



## Full wwPDB EM Validation Report ⓘ

Aug 5, 2025 – 01:29 pm BST

PDB ID : 9GD7 / pdb\_00009gd7  
EMDB ID : EMD-51249  
Title : DNA-PK Ku80 mediated dimer bound to DNA polymerase Lambda and DNA ligase 4/XRCC4  
Authors : Chaplin, A.K.; Amin, H.; Zahid, S.; Hardwick, S.W.  
Deposited on : 2024-08-05  
Resolution : 4.25 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.dev126  
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) : 2.45.1

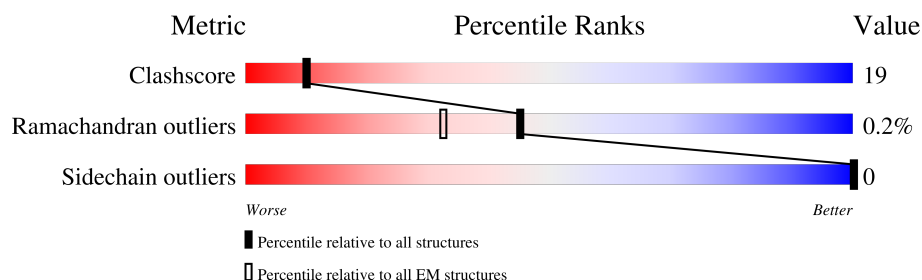
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.25 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	E	911	
2	L	732	
3	M	204	
4	P	336	
4	Q	336	
5	S	4128	
6	T	609	
7	i	25	

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Mol	Chain	Length	Quality of chain
8	j	25	<div><div></div><div>20%</div><div></div><div>80%</div></div>
9	A	575	<div><div></div><div>10%</div><div></div><div>7%</div><div></div><div>83%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 41717 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 DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	246	Total	C	N	O	S	0	0
			1956	1240	332	371	13		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	641	Total	C	N	O	S	0	0
			5084	3250	859	950	25		

- Molecule 3 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	23	Total	C	N	O	S	0	0
			160	102	27	30	1		

- Molecule 4 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	57	Total	C	N	O	S	0	0
			480	303	90	86	1		
4	Q	57	Total	C	N	O	S	0	0
			475	301	89	84	1		

- Molecule 5 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	3535	Total	C	N	O	S	0	0
			27773	17865	4705	5020	183		

- Molecule 6 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	501	Total 4001	C 2561	N 679	O 743	S 18	0	0

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	25	Total 510	C 247	N 92	O 146	P 25	0	0

- Molecule 8 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	25	Total 514	C 250	N 86	O 154	P 24	0	0

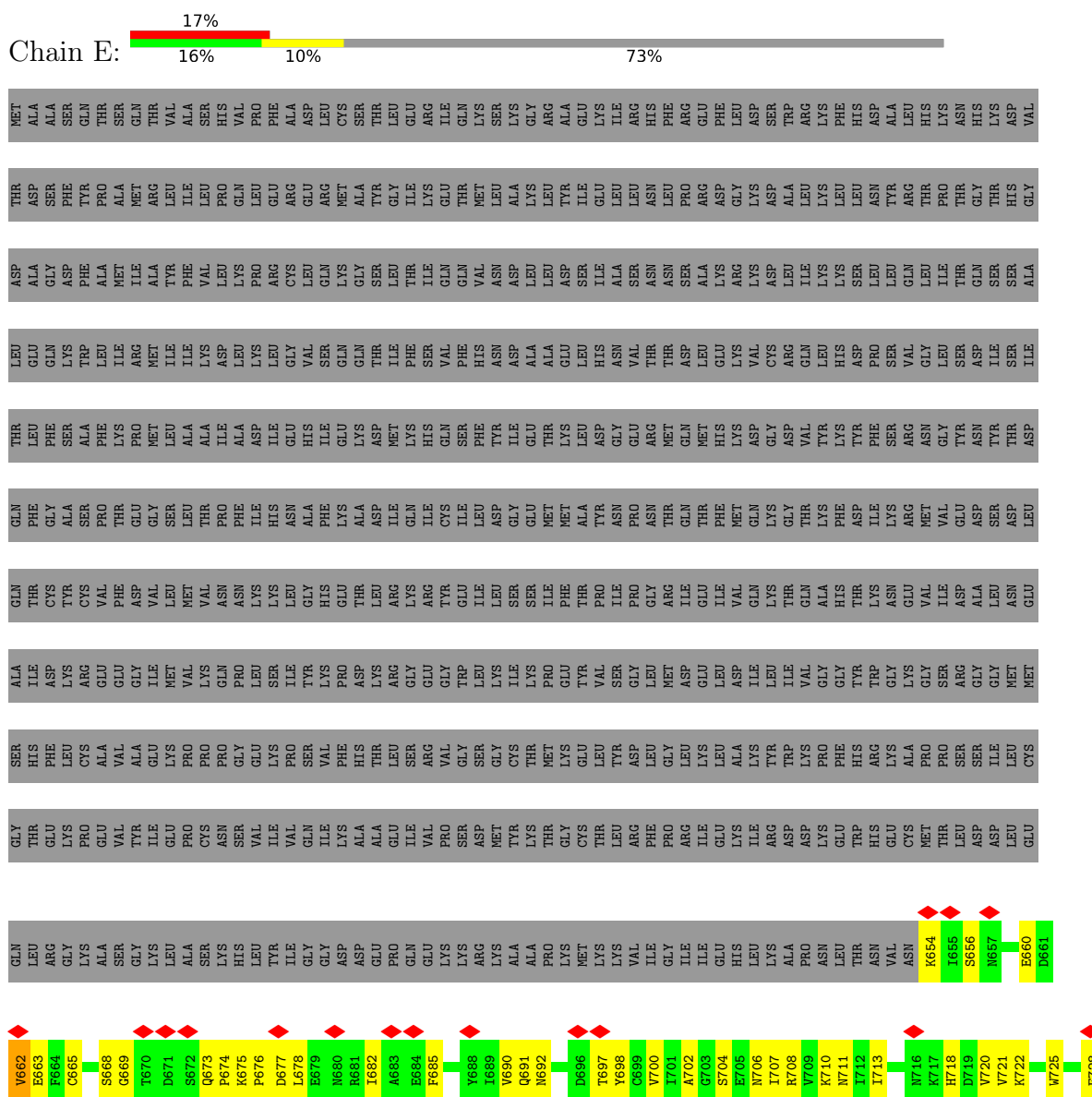
- Molecule 9 is a protein called DNA polymerase lambda.

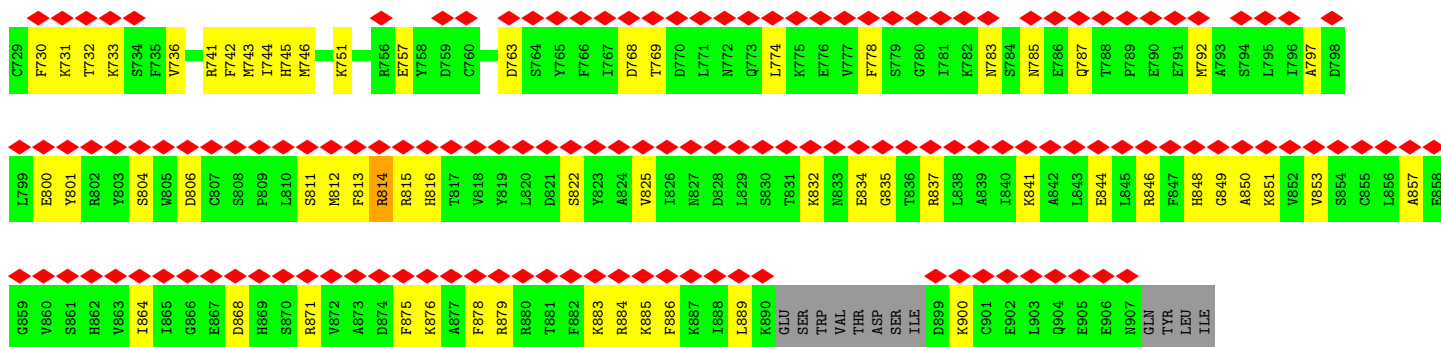
Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	98	Total 764	C 487	N 142	O 132	S 3	0	0

### 3 Residue-property plots

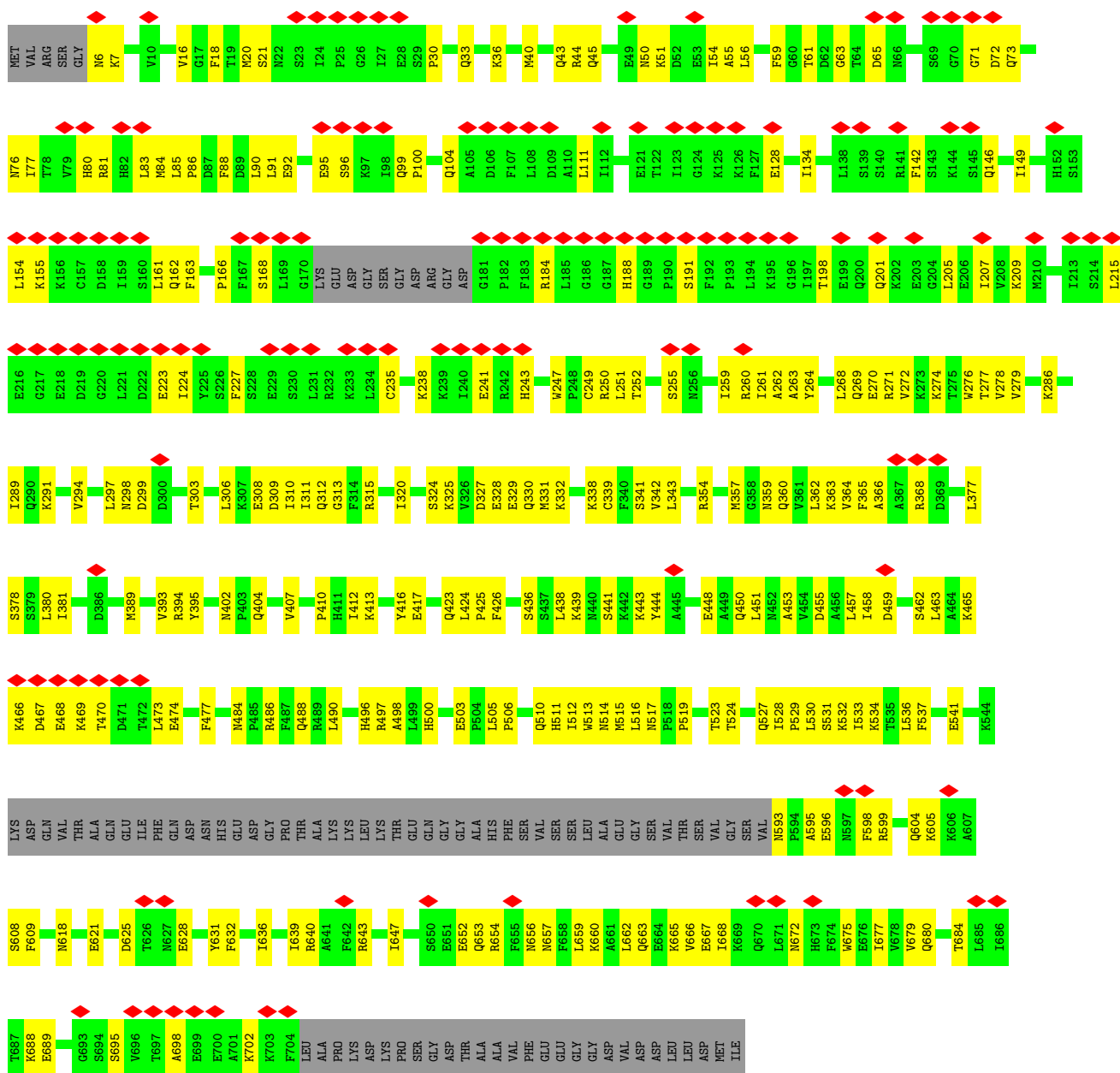
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA ligase 4



