2543	N2456	V2291	K2080	T1835	G1376	V1327	ALA	ALA	ALA
ASP	L2815	H2751	H2751	M2648	L2549	R2458	V2292	V2082	S1837	M1648	V1327	LEU	LEU	LEU
ASP	T2816	L2752	L2752	T2649	H2549	R2458	V2292	V2082	S1837	M1648	V1327	LYS	LYS	LYS
ASP	F2817	L2753	L2753	F2650	D2554	R2458	V2292	V2082	S1837	M1648	V1327	ILE	ILE	ILE
ASP	R2818	V2754	V2754	F2650	D2554	R2458	V2292	V2082	S1837	M1648	V1327	LEU	LEU	LEU
ASP	K2755	K2755	K2755	F2650	D2554	R2458	V2292	V2082	S1837	M1648	V1327	LYS	LYS	LYS
ASP	P2756	P2756	P2756	F2650	D2554	R2458	V2292	V2082	S1837	M1648	V1327	LEU	LEU	LEU
ASP	D2757	D2757	D2757	F2650	D2554	R2458	V2292	V2082	S1837	M1648	V1327	GLY	GLY	GLY
ASP	T2822	T2822	T2822	F2650	D2554	R2458	V2292	V2082	S1837	M1648	V1327	ILE	ILE	ILE
ASP	E2868	A2869	L2874	E2869	L2874	N2869	V2869	L2874	E2869	L2874	N2869	THR	THR	THR
ASP	D2870	L2870	L2871	L2870	L2871	N2870	V2870	L2871	E2870	L2871	N2870	THR	THR	THR
ASP	T2871	L2871	L2871	L2871	L2871	N2871	V2871	L2871	E2871	L2871	N2871	THR	THR	THR
ASP	E2872	A2873	L2874	E2872	L2873	N2872	V2872	L2873	E2872	L2873	N2872	THR	THR	THR
ASP	D2873	L2873	L2873	L2873	L2873	N2873	V2873	L2873	E2873	L2873	N2873	THR	THR	THR
ASP	T2874	L2874	L2874	L2874	L2874	N2874	V2874	L2874	E2874	L2874	N2874	THR	THR	THR
ASP	D2875	L2875	L2875	L2875	L2875	N2875	V2875	L2875	E2875	L2875	N2875	THR	THR	THR
ASP	T2876	L2876	L2876	L2876	L2876	N2876	V2876	L2876	E2876	L2876	N2876	THR	THR	THR
ASP	D2877	L2877	L2877	L2877	L2877	N2877	V2877	L2877	E2877	L2877	N2877	THR	THR	THR
ASP	T2878	L2878	L2878	L2878	L2878	N2878	V2878	L2878	E2878	L2878	N2878	THR	THR	THR
ASP	D2879	L2879	L2879	L2879	L2879	N2879	V2879	L2879	E2879	L2879	N2879	THR	THR	THR
ASP	T2880	L2880	L2880	L2880	L2880	N2880	V2880	L2880	E2880	L2880	N2880	THR	THR	THR
ASP	D2881	L2881	L2881	L2881	L2881	N2881	V2881	L2881	E2881	L2881	N2881	THR	THR	THR
ASP	T2882	L2882	L2882	L2882	L2882	N2882	V2882	L2882	E2882	L2882	N2882	THR	THR	THR
ASP	D2883	L2883	L2883	L2883	L2883	N2883	V2883	L2883	E2883	L2883	N2883	THR	THR	THR
ASP	T2884	L2884	L2884	L2884	L2884	N2884	V2884	L2884	E2884	L2884	N2884	THR	THR	THR
ASP	D2885	L2885	L2885	L2885	L2885	N2885	V2885	L2885	E2885	L2885	N2885	THR	THR	THR
ASP	T2886	L2886	L2886	L2886	L2886	N2886	V2886	L2886	E2886	L2886	N2886	THR	THR	THR
ASP	D2887	L2887	L2887	L2887	L2887	N2887	V2887	L2887	E2887	L2887	N2887	THR	THR	THR
ASP	T2888	L2888	L2888	L2888	L2888	N2888	V2888	L2888	E2888	L2888	N2888	THR	THR	THR
ASP	D2889	L2889	L2889	L2889	L2889	N2889	V2889	L2889	E2889	L2889	N2889	THR	THR	THR
ASP	T2890	L2890	L2890	L2890	L2890	N2890	V2890	L2890	E2890	L2890	N2890	THR	THR	THR
ASP	D2891	L2891	L2891	L2891	L2891	N2891	V2891	L2891	E2891	L2891	N2891	THR	THR	THR
ASP	T2892	L2892	L2892	L2892	L2892	N2892	V2892	L2892	E2892	L2892	N2892	THR	THR	THR
ASP	D2893	L2893	L2893	L2893	L2893	N2893	V2893	L2893	E2893	L2893	N2893	THR	THR	THR
ASP	T2894	L2894	L2894	L2894	L2894	N2894	V2894	L2894	E2894	L2894	N2894	THR	THR	THR
ASP	D2895	L2895	L2895	L2895	L2895	N2895	V2895	L2895	E2895	L2895	N2895	THR	THR	THR
ASP	T2896	L2896	L2896	L2896	L2896	N2896	V2896	L2896	E2896	L2896	N2896	THR	THR	THR
ASP	D2897	L2897	L2897	L2897	L2897	N2897	V2897	L2897	E2897	L2897	N2897	THR	THR	THR
ASP	T2898	L2898	L2898	L2898	L2898	N2898	V2898	L2898	E2898	L2898	N2898	THR	THR	THR
ASP	D2899	L2899	L2899	L2899	L2899	N2899	V2899	L2899	E2899	L2899	N2899	THR	THR	THR
ASP	T2900	L2900	L2900	L2900	L2900	N2900	V2900	L2900	E2900	L2900	N2900	THR	THR	THR
ASP	D2901	L2901	L2901	L2901	L2901	N2901	V2901	L2901	E2901	L2901	N2901	THR	THR	THR
ASP	T2902	L2902	L2902	L2902	L2902	N2902	V2902	L2902	E2902	L2902	N2902	THR	THR	THR
ASP	D2903	L2903	L2903	L2903	L2903	N2903	V2903	L2903	E2903	L2903	N2903	THR	THR	THR
ASP	T2904	L2904	L2904	L2904	L2904	N2904	V2904	L2904	E2904	L2904	N2904	THR	THR	THR
ASP	D2905	L2905	L2905	L2905	L2905	N2905	V2905	L2905	E2905	L2905	N2905	THR	THR	THR
ASP	T2906	L2906	L2906	L2906	L2906	N2906	V2906	L2906	E2906	L2906	N2906	THR	THR	THR
ASP	D2907	L2907	L2907	L2907	L2907	N2907	V2907	L2907	E2907	L2907	N2907	THR	THR	THR
ASP	T2908	L2908	L2908	L2908	L2908	N2908	V2908	L2908	E2908	L2908	N2908	THR	THR	THR
ASP	D2909	L2909	L2909	L2909	L2909	N2909	V2909	L2909	E2909	L2909	N2909	THR	THR	THR
ASP	T2910	L2910	L2910	L2910	L2910	N2910	V2910	L2910	E2910	L2910	N2910	THR	THR	THR
ASP	D2911	L2911	L2911	L2911	L2911	N2911	V2911	L2911	E2911	L2911	N2911	THR	THR	THR
ASP	T2912	L2912	L2912	L2912	L2912	N2912	V2912	L2912	E2912</					



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1100	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	43.996	Depositor
Minimum map value	-17.599	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.916	Depositor
Recommended contour level	3	Depositor
Map size ( $\text{\AA}$ )	378.4, 378.4, 378.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.946, 0.946, 0.946	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.24	0/22775	0.42	0/30861

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 [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	22338	0	22339	488	0
2	A	1	0	0	0	0
All	All	22339	0	22339	488	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (488) 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:2080:LYS:HG2	1:A:2198:ASN:HD22	1.28	0.95
1:A:3096:PRO:HA	1:A:3099:LEU:HD12	1.57	0.87

