



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:48 PM UTC

PDB ID : 7JGG / pdb_00007jgg
EMDB ID : EMD-22326
Title : Cryo-EM structure of P. falciparum VAR2CSA NF45 DBL5 and DBL6 domains at 4.88 Å
Authors : Ma, R.; Tolia, N.H.
Deposited on : 2020-07-19
Resolution : 4.88 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

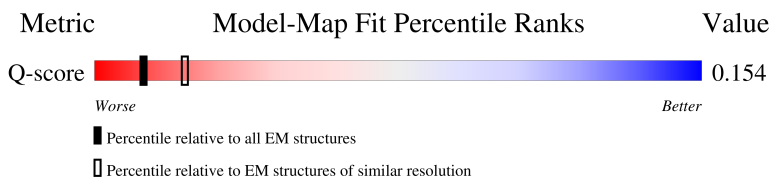
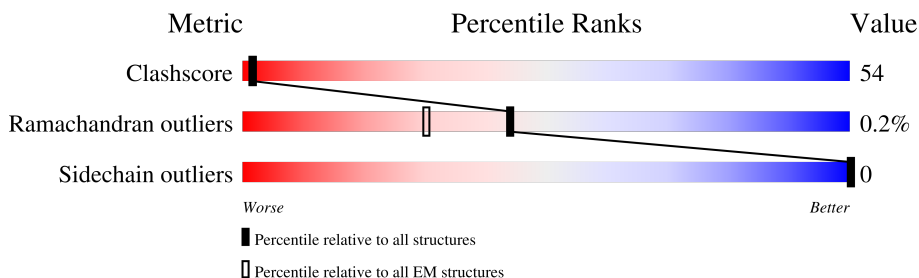
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.88 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	1260 (4.38 - 5.38)

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	2653	 7% 12% 81%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4210 atoms, of which 28 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 Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	506	4210	2643	28	713	799	27	0	0

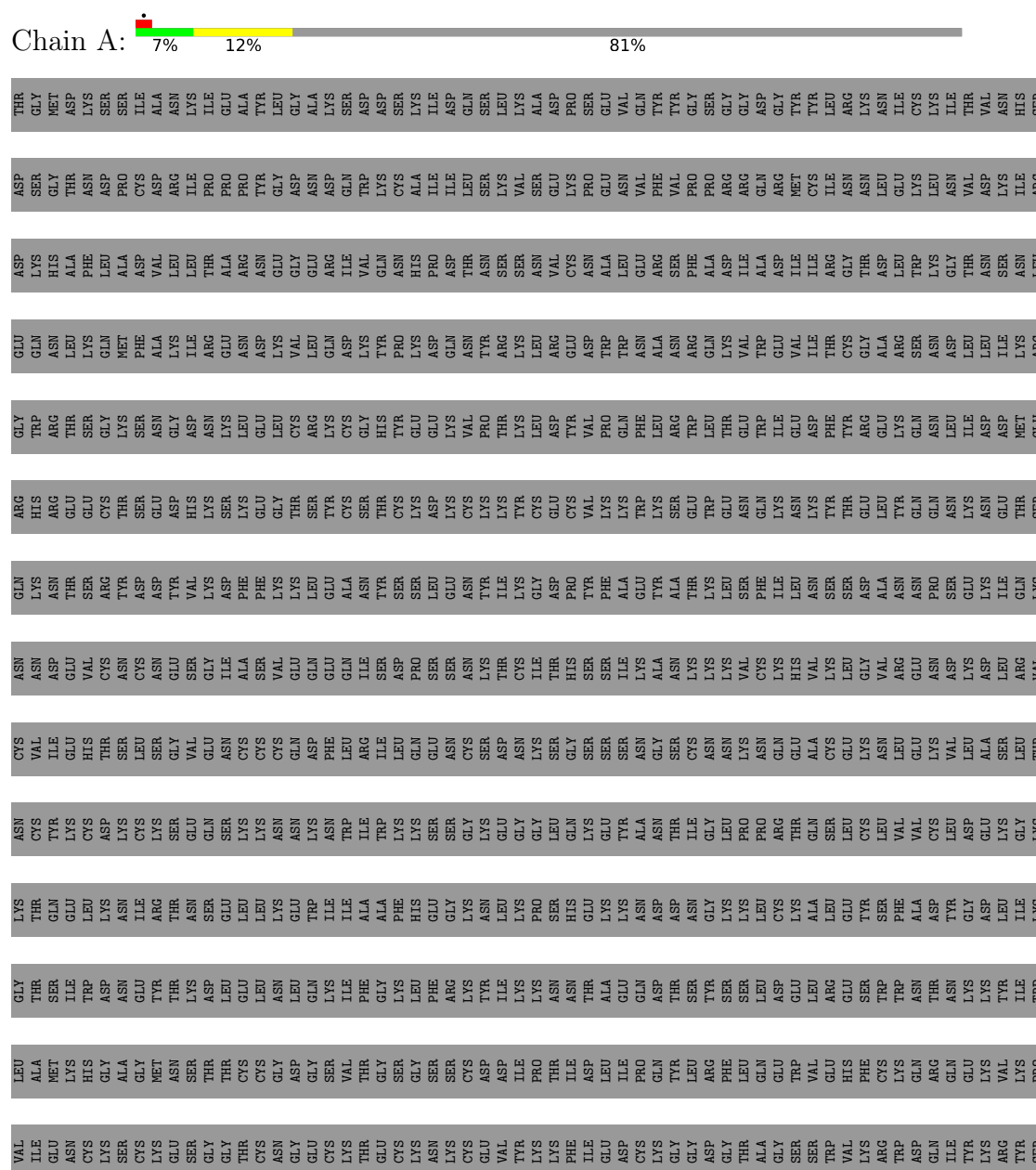
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	THR	-	expression tag	UNP W7K270
A	0	GLY	-	expression tag	UNP W7K270
A	2643	GLY	-	expression tag	UNP W7K270
A	2644	THR	-	expression tag	UNP W7K270
A	2645	LYS	-	expression tag	UNP W7K270
A	2646	HIS	-	expression tag	UNP W7K270
A	2647	HIS	-	expression tag	UNP W7K270
A	2648	HIS	-	expression tag	UNP W7K270
A	2649	HIS	-	expression tag	UNP W7K270
A	2650	HIS	-	expression tag	UNP W7K270
A	2651	HIS	-	expression tag	UNP W7K270

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: Erythrocyte membrane protein 1





THR	L2554	K2565	L2497	G2432	L2367	K2305	W2236	P2173	S2104	L2040
GLU	K2566	D2498	D2498	S2433	L2368	E2306	E2237	P2174	D2105	C2041
VAL	K2567	L2499	L2499	I2434	P2369	Q2307	A2238	P2175	M2106	F2042
LYS	E2568	P2500	P2500	I2435	R2370	V2308	I2239	F2176	L2107	S2043
ASN	Y2569	N2501	N2501	K2436	R2371	D2309	K2244	L2177	N2108	S2044
CYS	Q2570	D2503	D2503	D2438	R2372	T2310	K2245	R2178	N2109	R2044
MET	S2571	D2504	D2504	MET	K2373	P2311	Y2246	W2179	I2110	I2045
CYS	L2572	E2505	E2505	M2411	N2374	E2315	Y2247	I2180	Q2111	P2049
LYS	N2573	D2505	D2505	E2442	L2375	ASP	K2248	K2181	F2112	A2050
PRO	S2574	R2510	R2510	N2443	F2376	VAL	M2249	E2182	K2113	A2051
PRO	Q2575	W2511	W2511	N2444	L2377	ILE	ASP	W2183	D2114	L2052
PRO	Y2576	S2445	S2445	S2445	T2378	TYR	ASP	G2184	K2115	R2053
ALA	D2577	E2514	E2514	E2449	D2380	ARG	GLU	N2185	R2116	W2054
ALA	M2578	W2515	W2515	I2448	E2381	LEU	PHE	N2186	R2117	L2055
SER	N2579	T2516	T2516	K2449	S2382	LYS	LYS	W2187	L2118	E2056
ASN	Y2580	G2450	G2450	D2450	D2383	HIS	ASN	C2188	L2119	R2057
ASN	K2581	N2518	N2518	K2451	T2384	PHE	PHE	Q2189	R2120	F2058
GLY	F2582	F2519	F2519	I2452	T2385	GLU	LYS	Q2190	R2121	K2059
THR	E2582	C2520	C2520	L2453	K2386	TYR	ASN	E2192	L2122	E2060
LYS	T2583	T2521	T2521	G2454	Y2387	ASP	ILE	E2193	L2123	E2061
HIS	K2584	K2522	K2522	D2455	K2388	LYS	GLU	H2194	E2124	I2062
HIS	A2585	E2522	E2522	G2456	R2389	GLY	PRO	K2195	E2125	I2063
HIS	E2586	E2525	E2525	V2457	R2390	N2330	ASP	E2196	T2127	K2064
HIS	K2587	L2526	L2526	G2458	L2393	D2331	ALA	Y2197	N2128	G2065
HIS	E2588	Y2527	Y2527	Q2459	F2394	I2333	GLU	V2198	N2129	A2066
HIS	E2589	E2528	E2528	N2460	K2395	I2334	GLU	K2199	T2130	Q2067
HIS	S2590	N2529	N2529	E2461	K2396	C2334	PRO	S2200	E2131	S2068
HIS	P2591	W2530	W2530	E2462	T2398	N2335	ASN	K2201	K2132	E2069
HIS	E2592	V2531	V2531	K2463	Y2399	K2336	ALA	C2202	V2133	G2070
HIS	Y2593	T2532	T2532	R2464	A2402	Y2337	ASN	S2203	D2134	K2071
HIS	F2594	N2535	N2535	K2465	I2403	K2338	ASN	W2204	D2135	F2072
HIS	K2595	S2536	S2536	W2466	S2404	N2339	GLU	V2205	W2136	L2073
HIS	D2596	A2537	A2537	W2467	E2405	I2340	TYR	N2206	W2137	L2076
HIS	K2597	K2538	K2538	D2468	V2406	N2341	LEU	N2207	E2138	W2077
HIS	C2598	CYS	CYS	M2469	V2407	V2342	LYS	L2208	T2139	E2078
HIS	N2599	ASN	ASN	N2470	E2407	ASN	LYS	G2209	N2140	W2078
HIS	G2600	THR	THR	K2471	R2408	MET	HIS	Q2211	K2141	E2079
HIS	E2601	SER	SER	Y2472	L2409	LYS	CYS	E2212	K2142	D2082
HIS	C2602	ASN	ASN	H2473	K2410	LYS	LYS	S2213	S2143	D2083
HIS	L2605	G2544	G2544	I2474	K2411	ASN	CYS	S2214	I2144	E2084
HIS	S2606	S2545	S2545	W2475	Y2412	ASP	PRO	E2215	W2145	K2085
HIS	E2607	W2546	W2546	E2476	Y2413	ASP	CYS	S2216	K2153	A2086
HIS	TYR	D2547	D2547	S2477	G2414	THR	GLY	N2217	K2154	L2087
HIS	PHE	K2548	K2548	M2478	E2415	TRP	PHE	C2218	E2088	A2089
HIS	LYS	K2549	K2549	L2479	A2416	THR	ASN	T2219	K2158	M2090
HIS	ASP	E2549	E2549	K2483	K2417	D2354	ASP	T2222	I2159	K2091
HIS	GLU	E2550	E2550	Y2486	T2418	L2355	MET	K2223	I2160	W2092
HIS	THR	C2551	C2551	G2487	K2419	K2357	GLN	K2224	D2161	S2093
HIS	ARG	T2552	T2552	ASN	V2420	N2358	ILE	Y2225	P2162	F2094
HIS	TRP	E2553	E2553	ASN	W2421	S2359	THR	Q2226	S2163	W2095
HIS	LYS	K2556	K2556	ILE	M2424	S2360	LYS	E2227	W2164	D2096
HIS	ASN	W2557	W2557	SER	K2425	D2361	THR	W2228	C2165	W2097
HIS	PRO	Y2558	Y2558	GLU	Y2426	ILE	LYS	W2229	T2166	E2098
HIS	THR	S2559	S2559	ASN	F2427	ASN	LYS	S2230	I2167	Y2099
HIS	GLU	W2560	W2560	ASP	A2429	LYS	THR	K2231	P2168	I2100
HIS	THR	F2561	F2561	ARG	D2430	GLY	ASP	K2232	T2169	I2101
HIS	LEU	L2562	L2562	LYS	I2431	V2365	TYR	R2232	T2172	G2103
HIS	ASP	L2563	L2563	MET		V2366				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157702	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 ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.549	Depositor
Minimum map value	-4.473	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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	0.10	0/4264	0.30	0/5710