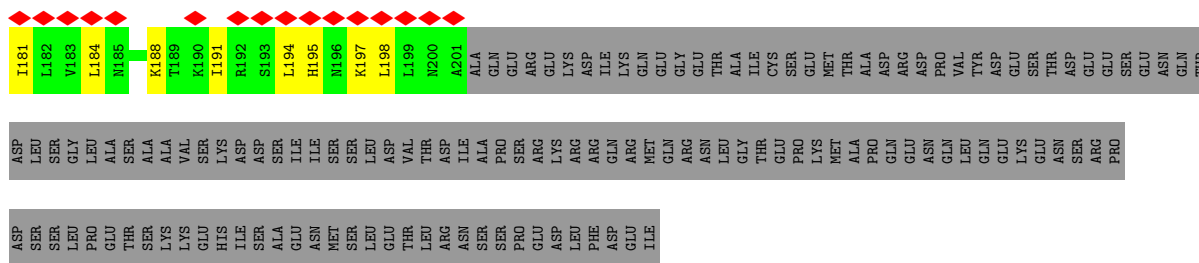


• Molecule 2: X-ray repair cross-complementing protein 5

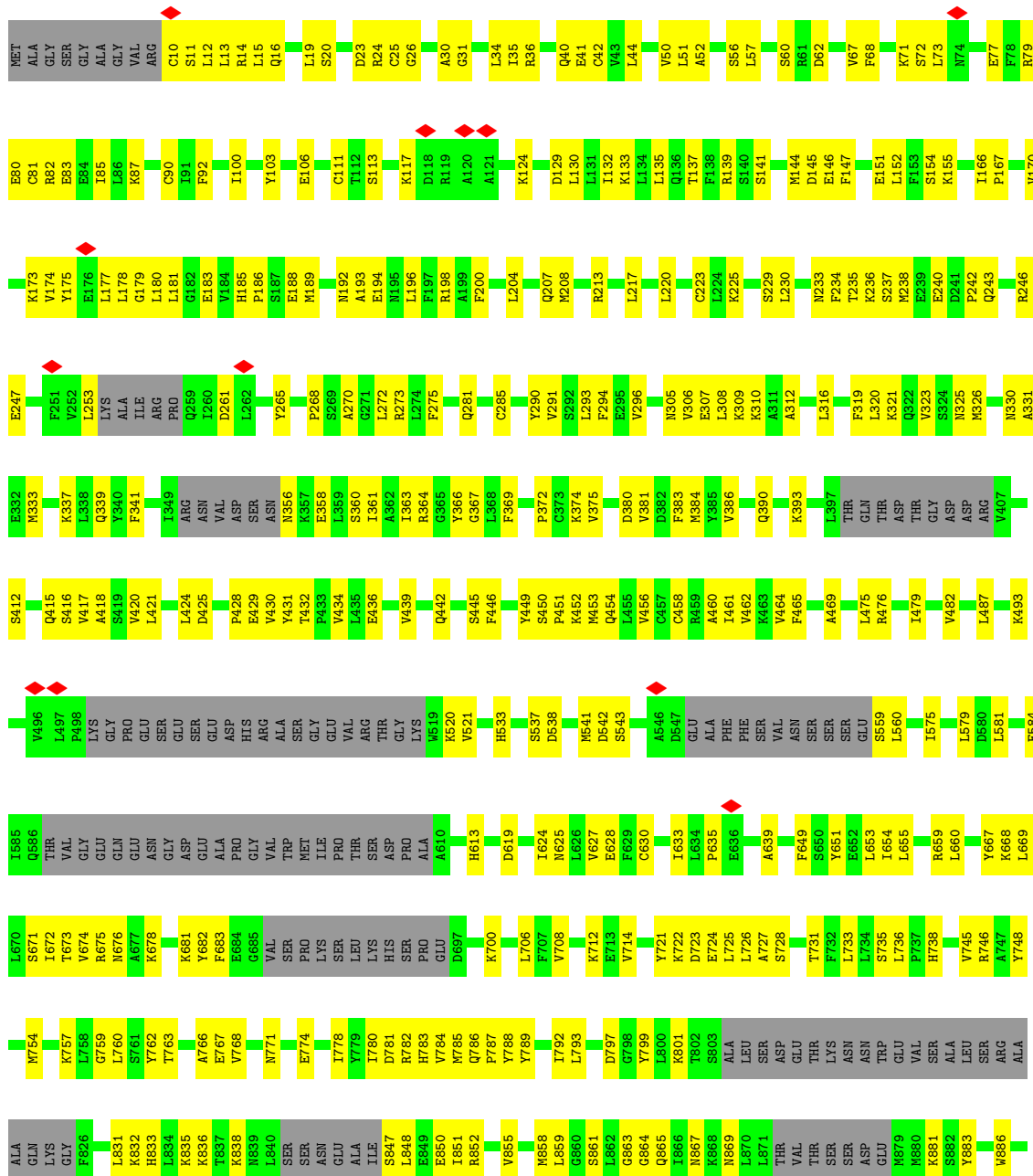








• Molecule 5: DNA-dependent protein kinase catalytic subunit





N3177	I3103	E3007	V2923	T2853	R2722	Q2495	V2405	K2313	V2210	ASP	G2048
I3178	Q3104	V3008	V2924	Q2834	T2723	E2497	E2406	Y2316	L2211	SER	V2049
N3179	N3105	L3011	E2925	R2835	D2724	F2498	G2407	A2317	R2214	VAL	Q2050
D3181	Q3106	E3012	Y2929	L2837	L2725	K2500	N2408	A2318		PRO	R2120
I3182	I3107	Y3013	Y2930	L2837	L2726	V2505	E2410		N2217	D2121	
N3185	F3110	T3016	E2935	F2840	R2727	L2506	L2411	E2321	F2218	W2125	
F3189	Y3114	E3022	Y2936	N2841	L2728	L2507	Y2412	V2322	L2219		
I3193	D3118	ASN	D2937	L2844	Q2751	Q2507	Q2414		K2221	L2129	
I3196	Q3119	PRO	V2938	F2848	R2750	Q2509	S2417	I2326	F2232	K2132	
L3197	L3120	PRO	R2940	F2851	K2752	L2510	K2418	L2327	V2230	L2133	
		ASP	Q2941	P2852	R2753	D2512		R2328	F2231	Q2134	
		LEU		P2852	K2755	N2514	V2421	Y2329	R2232		
		ASN	S2945	P2853		L2517	R2425	V2330	R2233	L2140	
		K3029	K2950	C2857	R2773	Q2518	R2425	M2331	R2232	R2143	
		E3033	Q2951	L2869	R2776		D2428	R2333	R2232	V2150	
		P3034	T2952	S2870	H2777	I2521	D2429	R2333	R2233	E2155	
		Q3037	Q2954	L2871	Q2778	R2522	E2430	K2334	W2234	E2154	
		Y3040	L2957	D2872	D2779	L2539	E2431	N2335	L2235	ARG	
		L3041	L2958	A2874	I2783	L2540	Q2432	I2336	E2236	ARG	
		M3044	E2960	A2875	Q2784	A2541	W2434	L2337	C2244	GLU	
		S3047	Y2965	C2880	I2785	L2542		E2338		GLN	
		K3048	E2968	Q2886	S2788	N2543	T2438	A2346	P2252	ARG	
		K3050	L2969	T2890	I2791	S2544	K2441	L2349	Y2253	ASP	
		L3051	K2970	R2891	T2792	L2545	W2442	Q2353	L2255	PRO	
		S3060	D2973	E2895	Q2795	Y2546		D2358	L2256	THR	
		L3061	E2974	A2896	V2797	S2547	W2449	K2359	F2260	VAL	
		F3064	N2977	R2899	L2798	P2548		F2360	S2261	LEU	
		K3067	K2978	L2900	R2800	P2549	E2460	L2364	G2262	N2176	
		A3068	Q2979	L2901	D2801	I2550		N2365	K2263	ASN	
		K3069	D2980	PRO	L2803	F2554	T2467	K2366	D2269	GLY	
		H3070	P2986	ALA	L2804	L2563	C2469	V2367	N2270	GLU	
		Q3074	T2987	GLU	A2805	M2565	R2470	T2368	S2271	LEU	
		A3076	E2988	LEU	Q2806	S2569	C2469	K2369		ASN	
		I3077	A2989	PRO	L2808	P2570	E2471	F2371	T2274		
		L3078	E2990	ALA		D2571	Q2472	P2372	Y2288		
		E3085	K2991	LYS		P2575	N2473	P2373			
		L3086	V2994	ARG	I2816	L2581	I2476	L2374	C2292		
		E3086	E2995	VAL	N2820	S2582		A2375	Q2293		
		L3086	L2996	GLY	F2823	E2583	D2486	D2376	I2294		
		Y3090	L2999	LYS	F2824	C2584	PRO	R2377	Q2295		
		D3095	D3000	ARG	T2825	E2585	GLU	L2386	S2297		
		K3172	C3001	P2917	L2826	F2586	SER	P2387	E2298		
		V3096	H3004	L2916	S2827	Q2587	GLU	K2388	Y2299		
		D3097	I3005	P2918	E2828	E2588	D2492	L2393	F2300		
		I3243	A3006	D2919	K2829	F2597	I2493		W2306		
		N3176		R2922	I2832	S2599	S2495	C2402	V2205		
								L2403	D2208		
								R2404	E2209		





[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14964	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 ( $e^-/\text{\AA}^2$ )	51.96	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.696	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.211	Depositor
Map size (Å)	417.28, 417.28, 417.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	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	E	0.14	0/1997	0.40	0/2695
2	L	0.14	0/5182	0.36	0/6990
3	M	0.17	0/164	0.44	0/220
4	P	0.11	0/485	0.34	0/647
4	Q	0.13	0/480	0.35	0/640
5	S	0.19	0/28315	0.48	0/38300
6	T	0.17	0/4079	0.41	0/5499
7	i	0.28	0/572	0.50	0/879
8	j	0.32	0/575	0.58	0/888
9	A	0.16	0/780	0.44	0/1057
All	All	0.18	0/42629	0.46	0/57815

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	E	1956	0	1905	76	0
2	L	5084	0	5080	206	0
3	M	160	0	148	6	0
4	P	480	0	501	27	0
4	Q	475	0	492	25	0
5	S	27773	0	27732	1057	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	4001	0	4050	188	0
7	i	510	0	285	18	0
8	j	514	0	290	20	0
9	A	764	0	785	35	0
All	All	41717	0	41268	1564	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 19.