*Continued on next page...*



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3068:ARG:HE	1:A:3075:ALA:HB1	1.40	0.85
1:A:2614:LEU:HD23	1:A:2615:ARG:HH21	1.40	0.84
1:A:545:MET:HE1	1:A:649:MET:HE1	1.59	0.84
1:A:2980:ARG:HH12	1:A:3088:ARG:HH22	1.27	0.81
1:A:2641:LEU:HD21	1:A:2664:LEU:HB3	1.61	0.81
1:A:3099:LEU:HB3	1:A:3160:MET:HE1	1.69	0.74
1:A:2795:ARG:HA	1:A:2821:PHE:HB2	1.70	0.73
1:A:397:TYR:HE2	1:A:835:PHE:CG	2.09	0.71
1:A:2648:MET:HG2	1:A:3084:ASP:HB2	1.72	0.71
1:A:1314:LEU:HD21	1:A:1319:LEU:HD12	1.74	0.69
1:A:378:ASN:HD21	1:A:1648:MET:HB3	1.57	0.69
1:A:769:ARG:HH12	1:A:782:ARG:HA	1.57	0.69
1:A:1189:VAL:HG22	1:A:1281:VAL:HG13	1.74	0.68
1:A:2527:ILE:HD13	1:A:2554:ASP:HB3	1.75	0.68
1:A:1870:SER:O	1:A:1874:VAL:HG23	1.93	0.68
1:A:2080:LYS:HG2	1:A:2198:ASN:ND2	2.05	0.68
1:A:1811:GLU:HB2	1:A:1828:ARG:HB2	1.75	0.67
1:A:2910:THR:HG23	1:A:2973:ILE:HD11	1.76	0.67
1:A:2642:MET:HE3	1:A:2642:MET:H	1.59	0.67
1:A:3005:ILE:HG23	1:A:3016:ARG:HB2	1.76	0.67
1:A:871:LEU:HD22	1:A:906:ILE:HG23	1.76	0.66
1:A:2776:ASP:HB3	1:A:2779:PHE:HB3	1.77	0.66
1:A:2096:SER:HB3	1:A:2141:PRO:HD2	1.77	0.66
1:A:2540:GLN:HE22	1:A:2542:ILE:HG23	1.60	0.66
1:A:2250:VAL:HB	1:A:2303:MET:HE1	1.77	0.65
1:A:3074:SER:O	1:A:3078:GLN:HG3	1.96	0.65
1:A:2754:VAL:HG12	1:A:2756:PRO:HD3	1.79	0.65
1:A:2990:ILE:HG22	1:A:3006:LEU:HB3	1.78	0.65
1:A:1797:PHE:HB3	1:A:1899:ILE:HD12	1.79	0.65
1:A:494:ILE:HG12	1:A:508:ILE:HG13	1.79	0.64
1:A:867:THR:HG21	1:A:912:ASP:HB2	1.79	0.64
1:A:2487:SER:HB3	1:A:2496:VAL:HG13	1.78	0.64
1:A:2562:LEU:HB3	1:A:2577:ALA:HB3	1.80	0.64
1:A:1626:GLU:HB2	1:A:1631:LEU:HD22	1.80	0.64
1:A:3155:TYR:HA	1:A:3200:VAL:O	1.98	0.64
1:A:2364:LEU:HD22	1:A:2371:HIS:CE1	2.33	0.64
1:A:494:ILE:HG13	1:A:498:GLN:HE21	1.64	0.63
1:A:2919:GLU:HG2	1:A:2936:TYR:HB2	1.80	0.63
1:A:2614:LEU:HD23	1:A:2615:ARG:NH2	2.12	0.63
1:A:2980:ARG:NH1	1:A:3088:ARG:HH22	1.96	0.63
1:A:1305:ILE:HD11	1:A:1323:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3184:GLU:HB3	1:A:3203:LYS:HB3	1.80	0.62
1:A:1315:ASN:H	1:A:1318:ASN:HD22	1.47	0.62
1:A:695:ARG:HH22	1:A:1392:ARG:HD2	1.64	0.62
1:A:900:ASP:OD2	1:A:1377:LEU:HD12	2.00	0.62
1:A:939:ASN:HB2	1:A:1257:LEU:HD13	1.81	0.62
1:A:2528:ILE:HG23	1:A:2558:ALA:HB2	1.82	0.62
1:A:1863:MET:HE2	1:A:1863:MET:HA	1.82	0.61
1:A:398:ASN:ND2	1:A:835:PHE:HE1	1.99	0.61
1:A:536:TYR:HB3	1:A:537:PRO:HD3	1.83	0.61
1:A:1815:LEU:HD13	1:A:1917:LYS:HD2	1.80	0.61
1:A:278:LYS:HA	1:A:281:MET:HE3	1.82	0.61
1:A:456:ILE:HG23	1:A:460:LEU:HD23	1.82	0.61
1:A:1489:GLN:HG2	1:A:1654:LEU:HD13	1.83	0.61
1:A:2941:MET:HE3	1:A:2942:ALA:N	2.15	0.61
1:A:549:LYS:HB2	1:A:680:ILE:HG21	1.83	0.61
1:A:3011:PRO:HG3	1:A:3078:GLN:HA	1.83	0.60
1:A:2503:TYR:HD1	1:A:2523:GLY:HA3	1.65	0.60
1:A:2739:MET:HE1	1:A:2741:LEU:HB2	1.82	0.60
1:A:760:ILE:O	1:A:764:MET:HG3	2.01	0.60
1:A:1481:MET:HE1	1:A:1575:LEU:HD13	1.83	0.60
1:A:2603:GLN:HB3	1:A:2606:ASP:HB3	1.83	0.60
1:A:2603:GLN:HE22	1:A:2634:THR:HB	1.66	0.60
1:A:276:LEU:O	1:A:280:ILE:HG13	2.02	0.60
1:A:2461:ALA:O	1:A:2465:ARG:HG2	2.01	0.60
1:A:862:GLN:HB2	1:A:914:ILE:HG21	1.83	0.59
1:A:1356:HIS:HE1	1:A:1368:ALA:HB2	1.67	0.59
1:A:246:ILE:HG23	1:A:250:ARG:HH21	1.68	0.59
1:A:245:ILE:O	1:A:248:ILE:HG22	2.02	0.59
1:A:2212:VAL:HG12	1:A:2214:PRO:HD3	1.83	0.59
1:A:3156:ARG:HH12	1:A:3158:ASP:HA	1.68	0.59
1:A:981:HIS:O	1:A:985:ILE:HG13	2.02	0.59
1:A:2563:VAL:HG21	1:A:2602:ILE:HD11	1.84	0.59
1:A:621:ILE:HA	1:A:624:ILE:HD12	1.85	0.58
1:A:2302:VAL:HG13	1:A:2303:MET:HG2	1.85	0.58
1:A:2525:ARG:HH22	1:A:2527:ILE:HB	1.68	0.58
1:A:630:LYS:HD2	1:A:630:LYS:C	2.27	0.58
1:A:2424:GLY:HA2	1:A:2447:ARG:HD3	1.84	0.58
1:A:3018:ILE:HG22	1:A:3030:VAL:HG22	1.84	0.58
1:A:2564:GLU:HG3	1:A:2625:GLY:HA2	1.85	0.58
1:A:1736:GLN:O	1:A:1740:ILE:HG12	2.04	0.58
1:A:2714:PHE:HD2	1:A:2720:VAL:HG11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:MET:HB3	1:A:812:ASN:HB3	1.84	0.58
1:A:3131:ASN:HB3	1:A:3176:THR:HB	1.85	0.58
1:A:2529:MET:HA	1:A:2557:GLU:HB2	1.85	0.57
1:A:2918:GLY:HA2	1:A:2937:LYS:HE2	1.85	0.57
1:A:1497:SER:O	1:A:1501:GLU:HG2	2.04	0.57
1:A:2532:VAL:HG13	1:A:2533:THR:HG23	1.87	0.57
1:A:2957:LEU:HB3	1:A:2976:LEU:HB2	1.86	0.57
1:A:1760:MET:HE3	1:A:1760:MET:HA	1.87	0.57
1:A:2082:VAL:HG22	1:A:2202:THR:HB	1.86	0.57
1:A:273:GLN:HA	1:A:276:LEU:HD12	1.87	0.56
1:A:792:VAL:HG23	1:A:807:GLU:HB2	1.86	0.56
1:A:2838:ARG:HH21	1:A:2879:GLN:HB3	1.71	0.56
1:A:3057:ARG:O	1:A:3061:MET:HG2	2.06	0.56
1:A:2688:LYS:HZ1	1:A:2695:VAL:H	1.54	0.56
1:A:1517:LYS:HE3	1:A:1984:THR:HG22	1.86	0.55
1:A:1824:ASN:HB3	1:A:1836:THR:HB	1.88	0.55
1:A:698:ARG:HH12	1:A:1392:ARG:CZ	2.19	0.55
1:A:1327:VAL:HG12	1:A:1375:VAL:HG11	1.88	0.55
1:A:2760:ALA:HB3	1:A:2856:HIS:CD2	2.42	0.55
1:A:2404:PRO:HG3	1:A:2410:LEU:HD13	1.88	0.55
1:A:2749:GLN:HE21	1:A:2750:GLU:H	1.54	0.55
1:A:397:TYR:CE2	1:A:835:PHE:CG	2.94	0.55
1:A:2512:ARG:HA	1:A:2536:ILE:HA	1.88	0.55
1:A:415:TYR:HB2	1:A:731:LEU:HB3	1.89	0.55
1:A:2384:LYS:HD2	1:A:2393:ILE:HG21	1.87	0.55
1:A:3032:PHE:H	1:A:3055:TYR:HB3	1.70	0.55
1:A:357:ALA:HB1	1:A:832:ASP:HB3	1.89	0.55
1:A:1121:PHE:HD2	1:A:1122:LYS:HE3	1.72	0.55
1:A:2531:PRO:HD2	1:A:2578:THR:HG21	1.89	0.55
1:A:240:LYS:HE2	1:A:241:TYR:HE1	1.72	0.55
1:A:2462:ILE:O	1:A:2466:LEU:HG	2.07	0.54
1:A:588:LEU:HD22	1:A:621:ILE:HD11	1.89	0.54
1:A:3065:LEU:HD11	1:A:3156:ARG:HB2	1.90	0.54
1:A:2800:ARG:HD3	1:A:2814:ARG:HH11	1.71	0.54
1:A:278:LYS:HD2	1:A:281:MET:HE3	1.88	0.54
1:A:1614:ILE:O	1:A:1618:ILE:HG13	2.07	0.54
1:A:311:ASP:HB2	1:A:643:ARG:HE	1.72	0.54
1:A:2941:MET:HE3	1:A:2942:ALA:H	1.71	0.54
1:A:1181:LEU:HD12	1:A:1186:ILE:HD12	1.88	0.54