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2039	GLN	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	4182	28	4095	450	0
All	All	4182	28	4095	450	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 54.

All (450) 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:2548:LYS:HE3	1:A:2550:GLU:HB3	1.38	1.04
1:A:2244:LYS:HG2	1:A:2247:LYS:HE2	1.37	1.03
1:A:2198:VAL:HG21	1:A:2222:ILE:HD13	1.42	1.01
1:A:2369:PRO:HG2	1:A:2372:ARG:HB3	1.44	0.98
1:A:2159:ILE:HG13	1:A:2167:ILE:HG22	1.47	0.97
1:A:2407:GLU:HA	1:A:2410:LYS:HZ3	1.30	0.97
1:A:2460:ASN:HB2	1:A:2463:ARG:HB2	1.43	0.96
1:A:2386:LYS:HE3	1:A:2393:LEU:HD13	1.48	0.92
1:A:2021:MET:HE1	1:A:2032:LEU:HA	1.53	0.90
1:A:2034:PRO:HG2	1:A:2037:ARG:HB3	1.55	0.88
1:A:2103:GLY:HA2	1:A:2175:GLN:HE22	1.38	0.88
1:A:2562:ILE:HG22	1:A:2566:LYS:HZ3	1.39	0.88
1:A:2111:GLN:HB3	1:A:2115:ILE:HD13	1.57	0.87
1:A:2563:LEU:HA	1:A:2566:LYS:HE2	1.56	0.85
1:A:2383:ASP:HA	1:A:2386:LYS:HD3	1.57	0.85
1:A:2224:LYS:O	1:A:2227:GLU:HG3	1.78	0.83
1:A:2188:CYS:O	1:A:2191:LYS:HG3	1.77	0.83
1:A:2465:LYS:HD2	1:A:2469:MET:HE2	1.60	0.82
1:A:2406:VAL:HG11	1:A:2474:ILE:HD12	1.61	0.81
1:A:2569:TYR:HA	1:A:2572:LEU:HD12	1.62	0.80
1:A:2199:LYS:O	1:A:2203:SER:OG	1.99	0.80
1:A:2588:LYS:HZ3	1:A:2592:GLU:HB3	1.47	0.79
1:A:2562:ILE:HG22	1:A:2566:LYS:NZ	1.98	0.78
1:A:2516:THR:HG22	1:A:2605:LEU:HD22	1.66	0.78
1:A:2023:ASP:HB3	1:A:2024:PRO:HD3	1.64	0.78
1:A:2176:PHE:CZ	1:A:2180:ILE:HD11	2.19	0.78
1:A:2436:LYS:HE2	1:A:2464:LYS:HA	1.66	0.78
1:A:2052:LEU:HD23	1:A:2057:GLU:HG2	1.66	0.77
1:A:2135:ASP:O	1:A:2138:GLU:HG3	1.84	0.77
1:A:2602:CYS:HA	1:A:2605:LEU:HG	1.65	0.76
1:A:2044:ARG:HE	1:A:2045:ILE:H	1.30	0.76
1:A:2376:PHE:HB2	1:A:2405:GLU:HG2	1.67	0.75
1:A:2053:ARG:HH21	1:A:2057:GLU:HG3	1.48	0.75
1:A:2236:TRP:O	1:A:2239:ILE:HG22	1.86	0.75
1:A:2428:PHE:CZ	1:A:2478:MET:HE1	2.20	0.75
1:A:2379:ILE:HD11	1:A:2444:ASN:HB2	1.69	0.74
1:A:2179:TRP:O	1:A:2182:GLU:HG3	1.88	0.74
1:A:2421:VAL:HA	1:A:2424:MET:HE3	1.69	0.74
1:A:2558:TYR:CE2	1:A:2562:ILE:HD11	2.22	0.74
1:A:2058:PHE:O	1:A:2061:GLU:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:LYS:O	1:A:2465:LYS:HG3	1.88	0.73
1:A:2100:ILE:O	1:A:2113:LYS:NZ	2.21	0.73
1:A:2044:ARG:HH21	1:A:2045:ILE:HG12	1.54	0.73
1:A:2222:ILE:HG21	1:A:2308:VAL:HG21	1.70	0.73
1:A:2521:THR:OG1	1:A:2522:LYS:NZ	2.20	0.73
1:A:2602:CYS:SG	1:A:2605:LEU:HD12	2.30	0.72
1:A:2069:GLU:O	1:A:2073:LEU:HG	1.89	0.72
1:A:2407:GLU:HB3	1:A:2411:LYS:HZ3	1.54	0.72
1:A:2355:LEU:HD21	1:A:2374:ASN:HD22	1.55	0.72
1:A:2453:LEU:HD22	1:A:2455:ASP:OD1	1.89	0.72
1:A:2186:ASN:O	1:A:2190:GLN:HG2	1.89	0.72
1:A:2084:GLU:OE2	1:A:2085:LYS:NZ	2.23	0.71
1:A:2077:TYR:CE2	1:A:2090:MET:HE2	2.25	0.71
1:A:2132:LYS:HA	1:A:2135:ASP:OD2	1.90	0.71
1:A:2370:PRO:O	1:A:2373:LYS:NZ	2.23	0.71
1:A:2173:PRO:HD2	1:A:2178:ARG:HD2	1.73	0.70
1:A:2435:ILE:HD11	1:A:2467:TRP:HB2	1.74	0.70
1:A:2394:PHE:CZ	1:A:2398:ILE:HD11	2.26	0.69
1:A:2466:TRP:HE3	1:A:2469:MET:HE3	1.54	0.69
1:A:2407:GLU:HB3	1:A:2411:LYS:NZ	2.08	0.69
1:A:2588:LYS:HZ3	1:A:2592:GLU:CB	2.06	0.69
1:A:2588:LYS:NZ	1:A:2592:GLU:HB3	2.07	0.69
1:A:2455:ASP:OD2	1:A:2463:ARG:NH1	2.26	0.69
1:A:2456:GLY:H	1:A:2459:GLN:HE21	1.41	0.69
1:A:2381:GLU:HA	1:A:2384:ILE:HG12	1.73	0.68
1:A:2572:LEU:HD23	1:A:2575:GLN:OE1	1.94	0.68
1:A:2066:ALA:HB1	1:A:2144:ILE:HD13	1.76	0.68
1:A:2077:TYR:HE2	1:A:2090:MET:HE2	1.58	0.68
1:A:2517:GLU:O	1:A:2521:THR:HG23	1.93	0.68
1:A:2059:LYS:O	1:A:2062:ILE:HG22	1.93	0.68
1:A:2153:LYS:HD2	1:A:2164:TRP:HA	1.75	0.68
1:A:2017:ASN:HB2	1:A:2020:ASP:HB3	1.75	0.68
1:A:2384:ILE:HD12	1:A:2451:LYS:HD2	1.76	0.67
1:A:2306:GLU:HA	1:A:2309:ASP:OD2	1.95	0.67
1:A:2471:LYS:HE3	1:A:2499:ILE:HG21	1.76	0.67
1:A:2058:PHE:HE2	1:A:2116:LYS:HD3	1.60	0.67
1:A:2330:ASN:OD1	1:A:2331:ASP:N	2.27	0.67
1:A:2475:TRP:HA	1:A:2478:MET:HE3	1.76	0.67
1:A:2130:THR:O	1:A:2133:VAL:HG22	1.94	0.67
1:A:2208:LEU:O	1:A:2211:GLN:NE2	2.28	0.67
1:A:2575:GLN:HA	1:A:2578:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2219:THR:O	1:A:2222:ILE:HG22	1.95	0.67
1:A:2450:GLY:HA2	1:A:2454:GLY:HA2	1.74	0.67
1:A:2566:LYS:O	1:A:2570:GLN:N	2.22	0.66
1:A:2189:ILE:O	1:A:2193:GLU:HG2	1.94	0.66
1:A:2562:ILE:O	1:A:2565:LYS:HB3	1.95	0.66
1:A:2053:ARG:NH2	1:A:2057:GLU:HG3	2.11	0.66
1:A:2575:GLN:HA	1:A:2578:MET:CE	2.26	0.66
1:A:2106:MET:HE1	1:A:2114:ASP:OD1	1.96	0.66
1:A:2416:ALA:HB3	1:A:2419:LYS:CG	2.26	0.66
1:A:2021:MET:HE1	1:A:2032:LEU:HD12	1.78	0.66
1:A:2421:VAL:HA	1:A:2424:MET:CE	2.26	0.65
1:A:2174:PRO:HG2	1:A:2177:LEU:HD12	1.79	0.65
1:A:2355:LEU:HA	1:A:2358:ASN:OD1	1.96	0.65
1:A:2589:GLU:O	1:A:2593:TYR:N	2.25	0.65
1:A:2305:LYS:HG2	1:A:2307:GLN:H	1.61	0.65
1:A:2035:PRO:HA	1:A:2038:ARG:HG2	1.78	0.65
1:A:2479:LEU:HD21	1:A:2497:LEU:HD22	1.77	0.65
1:A:2084:GLU:O	1:A:2087:LEU:HG	1.97	0.65
1:A:2460:ASN:O	1:A:2464:LYS:N	2.29	0.65
1:A:2129:ASN:ND2	1:A:2131:GLU:HB2	2.12	0.64
1:A:2158:LYS:HD2	1:A:2167:ILE:HG23	1.79	0.64
1:A:2453:LEU:HD23	1:A:2453:LEU:O	1.97	0.64
1:A:2448:LYS:HE3	1:A:2451:LYS:HZ1	1.62	0.64
1:A:2138:GLU:O	1:A:2142:LYS:HG2	1.98	0.64
1:A:2067:GLN:O	1:A:2071:LYS:HG2	1.98	0.64
1:A:2394:PHE:CE2	1:A:2398:ILE:HD11	2.33	0.64
1:A:2432:GLY:O	1:A:2436:LYS:HG2	1.98	0.64
1:A:2455:ASP:OD2	1:A:2463:ARG:HD2	1.98	0.64