All (1564) 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)
5:S:2806:LYS:HG3	5:S:2857:CYS:HB3	1.59	0.84
1:E:757:GLU:HB3	1:E:763:ASP:H	1.42	0.83
5:S:835:LYS:HA	5:S:838:LYS:HG2	1.62	0.81
5:S:1300:SER:HA	5:S:1304:HIS:HB2	1.65	0.79
5:S:1820:VAL:HA	5:S:1824:LEU:HD23	1.64	0.79
5:S:3913:ILE:HG21	5:S:3984:MET:HG2	1.64	0.78
5:S:111:CYS:HB2	5:S:130:LEU:HD11	1.64	0.77
5:S:2844:LEU:HD22	5:S:2875:ALA:HB1	1.66	0.77
5:S:3472:ILE:HD13	5:S:3479:THR:HB	1.67	0.76
5:S:3988:LEU:HD23	5:S:4100:GLU:HA	1.68	0.75
5:S:1307:ILE:HG13	5:S:1309:ALA:H	1.50	0.74
5:S:2256:ILE:HA	5:S:2259:LYS:HG2	1.68	0.74
5:S:3974:MET:HE2	5:S:3980:MET:HE1	1.69	0.73
5:S:667:TYR:HB2	5:S:728:SER:HB2	1.69	0.73
2:L:380:LEU:HD23	6:T:462:MET:HG3	1.71	0.73
5:S:931:CYS:HG	5:S:984:TYR:HH	1.35	0.72
2:L:628:GLU:HB2	2:L:631:TYR:HB3	1.72	0.72
5:S:487:LEU:HD11	5:S:575:ILE:HD13	1.71	0.72
6:T:273:ILE:HD11	6:T:366:LEU:HB3	1.71	0.72
5:S:913:ARG:HH11	5:S:2804:ILE:HG23	1.55	0.72
5:S:1536:ALA:O	5:S:1555:HIS:ND1	2.23	0.72
5:S:2217:ASN:HA	5:S:2220:MET:HE2	1.72	0.72
5:S:1235:ILE:HG13	5:S:1292:LYS:HE2	1.73	0.71
9:A:87:GLU:HA	9:A:111:LYS:HG2	1.73	0.71
5:S:2563:LEU:HD23	5:S:2795:GLN:HB3	1.70	0.71
1:E:663:GLU:HB3	1:E:697:THR:HA	1.72	0.70
5:S:2507:ILE:HA	5:S:2510:LEU:HD23	1.73	0.70
5:S:3064:PHE:HA	5:S:3067:LYS:HE3	1.72	0.70
2:L:462:SER:HA	6:T:350:PHE:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:656:ASN:HB3	2:L:688:LYS:HE3	1.72	0.70
5:S:738:HIS:HB2	5:S:780:ILE:HD11	1.73	0.70
5:S:1198:LEU:O	5:S:1202:ARG:NH2	2.24	0.70
5:S:25:CYS:SG	5:S:26:GLY:N	2.64	0.69
7:i:41:DT:H2''	7:i:42:DA:C8	2.27	0.69
5:S:1070:PRO:O	5:S:1075:ARG:NH2	2.26	0.69
5:S:1828:LEU:HD11	5:S:1880:MET:HB3	1.74	0.69
5:S:2965:TYR:HB3	5:S:3001:CYS:HB2	1.75	0.69
5:S:79:ARG:HA	5:S:82:ARG:HD2	1.74	0.69
5:S:1226:GLY:HA2	5:S:1259:LEU:HG	1.74	0.69
5:S:2405:VAL:HA	5:S:2441:LYS:HE3	1.73	0.69
5:S:3160:LEU:O	5:S:3167:ARG:NH2	2.26	0.69
6:T:351:LYS:HD2	6:T:355:LEU:HD13	1.75	0.69
5:S:2753:ARG:NH2	8:j:14:DT:O4	2.26	0.68
3:M:195:PRO:HG3	6:T:244:ARG:HE	1.58	0.68
1:E:813:PHE:H	1:E:848:HIS:HB2	1.58	0.68
6:T:458:GLN:HE21	6:T:528:LEU:HB3	1.59	0.68
5:S:917:LEU:O	5:S:927:LYS:NZ	2.26	0.68
2:L:497:ARG:NH2	2:L:503:GLU:O	2.26	0.67
5:S:3444:ALA:HB1	5:S:3482:LEU:HD12	1.76	0.67
5:S:2795:GLN:O	5:S:2799:GLN:NE2	2.27	0.67
5:S:170:VAL:O	5:S:173:LYS:NZ	2.28	0.67
5:S:2750:GLU:HA	5:S:2753:ARG:HD2	1.77	0.67
5:S:3161:LEU:HA	5:S:3167:ARG:HH12	1.58	0.67
5:S:757:LYS:HA	5:S:760:LEU:HD12	1.75	0.67
5:S:1934:LEU:HD13	5:S:1937:ARG:HH12	1.60	0.67
5:S:3130:GLN:NE2	5:S:3174:ASP:OD1	2.28	0.67
5:S:4039:TYR:HD2	5:S:4042:GLN:HG2	1.60	0.67
5:S:1178:ARG:NH2	5:S:1183:CYS:SG	2.63	0.67
5:S:1097:GLU:HG3	5:S:1149:LYS:HE2	1.77	0.67
5:S:1471:GLN:NE2	5:S:1475:LEU:O	2.28	0.67
5:S:722:LYS:NZ	5:S:1027:ASP:OD2	2.27	0.66
7:i:41:DT:H3	8:j:17:DT:H3	1.43	0.66
5:S:4082:ARG:NH2	5:S:4092:GLN:OE1	2.28	0.66
1:E:846:ARG:HB3	4:Q:166:VAL:HG11	1.78	0.66
6:T:482:VAL:HG12	6:T:486:HIS:HE1	1.61	0.66
1:E:673:GLN:HG3	1:E:678:LEU:HD21	1.78	0.66
1:E:692:ASN:ND2	6:T:290:ARG:O	2.25	0.66
5:S:1156:GLY:HA3	5:S:1171:TRP:HE1	1.59	0.66
2:L:20:MET:HB2	2:L:30:PRO:HB2	1.78	0.66
5:S:412:SER:O	5:S:415:GLN:NE2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:449:TYR:O	5:S:454:GLN:NE2	2.29	0.65
5:S:3274:VAL:HG13	5:S:3278:GLN:HE22	1.60	0.65
5:S:2328:ARG:HH21	5:S:2371:PHE:HA	1.60	0.65
2:L:249:CYS:SG	2:L:250:ARG:N	2.70	0.65
5:S:995:PHE:HD1	5:S:1000:LYS:HZ1	1.43	0.65
6:T:170:THR:HG22	6:T:172:GLU:H	1.61	0.65
5:S:2220:MET:HE1	5:S:2252:PRO:HG3	1.77	0.65
5:S:3885:ARG:HB3	5:S:3889:ARG:HH21	1.60	0.65
2:L:310:ILE:HD11	6:T:287:LYS:HD3	1.78	0.65
5:S:3884:LYS:NZ	5:S:3969:ASN:OD1	2.29	0.65
5:S:3239:LYS:NZ	5:S:3261:GLU:OE2	2.29	0.65
2:L:85:LEU:HD12	2:L:86:PRO:HD2	1.77	0.65
4:Q:166:VAL:HA	4:Q:169:LYS:HD2	1.77	0.65
5:S:1871:MET:HE1	5:S:1940:TYR:HA	1.78	0.65
5:S:992:ILE:HG23	5:S:1036:PHE:HD1	1.62	0.65
5:S:3006:ALA:O	5:S:3050:LYS:NZ	2.30	0.65
6:T:441:ASP:O	6:T:444:ARG:NH2	2.29	0.65
5:S:23:ASP:OD1	5:S:24:ARG:NH1	2.27	0.65
5:S:584:GLU:N	5:S:613:HIS:O	2.29	0.65
5:S:1504:ASP:H	5:S:1507:CYS:HB2	1.61	0.65
5:S:2349:LEU:O	5:S:2353:GLN:HB3	1.97	0.65
5:S:3730:ALA:HA	5:S:3734:ARG:HA	1.78	0.65
5:S:1783:ARG:NH1	5:S:1826:THR:O	2.29	0.64
5:S:2260:PHE:O	5:S:2306:ASN:ND2	2.29	0.64
6:T:485:GLN:O	6:T:489:ASN:ND2	2.30	0.64
5:S:1231:GLN:NE2	5:S:1287:GLN:OE1	2.30	0.64
5:S:1946:ASN:HA	5:S:1949:ILE:HD12	1.79	0.64
1:E:690:VAL:HG23	6:T:291:GLU:HG2	1.78	0.64
5:S:225:LYS:HZ1	5:S:273:ARG:HE	1.45	0.64
9:A:48:VAL:HA	9:A:84:VAL:HB	1.78	0.64
3:M:183:GLU:HA	3:M:191:LYS:HA	1.78	0.64
5:S:1178:ARG:H	5:S:1184:ARG:HD3	1.62	0.64
5:S:2327:LEU:O	5:S:2333:ARG:NH2	2.30	0.64
6:T:91:GLU:H	6:T:136:GLY:HA3	1.62	0.64
5:S:306:VAL:HA	5:S:309:LYS:HE2	1.79	0.64
2:L:466:LYS:NZ	2:L:470:THR:O	2.31	0.64
5:S:4055:ASN:HD22	5:S:4058:VAL:HG23	1.63	0.63
5:S:380:ASP:HB3	5:S:384:MET:HE1	1.78	0.63
5:S:2188:GLU:OE2	5:S:2729:ARG:NH2	2.31	0.63
5:S:913:ARG:NH1	5:S:2804:ILE:HG23	2.13	0.63
5:S:1630:ASP:HB3	5:S:1633:TRP:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1171:TRP:O	5:S:1175:HIS:ND1	2.31	0.63
5:S:2449:VAL:HA	5:S:2452:ARG:HE	1.63	0.63
5:S:2837:LEU:O	5:S:2841:ASN:ND2	2.31	0.63
5:S:3657:SER:N	5:S:3660:ASN:OD1	2.31	0.63
5:S:3741:ARG:HH11	5:S:3747:GLU:HB2	1.64	0.63
5:S:253:LEU:HD21	5:S:268:PRO:HA	1.80	0.63
9:A:45:ARG:HH21	9:A:70:GLY:HA2	1.63	0.63
5:S:13:LEU:HD21	5:S:3069:MET:HB3	1.81	0.63
5:S:767:GLU:O	5:S:771:ASN:ND2	2.32	0.63
5:S:3859:TYR:O	5:S:4119:ARG:NH2	2.32	0.63
5:S:3244:ASP:OD1	5:S:3247:ARG:NH2	2.31	0.63
6:T:81:ASP:O	6:T:110:ASN:ND2	2.31	0.63
2:L:465:LYS:H	2:L:474:GLU:HG2	1.63	0.63
6:T:396:ALA:HB3	6:T:413:LEU:HB2	1.81	0.63
2:L:271:ARG:HE	2:L:272:VAL:H	1.46	0.63