1:A:545:MET:HE3	1:A:545:MET:HA	1.88	0.54
1:A:3076:ARG:HG3	1:A:3139:ILE:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:MET:HG2	1:A:912:ASP:H	1.73	0.54
1:A:2640:ASN:HB3	1:A:2642:MET:SD	2.48	0.54
1:A:269:LEU:O	1:A:273:GLN:HG2	2.08	0.53
1:A:653:ARG:HD2	1:A:792:VAL:HG12	1.89	0.53
1:A:1802:ARG:HD3	1:A:1808:LEU:HD22	1.89	0.53
1:A:2730:PRO:HA	1:A:2751:HIS:O	2.08	0.53
1:A:3068:ARG:NE	1:A:3075:ALA:HB1	2.17	0.53
1:A:2312:THR:O	1:A:2312:THR:HG22	2.06	0.53
1:A:3017:THR:HG23	1:A:3031:SER:HB2	1.90	0.53
1:A:2594:LEU:HD12	1:A:2614:LEU:HD22	1.91	0.53
1:A:2699:ILE:HD12	1:A:2702:LEU:HD11	1.90	0.53
1:A:254:GLU:HB3	1:A:269:LEU:HD13	1.91	0.53
1:A:339:THR:HG21	1:A:637:PHE:HB2	1.90	0.53
1:A:828:ARG:HD2	1:A:831:ASP:HB2	1.91	0.53
1:A:1333:THR:O	1:A:1337:ILE:HG13	2.09	0.53
1:A:3058:GLU:HG2	1:A:3059:GLU:N	2.24	0.53
1:A:286:VAL:HG13	1:A:290:THR:HB	1.90	0.53
1:A:397:TYR:HE2	1:A:835:PHE:CD2	2.26	0.53
1:A:973:ILE:HB	1:A:1147:ILE:HD13	1.90	0.52
1:A:392:GLU:HA	1:A:395:LYS:HZ1	1.74	0.52
1:A:3087:VAL:HG12	1:A:3087:VAL:O	2.08	0.52
1:A:3061:MET:SD	1:A:3201:THR:HG21	2.50	0.52
1:A:3197:ILE:C	1:A:3198:ILE:HD12	2.35	0.52
1:A:1303:TYR:O	1:A:1307:VAL:HG12	2.09	0.52
1:A:2560:PRO:HA	1:A:2576:ILE:HD11	1.90	0.52
1:A:1754:ARG:HG2	1:A:1978:ILE:HD13	1.91	0.52
1:A:2409:LYS:HG3	1:A:2412:HIS:HB2	1.92	0.52
1:A:2714:PHE:CD2	1:A:2720:VAL:HG11	2.45	0.52
1:A:2980:ARG:HH21	1:A:3081:TRP:CG	2.27	0.52
1:A:3035:THR:HG22	1:A:3046:TYR:HD2	1.73	0.52
1:A:3085:ALA:HA	1:A:3088:ARG:NE	2.24	0.52
1:A:1319:LEU:HD11	1:A:1340:LEU:HD23	1.91	0.52
1:A:3006:LEU:HB2	1:A:3015:VAL:HG23	1.92	0.52
1:A:3082:LEU:HD11	1:A:3102:THR:HG22	1.91	0.52
1:A:2080:LYS:HD3	1:A:2200:GLN:HB3	1.90	0.51
1:A:2425:MET:HE3	1:A:2466:LEU:HD21	1.91	0.51
1:A:404:GLN:HE22	1:A:830:VAL:HA	1.75	0.51
1:A:929:LYS:O	1:A:933:MET:HG2	2.10	0.51
1:A:2276:GLU:HA	1:A:2317:ALA:HB3	1.93	0.51
1:A:2543:LEU:HD13	1:A:2595:PRO:HG2	1.93	0.51
1:A:3085:ALA:HA	1:A:3088:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:VAL:HG21	1:A:637:PHE:CE2	2.45	0.51
1:A:3065:LEU:HD21	1:A:3156:ARG:HG2	1.93	0.51
1:A:269:LEU:HA	1:A:272:LYS:HE3	1.91	0.51
1:A:1427:SER:HB2	1:A:1547:THR:HG21	1.93	0.51
1:A:1182:HIS:CE1	1:A:1282:SER:HB2	2.46	0.51
1:A:2605:GLN:HE22	1:A:2638:LEU:H	1.59	0.51
1:A:3056:SER:H	1:A:3059:GLU:HG3	1.75	0.51
1:A:1742:LYS:O	1:A:1746:THR:HG23	2.10	0.51
1:A:2846:HIS:HA	1:A:2849:ILE:HB	1.93	0.51
1:A:406:GLU:O	1:A:410:LYS:HE2	2.11	0.51
1:A:248:ILE:O	1:A:251:ILE:HG22	2.11	0.50
1:A:878:LEU:HD21	1:A:902:MET:SD	2.51	0.50
1:A:907:MET:HE1	1:A:923:GLN:HE22	1.76	0.50
1:A:1131:LYS:O	1:A:1135:ILE:HG22	2.11	0.50
1:A:3076:ARG:HA	1:A:3139:ILE:HG13	1.93	0.50
1:A:576:THR:HG22	1:A:620:ILE:HD11	1.92	0.50
1:A:1825:LEU:H	1:A:1836:THR:HA	1.77	0.50
1:A:2226:THR:O	1:A:2230:ILE:HG12	2.11	0.50
1:A:2838:ARG:O	1:A:2842:ILE:HG13	2.11	0.50
1:A:2563:VAL:HB	1:A:2627:PHE:HB3	1.93	0.50
1:A:2959:ILE:HB	1:A:2974:VAL:HB	1.93	0.50
1:A:632:PRO:O	1:A:633:GLU:C	2.55	0.50
1:A:2465:ARG:HG3	1:A:2465:ARG:HH11	1.77	0.50
1:A:2477:VAL:HB	1:A:2488:TYR:HB3	1.92	0.50
1:A:2948:LEU:HD23	1:A:2960:ILE:HG21	1.93	0.50
1:A:451:LYS:HD3	1:A:917:ARG:HH21	1.77	0.50
1:A:1849:LYS:HB3	1:A:1867:LEU:HD11	1.92	0.50
1:A:2963:VAL:HG13	1:A:2965:THR:H	1.76	0.50
1:A:3113:TRP:CZ3	1:A:3198:ILE:HG12	2.47	0.50
1:A:871:LEU:HD13	1:A:910:MET:HE2	1.94	0.49
1:A:947:LEU:HD11	1:A:975:TYR:HB2	1.94	0.49
1:A:2573:ILE:O	1:A:2573:ILE:HG13	2.12	0.49
1:A:3136:LEU:HD22	1:A:3173:THR:HG21	1.93	0.49
1:A:2641:LEU:HD12	1:A:2666:ASN:HB2	1.92	0.49
1:A:2805:ARG:HH12	1:A:2809:GLY:C	2.20	0.49
1:A:1871:VAL:O	1:A:1875:VAL:HG12	2.12	0.49
1:A:1608:ILE:O	1:A:1612:LYS:HG3	2.13	0.49
1:A:2505:GLU:HG2	1:A:2525:ARG:HE	1.77	0.49
1:A:2983:TRP:H	1:A:2983:TRP:CD1	2.30	0.49
1:A:3117:TRP:CH2	1:A:3216:PRO:HD3	2.47	0.49
1:A:3117:TRP:CZ3	1:A:3216:PRO:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3188:VAL:HG23	1:A:3200:VAL:HG22	1.93	0.49
1:A:2650:PHE:CE1	1:A:2721:LEU:HB2	2.48	0.49
1:A:2682:LYS:HD2	1:A:2682:LYS:C	2.38	0.49
1:A:2394:TYR:H	1:A:2399:ASN:HB3	1.78	0.49
1:A:848:GLU:HG3	1:A:928:GLU:OE2	2.13	0.49
1:A:2456:ASN:HB3	1:A:2458:ARG:NE	2.27	0.49
1:A:793:TYR:CD1	1:A:806:PRO:HB3	2.48	0.48
1:A:1764:THR:HG21	1:A:1772:GLN:HG3	1.94	0.48
1:A:2036:VAL:HG13	1:A:2045:GLN:HB3	1.94	0.48
1:A:3197:ILE:O	1:A:3197:ILE:HG13	2.12	0.48
1:A:753:GLN:HE21	1:A:753:GLN:HA	1.78	0.48
1:A:2642:MET:H	1:A:2642:MET:CE	2.25	0.48
1:A:1822:ARG:HH22	1:A:1837:SER:HA	1.77	0.48
1:A:1823:PHE:HB2	1:A:1838:VAL:HG12	1.95	0.48
1:A:2115:ILE:O	1:A:2119:VAL:HG12	2.13	0.48
1:A:1488:LEU:HD11	1:A:1573:ARG:HB3	1.94	0.48
1:A:2618:PRO:HB2	1:A:2620:ASN:OD1	2.13	0.48
1:A:390:TYR:CZ	1:A:394:ARG:HD2	2.48	0.48
1:A:1332:LEU:HD23	1:A:1332:LEU:HA	1.69	0.48
1:A:2280:LEU:HD12	1:A:2281:THR:N	2.29	0.48
1:A:2392:LEU:O	1:A:2399:ASN:HB2	2.13	0.48
1:A:2465:ARG:O	1:A:2469:MET:HG3	2.14	0.48
1:A:2516:THR:OG1	1:A:2539:THR:HG23	2.13	0.48
1:A:1626:GLU:HA	1:A:1631:LEU:HB2	1.95	0.48
1:A:3192:HIS:CD2	1:A:3195:TRP:HD1	2.31	0.48
1:A:451:LYS:HD3	1:A:917:ARG:NH2	2.29	0.48
1:A:588:LEU:O	1:A:592:ILE:HG13	2.13	0.48
1:A:1775:LEU:HD12	1:A:1869:MET:HE3	1.96	0.48
1:A:265:ASN:O	1:A:269:LEU:HG	2.14	0.48
1:A:1128:ILE:HA	1:A:1131:LYS:HZ3	1.78	0.48
1:A:2802:PHE:HZ	1:A:3042:GLN:HG2	1.78	0.48
1:A:646:ARG:HG2	1:A:647:ASP:OD1	2.14	0.47
1:A:769:ARG:HH22	1:A:782:ARG:HB2	1.79	0.47
1:A:2329:ASP:HA	1:A:2347:ASN:O	2.14	0.47
1:A:2556:LEU:HD22	1:A:2604:PRO:HD3	1.96	0.47
1:A:2834:GLU:O	1:A:2838:ARG:HG3	2.13	0.47
1:A:2508:LEU:HD12	1:A:2509:ALA:H	1.79	0.47
1:A:466:LYS:HG2	1:A:471:LEU:HB2	1.95	0.47
1:A:796:THR:HB	1:A:802:ASP:HB3	1.96	0.47