1:A:2191:LYS:HE3	1:A:2192:GLU:OE2	1.97	0.63
1:A:2372:ARG:HB2	1:A:2430:ASP:OD1	1.98	0.63
1:A:2420:VAL:HG12	1:A:2424:MET:HE2	1.81	0.63
1:A:2594:PHE:O	1:A:2597:LYS:HG2	1.98	0.63
1:A:2474:ILE:HG22	1:A:2478:MET:CE	2.29	0.63
1:A:2176:PHE:O	1:A:2180:ILE:HG13	1.99	0.62
1:A:2590:SER:HB2	1:A:2591:PRO:HD3	1.81	0.62
1:A:2018:ASP:O	1:A:2022:ARG:HG2	2.00	0.62
1:A:2161:ASP:HB2	1:A:2164:TRP:O	2.00	0.62
1:A:2088:GLU:HA	1:A:2091:LYS:HE3	1.80	0.62
1:A:2435:ILE:O	1:A:2463:ARG:NE	2.25	0.61
1:A:2141:LYS:O	1:A:2144:ILE:HG22	1.99	0.61
1:A:2407:GLU:HA	1:A:2410:LYS:NZ	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2405:GLU:O	1:A:2409:LEU:HD23	1.99	0.61
1:A:2415:GLU:OE2	1:A:2486:TYR:OH	2.08	0.61
1:A:2103:GLY:HA2	1:A:2175:GLN:NE2	2.12	0.61
1:A:2228:TRP:CZ3	1:A:2231:LYS:HD2	2.36	0.61
1:A:2522:LYS:O	1:A:2526:LEU:HD23	2.01	0.61
1:A:2099:TYR:CE1	1:A:2178:ARG:HB3	2.36	0.61
1:A:2124:GLU:HG3	1:A:2132:LYS:HD3	1.82	0.61
1:A:2103:GLY:CA	1:A:2175:GLN:HE22	2.12	0.61
1:A:2563:LEU:HA	1:A:2566:LYS:CE	2.28	0.60
1:A:2429:ALA:HB2	1:A:2510:ARG:HH12	1.65	0.60
1:A:2119:LEU:HD12	1:A:2120:ASP:N	2.17	0.60
1:A:2121:ARG:HA	1:A:2128:ASN:HB3	1.82	0.60
1:A:2053:ARG:HH22	1:A:2061:GLU:HG2	1.66	0.60
1:A:2473:HIS:O	1:A:2476:GLU:HG3	2.02	0.60
1:A:2058:PHE:CE2	1:A:2116:LYS:HD3	2.36	0.60
1:A:2073:LEU:HD13	1:A:2093:SER:HB2	1.84	0.59
1:A:2138:GLU:O	1:A:2142:LYS:NZ	2.34	0.59
1:A:2116:LYS:O	1:A:2119:LEU:HG	2.01	0.59
1:A:2413:TYR:HB3	1:A:2420:VAL:HG22	1.84	0.59
1:A:2416:ALA:HB3	1:A:2419:LYS:HG3	1.83	0.59
1:A:2475:TRP:O	1:A:2478:MET:HG2	2.02	0.59
1:A:2099:TYR:HE1	1:A:2178:ARG:HB3	1.68	0.59
1:A:2518:ASN:O	1:A:2522:LYS:HG2	2.03	0.59
1:A:2183:TRP:NE1	1:A:2239:ILE:HG21	2.17	0.59
1:A:2518:ASN:OD1	1:A:2519:PHE:N	2.35	0.59
1:A:2034:PRO:HG2	1:A:2037:ARG:CB	2.28	0.59
1:A:2137:TRP:HA	1:A:2140:ASN:ND2	2.18	0.58
1:A:2124:GLU:HG3	1:A:2132:LYS:CD	2.33	0.58
1:A:2033:ILE:O	1:A:2038:ARG:NH2	2.35	0.58
1:A:2190:GLN:HB3	1:A:2232:ARG:HH22	1.68	0.58
1:A:2385:CYS:SG	1:A:2389:ARG:NE	2.76	0.58
1:A:2502:ASN:O	1:A:2510:ARG:HD3	2.02	0.58
1:A:2408:ARG:NH1	1:A:2412:VAL:HG11	2.18	0.58
1:A:2516:THR:HG21	1:A:2605:LEU:HB3	1.85	0.58
1:A:2407:GLU:HG2	1:A:2410:LYS:NZ	2.19	0.58
1:A:2408:ARG:O	1:A:2412:VAL:HG22	2.04	0.58
1:A:2428:PHE:O	1:A:2431:ILE:HG12	2.04	0.58
1:A:2114:ASP:O	1:A:2118:LYS:HD3	2.03	0.57
1:A:2336:LYS:NZ	1:A:2476:GLU:OE2	2.26	0.57
1:A:2460:ASN:CB	1:A:2463:ARG:HB2	2.27	0.57
1:A:2516:THR:CG2	1:A:2605:LEU:HD13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2418:THR:O	1:A:2421:VAL:HG12	2.04	0.57
1:A:2511:TRP:O	1:A:2514:GLU:HG2	2.04	0.57
1:A:2216:LYS:O	1:A:2219:THR:OG1	2.22	0.57
1:A:2213:SER:HA	1:A:2216:LYS:HD3	1.86	0.56
1:A:2053:ARG:NH2	1:A:2061:GLU:HG2	2.20	0.56
1:A:2372:ARG:HH21	1:A:2442:GLU:HB3	1.70	0.56
1:A:2098:GLU:HA	1:A:2101:ILE:HG12	1.88	0.56
1:A:2124:GLU:HB3	1:A:2132:LYS:HZ3	1.69	0.56
1:A:2173:PRO:HD2	1:A:2178:ARG:HH11	1.69	0.56
1:A:2305:LYS:O	1:A:2308:VAL:HG12	2.06	0.56
1:A:2414:GLY:HA3	1:A:2419:LYS:NZ	2.20	0.56
1:A:2173:PRO:HD2	1:A:2178:ARG:CD	2.36	0.56
1:A:2442:GLU:HG3	1:A:2445:SER:HB3	1.87	0.56
1:A:2525:GLU:O	1:A:2528:GLU:HG3	2.06	0.56
1:A:2069:GLU:HB3	1:A:2097:TYR:OH	2.06	0.56
1:A:2055:LEU:HB2	1:A:2123:LEU:HD22	1.86	0.56
1:A:2427:SER:O	1:A:2431:ILE:HG23	2.05	0.56
1:A:2434:ILE:HD11	1:A:2442:GLU:HG3	1.86	0.56
1:A:2049:PRO:HB2	1:A:2052:LEU:HB3	1.88	0.55
1:A:2124:GLU:HB3	1:A:2132:LYS:NZ	2.20	0.55
1:A:2367:LEU:HB3	1:A:2567:LYS:NZ	2.21	0.55
1:A:2448:LYS:HE3	1:A:2451:LYS:NZ	2.21	0.55
1:A:2466:TRP:CE3	1:A:2469:MET:HE3	2.39	0.55
1:A:2188:CYS:SG	1:A:2189:ILE:N	2.79	0.55
1:A:2449:ILE:HG23	1:A:2455:ASP:OD2	2.06	0.55
1:A:2531:VAL:HA	1:A:2535:ASN:OD1	2.05	0.55
1:A:2340:ILE:HD12	1:A:2403:ILE:HD11	1.88	0.55
1:A:2448:LYS:O	1:A:2451:LYS:HG2	2.06	0.55
1:A:2566:LYS:O	1:A:2570:GLN:HG2	2.06	0.55
1:A:2021:MET:CE	1:A:2032:LEU:HD12	2.37	0.55
1:A:2183:TRP:HE1	1:A:2239:ILE:HG21	1.72	0.55
1:A:2435:ILE:HD11	1:A:2467:TRP:CD1	2.42	0.55
1:A:2528:GLU:HA	1:A:2531:VAL:HG22	1.88	0.55
1:A:2118:LYS:O	1:A:2122:LEU:HD23	2.07	0.54
1:A:2158:LYS:HB3	1:A:2167:ILE:HG23	1.88	0.54
1:A:2182:GLU:O	1:A:2185:THR:HG22	2.07	0.54
1:A:2586:GLU:OE2	1:A:2590:SER:OG	2.23	0.54
1:A:2055:LEU:HG	1:A:2059:LYS:NZ	2.23	0.54
1:A:2059:LYS:HG2	1:A:2136:TRP:CZ2	2.42	0.54
1:A:2413:TYR:O	1:A:2419:LYS:NZ	2.40	0.54
1:A:2470:ASN:O	1:A:2474:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2137:TRP:HA	1:A:2140:ASN:HD22	1.73	0.54
1:A:2602:CYS:HA	1:A:2605:LEU:CG	2.38	0.54
1:A:2576:TYR:O	1:A:2580:TYR:N	2.41	0.54
1:A:2164:TRP:NE1	1:A:2166:THR:OG1	2.41	0.54
1:A:2017:ASN:ND2	1:A:2020:ASP:OD1	2.40	0.53
1:A:2196:GLU:HA	1:A:2199:LYS:HG2	1.91	0.53
1:A:2409:LEU:HD12	1:A:2413:TYR:CZ	2.43	0.53
1:A:2479:LEU:HD11	1:A:2483:LYS:HE3	1.89	0.53
1:A:2461:GLU:HG2	1:A:2462:LYS:N	2.24	0.53
1:A:2027:LYS:NZ	1:A:2029:LYS:HB2	2.23	0.53
1:A:2201:LYS:HZ1	1:A:2218:CYS:HA	1.73	0.53
1:A:2205:VAL:O	1:A:2209:GLY:HA3	2.08	0.53
1:A:2407:GLU:CB	1:A:2411:LYS:HZ3	2.22	0.53
1:A:2475:TRP:CH2	1:A:2500:PRO:HD2	2.43	0.53
1:A:2118:LYS:NZ	1:A:2121:ARG:HH12	2.07	0.52
1:A:2111:GLN:O	1:A:2115:ILE:HG12	2.09	0.52
1:A:2159:ILE:HD12	1:A:2168:PRO:CD	2.39	0.52
1:A:2033:ILE:HG13	1:A:2038:ARG:HB3	1.90	0.52
1:A:2336:LYS:O	1:A:2340:ILE:HG12	2.09	0.52