5:S:907:LEU:HD13	5:S:937:MET:HG2	1.81	0.63
6:T:287:LYS:NZ	6:T:296:VAL:O	2.30	0.63
5:S:1707:LEU:O	5:S:1711:ARG:NH1	2.32	0.62
5:S:2233:HIS:NE2	5:S:2727:ARG:O	2.30	0.62
5:S:2328:ARG:O	5:S:2333:ARG:NE	2.32	0.62
1:E:654:LYS:N	1:E:660:GLU:OE2	2.33	0.62
5:S:958:MET:O	5:S:962:TYR:N	2.29	0.62
5:S:1227:GLY:O	5:S:1292:LYS:NZ	2.32	0.62
6:T:65:GLN:HB3	6:T:123:LYS:HD3	1.81	0.62
1:E:783:ASN:HA	4:Q:179:ARG:HH21	1.64	0.62
3:M:193:LYS:O	6:T:244:ARG:NH2	2.32	0.62
5:S:3997:LEU:O	5:S:4000:ASN:ND2	2.32	0.62
6:T:164:LYS:HG3	6:T:198:ILE:HA	1.81	0.62
9:A:96:ARG:O	9:A:99:ARG:NH1	2.32	0.62
4:P:176:LEU:HD11	4:Q:173:GLU:HG3	1.80	0.62
9:A:114:TRP:NE1	9:A:125:VAL:O	2.33	0.62
6:T:363:ARG:NH1	8:j:28:DA:OP1	2.33	0.62
5:S:10:CYS:SG	5:S:11:SER:N	2.72	0.62
5:S:1031:ARG:HH22	5:S:1034:ARG:HH11	1.47	0.62
5:S:193:ALA:HA	5:S:196:LEU:HD12	1.81	0.62
5:S:797:ASP:O	5:S:801:LYS:NZ	2.32	0.62
6:T:168:LEU:HD11	6:T:202:LEU:HG	1.81	0.62
2:L:44:ARG:HH12	2:L:488:GLN:HA	1.63	0.62
5:S:2218:PHE:HA	5:S:2221:LYS:HE3	1.82	0.62
5:S:2725:LEU:HD13	5:S:2728:LEU:HD21	1.82	0.62
2:L:146:GLN:HG3	2:L:149:ILE:HD12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3278:GLN:NE2	5:S:3326:GLN:HE21	1.97	0.61
2:L:377:LEU:HD23	2:L:380:LEU:HD12	1.81	0.61
5:S:217:LEU:HA	5:S:220:LEU:HD13	1.82	0.61
5:S:1360:LYS:HZ3	5:S:1363:LEU:HB3	1.64	0.61
5:S:174:VAL:HA	5:S:177:LEU:HB2	1.83	0.61
6:T:94:LYS:H	6:T:103:TYR:HA	1.64	0.61
6:T:167:MET:HE2	6:T:203:MET:HB2	1.82	0.61
5:S:67:VAL:HA	5:S:71:LYS:HD3	1.83	0.61
5:S:799:TYR:O	5:S:852:ARG:NH1	2.32	0.61
5:S:890:LYS:HD2	5:S:906:PHE:HB3	1.82	0.61
5:S:3962:ARG:NH1	5:S:4124:TRP:O	2.33	0.61
1:E:778:PHE:O	4:Q:179:ARG:NH1	2.33	0.61
5:S:2094:MET:HB2	5:S:2097:LEU:HD12	1.83	0.61
5:S:2896:ALA:HB1	5:S:2922:ARG:HH21	1.66	0.61
5:S:3974:MET:HG3	5:S:3976:GLU:H	1.66	0.61
5:S:3880:ALA:O	5:S:3885:ARG:NH2	2.34	0.61
5:S:2473:MET:HA	5:S:2476:ILE:HD12	1.82	0.61
9:A:50:ARG:NH1	9:A:53:ILE:O	2.34	0.61
1:E:697:THR:O	1:E:718:HIS:NE2	2.31	0.60
2:L:184:ARG:NH1	2:L:514:ASN:O	2.34	0.60
5:S:2587:GLN:O	5:S:2777:HIS:N	2.28	0.60
5:S:3728:VAL:HA	5:S:3736:LYS:HG3	1.82	0.60
5:S:4046:TYR:HA	5:S:4049:ARG:HH11	1.65	0.60
5:S:867:ASN:HB2	5:S:3129:LEU:HD21	1.83	0.60
6:T:488:ARG:HE	6:T:501:GLU:HG3	1.66	0.60
2:L:269:GLN:NE2	2:L:359:ASN:O	2.26	0.60
5:S:1326:GLU:O	5:S:1329:ARG:NH1	2.33	0.60
5:S:2588:GLU:HA	5:S:2776:ARG:HA	1.81	0.60
5:S:3154:GLN:O	5:S:3159:ARG:NH2	2.35	0.60
5:S:3789:ARG:HH12	5:S:3938:ILE:HB	1.67	0.60
6:T:482:VAL:O	6:T:486:HIS:ND1	2.35	0.60
5:S:984:TYR:HA	5:S:987:LEU:HD12	1.84	0.60
5:S:2547:SER:H	5:S:2554:PHE:HE2	1.48	0.60
5:S:3686:TRP:HB2	5:S:3696:ARG:HH22	1.67	0.60
5:S:3924:HIS:N	5:S:3927:ASN:OD1	2.35	0.60
2:L:541:GLU:HG3	6:T:375:VAL:HG13	1.84	0.60
5:S:678:LYS:NZ	5:S:735:SER:O	2.35	0.60
5:S:1881:TYR:HB2	5:S:1950:SER:HB2	1.84	0.60
5:S:2511:ILE:HD11	5:S:2550:ILE:HG23	1.84	0.60
5:S:14:ARG:HH12	5:S:3070:HIS:HA	1.66	0.60
5:S:881:LYS:NZ	5:S:883:TYR:O	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1322:THR:O	5:S:1326:GLU:N	2.34	0.60
5:S:1621:THR:O	5:S:1625:HIS:ND1	2.33	0.60
5:S:2358:ASP:OD1	5:S:2359:LYS:N	2.35	0.60
5:S:2467:THR:HG22	5:S:2470:ARG:HH21	1.65	0.60
5:S:4094:PRO:HB3	5:S:4103:GLN:HG2	1.82	0.60
2:L:477:PHE:CZ	2:L:519:PRO:HD2	2.37	0.60
5:S:538:ASP:HA	5:S:541:MET:HG3	1.84	0.60
5:S:3772:ASN:ND2	5:S:3788:LEU:O	2.34	0.60
2:L:510:GLN:HA	2:L:513:TRP:HD1	1.67	0.60
2:L:628:GLU:O	2:L:632:PHE:N	2.30	0.60
5:S:393:LYS:HD2	5:S:434:VAL:HG11	1.83	0.60
5:S:3690:PHE:O	5:S:3696:ARG:NH1	2.35	0.60
5:S:1961:PHE:HB2	5:S:2125:TRP:CZ2	2.36	0.59
5:S:40:GLN:NE2	5:S:2425:ARG:O	2.36	0.59
6:T:213:ILE:HG13	6:T:218:ARG:HH21	1.67	0.59
2:L:659:LEU:HD23	2:L:662:LEU:HD21	1.84	0.59
5:S:895:ALA:HA	5:S:904:VAL:HA	1.85	0.59
5:S:1232:PRO:HA	5:S:1235:ILE:HD12	1.85	0.59
5:S:2134:GLY:HA2	5:S:2167:PRO:HB3	1.83	0.59
4:P:150:ARG:NH1	4:P:154:ASP:OD2	2.35	0.59
5:S:1783:ARG:HH12	5:S:1829:TRP:HB2	1.68	0.59
5:S:2388:LYS:NZ	6:T:157:VAL:O	2.35	0.59
1:E:720:VAL:HB	1:E:745:HIS:H	1.67	0.59
1:E:813:PHE:N	1:E:848:HIS:HB2	2.17	0.59
2:L:198:THR:HG23	2:L:201:GLN:HE21	1.68	0.59
5:S:1611:GLN:NE2	5:S:1614:GLN:OE1	2.36	0.59
5:S:1634:ALA:O	5:S:1642:LYS:NZ	2.34	0.59
5:S:2973:ASP:O	5:S:2977:ASN:ND2	2.34	0.59
1:E:704:SER:O	1:E:708:ARG:NH2	2.36	0.59
2:L:463:LEU:HG	6:T:350:PHE:H	1.67	0.59
6:T:363:ARG:HH22	8:j:27:DT:H5"	1.67	0.59
2:L:359:ASN:OD1	2:L:360:GLN:N	2.35	0.59
7:i:41:DT:H2"	7:i:42:DA:H8	1.68	0.59
1:E:674:PRO:HB2	1:E:676:PRO:HD2	1.85	0.59
6:T:351:LYS:O	6:T:395:ALA:N	2.35	0.59
1:E:721:VAL:HG22	1:E:743:MET:HE1	1.84	0.58
5:S:330:ASN:HB3	5:S:333:MET:HE3	1.85	0.58
5:S:859:LEU:O	5:S:867:ASN:ND2	2.36	0.58
5:S:1222:ASN:OD1	5:S:1223:THR:N	2.34	0.58
5:S:1231:GLN:O	5:S:1292:LYS:NZ	2.33	0.58
5:S:3569:GLN:HA	5:S:3572:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:268:LEU:O	6:T:444:ARG:NH1	2.36	0.58
5:S:1922:ALA:HB2	5:S:1944:ALA:HB3	1.85	0.58
6:T:203:MET:HE1	6:T:238:LYS:H	1.68	0.58
6:T:363:ARG:HB3	6:T:436:PHE:CD2	2.38	0.58
2:L:412:ILE:HA	2:L:417:GLU:HA	1.85	0.58
5:S:651:TYR:HE1	5:S:1388:ASP:HB3	1.69	0.58
5:S:1663:THR:OG1	5:S:1665:HIS:NE2	2.37	0.58
5:S:2507:ILE:HD12	5:S:2545:LEU:HB2	1.84	0.58
8:j:30:DT:H2'	8:j:31:DT:H71	1.86	0.58
2:L:647:ILE:HA	2:L:652:GLU:HB3	1.84	0.58
5:S:2880:CYS:HB3	5:S:2886:GLN:HA	1.85	0.58
5:S:3313:SER:HB3	5:S:3316:LEU:HA	1.85	0.58
6:T:357:LYS:HB2	6:T:360:HIS:CD2	2.38	0.58
1:E:682:ILE:HG13	1:E:730:PHE:HZ	1.68	0.58
1:E:728:GLU:OE1	1:E:741:ARG:NH2	2.37	0.58
5:S:1420:ARG:NH2	5:S:1466:ASN:O	2.36	0.58
5:S:3912:CYS:HA	5:S:3915:HIS:CD2	2.38	0.58
6:T:418:GLU:HB2	6:T:430:PRO:HB3	1.85	0.58
2:L:96:SER:O	2:L:99:GLN:NE2	2.37	0.58
2:L:324:SER:OG	2:L:325:LYS:N	2.36	0.58
5:S:3545:THR:OG1	5:S:3549:HIS:N	2.37	0.58
6:T:141:TYR:O	6:T:182:LYS:NZ	2.37	0.58