1:A:2307:GLN:HB2	1:A:2310:ILE:HG13	1.95	0.47
1:A:2605:GLN:HE22	1:A:2637:ARG:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:HA	1:A:271:GLN:OE1	2.14	0.47
1:A:292:LYS:HA	1:A:292:LYS:HD3	1.79	0.47
1:A:567:GLN:HE21	1:A:571:LYS:HD2	1.79	0.47
1:A:2942:ALA:HB2	1:A:2993:GLU:HB3	1.96	0.47
1:A:2944:LYS:HE2	1:A:2962:GLN:HB3	1.95	0.47
1:A:281:MET:HE1	1:A:298:ILE:HD11	1.96	0.47
1:A:409:ASN:O	1:A:413:GLU:HG2	2.14	0.47
1:A:638:THR:OG1	1:A:639:LYS:N	2.46	0.47
1:A:2603:GLN:CD	1:A:2604:PRO:HD2	2.39	0.47
1:A:246:ILE:HG23	1:A:250:ARG:NH2	2.30	0.47
1:A:252:MET:HE2	1:A:252:MET:HB2	1.84	0.47
1:A:981:HIS:HD1	1:A:981:HIS:C	2.22	0.47
1:A:2868:LEU:O	1:A:2868:LEU:HD12	2.15	0.47
1:A:3058:GLU:O	1:A:3062:MET:HG2	2.15	0.47
1:A:624:ILE:O	1:A:628:ILE:HG22	2.15	0.47
1:A:936:PRO:HB3	1:A:1537:MET:SD	2.55	0.47
1:A:3060:TYR:O	1:A:3064:GLU:HG3	2.14	0.47
1:A:3089:ASN:HD21	1:A:3093:LYS:HB3	1.80	0.47
1:A:1974:TYR:HA	1:A:1978:ILE:HB	1.96	0.47
1:A:2503:TYR:CD1	1:A:2523:GLY:HA3	2.48	0.47
1:A:2689:ALA:HB3	1:A:2692:GLU:HB3	1.97	0.47
1:A:569:ILE:HA	1:A:572:ILE:HG22	1.97	0.46
1:A:2270:SER:HA	1:A:2314:VAL:HB	1.95	0.46
1:A:836:LYS:HA	1:A:836:LYS:HE2	1.96	0.46
1:A:1177:SER:O	1:A:1181:LEU:HD23	2.15	0.46
1:A:1963:VAL:HB	1:A:1968:LEU:HD11	1.97	0.46
1:A:2291:VAL:HB	1:A:2303:MET:HB2	1.97	0.46
1:A:3071:GLU:OE1	1:A:3071:GLU:HA	2.15	0.46
1:A:2741:LEU:HD12	1:A:2741:LEU:HA	1.79	0.46
1:A:2967:MET:HE2	1:A:2967:MET:C	2.40	0.46
1:A:267:LEU:HB3	1:A:305:TYR:CZ	2.50	0.46
1:A:1454:PHE:CE2	1:A:2142:ARG:HD3	2.50	0.46
1:A:1699:LEU:HG	1:A:1716:LEU:HD23	1.97	0.46
1:A:1248:PRO:HD2	1:A:1251:GLU:HG3	1.97	0.46
1:A:1865:PHE:CZ	1:A:1869:MET:HE2	2.51	0.46
1:A:777:GLU:HG3	1:A:778:PHE:HD1	1.81	0.46
1:A:3065:LEU:HD12	1:A:3199:TYR:HB3	1.98	0.46
1:A:986:LYS:HD3	1:A:1169:VAL:HG11	1.98	0.46
1:A:1274:LYS:HB2	1:A:1274:LYS:HE2	1.76	0.46
1:A:1386:ARG:HD2	1:A:1386:ARG:HA	1.70	0.46
1:A:1649:VAL:HG12	1:A:1653:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2343:SER:HB2	1:A:2348:ASN:OD1	2.16	0.46
1:A:697:ILE:HD12	1:A:719:THR:HG21	1.99	0.46
1:A:2563:VAL:HG12	1:A:2626:ILE:HD11	1.98	0.46
1:A:2512:ARG:HG2	1:A:2533:THR:OG1	2.16	0.45
1:A:2789:MET:HE1	1:A:2799:VAL:HG13	1.98	0.45
1:A:545:MET:CE	1:A:680:ILE:HG23	2.47	0.45
1:A:2239:LEU:HD12	1:A:2258:ILE:HG12	1.98	0.45
1:A:2539:THR:HB	1:A:2585:LEU:HD12	1.98	0.45
1:A:2943:ARG:HD3	1:A:2961:TYR:CD1	2.50	0.45
1:A:248:ILE:HA	1:A:251:ILE:HG22	1.99	0.45
1:A:559:ASP:OD1	1:A:560:MET:HE2	2.15	0.45
1:A:2750:GLU:OE1	1:A:2751:HIS:HB2	2.15	0.45
1:A:2777:LYS:HE2	1:A:2777:LYS:HB2	1.90	0.45
1:A:251:ILE:HD11	1:A:269:LEU:HB3	1.99	0.45
1:A:759:LEU:HD12	1:A:762:ARG:HH21	1.81	0.45
1:A:449:ILE:HD13	1:A:1386:ARG:HB3	1.98	0.45
1:A:795:THR:HA	1:A:801:TYR:HA	1.99	0.45
1:A:1828:ARG:HH22	1:A:1832:THR:HG22	1.81	0.45
1:A:1873:GLY:HA3	1:A:1998:PHE:CZ	2.52	0.45
1:A:582:PHE:CD1	1:A:588:LEU:HD13	2.52	0.45
1:A:873:LYS:HA	1:A:873:LYS:HE2	1.99	0.45
1:A:2159:TYR:HE1	1:A:2215:LEU:HB3	1.82	0.45
1:A:2734:THR:HG22	1:A:2755:LYS:HB3	1.99	0.45
1:A:540:SER:HB3	1:A:543:LEU:HD12	1.99	0.45
1:A:1592:TYR:CE2	1:A:1607:PRO:HG3	2.52	0.45
1:A:1685:ILE:O	1:A:1685:ILE:HD12	2.17	0.45
1:A:2503:TYR:HB3	1:A:3146:ARG:HH22	1.81	0.45
1:A:3064:GLU:O	1:A:3067:GLN:HG2	2.16	0.45
1:A:3122:THR:HG22	1:A:3123:ILE:H	1.81	0.45
1:A:616:ALA:O	1:A:620:ILE:HG22	2.16	0.45
1:A:693:GLU:OE1	1:A:716:LEU:HD12	2.16	0.45
1:A:1122:LYS:H	1:A:1122:LYS:HD2	1.82	0.45
1:A:1273:GLY:HA2	1:A:1414:PHE:CE1	2.52	0.45
1:A:976:SER:O	1:A:980:GLU:HG2	2.16	0.45
1:A:1652:LYS:HB3	1:A:1652:LYS:HE2	1.74	0.45
1:A:1832:THR:HA	1:A:1834:HIS:CE1	2.52	0.45
1:A:2957:LEU:HD23	1:A:2976:LEU:HD13	1.98	0.45
1:A:3008:VAL:HG12	1:A:3013:MET:SD	2.57	0.45
1:A:3015:VAL:HG12	1:A:3033:SER:HB2	1.98	0.45
1:A:397:TYR:CE2	1:A:835:PHE:CD1	3.05	0.45
1:A:947:LEU:HD13	1:A:1128:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2753:ILE:HD11	1:A:2818:ARG:HD3	1.98	0.45
1:A:2966:LYS:HB2	1:A:2966:LYS:HE2	1.75	0.45
1:A:866:LYS:HA	1:A:869:LYS:HG2	1.99	0.44
1:A:1160:LEU:HD12	1:A:1164:TYR:CZ	2.52	0.44
1:A:2426:THR:HB	1:A:2442:LEU:HB2	1.99	0.44
1:A:773:VAL:O	1:A:776:GLU:HG3	2.17	0.44
1:A:981:HIS:CE1	1:A:985:ILE:HD11	2.53	0.44
1:A:1210:HIS:ND1	1:A:1240:ILE:HD11	2.33	0.44
1:A:3034:ASP:HB3	1:A:3060:TYR:OH	2.17	0.44
1:A:325:PRO:O	1:A:329:ILE:HG12	2.17	0.44
1:A:2502:ARG:HG3	1:A:2503:TYR:CD2	2.53	0.44
1:A:494:ILE:HD11	1:A:506:ILE:HG12	2.00	0.44
1:A:631:MET:HG2	1:A:632:PRO:HD2	1.98	0.44
1:A:774:LEU:HD22	1:A:774:LEU:H	1.82	0.44
1:A:966:ASN:HB2	1:A:1255:PRO:HB3	2.00	0.44
1:A:1212:ASN:HB2	1:A:1214:ASP:OD1	2.18	0.44
1:A:2960:ILE:HD13	1:A:2960:ILE:HA	1.86	0.44
1:A:2807:GLN:H	1:A:2807:GLN:HG3	1.60	0.44
1:A:2915:THR:HG22	1:A:2986:TYR:HE1	1.83	0.44
1:A:869:LYS:HB2	1:A:869:LYS:HE2	1.64	0.44
1:A:3057:ARG:CZ	1:A:3057:ARG:HA	2.47	0.44
1:A:657:LEU:HD13	1:A:662:TRP:CE2	2.52	0.43
1:A:2166:ASN:ND2	1:A:2191:ARG:HG3	2.33	0.43
1:A:3203:LYS:HD2	1:A:3203:LYS:HA	1.69	0.43
1:A:1645:GLU:H	1:A:1645:GLU:CD	2.25	0.43
1:A:2258:ILE:HG21	1:A:2310:ILE:HD11	2.01	0.43
1:A:2534:THR:HG22	1:A:2581:TYR:HE1	1.83	0.43
1:A:2654:VAL:HG12	1:A:2657:SER:H	1.82	0.43
1:A:3160:MET:C	1:A:3160:MET:HE2	2.42	0.43
1:A:1195:LEU:HD11	1:A:1279:VAL:CG2	2.48	0.43
1:A:2400:ILE:HD12	1:A:2400:ILE:H	1.84	0.43
1:A:2563:VAL:HG22	1:A:2576:ILE:HD13	1.99	0.43
1:A:3183:PHE:HB3	1:A:3202:LEU:HB3	2.01	0.43
1:A:620:ILE:O	1:A:623:LYS:HG2	2.18	0.43
1:A:753:GLN:HG2	1:A:756:GLY:HA3	2.01	0.43
1:A:1545:TYR:CE2	1:A:1653:LEU:HB3	2.53	0.43
1:A:1618:ILE:O	1:A:1625:GLN:HG3	2.19	0.43
1:A:2509:ALA:HB2	1:A:2529:MET:HE1	2.00	0.43
1:A:447:TYR:HA	1:A:450:VAL:HG12	2.01	0.43