1:A:2589:GLU:O	1:A:2593:TYR:HB2	2.09	0.52
1:A:2153:LYS:HG3	1:A:2165:CYS:N	2.25	0.52
1:A:2173:PRO:HD2	1:A:2178:ARG:CG	2.40	0.52
1:A:2244:LYS:O	1:A:2247:LYS:HG2	2.09	0.52
1:A:2407:GLU:CA	1:A:2410:LYS:HZ3	2.14	0.52
1:A:2101:ILE:HB	1:A:2137:TRP:CE3	2.44	0.52
1:A:2141:LYS:HZ1	1:A:2145:TRP:HB2	1.75	0.52
1:A:2449:ILE:HA	1:A:2452:ILE:HD11	1.91	0.52
1:A:2158:LYS:HD2	1:A:2167:ILE:CG2	2.40	0.52
1:A:2471:LYS:HE3	1:A:2499:ILE:HD13	1.92	0.52
1:A:2379:ILE:HA	1:A:2448:LYS:NZ	2.25	0.52
1:A:2562:ILE:C	1:A:2566:LYS:HZ3	2.17	0.52
1:A:2598:CYS:HB3	1:A:2601:GLU:H	1.75	0.52
1:A:2355:LEU:HD22	1:A:2373:LYS:HZ3	1.75	0.51
1:A:2461:GLU:HG2	1:A:2462:LYS:H	1.75	0.51
1:A:2027:LYS:HZ3	1:A:2029:LYS:HB2	1.74	0.51
1:A:2052:LEU:CD2	1:A:2057:GLU:HG2	2.38	0.51
1:A:2227:GLU:HA	1:A:2230:ARG:HD2	1.91	0.51
1:A:2357:LYS:HD2	1:A:2357:LYS:N	2.24	0.51
1:A:2039:GLN:O	1:A:2040:LEU:CD1	2.59	0.51
1:A:2355:LEU:HD13	1:A:2374:ASN:HB3	1.93	0.51
1:A:2402:ALA:O	1:A:2406:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2403:ILE:O	1:A:2406:VAL:HG22	2.11	0.51
1:A:2195:LYS:HA	1:A:2198:VAL:HG12	1.93	0.51
1:A:2414:GLY:HA3	1:A:2419:LYS:HZ1	1.74	0.51
1:A:2435:ILE:CD1	1:A:2467:TRP:HB2	2.40	0.51
1:A:2308:VAL:O	1:A:2311:PRO:HD2	2.11	0.51
1:A:2213:SER:HA	1:A:2216:LYS:CD	2.40	0.51
1:A:2381:GLU:HA	1:A:2384:ILE:CG1	2.41	0.51
1:A:2044:ARG:NH2	1:A:2045:ILE:HG12	2.24	0.50
1:A:2069:GLU:HB3	1:A:2097:TYR:CZ	2.46	0.50
1:A:2355:LEU:HD11	1:A:2374:ASN:ND2	2.26	0.50
1:A:2386:LYS:HE3	1:A:2393:LEU:CD1	2.31	0.50
1:A:2530:MET:SD	1:A:2531:VAL:HG13	2.51	0.50
1:A:2568:GLU:O	1:A:2572:LEU:HG	2.11	0.50
1:A:2407:GLU:O	1:A:2411:LYS:HE2	2.11	0.50
1:A:2516:THR:CG2	1:A:2605:LEU:HB3	2.41	0.50
1:A:2409:LEU:HA	1:A:2412:VAL:HG22	1.93	0.50
1:A:2371:ARG:HG3	1:A:2426:TYR:HD2	1.76	0.50
1:A:2431:ILE:HA	1:A:2434:ILE:HG22	1.92	0.50
1:A:2569:TYR:HA	1:A:2572:LEU:HB2	1.93	0.50
1:A:2436:LYS:HB3	1:A:2460:ASN:ND2	2.27	0.50
1:A:2159:ILE:HB	1:A:2166:THR:O	2.12	0.50
1:A:2247:LYS:O	1:A:2249:MET:HE2	2.11	0.50
1:A:2449:ILE:HG12	1:A:2463:ARG:NH2	2.26	0.50
1:A:2176:PHE:HB2	1:A:2246:TYR:HE2	1.77	0.50
1:A:2116:LYS:HA	1:A:2119:LEU:CD2	2.41	0.49
1:A:2076:TYR:O	1:A:2079:GLU:HB3	2.12	0.49
1:A:2173:PRO:CD	1:A:2178:ARG:HH11	2.25	0.49
1:A:2304:ILE:HG21	1:A:2308:VAL:HG11	1.93	0.49
1:A:2385:CYS:O	1:A:2389:ARG:HG3	2.12	0.49
1:A:2102:LYS:NZ	1:A:2134:ASP:O	2.46	0.49
1:A:2087:LEU:HD12	1:A:2088:GLU:N	2.27	0.49
1:A:2121:ARG:HA	1:A:2128:ASN:HD22	1.77	0.49
1:A:2109:ASN:HB3	1:A:2112:PHE:HD1	1.77	0.48
1:A:2145:TRP:CZ2	1:A:2169:THR:HA	2.48	0.48
1:A:2055:LEU:O	1:A:2059:LYS:HG3	2.13	0.48
1:A:2303:GLN:C	1:A:2304:ILE:HD13	2.38	0.48
1:A:2431:ILE:O	1:A:2435:ILE:HG23	2.14	0.48
1:A:2505:GLU:HB2	1:A:2510:ARG:HG3	1.95	0.48
1:A:2159:ILE:HD12	1:A:2168:PRO:HD3	1.95	0.48
1:A:2436:LYS:CE	1:A:2464:LYS:HA	2.40	0.48
1:A:2431:ILE:O	1:A:2434:ILE:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2044:ARG:HE	1:A:2045:ILE:N	2.05	0.48
1:A:2106:MET:O	1:A:2107:LEU:HD22	2.14	0.48
1:A:2387:TYR:CD1	1:A:2394:PHE:HB2	2.49	0.48
1:A:2528:GLU:O	1:A:2532:THR:HG22	2.13	0.48
1:A:2018:ASP:OD2	1:A:2018:ASP:N	2.45	0.47
1:A:2125:LYS:HE3	1:A:2128:ASN:HA	1.96	0.47
1:A:2338:LYS:HA	1:A:2341:ASN:OD1	2.14	0.47
1:A:2055:LEU:HG	1:A:2059:LYS:HZ2	1.78	0.47
1:A:2164:TRP:CZ2	1:A:2166:THR:HG21	2.49	0.47
1:A:2183:TRP:O	1:A:2187:VAL:HG12	2.14	0.47
1:A:2394:PHE:O	1:A:2398:ILE:HG13	2.14	0.47
1:A:2104:SER:H	1:A:2117:ARG:HH22	1.61	0.47
1:A:2158:LYS:N	1:A:2165:CYS:SG	2.83	0.47
1:A:2172:THR:HG23	1:A:2172:THR:O	2.14	0.47
1:A:2435:ILE:HD11	1:A:2467:TRP:CB	2.43	0.47
1:A:2516:THR:HG22	1:A:2605:LEU:HD13	1.96	0.47
1:A:2055:LEU:C	1:A:2059:LYS:HZ3	2.22	0.47
1:A:2355:LEU:HB3	1:A:2373:LYS:NZ	2.29	0.47
1:A:2426:TYR:HA	1:A:2514:GLU:OE1	2.14	0.47
1:A:2153:LYS:HG3	1:A:2165:CYS:H	1.80	0.47
1:A:2052:LEU:HD23	1:A:2052:LEU:O	2.15	0.47
1:A:2110:ILE:H	1:A:2110:ILE:HD12	1.80	0.47
1:A:2116:LYS:HA	1:A:2119:LEU:HD21	1.96	0.47
1:A:2141:LYS:HB3	1:A:2142:LYS:NZ	2.30	0.46
1:A:2217:ASN:OD1	1:A:2218:CYS:N	2.48	0.46
1:A:2449:ILE:HG12	1:A:2463:ARG:CZ	2.44	0.46
1:A:2475:TRP:CA	1:A:2478:MET:HE3	2.44	0.46
1:A:2035:PRO:CA	1:A:2038:ARG:HG2	2.45	0.46
1:A:2082:ASP:HB3	1:A:2085:LYS:HB2	1.96	0.46
1:A:2479:LEU:O	1:A:2483:LYS:HG3	2.16	0.46
1:A:2371:ARG:HG3	1:A:2426:TYR:CD2	2.50	0.46
1:A:2331:ASP:CG	1:A:2334:CYS:HB3	2.41	0.46
1:A:2379:ILE:HD13	1:A:2448:LYS:HD2	1.97	0.46
1:A:2449:ILE:HA	1:A:2452:ILE:CD1	2.45	0.46
1:A:2588:LYS:NZ	1:A:2596:ASP:OD2	2.41	0.46
1:A:2315:GLU:N	1:A:2315:GLU:OE1	2.49	0.46
1:A:2409:LEU:HD12	1:A:2413:TYR:CE2	2.50	0.46
1:A:2583:THR:O	1:A:2583:THR:HG23	2.15	0.46
1:A:2128:ASN:OD1	1:A:2132:LYS:HE3	2.16	0.46
1:A:2474:ILE:C	1:A:2478:MET:HE3	2.40	0.46
1:A:2575:GLN:HA	1:A:2578:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2173:PRO:CD	1:A:2178:ARG:HD2	2.44	0.46
1:A:2403:ILE:O	1:A:2407:GLU:HG3	2.16	0.46
1:A:2515:TRP:HZ3	1:A:2575:GLN:NE2	2.14	0.46
1:A:2553:GLU:HA	1:A:2556:LYS:HD3	1.98	0.46
1:A:2205:VAL:HG21	1:A:2311:PRO:HG3	1.97	0.45
1:A:2569:TYR:O	1:A:2573:ASN:N	2.37	0.45
1:A:2053:ARG:HH22	1:A:2058:PHE:HA	1.80	0.45
1:A:2425:LYS:HG3	1:A:2503:ASP:OD1	2.16	0.45
1:A:2035:PRO:HA	1:A:2038:ARG:HD2	1.97	0.45
1:A:2442:GLU:O	1:A:2442:GLU:HG2	2.16	0.45
1:A:2474:ILE:HG22	1:A:2478:MET:HE2	1.98	0.45