2:L:423:GLN:NE2	2:L:424:LEU:O	2.37	0.58
5:S:1117:ASP:OD1	5:S:1118:GLU:N	2.37	0.58
5:S:3870:SER:OG	5:S:4117:LEU:O	2.21	0.58
5:S:4012:ASP:O	5:S:4014:LYS:N	2.36	0.58
1:E:774:LEU:HD22	4:P:181:ILE:HG23	1.85	0.58
5:S:649:PHE:O	5:S:653:LEU:HG	2.04	0.58
5:S:782:ARG:HG2	5:S:786:GLN:HE22	1.68	0.58
5:S:1747:LEU:HD21	5:S:1778:PHE:HD1	1.69	0.58
5:S:1000:LYS:NZ	5:S:1005:ASP:OD1	2.37	0.58
5:S:2161:ALA:HA	5:S:2164:TRP:HB2	1.85	0.58
5:S:2269:ASP:OD1	5:S:2270:ASN:N	2.37	0.58
6:T:46:LYS:NZ	6:T:137:HIS:O	2.37	0.58
2:L:640:ARG:NH2	2:L:684:THR:OG1	2.34	0.57
5:S:891:ARG:NH1	5:S:956:PRO:O	2.36	0.57
5:S:899:ARG:NH1	5:S:2565:MET:O	2.36	0.57
5:S:3155:VAL:HG22	5:S:3158:LYS:HZ1	1.69	0.57
6:T:85:VAL:HG21	6:T:119:LEU:HD11	1.86	0.57
2:L:463:LEU:HD11	6:T:349:GLY:HA3	1.85	0.57
6:T:416:GLN:OE1	6:T:433:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2129:LEU:HD23	5:S:2132:LYS:HZ3	1.69	0.57
5:S:2257:PHE:HA	5:S:2260:PHE:CE2	2.39	0.57
5:S:4082:ARG:HG3	5:S:4089:ILE:HG22	1.85	0.57
2:L:354:ARG:HD3	6:T:433:GLN:HE21	1.70	0.57
2:L:490:LEU:HA	6:T:337:LEU:HD21	1.84	0.57
5:S:2936:TYR:HA	5:S:2939:LEU:HD13	1.86	0.57
9:A:93:ARG:HE	9:A:97:LEU:HG	1.68	0.57
2:L:277:THR:OG1	6:T:319:SER:OG	2.21	0.57
2:L:278:VAL:HG22	6:T:318:ARG:HH21	1.68	0.57
5:S:243:GLN:O	5:S:246:ARG:NH1	2.37	0.57
5:S:321:LYS:NZ	5:S:325:ASN:OD1	2.37	0.57
5:S:1182:GLU:OE2	5:S:1185:HIS:ND1	2.37	0.57
5:S:1389:VAL:HG23	5:S:1391:VAL:HG22	1.86	0.57
5:S:1490:GLY:O	5:S:1502:SER:N	2.37	0.57
5:S:1592:MET:SD	5:S:1592:MET:N	2.77	0.57
5:S:1803:GLU:OE1	5:S:1806:ARG:NH2	2.36	0.57
5:S:682:TYR:O	5:S:700:LYS:NZ	2.32	0.57
5:S:3706:ASP:OD2	5:S:3708:ARG:NH2	2.38	0.57
6:T:176:HIS:HD2	6:T:182:LYS:HD3	1.70	0.57
2:L:497:ARG:HG2	2:L:505:LEU:HD11	1.86	0.57
5:S:1082:PHE:HA	5:S:1085:ILE:HG12	1.87	0.57
5:S:2986:PRO:O	5:S:2991:LYS:NZ	2.38	0.57
6:T:318:ARG:N	6:T:329:LEU:O	2.38	0.57
5:S:2832:ILE:HA	5:S:2835:LYS:HD2	1.85	0.57
1:E:785:ASN:HA	1:E:792:MET:HE1	1.87	0.57
2:L:81:ARG:NH2	2:L:85:LEU:O	2.38	0.57
4:Q:151:LEU:HA	4:Q:154:ASP:HB2	1.87	0.57
5:S:926:THR:HG22	5:S:2800:ARG:HB3	1.87	0.57
5:S:1623:LEU:HD12	5:S:1624:GLN:HG3	1.87	0.57
5:S:3118:ASP:OD1	5:S:3119:VAL:N	2.38	0.57
5:S:3668:LEU:O	5:S:3672:LYS:NZ	2.35	0.57
5:S:3675:LYS:NZ	5:S:3676:PRO:O	2.37	0.57
5:S:579:LEU:HD11	5:S:619:ASP:HB3	1.87	0.57
5:S:1019:ASP:O	5:S:1026:ARG:NH2	2.31	0.57
8:j:29:DG:H2''	8:j:30:DT:H5''	1.87	0.57
2:L:44:ARG:HH22	2:L:488:GLN:HB2	1.71	0.56
5:S:913:ARG:CZ	5:S:2803:ILE:HB	2.35	0.56
6:T:502:GLN:NE2	6:T:503:ALA:O	2.38	0.56
8:j:18:DA:H2''	8:j:19:DA:C8	2.40	0.56
1:E:814:ARG:N	1:E:850:ALA:H	2.04	0.56
2:L:270:GLU:OE1	6:T:444:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1182:GLU:HG3	5:S:1186:LYS:HZ3	1.70	0.56
5:S:1611:GLN:OE1	5:S:1613:HIS:ND1	2.38	0.56
5:S:2510:LEU:HA	5:S:2521:ILE:HD12	1.87	0.56
5:S:2954:GLN:HE21	5:S:2958:LEU:HD23	1.69	0.56
5:S:3965:ARG:O	5:S:3969:ASN:ND2	2.38	0.56
8:j:23:DT:H2'	8:j:24:DT:H71	1.86	0.56
2:L:643:ARG:HH11	2:L:659:LEU:HD12	1.70	0.56
4:Q:191:ILE:O	4:Q:195:HIS:ND1	2.29	0.56
5:S:20:SER:O	5:S:24:ARG:NH1	2.38	0.56
5:S:2470:ARG:NH1	5:S:2512:ASP:OD1	2.39	0.56
5:S:3830:SER:O	5:S:3833:ARG:NH1	2.38	0.56
6:T:203:MET:HE2	6:T:239:LEU:HD23	1.88	0.56
6:T:352:PRO:HA	6:T:394:VAL:HA	1.88	0.56
2:L:81:ARG:HD3	2:L:90:LEU:HD11	1.87	0.56
5:S:998:ASN:HA	5:S:1001:PHE:HB2	1.88	0.56
8:j:16:DA:H2''	8:j:17:DT:C5	2.40	0.56
5:S:229:SER:O	5:S:233:ASN:ND2	2.38	0.56
5:S:1864:ASP:HA	5:S:1867:ILE:HD12	1.87	0.56
5:S:3667:LEU:HD12	5:S:3670:MET:HG2	1.88	0.56
5:S:3707:GLY:HA3	5:S:3712:LEU:HD21	1.86	0.56
5:S:520:LYS:NZ	5:S:521:VAL:O	2.39	0.56
5:S:1251:GLN:HA	5:S:1254:LEU:HD12	1.87	0.56
5:S:2197:THR:HG23	5:S:2244:CYS:HB2	1.86	0.56
5:S:3064:PHE:HD1	5:S:3067:LYS:HZ1	1.54	0.56
5:S:4012:ASP:O	5:S:4013:TRP:C	2.49	0.56
6:T:482:VAL:HG12	6:T:486:HIS:CE1	2.40	0.56
5:S:669:LEU:O	5:S:673:THR:HG23	2.06	0.56
5:S:893:SER:H	5:S:944:LYS:HZ1	1.54	0.56
5:S:2987:THR:HG23	5:S:2990:GLU:H	1.70	0.56
5:S:913:ARG:NH1	5:S:2801:ASP:OD2	2.39	0.56
5:S:2788:SER:HA	5:S:2791:ILE:HG12	1.88	0.56
5:S:2945:SER:HB2	5:S:3975:LYS:HD3	1.87	0.56
5:S:3814:ASP:O	5:S:3818:ASN:ND2	2.39	0.56
5:S:1071:ASN:HD22	5:S:1074:LYS:HG3	1.71	0.56
1:E:871:ARG:O	1:E:875:PHE:N	2.35	0.56
2:L:33:GLN:HA	2:L:36:LYS:HE2	1.88	0.56
5:S:246:ARG:NH2	5:S:281:GLN:O	2.39	0.56
5:S:1379:PRO:HB3	5:S:1385:ASN:HB3	1.88	0.56
5:S:1589:ASN:HB3	5:S:1592:MET:SD	2.46	0.56
5:S:1651:LYS:NZ	5:S:2045:PHE:O	2.39	0.56
2:L:466:LYS:NZ	2:L:467:ASP:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:593:ASN:HB2	5:S:1723:PRO:HG3	1.88	0.55
3:M:196:ALA:HA	6:T:477:SER:HA	1.88	0.55
5:S:2549:LYS:HG3	5:S:2550:ILE:HG13	1.88	0.55
5:S:3261:GLU:HA	5:S:3264:LYS:HB2	1.88	0.55
2:L:484:ASN:HD21	2:L:486:ARG:HB3	1.71	0.55
2:L:595:ALA:HA	2:L:598:PHE:CE1	2.40	0.55
5:S:1611:GLN:HB2	5:S:1613:HIS:HD1	1.70	0.55
5:S:1762:MET:O	5:S:1766:LEU:HB2	2.06	0.55
5:S:1837:ARG:HH22	5:S:1884:LEU:HD22	1.70	0.55
5:S:3033:GLU:OE1	5:S:3033:GLU:N	2.29	0.55
5:S:3578:LEU:HD11	5:S:3752:VAL:HG21	1.88	0.55
5:S:3684:SER:HB3	5:S:3687:MET:HB2	1.88	0.55
2:L:459:ASP:OD1	6:T:392:LYS:NZ	2.40	0.55
5:S:307:GLU:HA	5:S:310:LYS:HG2	1.88	0.55
5:S:668:LYS:NZ	5:S:728:SER:HB3	2.21	0.55
5:S:2467:THR:HA	5:S:2470:ARG:HE	1.71	0.55
2:L:378:SER:HA	2:L:381:ILE:HD12	1.88	0.55
5:S:4125:GLU:HA	5:S:4127:TRP:CZ3	2.41	0.55
1:E:662:VAL:HG13	1:E:698:TYR:HB2	1.88	0.55
2:L:297:LEU:HB2	2:L:303:THR:HB	1.89	0.55
5:S:330:ASN:OD1	5:S:331:ALA:N	2.40	0.55
5:S:453:MET:HA	5:S:456:VAL:HB	1.89	0.55
5:S:1657:SER:O	5:S:1660:SER:OG	2.21	0.55
5:S:1734:PRO:O	5:S:1738:ASN:ND2	2.40	0.55
5:S:2254:ARG:HD3	5:S:2293:GLY:H	1.71	0.55
5:S:3097:ASP:N	5:S:3097:ASP:OD1	2.39	0.55
5:S:3829:LEU:HA	5:S:3833:ARG:HD2	1.89	0.55
5:S:2129:LEU:HA	5:S:2132:LYS:HZ3	1.71	0.55