1:A:2320:LYS:NZ	1:A:2358:THR:HG21	2.34	0.43
1:A:2493:ARG:HH21	1:A:2513:HIS:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3177:LEU:HD23	1:A:3177:LEU:HA	1.89	0.43
1:A:292:LYS:O	1:A:296:ILE:HG12	2.19	0.43
1:A:483:ILE:HG22	1:A:487:LYS:HZ2	1.83	0.43
1:A:494:ILE:HD12	1:A:494:ILE:HA	1.71	0.43
1:A:2280:LEU:HD12	1:A:2281:THR:H	1.82	0.43
1:A:1799:ASN:OD1	1:A:1799:ASN:C	2.62	0.42
1:A:3107:ARG:HE	1:A:3107:ARG:HB3	1.54	0.42
1:A:590:ARG:HD3	1:A:821:THR:HG21	2.01	0.42
1:A:2460:ASP:OD2	1:A:2509:ALA:HB3	2.19	0.42
1:A:3088:ARG:HA	1:A:3088:ARG:HD3	1.66	0.42
1:A:3110:VAL:HG21	1:A:3113:TRP:HE1	1.83	0.42
1:A:2742:SER:HA	1:A:2766:SER:HB2	2.01	0.42
1:A:3157:ILE:CD1	1:A:3202:LEU:HB2	2.49	0.42
1:A:1211:TYR:CZ	1:A:1219:LYS:HG2	2.54	0.42
1:A:1220:LEU:HD23	1:A:1220:LEU:HA	1.93	0.42
1:A:1485:LEU:HD23	1:A:1485:LEU:HA	1.87	0.42
1:A:1861:GLY:HA2	1:A:1943:ARG:HH12	1.84	0.42
1:A:3177:LEU:HD13	1:A:3183:PHE:HZ	1.85	0.42
1:A:536:TYR:CE2	1:A:828:ARG:HG2	2.54	0.42
1:A:708:LYS:H	1:A:708:LYS:HG2	1.59	0.42
1:A:2320:LYS:HE2	1:A:2320:LYS:HB2	1.89	0.42
1:A:630:LYS:HZ1	1:A:631:MET:HG3	1.84	0.42
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.83	0.42
1:A:1230:LYS:HE3	1:A:1230:LYS:HA	2.01	0.42
1:A:2169:ILE:HD13	1:A:2169:ILE:HA	1.92	0.42
1:A:2226:THR:HG23	1:A:2293:LEU:HD21	2.02	0.42
1:A:2236:LYS:HE2	1:A:2236:LYS:HB2	1.83	0.42
1:A:2268:THR:HG23	1:A:2312:THR:HG22	2.01	0.42
1:A:2459:PRO:HB3	1:A:2479:PHE:CD2	2.54	0.42
1:A:2517:ALA:HA	1:A:2540:GLN:O	2.19	0.42
1:A:3013:MET:O	1:A:3034:ASP:HA	2.19	0.42
1:A:3085:ALA:O	1:A:3088:ARG:HG2	2.20	0.42
1:A:354:PHE:HD1	1:A:354:PHE:HA	1.76	0.42
1:A:374:THR:O	1:A:378:ASN:HB2	2.19	0.42
1:A:587:LYS:HE3	1:A:587:LYS:HB2	1.91	0.42
1:A:704:GLU:HG3	1:A:707:PHE:CZ	2.55	0.42
1:A:2555:LEU:HD12	1:A:2602:ILE:HG13	2.01	0.42
1:A:3107:ARG:HB2	1:A:3144:PHE:CD1	2.54	0.42
1:A:393:ILE:HD11	1:A:410:LYS:HE3	2.01	0.42
1:A:950:LYS:N	1:A:950:LYS:HD2	2.34	0.42
1:A:2542:ILE:HB	1:A:2590:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:ILE:HD12	1:A:809:ILE:H	1.84	0.42
1:A:1295:ILE:HD11	1:A:1369:THR:HG22	2.02	0.42
1:A:633:GLU:HA	1:A:636:ILE:HD12	2.02	0.41
1:A:470:LYS:HA	1:A:470:LYS:HD2	1.85	0.41
1:A:894:LYS:HB3	1:A:894:LYS:HE3	1.71	0.41
1:A:902:MET:HE3	1:A:902:MET:HB2	1.81	0.41
1:A:1308:ARG:HD2	1:A:1322:LEU:HD11	2.01	0.41
1:A:3153:VAL:HB	1:A:3155:TYR:HE1	1.85	0.41
1:A:886:ILE:HD13	1:A:886:ILE:HA	1.91	0.41
1:A:3151:TYR:N	1:A:3151:TYR:CD1	2.89	0.41
1:A:469:ILE:HD12	1:A:469:ILE:HA	1.84	0.41
1:A:561:MET:SD	1:A:597:LEU:HD13	2.61	0.41
1:A:694:LEU:O	1:A:697:ILE:HG22	2.21	0.41
1:A:2632:THR:HA	1:A:2687:TRP:CH2	2.55	0.41
1:A:3110:VAL:HG21	1:A:3113:TRP:NE1	2.36	0.41
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.91	0.41
1:A:2825:MET:HG3	1:A:2848:PHE:HB3	2.02	0.41
1:A:3203:LYS:HG3	1:A:3204:THR:H	1.86	0.41
1:A:389:LEU:O	1:A:393:ILE:HG22	2.21	0.41
1:A:994:MET:HE2	1:A:994:MET:HB2	1.86	0.41
1:A:2768:PHE:HE1	1:A:2770:ARG:HD2	1.85	0.41
1:A:2868:LEU:HA	1:A:2871:ILE:HG12	2.03	0.41
1:A:3089:ASN:ND2	1:A:3093:LYS:HB3	2.35	0.41
1:A:496:ASP:OD1	1:A:496:ASP:C	2.64	0.41
1:A:609:ASN:OD1	1:A:609:ASN:C	2.63	0.41
1:A:2522:PRO:HB3	1:A:2549:HIS:HB2	2.03	0.41
1:A:2743:GLU:OE1	1:A:2747:GLN:HB3	2.20	0.41
1:A:2797:LEU:O	1:A:2816:THR:HA	2.20	0.41
1:A:2990:ILE:HD12	1:A:2990:ILE:HA	1.87	0.41
1:A:495:LEU:O	1:A:495:LEU:HD12	2.21	0.41
1:A:519:LYS:HG2	1:A:521:GLU:OE1	2.21	0.41
1:A:534:TRP:CZ2	1:A:753:GLN:NE2	2.89	0.41
1:A:1454:PHE:CD1	1:A:1454:PHE:C	2.97	0.41
1:A:2494:GLN:HE22	1:A:2517:ALA:HB2	1.86	0.41
1:A:3066:GLN:HA	1:A:3199:TYR:CE2	2.56	0.41
1:A:274:ALA:O	1:A:278:LYS:HG2	2.21	0.41
1:A:532:LEU:HD13	1:A:694:LEU:HD21	2.02	0.41
1:A:645:PRO:HB2	1:A:648:THR:HG21	2.03	0.41
1:A:908:LEU:HD23	1:A:908:LEU:HA	1.87	0.41
1:A:1195:LEU:HD13	1:A:1403:PHE:CG	2.56	0.41
1:A:1816:ALA:HB2	1:A:1824:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2140:TRP:HB2	1:A:2141:PRO:HD3	2.02	0.41
1:A:2223:PRO:O	1:A:2227:GLU:HG2	2.20	0.41
1:A:2738:GLU:HA	1:A:2762:SER:HB2	2.02	0.41
1:A:2741:LEU:HD23	1:A:2746:TRP:HD1	1.86	0.41
1:A:2908:ILE:HG13	1:A:2970:GLN:HB2	2.03	0.41
1:A:329:ILE:HD12	1:A:558:THR:HG21	2.02	0.41
1:A:599:TYR:CE2	1:A:629:SER:HA	2.56	0.41
1:A:1207:LEU:HD23	1:A:1207:LEU:HA	1.85	0.41
1:A:271:GLN:HG3	1:A:774:LEU:HD23	2.02	0.40
1:A:1709:THR:O	1:A:1713:ILE:HG12	2.21	0.40
1:A:2303:MET:HE3	1:A:2305:ILE:HD11	2.03	0.40
1:A:2664:LEU:HD13	1:A:2674:VAL:HG21	2.03	0.40
1:A:432:PHE:O	1:A:433:PHE:C	2.64	0.40
1:A:847:PRO:HB3	1:A:925:GLN:HG3	2.03	0.40
1:A:1742:LYS:HE3	1:A:1742:LYS:HB2	1.80	0.40
1:A:2121:TYR:HB2	1:A:2169:ILE:HG21	2.03	0.40
1:A:2137:ASN:OD1	1:A:2137:ASN:C	2.64	0.40
1:A:2798:SER:HB2	1:A:2814:ARG:HD2	2.03	0.40
1:A:2950:HIS:CE1	1:A:2952:THR:HG22	2.55	0.40
1:A:1262:ASN:HD22	1:A:1264:LEU:HB2	1.86	0.40
1:A:1479:ARG:HH22	1:A:1577:SER:HB3	1.87	0.40
1:A:1754:ARG:HG2	1:A:1978:ILE:CD1	2.50	0.40
1:A:2460:ASP:HA	1:A:2463:LEU:HG	2.03	0.40
1:A:2937:LYS:HA	1:A:2937:LYS:HD3	1.62	0.40
1:A:650:PRO:HB3	1:A:790:ILE:HG23	2.04	0.40
1:A:1315:ASN:OD1	1:A:1315:ASN:C	2.64	0.40
1:A:1957:ARG:O	1:A:1957:ARG:HD3	2.21	0.40
1:A:2411:ASN:HA	1:A:2436:ILE:HD11	2.02	0.40
1:A:2564:GLU:O	1:A:2574:LEU:HD23	2.22	0.40
1:A:3163:ALA:HB2	1:A:3177:LEU:HD23	2.03	0.40
1:A:375:ILE:HD13	1:A:428:MET:HE3	2.03	0.40
1:A:569:ILE:HA	1:A:569:ILE:HD12	1.97	0.40
1:A:804:LEU:HG	1:A:805:THR:HG23	2.03	0.40
1:A:1716:LEU:HD23	1:A:1716:LEU:HA	1.92	0.40
1:A:2877:ARG:HH12	1:A:2880:LYS:HD2	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2791/3223 (87%)	2688 (96%)	102 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	812	ASN