1:A:2591:PRO:O	1:A:2595:LYS:HG2	2.16	0.45
1:A:2016:TRP:HD1	1:A:2038:ARG:HH12	1.63	0.45
1:A:2141:LYS:NZ	1:A:2145:TRP:HB2	2.31	0.45
1:A:2367:LEU:HB3	1:A:2567:LYS:HZ3	1.80	0.45
1:A:2527:TYR:OH	1:A:2558:TYR:OH	2.35	0.45
1:A:2409:LEU:HD12	1:A:2413:TYR:OH	2.16	0.45
1:A:2475:TRP:HA	1:A:2478:MET:HG2	1.98	0.45
1:A:2455:ASP:CG	1:A:2463:ARG:HD2	2.42	0.45
1:A:2370:PRO:O	1:A:2373:LYS:HG2	2.16	0.45
1:A:2099:TYR:HE1	1:A:2178:ARG:HE	1.65	0.45
1:A:2304:ILE:CG2	1:A:2308:VAL:HG11	2.47	0.44
1:A:2073:LEU:HD13	1:A:2093:SER:CB	2.47	0.44
1:A:2515:TRP:HZ3	1:A:2575:GLN:HE22	1.65	0.44
1:A:2033:ILE:HD12	1:A:2038:ARG:HA	1.99	0.44
1:A:2064:LYS:C	1:A:2064:LYS:HD3	2.42	0.44
1:A:2188:CYS:O	1:A:2192:GLU:OE1	2.36	0.44
1:A:2205:VAL:HG21	1:A:2311:PRO:CG	2.47	0.44
1:A:2237:GLU:HA	1:A:2237:GLU:OE1	2.16	0.44
1:A:2244:LYS:HG2	1:A:2247:LYS:CE	2.27	0.44
1:A:2029:LYS:HD2	1:A:2029:LYS:HA	1.76	0.44
1:A:2333:ILE:HG13	1:A:2334:CYS:N	2.33	0.44
1:A:2465:LYS:HD2	1:A:2469:MET:CE	2.39	0.44
1:A:2035:PRO:O	1:A:2038:ARG:HG2	2.18	0.44
1:A:2016:TRP:CD1	1:A:2038:ARG:HH12	2.35	0.44
1:A:2090:MET:SD	1:A:2094:PHE:CZ	3.11	0.44
1:A:2159:ILE:HD12	1:A:2168:PRO:HD2	2.00	0.44
1:A:2357:LYS:HD2	1:A:2357:LYS:H	1.82	0.44
1:A:2355:LEU:HB3	1:A:2373:LYS:HZ1	1.83	0.44
1:A:2379:ILE:HA	1:A:2448:LYS:HZ2	1.82	0.44
1:A:2418:THR:HG23	1:A:2419:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2069:GLU:HB3	1:A:2097:TYR:CE2	2.53	0.44
1:A:2077:TYR:HE2	1:A:2090:MET:CE	2.29	0.44
1:A:2176:PHE:CE2	1:A:2180:ILE:HD11	2.51	0.44
1:A:2376:PHE:CZ	1:A:2408:ARG:HD2	2.53	0.44
1:A:2068:SER:O	1:A:2072:PHE:CD1	2.71	0.43
1:A:2102:LYS:NZ	1:A:2137:TRP:HB2	2.33	0.43
1:A:2522:LYS:HA	1:A:2522:LYS:HD3	1.87	0.43
1:A:2595:LYS:HA	1:A:2595:LYS:HE3	2.00	0.43
1:A:2053:ARG:HA	1:A:2053:ARG:NE	2.33	0.43
1:A:2304:ILE:HG22	1:A:2305:LYS:N	2.33	0.43
1:A:2475:TRP:HA	1:A:2478:MET:CE	2.45	0.43
1:A:2528:GLU:HA	1:A:2531:VAL:CG2	2.47	0.43
1:A:2068:SER:HB2	1:A:2072:PHE:CZ	2.53	0.43
1:A:2310:ILE:HD12	1:A:2310:ILE:H	1.83	0.43
1:A:2355:LEU:HD11	1:A:2374:ASN:HD22	1.82	0.43
1:A:2527:TYR:O	1:A:2530:MET:HG3	2.18	0.43
1:A:2569:TYR:O	1:A:2572:LEU:HB2	2.17	0.43
1:A:2211:GLN:HE21	1:A:2214:GLU:CB	2.32	0.43
1:A:2310:ILE:HB	1:A:2311:PRO:HD3	1.98	0.43
1:A:2191:LYS:HD3	1:A:2195:LYS:NZ	2.33	0.43
1:A:2161:ASP:HB3	1:A:2162:PRO:HD2	2.00	0.43
1:A:2230:ARG:HG2	1:A:2302:LYS:NZ	2.33	0.43
1:A:2424:MET:HB3	1:A:2428:PHE:CZ	2.54	0.43
1:A:2520:CYS:HB2	1:A:2605:LEU:CD2	2.49	0.43
1:A:2035:PRO:C	1:A:2038:ARG:HG2	2.43	0.43
1:A:2035:PRO:HA	1:A:2038:ARG:CG	2.46	0.43
1:A:2055:LEU:HB2	1:A:2123:LEU:CD2	2.49	0.43
1:A:2211:GLN:CD	1:A:2211:GLN:H	2.26	0.43
1:A:2528:GLU:O	1:A:2531:VAL:HG22	2.18	0.43
1:A:2025:TYR:HB3	1:A:2027:LYS:HG2	2.00	0.43
1:A:2377:LEU:O	1:A:2377:LEU:HG	2.18	0.43
1:A:2456:GLY:N	1:A:2459:GLN:HE21	2.11	0.43
1:A:2213:SER:O	1:A:2216:LYS:NZ	2.51	0.42
1:A:2395:LYS:HE2	1:A:2399:TYR:OH	2.19	0.42
1:A:2515:TRP:O	1:A:2518:ASN:OD1	2.37	0.42
1:A:2039:GLN:O	1:A:2040:LEU:HD13	2.19	0.42
1:A:2073:LEU:HD11	1:A:2097:TYR:CE2	2.54	0.42
1:A:2126:GLU:O	1:A:2127:THR:OG1	2.28	0.42
1:A:2153:LYS:HG3	1:A:2165:CYS:HB3	2.00	0.42
1:A:2191:LYS:HE3	1:A:2192:GLU:CD	2.44	0.42
1:A:2222:ILE:HD12	1:A:2225:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:GLN:O	1:A:2229:SER:OG	2.35	0.42
1:A:2354:ASP:OD2	1:A:2357:LYS:HB2	2.20	0.42
1:A:2475:TRP:CZ3	1:A:2499:ILE:HG23	2.54	0.42
1:A:2190:GLN:HB2	1:A:2232:ARG:HH12	1.84	0.42
1:A:2020:ASP:O	1:A:2024:PRO:HD2	2.20	0.42
1:A:2436:LYS:HD2	1:A:2460:ASN:CG	2.45	0.42
1:A:2097:TYR:O	1:A:2101:ILE:HG12	2.19	0.42
1:A:2375:LEU:HB3	1:A:2377:LEU:HD22	2.02	0.42
1:A:2471:LYS:NZ	1:A:2503:ASP:OD2	2.51	0.42
1:A:2098:GLU:HA	1:A:2101:ILE:CG1	2.50	0.42
1:A:2448:LYS:O	1:A:2452:ILE:HG12	2.19	0.42
1:A:2022:ARG:NE	1:A:2022:ARG:HA	2.35	0.41
1:A:2090:MET:O	1:A:2093:SER:OG	2.32	0.41
1:A:2426:TYR:HD1	1:A:2514:GLU:CD	2.28	0.41
1:A:2569:TYR:HA	1:A:2572:LEU:CD1	2.42	0.41
1:A:2118:LYS:HZ3	1:A:2121:ARG:HH12	1.68	0.41
1:A:2211:GLN:HG2	1:A:2211:GLN:O	2.20	0.41
1:A:2384:ILE:HD12	1:A:2451:LYS:CD	2.46	0.41
1:A:2516:THR:HG22	1:A:2605:LEU:CD2	2.44	0.41
1:A:2035:PRO:HA	1:A:2038:ARG:CD	2.51	0.41
1:A:2384:ILE:CD1	1:A:2451:LYS:HE3	2.51	0.41
1:A:2442:GLU:CG	1:A:2445:SER:HB3	2.51	0.41
1:A:2017:ASN:HB2	1:A:2020:ASP:CB	2.47	0.41
1:A:2435:ILE:HD11	1:A:2467:TRP:CG	2.56	0.41
1:A:2475:TRP:HA	1:A:2478:MET:SD	2.61	0.41
1:A:2377:LEU:H	1:A:2377:LEU:HD23	1.84	0.41
1:A:2053:ARG:NH2	1:A:2058:PHE:HA	2.35	0.41
1:A:2191:LYS:HD3	1:A:2195:LYS:HZ1	1.86	0.41
1:A:2218:CYS:SG	1:A:2219:THR:N	2.94	0.41
1:A:2413:TYR:HE1	1:A:2424:MET:HG2	1.85	0.41
1:A:2449:ILE:O	1:A:2452:ILE:HG12	2.21	0.41
1:A:2195:LYS:HA	1:A:2198:VAL:CG1	2.51	0.41
1:A:2037:ARG:O	1:A:2037:ARG:HD2	2.21	0.40
1:A:2399:TYR:O	1:A:2403:ILE:HG13	2.21	0.40
1:A:2185:THR:O	1:A:2189:ILE:HG12	2.21	0.40
1:A:2035:PRO:HA	1:A:2038:ARG:HH11	1.86	0.40
1:A:2179:TRP:HA	1:A:2182:GLU:CG	2.51	0.40
1:A:2560:ASN:O	1:A:2563:LEU:HB3	2.22	0.40
1:A:2091:LYS:HB2	1:A:2095:TYR:CZ	2.56	0.40
1:A:2585:ALA:O	1:A:2586:GLU:HG3	2.22	0.40
1:A:2528:GLU:CA	1:A:2531:VAL:HG22	2.52	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	490/2653 (18%)	473 (96%)	16 (3%)	1 (0%)	43 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2040	LEU