5:S:3576:ASP:O	5:S:3629:ARG:NH1	2.39	0.55
5:S:3707:GLY:HA2	5:S:3710:LYS:HE2	1.88	0.55
5:S:3793:VAL:HG23	5:S:3803:ILE:HG13	1.89	0.55
5:S:3812:LEU:HB2	5:S:3925:LEU:HB3	1.88	0.55
6:T:64:ILE:HG22	6:T:123:LYS:HE2	1.88	0.55
5:S:316:LEU:HD13	5:S:361:ILE:HG21	1.88	0.55
5:S:3263:HIS:O	5:S:3267:LYS:NZ	2.33	0.55
6:T:35:ARG:N	6:T:160:LYS:O	2.40	0.55
5:S:129:ASP:HA	5:S:132:ILE:HG22	1.88	0.55
5:S:364:ARG:HA	5:S:415:GLN:HE22	1.72	0.55
5:S:417:VAL:HA	5:S:420:VAL:HG12	1.89	0.55
5:S:1346:THR:O	5:S:1350:ASN:ND2	2.39	0.55
5:S:2349:LEU:O	5:S:2353:GLN:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:311:ILE:O	6:T:288:LEU:N	2.35	0.55
4:P:151:LEU:HA	4:P:154:ASP:HB2	1.88	0.55
5:S:3813:LYS:HG3	5:S:3925:LEU:HB2	1.89	0.55
9:A:76:GLN:NE2	9:A:98:LEU:O	2.40	0.55
2:L:513:TRP:HA	2:L:516:LEU:HB3	1.89	0.55
5:S:72:SER:HA	5:S:117:LYS:HE2	1.88	0.55
5:S:1342:MET:HE1	5:S:1398:VAL:HG13	1.87	0.55
5:S:1640:GLU:HA	5:S:1643:MET:HE3	1.89	0.55
5:S:2410:GLU:O	5:S:2414:GLN:NE2	2.40	0.55
5:S:2940:ARG:NH1	5:S:3977:THR:O	2.40	0.55
2:L:247:TRP:HZ2	2:L:338:LYS:HB2	1.72	0.54
5:S:1608:ARG:O	5:S:1608:ARG:NE	2.41	0.54
5:S:1806:ARG:HA	5:S:1869:LYS:HZ1	1.71	0.54
5:S:3130:GLN:HB3	5:S:3178:ILE:HG12	1.89	0.54
6:T:90:THR:OG1	6:T:92:LYS:O	2.25	0.54
6:T:207:LYS:HD2	6:T:208:PRO:HD2	1.89	0.54
6:T:245:LYS:NZ	6:T:246:VAL:O	2.41	0.54
5:S:1798:LEU:HD22	5:S:1827:LEU:HD13	1.89	0.54
7:i:19:DC:O2	7:i:20:DT:N3	2.40	0.54
5:S:1233:SER:O	5:S:1237:ALA:N	2.40	0.54
5:S:1608:ARG:HD2	5:S:1612:LYS:HG3	1.89	0.54
5:S:3044:MET:O	5:S:3047:SER:OG	2.21	0.54
6:T:210:GLY:HA2	6:T:233:PHE:HA	1.88	0.54
2:L:76:ASN:ND2	2:L:104:GLN:O	2.41	0.54
5:S:68:PHE:O	5:S:72:SER:OG	2.25	0.54
5:S:1697:PRO:HG2	5:S:1752:LEU:HD23	1.90	0.54
5:S:2803:ILE:O	5:S:2806:LYS:HB3	2.07	0.54
6:T:316:THR:HB	6:T:318:ARG:HH22	1.72	0.54
2:L:251:LEU:N	2:L:259:ILE:O	2.33	0.54
2:L:531:SER:HA	2:L:534:LYS:HG2	1.89	0.54
5:S:50:VAL:HG13	5:S:51:LEU:HG	1.90	0.54
5:S:998:ASN:HB3	5:S:1044:ILE:HG23	1.89	0.54
5:S:1271:ILE:O	5:S:1274:ARG:NH1	2.38	0.54
5:S:1295:ALA:HA	5:S:1298:LEU:HD12	1.89	0.54
5:S:2919:ASP:N	5:S:2919:ASP:OD1	2.40	0.54
6:T:419:GLU:HB2	6:T:428:THR:HB	1.89	0.54
5:S:1050:GLU:HA	5:S:1055:ASN:HD22	1.73	0.54
5:S:1471:GLN:HE22	5:S:1476:HIS:HA	1.73	0.54
5:S:3177:ASN:OD1	5:S:3178:ILE:HD12	2.07	0.54
5:S:360:SER:HA	5:S:363:ILE:HD12	1.89	0.54
5:S:1952:ILE:HD12	5:S:1961:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3684:SER:O	5:S:3688:SER:OG	2.24	0.54
5:S:3758:LEU:HB2	5:S:3795:PRO:HB3	1.88	0.54
5:S:3780:ALA:HB1	5:S:3784:ARG:HH12	1.73	0.54
6:T:363:ARG:HB3	6:T:436:PHE:HD2	1.72	0.54
9:A:123:ARG:HH12	9:A:125:VAL:HG22	1.72	0.54
2:L:455:ASP:HB2	6:T:388:LYS:HD2	1.90	0.54
5:S:42:CYS:HA	5:S:92:PHE:HZ	1.73	0.54
5:S:2313:LYS:HA	5:S:2316:TYR:CZ	2.42	0.54
5:S:2373:PRO:HA	5:S:2404:ARG:HH22	1.72	0.54
5:S:2408:MET:N	5:S:2408:MET:SD	2.81	0.54
5:S:3158:LYS:HG3	5:S:3159:ARG:HD3	1.89	0.54
5:S:3455:LYS:NZ	5:S:3489:SER:O	2.41	0.54
6:T:230:ARG:NH1	6:T:234:GLU:OE1	2.40	0.54
5:S:1342:MET:HG2	5:S:1402:LEU:HD22	1.90	0.53
5:S:1565:GLU:O	5:S:1569:THR:OG1	2.22	0.53
5:S:1726:SER:HA	5:S:1729:PHE:HD2	1.73	0.53
5:S:3181:ASP:O	5:S:3185:ASN:ND2	2.41	0.53
5:S:3962:ARG:NH2	5:S:4125:GLU:O	2.38	0.53
1:E:691:GLN:NE2	6:T:291:GLU:O	2.40	0.53
2:L:533:ILE:HG23	2:L:537:PHE:HD2	1.73	0.53
5:S:1264:LEU:HD11	5:S:1340:ARG:HB3	1.89	0.53
5:S:2973:ASP:OD1	5:S:2977:ASN:ND2	2.40	0.53
5:S:3136:THR:HA	5:S:3139:GLN:HG3	1.89	0.53
5:S:3179:TRP:HB3	5:S:3242:MET:SD	2.48	0.53
5:S:3587:ASP:OD2	5:S:3799:ARG:NH1	2.41	0.53
5:S:3891:SER:HB2	5:S:3900:LEU:HD21	1.89	0.53
2:L:7:LYS:O	2:L:128:GLU:N	2.33	0.53
5:S:1220:LEU:HD11	5:S:1287:GLN:HB2	1.91	0.53
5:S:1428:ILE:HD12	5:S:1431:LEU:HD12	1.89	0.53
5:S:1656:ASP:OD2	5:S:1660:SER:OG	2.27	0.53
5:S:2940:ARG:HH22	5:S:3981:TYR:HB3	1.74	0.53
5:S:3728:VAL:HG13	5:S:3736:LYS:HD2	1.89	0.53
1:E:868:ASP:HB3	1:E:871:ARG:HG3	1.91	0.53
5:S:894:PHE:N	5:S:905:ILE:O	2.38	0.53
5:S:1070:PRO:HG3	5:S:3715:TYR:HB2	1.90	0.53
5:S:2425:ARG:NH1	5:S:2457:PRO:O	2.42	0.53
5:S:2941:GLY:O	5:S:3975:LYS:NZ	2.38	0.53
1:E:792:MET:HE3	4:Q:178:LYS:HD2	1.90	0.53
5:S:2996:LEU:HA	5:S:2999:LEU:HD12	1.91	0.53
5:S:3090:TYR:O	5:S:3095:ASP:N	2.38	0.53
5:S:3145:ILE:HG23	5:S:3196:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:15:LEU:HB3	5:S:41:GLU:OE2	2.08	0.53
5:S:3104:GLN:NE2	5:S:3105:ASN:OD1	2.41	0.53
4:Q:158:VAL:HA	4:Q:161:ARG:HB2	1.90	0.53
5:S:865:GLN:HB2	5:S:3168:TYR:HE2	1.74	0.53
5:S:1608:ARG:HB2	5:S:1612:LYS:HE3	1.91	0.53
5:S:1627:LYS:HG3	5:S:1628:LYS:HD3	1.90	0.53
5:S:2346:ALA:HB2	5:S:2377:ARG:HH21	1.74	0.53
2:L:168:SER:HB3	2:L:191:SER:HB3	1.90	0.53
5:S:420:VAL:O	5:S:424:LEU:N	2.37	0.53
5:S:2133:LEU:HG	5:S:2167:PRO:HB2	1.89	0.53
5:S:2970:LYS:NZ	5:S:2974:GLU:OE1	2.41	0.53
5:S:3751:LEU:N	5:S:3803:ILE:O	2.39	0.53
6:T:308:GLY:O	9:A:57:ARG:NH1	2.42	0.53
2:L:142:PHE:HZ	2:L:207:ILE:HG13	1.73	0.53
2:L:308:GLU:O	6:T:290:ARG:NH2	2.42	0.53
5:S:1570:GLU:HG3	5:S:1571:LEU:HD22	1.89	0.53
5:S:3048:LYS:NZ	5:S:3060:SER:OG	2.37	0.53
2:L:451:LEU:HB3	6:T:388:LYS:HE3	1.89	0.52
4:P:181:ILE:O	4:P:185:ASN:ND2	2.42	0.52
5:S:236:LYS:HE3	5:S:243:GLN:HE22	1.72	0.52
5:S:1071:ASN:HD21	5:S:1073:PHE:HB2	1.74	0.52
5:S:3774:ILE:O	5:S:3777:GLN:NE2	2.36	0.52
6:T:362:LEU:HD11	6:T:438:PRO:HA	1.90	0.52
5:S:152:LEU:HA	5:S:155:LYS:HE2	1.91	0.52
5:S:305:ASN:O	5:S:308:LEU:N	2.33	0.52
5:S:913:ARG:HH12	5:S:2801:ASP:CG	2.17	0.52
5:S:1725:GLN:H	5:S:1768:ARG:CZ	2.22	0.52
5:S:1936:ARG:HH21	5:S:1937:ARG:HH22	1.55	0.52
5:S:2331:MET:O	5:S:2334:LYS:NZ	2.36	0.52
2:L:652:GLU:O	2:L:656:ASN:ND2	2.42	0.52
5:S:100:ILE:HG22	5:S:103:TYR:HB2	1.91	0.52
5:S:358:GLU:HA	5:S:361:ILE:HD12	1.90	0.52
5:S:1228:GLY:HA3	5:S:1234:GLY:H	1.74	0.52