### 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	2490/2880 (86%)	2479 (100%)	11 (0%)	89	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	ILE
1	A	535	ASN
1	A	700	ASN
1	A	753	GLN
1	A	815	THR
1	A	832	ASP
1	A	834	LEU
1	A	1528	MET
1	A	1764	THR
1	A	2541	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2613	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	378	ASN
1	A	388	ASN
1	A	404	GLN
1	A	405	GLN
1	A	463	ASN
1	A	498	GLN
1	A	753	GLN
1	A	966	ASN
1	A	1318	ASN
1	A	1586	GLN
1	A	1772	GLN
1	A	1796	HIS
1	A	1824	ASN
1	A	1901	GLN
1	A	1981	GLN
1	A	1995	GLN
1	A	2164	GLN
1	A	2166	ASN
1	A	2198	ASN
1	A	2228	GLN
1	A	2348	ASN
1	A	2371	HIS
1	A	2540	GLN
1	A	2603	GLN
1	A	2786	HIS
1	A	2787	GLN
1	A	3042	GLN
1	A	3168	ASN
1	A	3196	ASN
1	A	3220	ASN

### 5.3.3 RNA ⓘ

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 1 ligands modelled in this entry, 1 is 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.

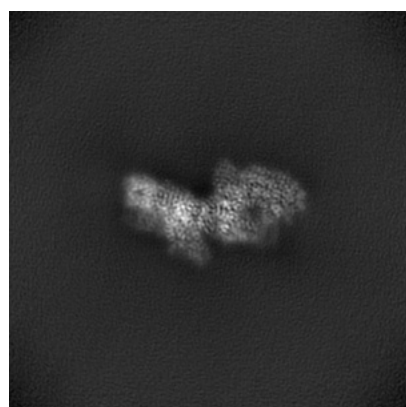
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52990. These allow visual inspection of the internal detail of the map and identification of artifacts.

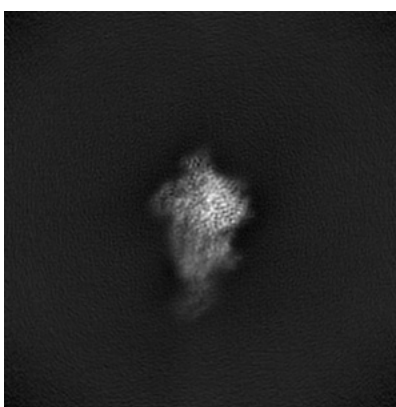
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

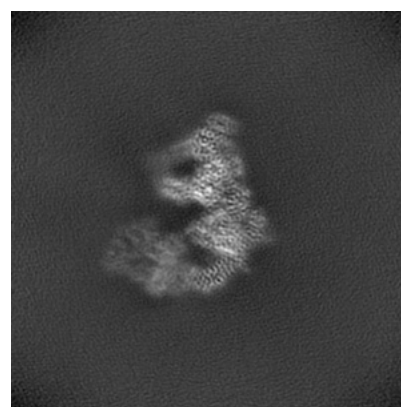
#### 6.1.1 Primary map



X



Y

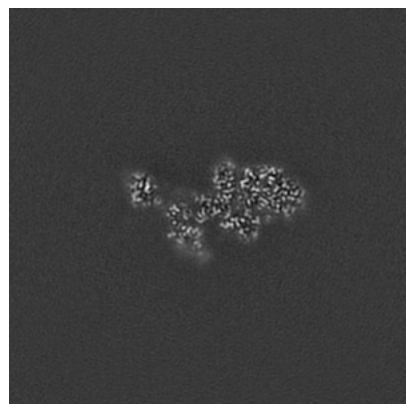


Z

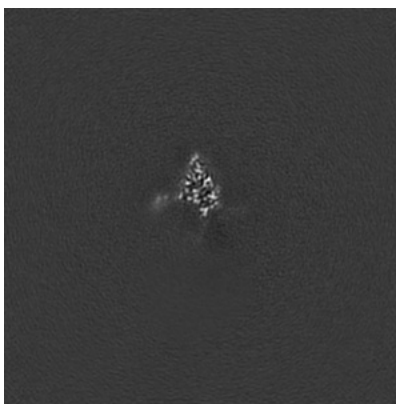
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

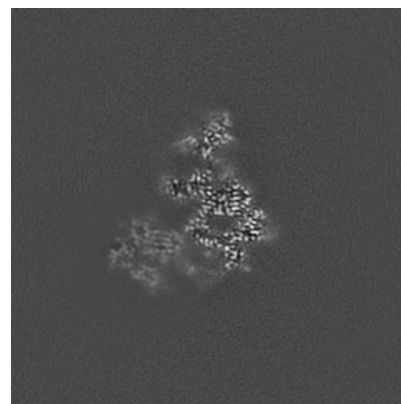
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



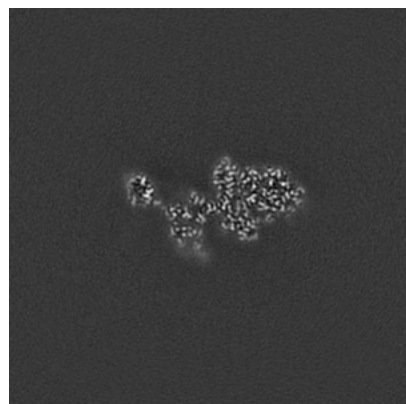
Z Index: 200



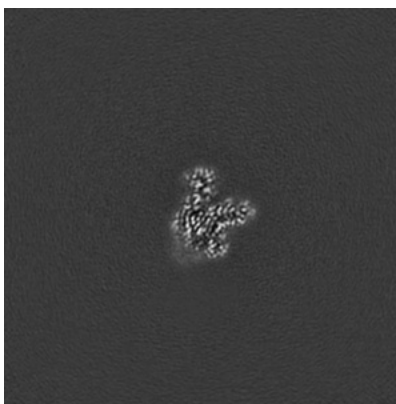
The images above show central slices of the map in three orthogonal directions.

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

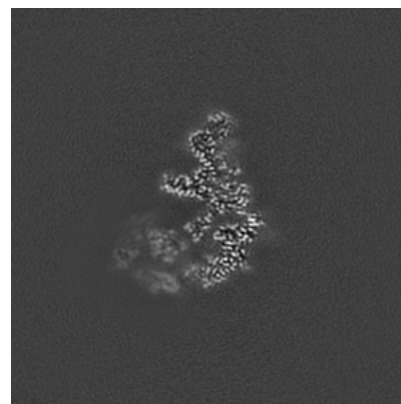
### 6.3.1 Primary map



X Index: 198



Y Index: 218

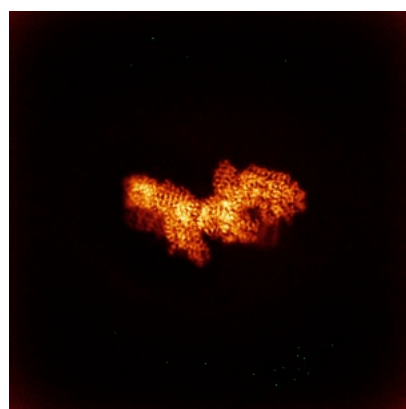


Z Index: 206

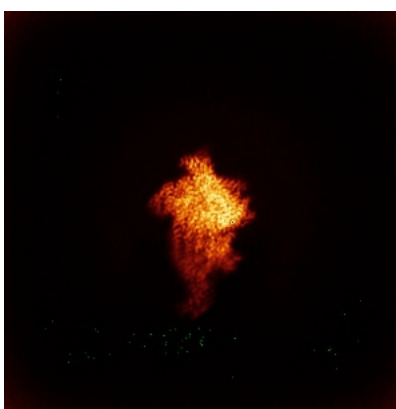
The images above show the largest variance slices of the map in three orthogonal directions.