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	461/2419 (19%)	461 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2140	ASN
1	A	2175	GLN
1	A	2374	ASN
1	A	2422	HIS
1	A	2459	GLN

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Mol	Chain	Res	Type
1	A	2470	ASN
1	A	2506	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.

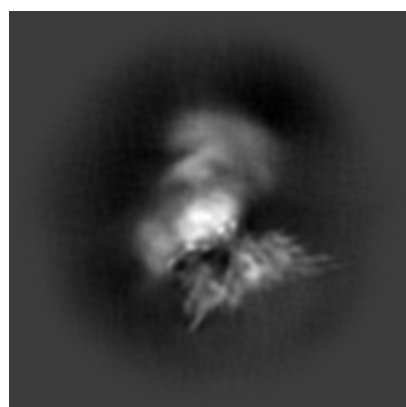
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22326. These allow visual inspection of the internal detail of the map and identification of artifacts.

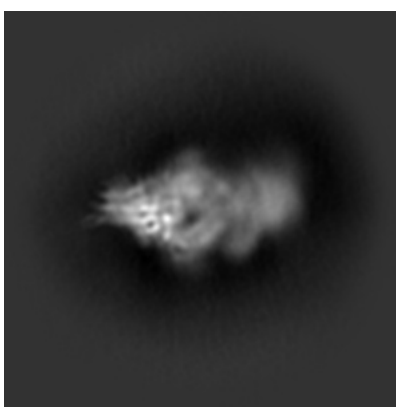
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

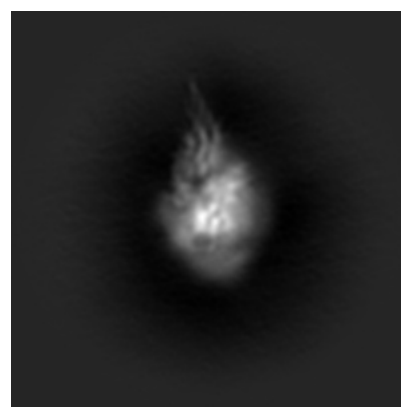
6.1.1 Primary map



X



Y

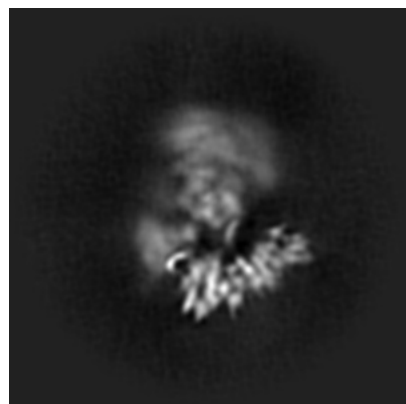


Z

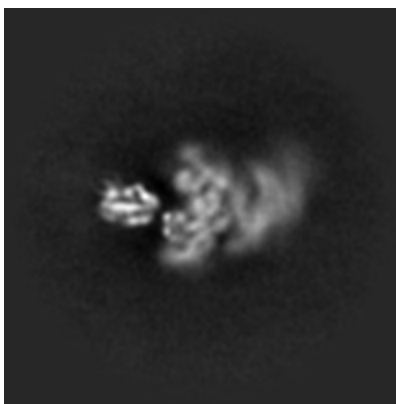
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

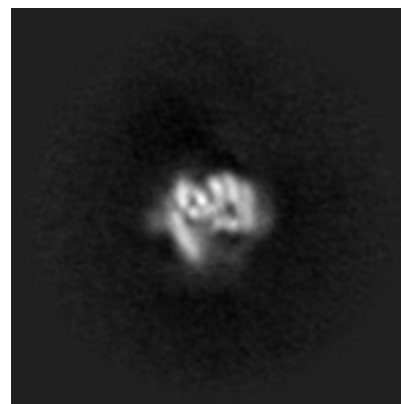
6.2.1 Primary map



X Index: 150



Y Index: 150

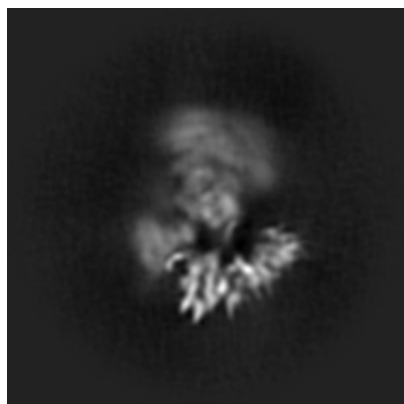


Z Index: 150

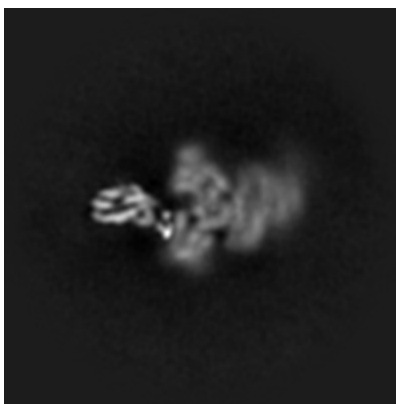
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

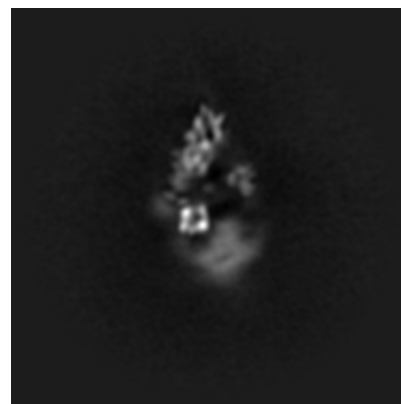
6.3.1 Primary map



X Index: 152



Y Index: 144

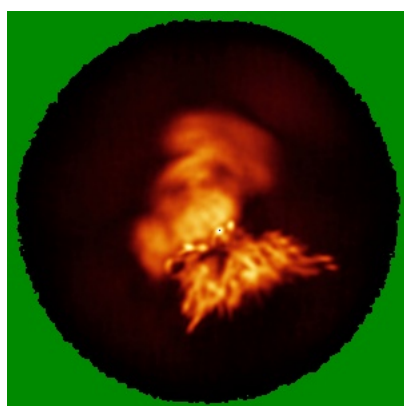


Z Index: 122

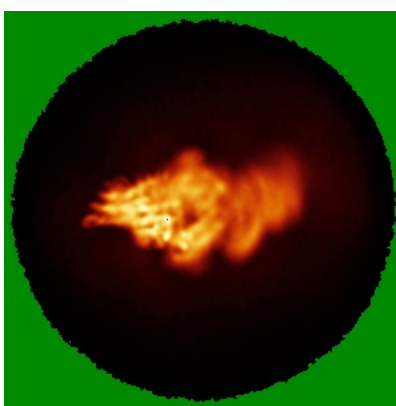
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