5:S:2550:ILE:HB	5:S:2554:PHE:CE1	2.44	0.52
5:S:3603:LYS:NZ	5:S:3607:GLU:OE1	2.39	0.52
2:L:269:GLN:HG3	6:T:362:LEU:HD22	1.92	0.52
5:S:963:LYS:HG2	5:S:1007:VAL:HG11	1.91	0.52
5:S:1633:TRP:CE2	5:S:1674:THR:HG21	2.44	0.52
5:S:1697:PRO:HG3	5:S:1753:SER:HB3	1.91	0.52
5:S:3506:LEU:HD21	5:S:3514:VAL:HG23	1.90	0.52
5:S:3706:ASP:O	5:S:3708:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:812:MET:H	1:E:849:GLY:H	1.57	0.52
2:L:250:ARG:HH21	6:T:536:PRO:HB2	1.74	0.52
2:L:463:LEU:HD22	2:L:477:PHE:HE2	1.74	0.52
5:S:985:GLU:HA	5:S:988:VAL:HG22	1.90	0.52
5:S:1564:SER:O	5:S:1568:ASN:ND2	2.42	0.52
5:S:1583:MET:HE2	5:S:1628:LYS:HB2	1.91	0.52
5:S:3469:LEU:HD11	5:S:3502:MET:HE1	1.91	0.52
5:S:180:LEU:O	5:S:185:HIS:NE2	2.43	0.52
5:S:272:LEU:HD23	5:S:312:ALA:HA	1.91	0.52
5:S:1457:GLN:HG2	5:S:1460:ARG:HH21	1.75	0.52
5:S:624:ILE:HA	5:S:627:VAL:HG12	1.92	0.52
5:S:1017:ILE:HG13	5:S:1018:VAL:HG23	1.91	0.52
5:S:1225:GLU:O	5:S:1230:GLY:N	2.40	0.52
5:S:2140:LEU:HD23	5:S:2143:ARG:HD2	1.92	0.52
5:S:3156:PRO:HA	5:S:3159:ARG:HE	1.75	0.52
6:T:416:GLN:NE2	6:T:429:PRO:O	2.26	0.52
1:E:668:SER:HB3	1:E:702:ALA:HA	1.92	0.52
2:L:625:ASP:HA	2:L:672:ASN:HD21	1.75	0.52
5:S:320:LEU:HA	5:S:323:VAL:HG22	1.91	0.52
5:S:681:LYS:NZ	5:S:683:PHE:O	2.34	0.52
5:S:958:MET:HB3	5:S:961:LEU:HB2	1.92	0.52
5:S:1115:HIS:HD2	5:S:1119:LYS:HE3	1.73	0.52
5:S:1775:GLU:HA	5:S:1778:PHE:CD2	2.45	0.52
5:S:2582:SER:OG	5:S:2583:GLU:N	2.42	0.52
5:S:3806:LEU:HG	5:S:3808:ASN:H	1.74	0.52
2:L:498:ALA:O	6:T:325:ARG:NH2	2.33	0.52
4:P:189:THR:O	4:P:193:SER:N	2.43	0.52
5:S:1052:SER:OG	5:S:1054:VAL:O	2.28	0.52
5:S:1603:GLN:HG2	5:S:1606:ARG:HH21	1.75	0.52
5:S:2988:GLU:HA	5:S:2991:LYS:HE2	1.92	0.52
1:E:822:SER:HA	1:E:841:LYS:HD2	1.92	0.52
5:S:1601:LEU:HB2	5:S:1655:ILE:HD11	1.91	0.52
6:T:258:ARG:NH1	6:T:259:LEU:O	2.42	0.52
1:E:879:ARG:HB2	1:E:886:PHE:HB2	1.91	0.51
2:L:313:GLY:O	6:T:286:ILE:N	2.34	0.51
4:Q:188:LYS:HA	4:Q:191:ILE:HB	1.91	0.51
5:S:1400:VAL:HA	5:S:1403:MET:HE2	1.92	0.51
5:S:3751:LEU:HB2	5:S:3803:ILE:HB	1.91	0.51
5:S:275:PHE:HE2	5:S:319:PHE:HB2	1.75	0.51
5:S:1805:PHE:O	5:S:1869:LYS:NZ	2.43	0.51
5:S:3753:LYS:HD3	5:S:3756:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:4054:ALA:HA	5:S:4095:GLU:HA	1.91	0.51
2:L:81:ARG:HE	2:L:84:MET:HB2	1.75	0.51
5:S:542:ASP:OD1	5:S:543:SER:N	2.42	0.51
5:S:1164:CYS:SG	5:S:1165:LEU:N	2.83	0.51
5:S:1296:PHE:O	5:S:1300:SER:OG	2.24	0.51
5:S:2234:ASN:HA	5:S:2237:ILE:HD12	1.92	0.51
5:S:2834:GLN:HA	5:S:2837:LEU:HD12	1.92	0.51
5:S:4125:GLU:HB3	5:S:4128:MET:HB2	1.91	0.51
1:E:837:ARG:HG2	4:P:153:ARG:NH2	2.25	0.51
2:L:161:LEU:HD12	2:L:163:PHE:HE1	1.75	0.51
2:L:184:ARG:NH1	2:L:517:ASN:O	2.37	0.51
2:L:272:VAL:HG22	2:L:274:LYS:H	1.76	0.51
2:L:463:LEU:HD22	2:L:477:PHE:CE2	2.44	0.51
5:S:1474:ASP:OD1	5:S:1474:ASP:N	2.44	0.51
6:T:107:GLU:O	6:T:115:ARG:NH2	2.34	0.51
2:L:689:GLU:HA	2:L:695:SER:HB3	1.92	0.51
5:S:146:GLU:HB3	5:S:183:GLU:HG3	1.92	0.51
5:S:186:PRO:HD2	5:S:189:MET:HE1	1.92	0.51
5:S:1502:SER:OG	5:S:1503:LEU:N	2.41	0.51
2:L:88:PHE:HD2	6:T:325:ARG:HD3	1.75	0.51
2:L:608:SER:HB2	2:L:654:ARG:HH12	1.76	0.51
5:S:955:ALA:O	5:S:957:PRO:HD3	2.10	0.51
5:S:2121:ASP:OD1	5:S:2121:ASP:N	2.43	0.51
5:S:3008:TRP:HB2	5:S:3051:LEU:HD23	1.93	0.51
5:S:3176:MET:HA	5:S:3179:TRP:HD1	1.75	0.51
5:S:3923:ARG:HH21	5:S:3924:HIS:HB3	1.76	0.51
5:S:3970:LEU:HD21	5:S:3974:MET:HG2	1.93	0.51
5:S:1786:ALA:HB3	5:S:1830:HIS:HB3	1.92	0.51
5:S:3927:ASN:O	5:S:3940:ILE:N	2.43	0.51
6:T:299:LYS:NZ	6:T:300:THR:O	2.43	0.51
7:i:36:DA:H2"	7:i:37:DT:C5	2.45	0.51
9:A:45:ARG:HE	9:A:71:GLN:H	1.58	0.51
1:E:879:ARG:HD3	1:E:885:LYS:HA	1.92	0.51
2:L:605:LYS:HE3	2:L:609:PHE:HZ	1.76	0.51
5:S:372:PRO:HA	5:S:375:VAL:HB	1.92	0.51
5:S:430:VAL:HG11	5:S:1643:MET:HG3	1.92	0.51
5:S:1602:ASP:HB3	5:S:1606:ARG:HH12	1.75	0.51
5:S:1626:TRP:HH2	5:S:1632:TRP:HB2	1.76	0.51
5:S:3142:ILE:O	5:S:3147:LYS:NZ	2.39	0.51
6:T:414:VAL:O	6:T:433:GLN:N	2.37	0.51
2:L:261:ILE:HA	2:L:366:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1621:THR:O	5:S:1625:HIS:N	2.44	0.51
9:A:90:ASP:HB3	9:A:93:ARG:HB3	1.93	0.51
5:S:35:ILE:HG12	5:S:36:ARG:HH21	1.76	0.51
5:S:493:LYS:O	5:S:625:ASN:ND2	2.44	0.51
5:S:886:TRP:O	5:S:964:ARG:NH1	2.43	0.51
5:S:1538:LEU:HB2	5:S:1555:HIS:CE1	2.46	0.51
5:S:2505:VAL:HA	5:S:2508:GLN:HG2	1.93	0.51
6:T:147:LEU:HD11	6:T:193:LEU:HD23	1.93	0.51
6:T:307:THR:HG22	6:T:309:GLY:H	1.75	0.51
6:T:414:VAL:HB	6:T:433:GLN:HB2	1.92	0.51
2:L:235:CYS:HA	2:L:238:LYS:HB2	1.93	0.50
2:L:458:ILE:O	2:L:462:SER:N	2.44	0.50
5:S:833:HIS:O	5:S:838:LYS:NZ	2.43	0.50
5:S:863:GLY:O	5:S:867:ASN:N	2.40	0.50
5:S:2376:ASP:N	5:S:2376:ASP:OD1	2.43	0.50
5:S:2890:ILE:HD11	5:S:2929:LEU:HB3	1.94	0.50
6:T:413:LEU:HB3	6:T:432:PHE:CD2	2.45	0.50
1:E:816:HIS:HB2	1:E:850:ALA:HA	1.93	0.50
5:S:129:ASP:O	5:S:133:LYS:HG2	2.12	0.50
5:S:1576:ASP:OD1	5:S:1576:ASP:N	2.44	0.50
5:S:3037:GLN:N	5:S:3037:GLN:OE1	2.44	0.50
5:S:3311:ASN:HB3	5:S:3315:TYR:CZ	2.46	0.50
5:S:3657:SER:OG	5:S:3658:ASP:N	2.41	0.50
1:E:746:MET:O	1:E:751:LYS:NZ	2.44	0.50
5:S:3266:SER:HA	5:S:3272:TRP:CD1	2.46	0.50
5:S:2232:ARG:HA	5:S:2235:LEU:HD12	1.93	0.50
5:S:2510:LEU:O	5:S:2518:GLN:NE2	2.31	0.50
5:S:3828:TYR:HD2	5:S:3829:LEU:HD22	1.77	0.50
6:T:389:CYS:O	6:T:393:GLU:N	2.44	0.50
2:L:450:GLN:NE2	2:L:536:LEU:O	2.36	0.50
4:P:161:ARG:HA	4:P:164:LYS:HE2	1.93	0.50
5:S:1479:VAL:O	5:S:1482:GLU:HG2	2.11	0.50
5:S:2255:LEU:HD23	5:S:2255:LEU:H	1.77	0.50
5:S:3321:LEU:O	5:S:3324:ARG:HG2	2.12	0.50
1:E:857:ALA:O	1:E:884:ARG:NH1	2.44	0.50
5:S:668:LYS:HZ2	5:S:728:SER:HB3	1.77	0.50
5:S:1776:GLU:O	5:S:1779:GLN:NE2	2.45	0.50
5:S:3228:SER:HA	5:S:3231:ILE:HG12	1.94	0.50
5:S:3806:LEU:HD23	5:S:3809:THR:HB	1.93	0.50