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

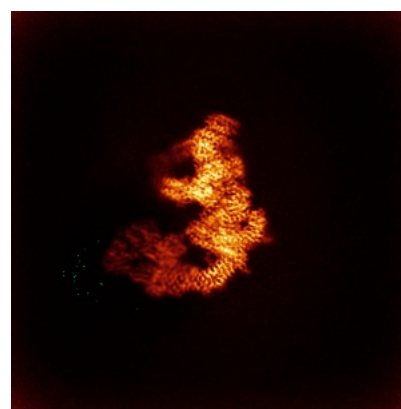
### 6.4.1 Primary map



X



Y

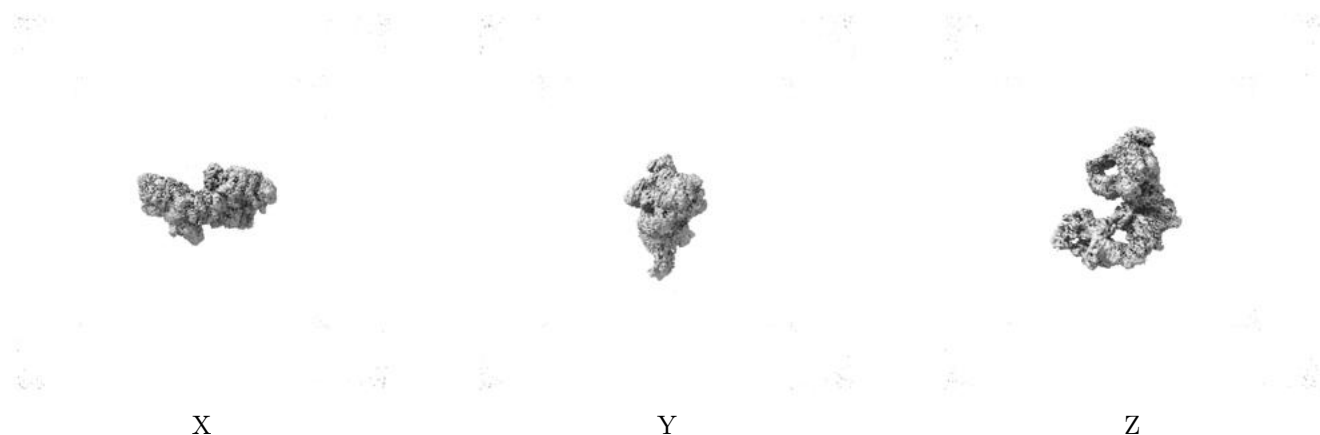


Z

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

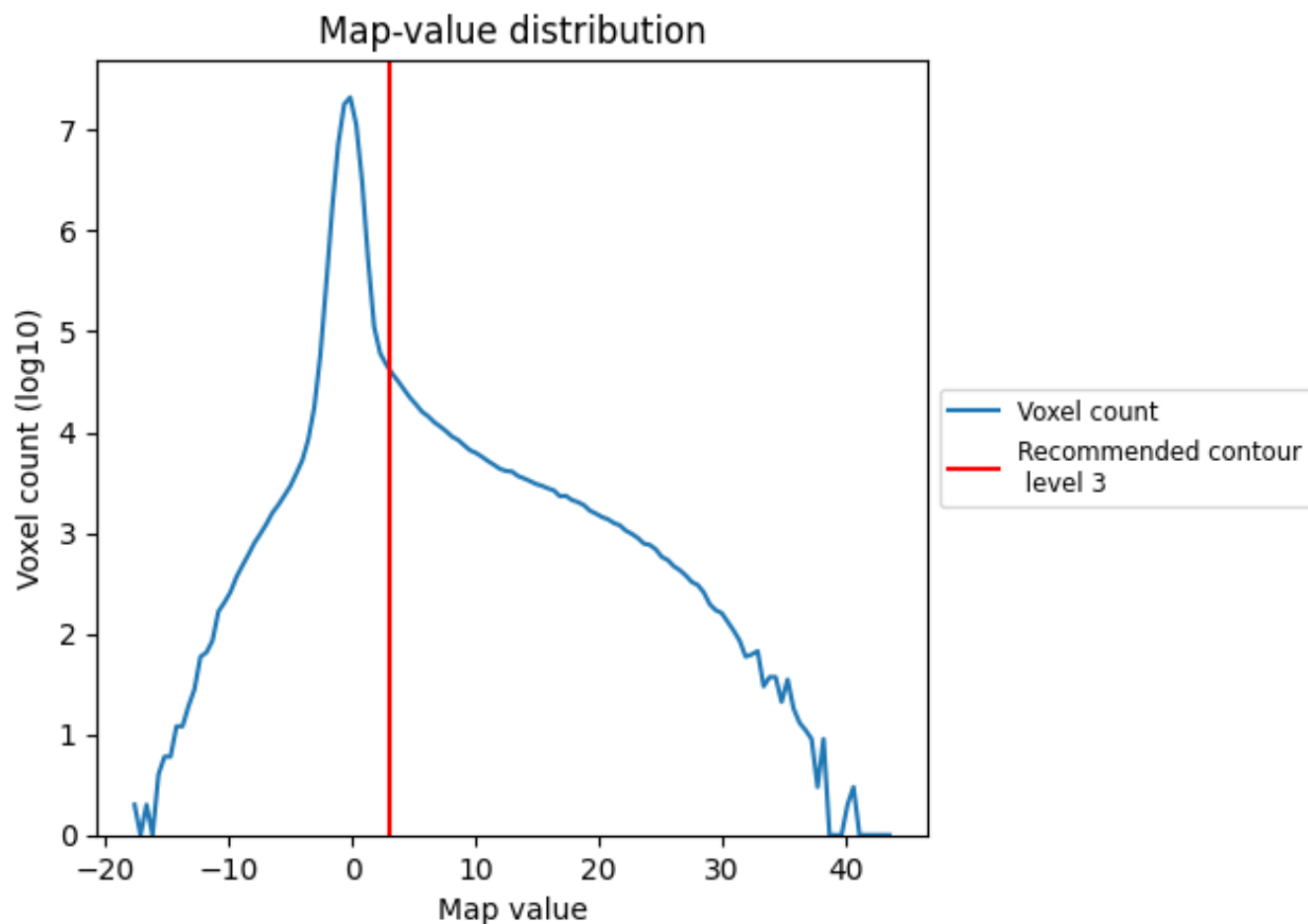
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

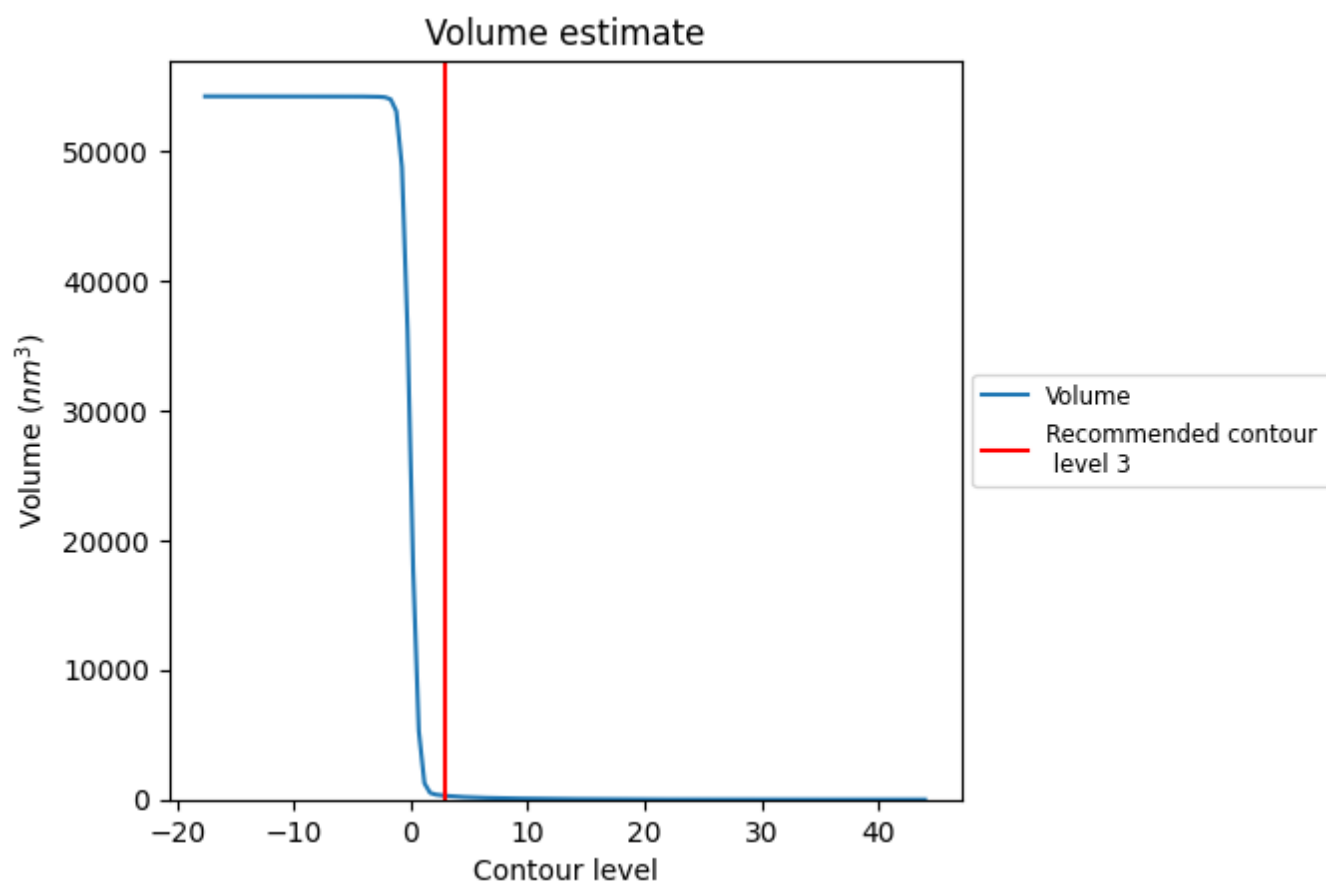
This section contains the results of statistical analysis of the map.

### 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.

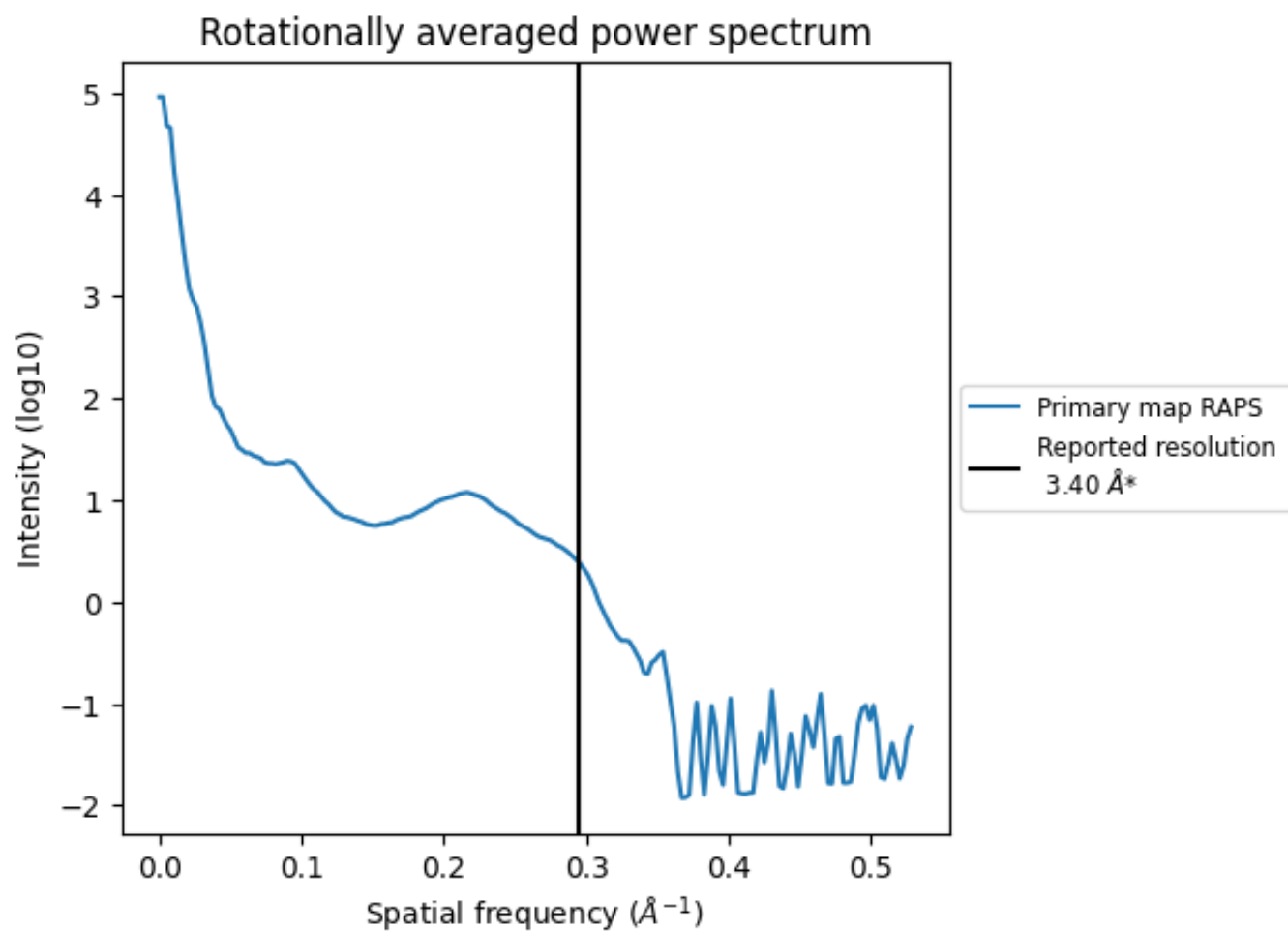
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290  $\text{nm}^3$ ; this corresponds to an approximate mass of 262 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 0.294 Å<sup>-1</sup>