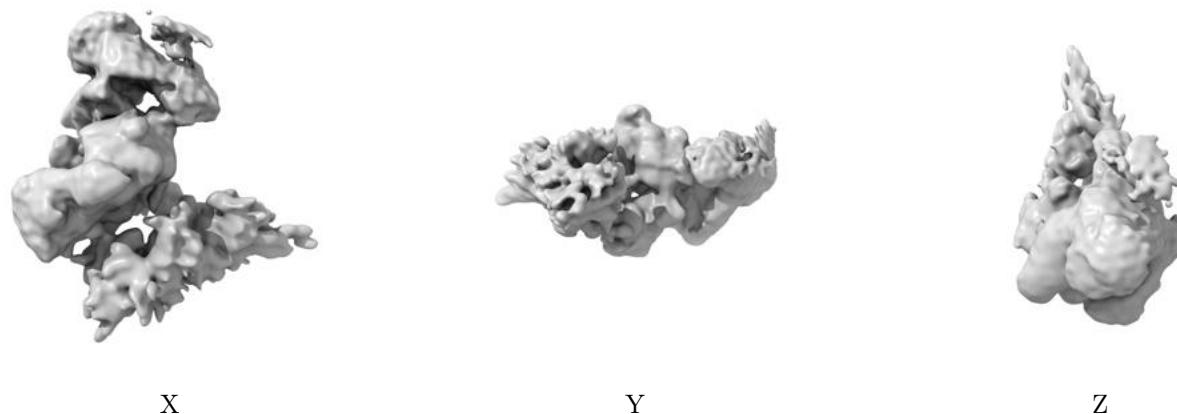


Z

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

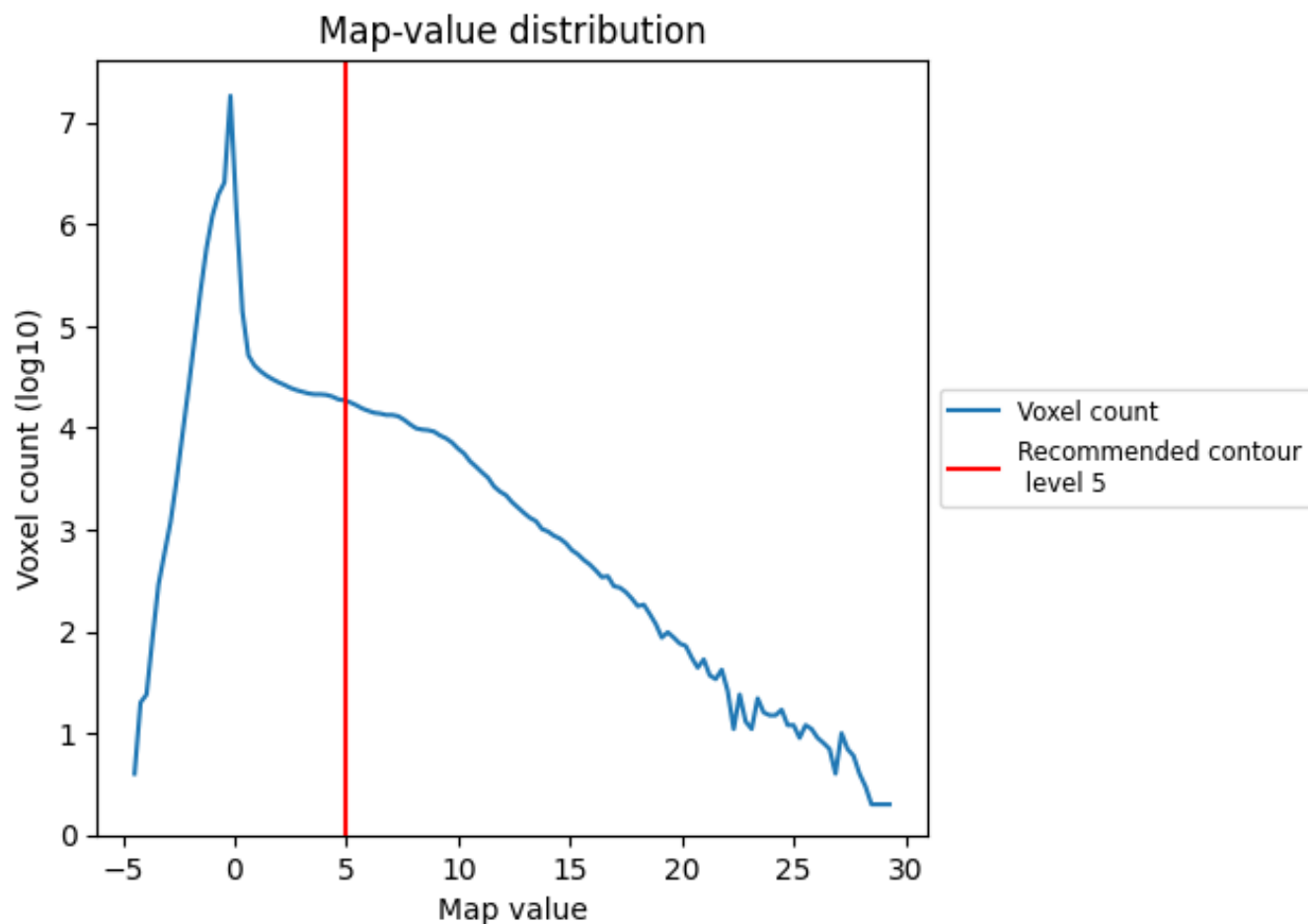
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

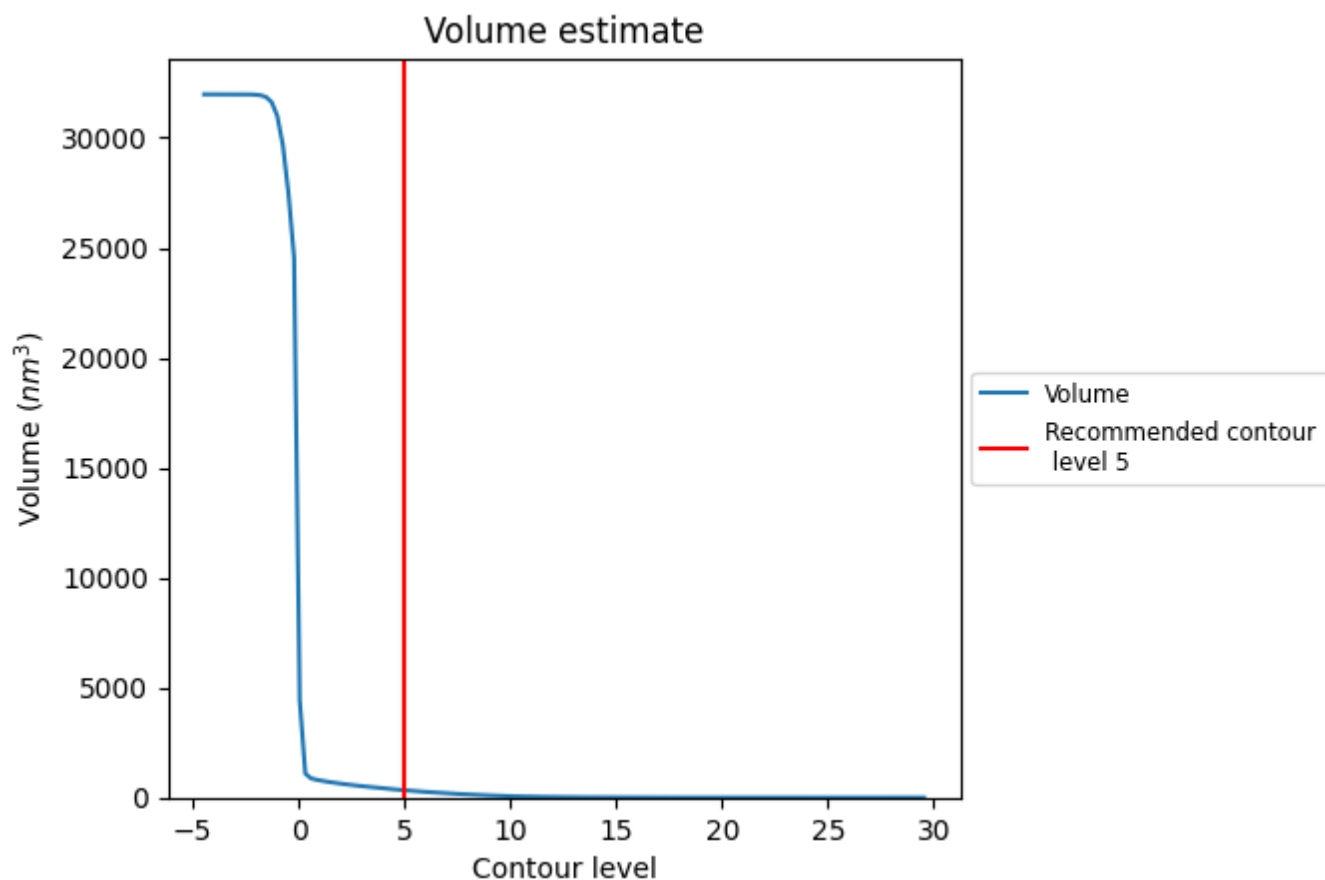
This section contains the results of statistical analysis of the map.

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.

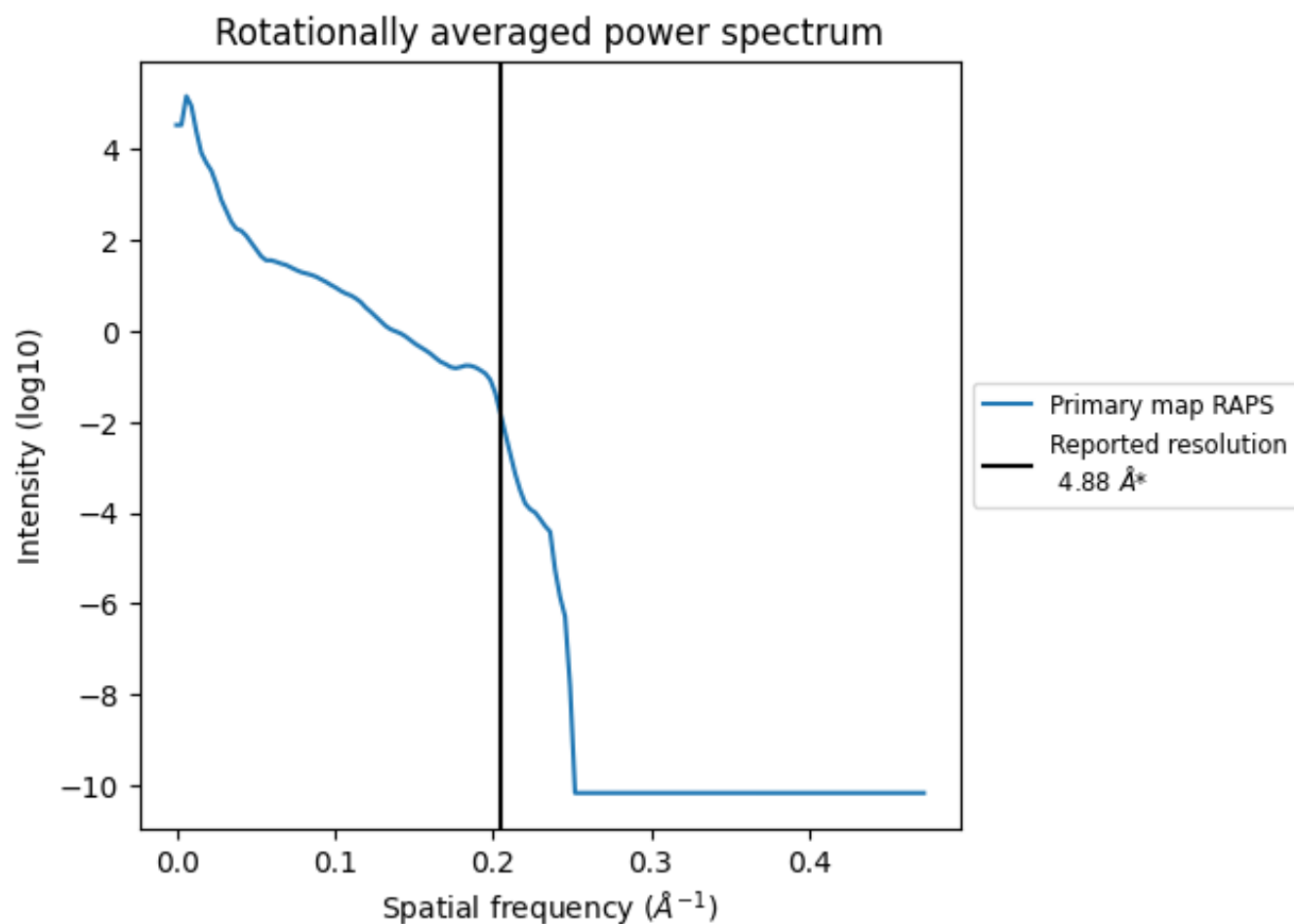
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm^3 ; this corresponds to an approximate mass of 300 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 0.205 Å⁻¹

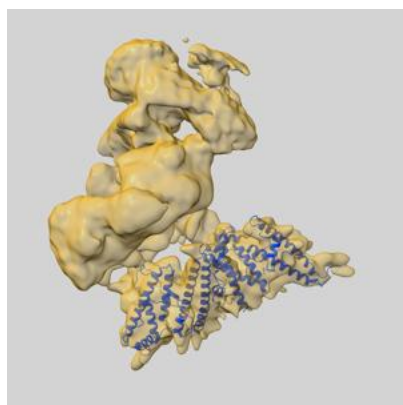
8 Fourier-Shell correlation

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

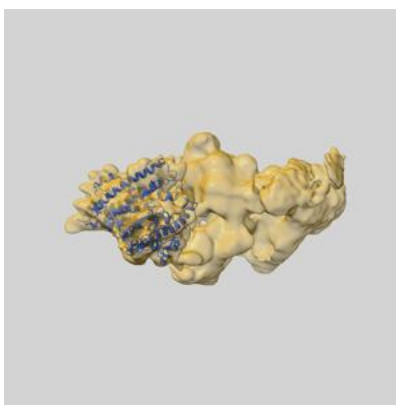
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22326 and PDB model 7JGG. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

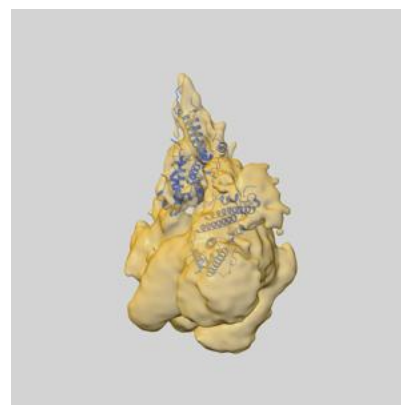
9.1 Map-model overlay [i](#)



X



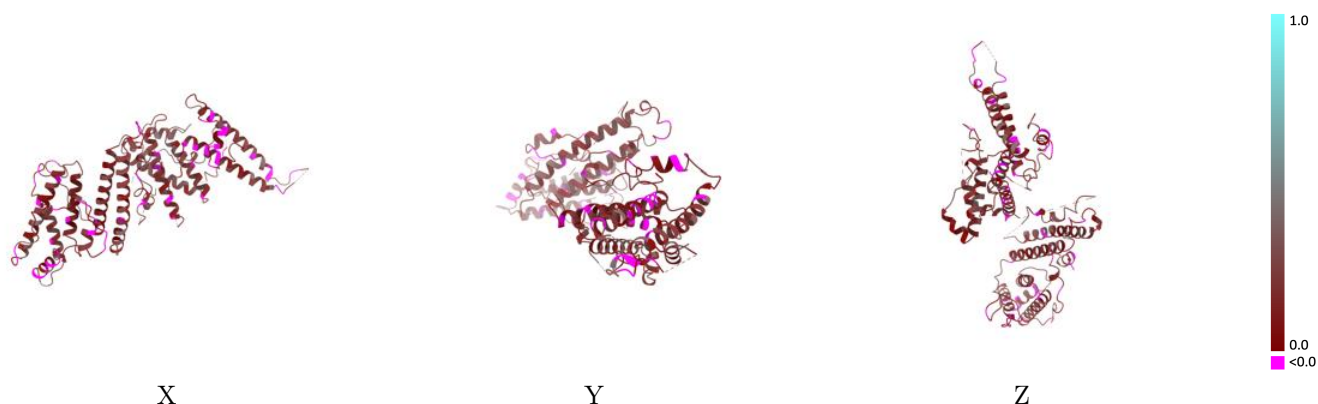
Y



Z

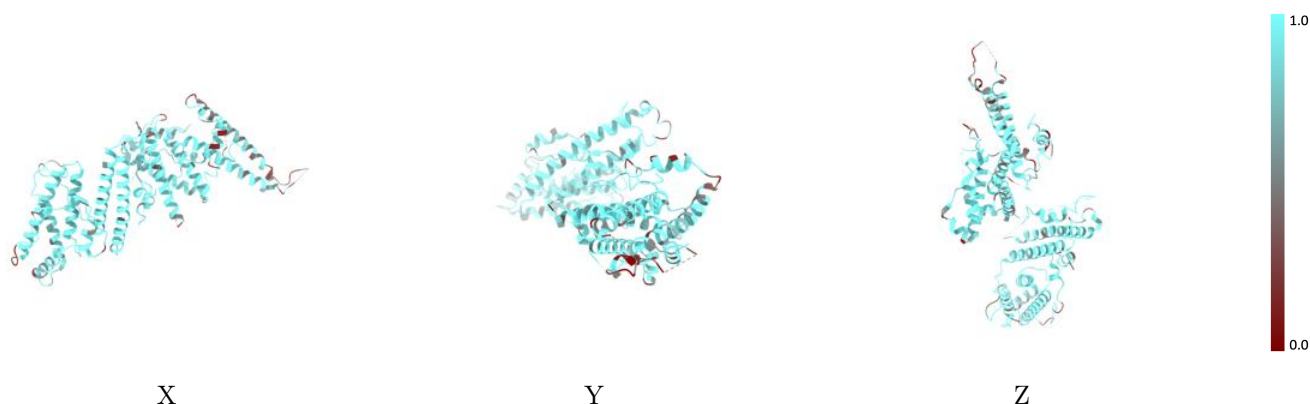
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



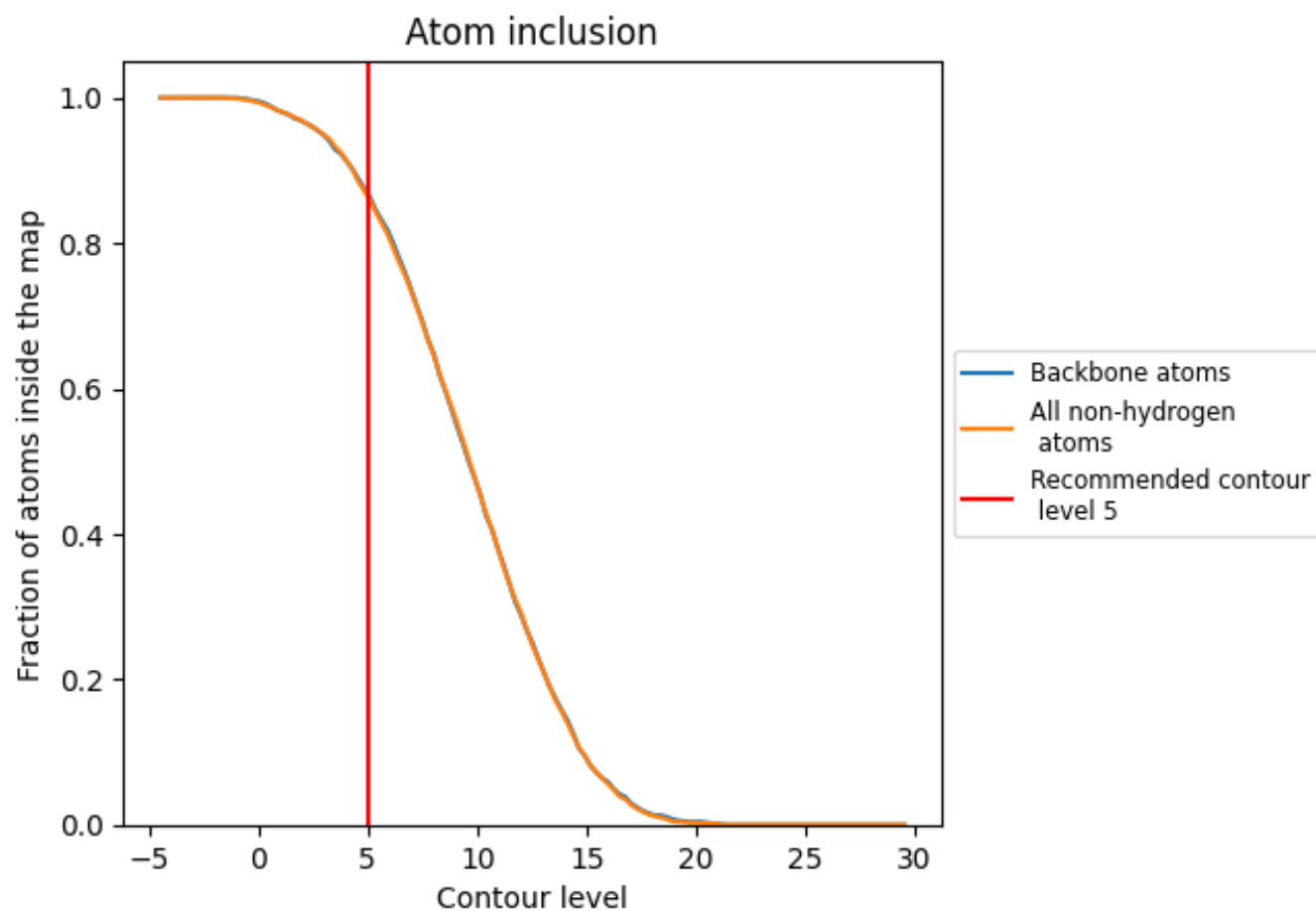
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8640	0.1540
A	0.8660	0.1540