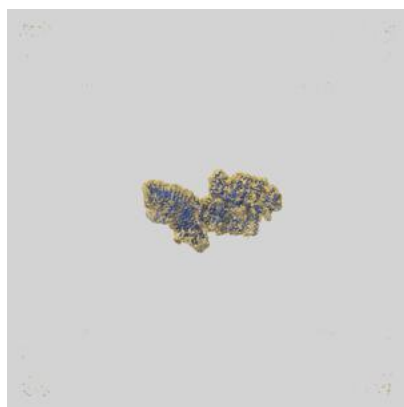
## 8 Fourier-Shell correlation

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

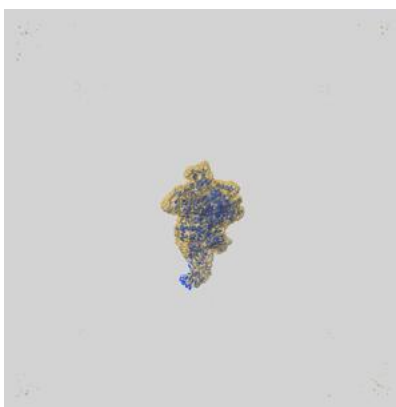
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52990 and PDB model 9QB8. Per-residue inclusion information can be found in section [3](#) on page [4](#).

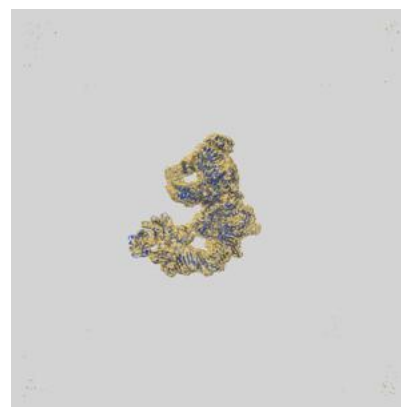
### 9.1 Map-model overlay [i](#)



X



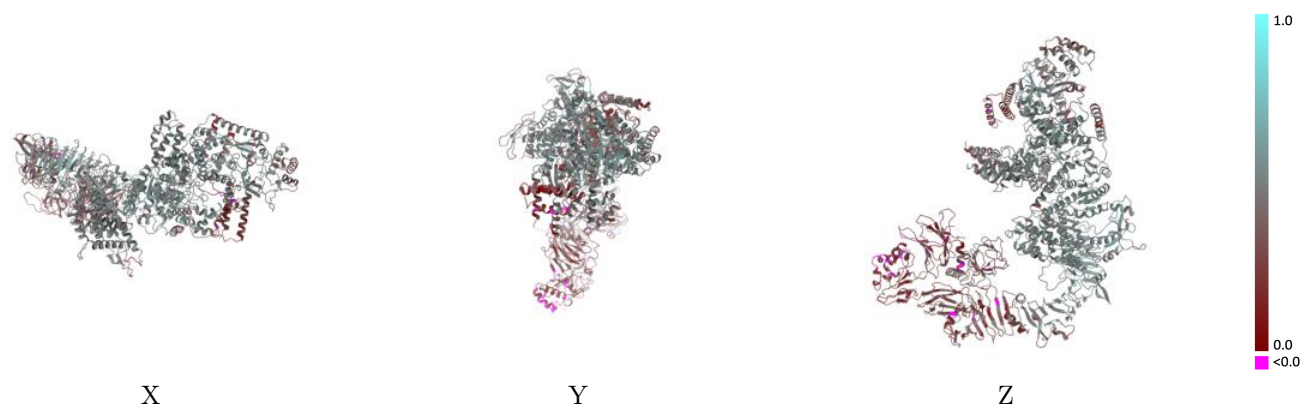
Y



Z

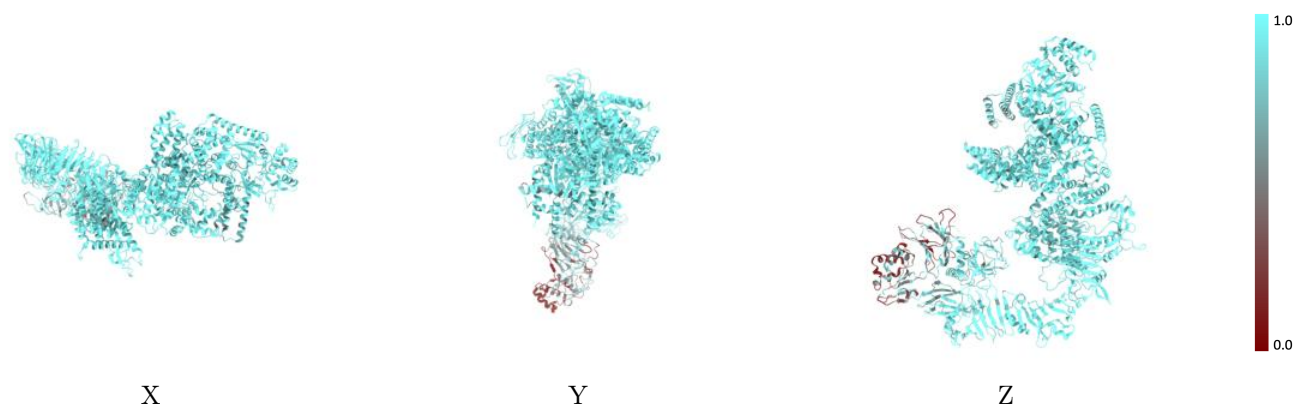
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

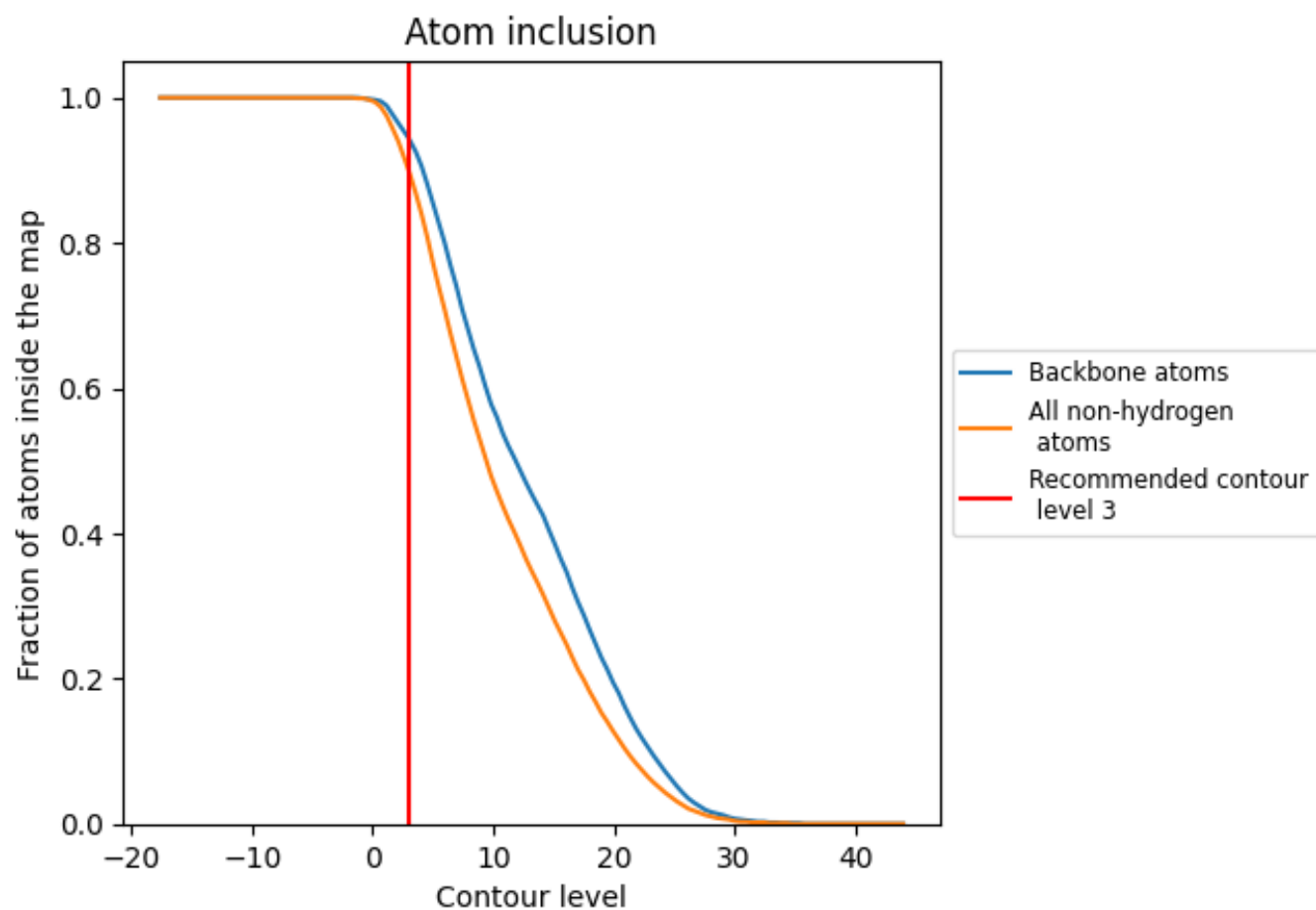
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (3).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 90% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9000	<div><div></div></div> 0.4230
A	<div><div></div></div> 0.9000	<div><div></div></div> 0.4230