6:T:261:LEU:HB3	6:T:269:ILE:HB	1.94	0.50
2:L:33:GLN:HB3	2:L:227:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:137:THR:O	5:S:141:SER:OG	2.29	0.50
5:S:931:CYS:O	5:S:935:HIS:ND1	2.45	0.50
5:S:1075:ARG:NH1	5:S:1117:ASP:OD2	2.41	0.50
5:S:2470:ARG:O	5:S:2473:MET:HG2	2.12	0.50
5:S:3132:VAL:HA	5:S:3135:LEU:HD12	1.94	0.50
5:S:3133:GLN:NE2	5:S:3137:GLU:OE2	2.44	0.50
5:S:3796:MET:HB2	5:S:3800:LEU:HB3	1.92	0.50
6:T:343:PRO:HA	6:T:401:THR:HB	1.91	0.50
5:S:630:CYS:HA	5:S:633:ILE:HG12	1.94	0.50
5:S:1057:LYS:HA	5:S:1060:PHE:HD2	1.76	0.50
5:S:1949:ILE:HD13	5:S:2096:PRO:HB2	1.94	0.50
6:T:42:VAL:HG22	6:T:169:PHE:HB2	1.93	0.50
6:T:263:LEU:HD12	6:T:267:ILE:HG21	1.94	0.50
1:E:668:SER:OG	1:E:708:ARG:NH2	2.40	0.49
1:E:707:ILE:HA	1:E:710:LYS:HD3	1.94	0.49
5:S:469:ALA:HA	5:S:475:LEU:HD13	1.93	0.49
5:S:759:GLY:O	5:S:799:TYR:OH	2.28	0.49
5:S:1062:ARG:NH2	5:S:3745:GLU:OE1	2.43	0.49
5:S:189:MET:HA	5:S:192:ASN:HB2	1.94	0.49
5:S:451:PRO:HA	5:S:454:GLN:HB2	1.94	0.49
5:S:1708:GLU:HA	5:S:1711:ARG:HD2	1.94	0.49
5:S:2322:VAL:O	5:S:2326:ILE:HG12	2.12	0.49
5:S:2870:SER:OG	5:S:2899:ARG:NH2	2.43	0.49
5:S:3013:TYR:HA	5:S:3016:THR:HG23	1.94	0.49
6:T:372:GLU:OE1	6:T:377:GLY:N	2.37	0.49
2:L:448:GLU:HA	2:L:451:LEU:HD12	1.93	0.49
2:L:643:ARG:HE	2:L:647:ILE:HG13	1.77	0.49
5:S:425:ASP:OD1	5:S:425:ASP:N	2.43	0.49
5:S:3619:ASP:OD1	5:S:3619:ASP:N	2.45	0.49
6:T:357:LYS:HB3	6:T:359:HIS:CE1	2.47	0.49
2:L:294:VAL:HB	6:T:299:LYS:HB3	1.94	0.49
2:L:298:ASN:OD1	2:L:299:ASP:N	2.46	0.49
5:S:672:ILE:HD12	5:S:675:ARG:HH21	1.78	0.49
5:S:938:VAL:HA	5:S:941:MET:HG3	1.94	0.49
5:S:1118:GLU:OE2	5:S:1120:SER:OG	2.28	0.49
5:S:1250:LEU:O	5:S:1253:THR:OG1	2.25	0.49
5:S:2978:LYS:NZ	5:S:2980:ASP:O	2.37	0.49
5:S:3965:ARG:HA	5:S:3968:ILE:HD12	1.93	0.49
6:T:363:ARG:HH22	8:j:27:DT:H3'	1.77	0.49
7:i:35:DT:O4	7:i:36:DA:N6	2.44	0.49
4:P:187:LYS:O	4:P:191:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1142:HIS:O	5:S:1146:ASN:N	2.44	0.49
5:S:3753:LYS:NZ	5:S:3755:GLY:O	2.32	0.49
6:T:74:LYS:HZ1	6:T:81:ASP:H	1.58	0.49
6:T:147:LEU:HD13	6:T:189:LYS:HB3	1.94	0.49
1:E:853:VAL:HG11	1:E:857:ALA:HB2	1.95	0.49
5:S:52:ALA:O	5:S:56:SER:OG	2.25	0.49
5:S:649:PHE:CE2	5:S:653:LEU:HD11	2.48	0.49
5:S:1181:THR:OG1	5:S:1184:ARG:NH2	2.46	0.49
5:S:1357:LYS:HE3	5:S:1410:PRO:HG2	1.95	0.49
5:S:1571:LEU:HD12	5:S:1578:ALA:HB2	1.94	0.49
5:S:3269:ARG:CZ	5:S:3272:TRP:HB2	2.42	0.49
5:S:3413:TYR:O	5:S:3449:LYS:NZ	2.45	0.49
6:T:301:ARG:HH22	9:A:57:ARG:HE	1.61	0.49
2:L:342:VAL:HG23	2:L:393:VAL:HG22	1.95	0.49
2:L:654:ARG:HA	2:L:657:ASN:HD21	1.77	0.49
5:S:793:LEU:HD22	5:S:869:ASN:HB2	1.94	0.49
5:S:1769:GLU:O	5:S:1772:HIS:ND1	2.33	0.49
5:S:2569:SER:OG	5:S:2571:ASP:OD1	2.29	0.49
5:S:2796:ALA:O	5:S:2800:ARG:HG2	2.11	0.49
5:S:2924:VAL:HG11	5:S:2989:ALA:HB1	1.95	0.49
5:S:3538:GLU:OE1	5:S:3538:GLU:N	2.42	0.49
2:L:473:LEU:HD21	6:T:352:PRO:HG2	1.94	0.49
3:M:198:GLY:H	6:T:477:SER:HB3	1.78	0.49
4:P:194:LEU:HD22	4:Q:194:LEU:HD22	1.95	0.49
5:S:87:LYS:HG3	5:S:831:LEU:HD22	1.95	0.49
5:S:1643:MET:HA	5:S:1646:LEU:HG	1.95	0.49
5:S:2495:SER:HA	5:S:2498:ILE:HD12	1.94	0.49
5:S:2541:ALA:O	5:S:2544:SER:OG	2.26	0.49
5:S:3034:PRO:HD2	5:S:3037:GLN:HB2	1.95	0.49
6:T:266:ASP:N	6:T:266:ASP:OD1	2.44	0.49
6:T:422:ASP:OD1	6:T:422:ASP:N	2.44	0.49
9:A:40:TRP:HE1	9:A:122:ARG:CZ	2.25	0.49
2:L:660:LYS:HZ1	2:L:698:ALA:HB1	1.78	0.49
5:S:3169:PRO:HG3	5:S:3241:LYS:HD2	1.95	0.49
6:T:103:TYR:CG	6:T:135:MET:HE1	2.48	0.49
6:T:142:SER:HB3	6:T:145:GLU:HG2	1.94	0.49
2:L:241:GLU:HG3	6:T:445:LYS:HE2	1.95	0.49
5:S:135:LEU:O	5:S:139:ARG:HG2	2.12	0.49
5:S:672:ILE:HG23	5:S:675:ARG:HH21	1.78	0.49
5:S:3104:GLN:HA	5:S:3107:ILE:HG12	1.94	0.49
9:A:109:LEU:HG	9:A:132:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:402:ASN:O	2:L:404:GLN:NE2	2.46	0.48
2:L:407:VAL:HG12	2:L:424:LEU:HD21	1.94	0.48
5:S:31:GLY:HA2	5:S:34:LEU:HD12	1.95	0.48
5:S:1191:PHE:O	5:S:1195:VAL:HG23	2.13	0.48
5:S:1828:LEU:HD21	5:S:1880:MET:HA	1.95	0.48
5:S:3119:VAL:HG23	5:S:3120:LEU:HD23	1.95	0.48
2:L:329:GLU:HA	2:L:332:LYS:HG2	1.94	0.48
2:L:663:GLN:HA	2:L:666:VAL:HG12	1.95	0.48
2:L:667:GLU:OE2	2:L:702:LYS:NZ	2.46	0.48
5:S:321:LYS:O	5:S:325:ASN:ND2	2.46	0.48
5:S:847:SER:N	5:S:850:GLU:OE2	2.46	0.48
5:S:3037:GLN:O	5:S:3041:LEU:HG	2.13	0.48
5:S:3476:PRO:O	5:S:3480:LEU:HB2	2.13	0.48
7:i:36:DA:H2"	7:i:37:DT:C4	2.48	0.48
5:S:390:GLN:HA	5:S:393:LYS:HE2	1.96	0.48
5:S:768:VAL:HA	5:S:771:ASN:HD22	1.79	0.48
5:S:3193:ILE:HG13	5:S:3196:LYS:HZ3	1.78	0.48
5:S:3780:ALA:HB1	5:S:3784:ARG:NH1	2.28	0.48
5:S:4086:ASP:OD1	5:S:4086:ASP:N	2.45	0.48
6:T:35:ARG:O	6:T:162:SER:N	2.45	0.48
2:L:55:ALA:HB2	2:L:83:LEU:HG	1.95	0.48
5:S:847:SER:OG	5:S:848:LEU:N	2.29	0.48
2:L:277:THR:OG1	6:T:319:SER:O	2.32	0.48
2:L:389:MET:HG2	6:T:466:VAL:HG21	1.96	0.48
4:P:190:LYS:HG3	4:Q:191:ILE:HD13	1.96	0.48
5:S:243:GLN:O	5:S:246:ARG:HD3	2.14	0.48
5:S:1711:ARG:HE	5:S:1757:MET:HE2	1.78	0.48
5:S:2486:ASP:OD1	5:S:2486:ASP:N	2.42	0.48
5:S:2547:SER:HB3	5:S:2554:PHE:HZ	1.79	0.48
2:L:260:ARG:NE	6:T:536:PRO:O	2.37	0.48
4:P:198:LEU:HD12	4:Q:198:LEU:HD13	1.95	0.48
5:S:1150:LYS:HA	5:S:1162:SER:HA	1.96	0.48
5:S:1196:PRO:HA	5:S:1202:ARG:HA	1.95	0.48
5:S:1591:LYS:O	5:S:1594:SER:OG	2.27	0.48
5:S:2406:GLU:N	5:S:2406:GLU:OE1	2.46	0.48
5:S:261:ASP:HB3	5:S:265:TYR:H	1.79	0.48
5:S:625:ASN:O	5:S:628:GLU:HG2	2.13	0.48
5:S:1257:LEU:HA	5:S:1260:LEU:HD12	1.94	0.48
5:S:1867:ILE:O	5:S:1871:MET:HG2	2.14	0.48
5:S:2522:ARG:HH12	5:S:2564:GLU:HG2	1.79	0.48
5:S:3236:PHE:HD2	5:S:3269:ARG:HH12	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3923:ARG:HG2	5:S:4124:TRP:HA	1.96	0.48
5:S:3964:THR:HG23	5:S:3966:GLN:H	1.77	0.48
2:L:457:LEU:HD22	2:L:533:ILE:HD13	1.94	0.48
5:S:476:ARG:HH21	5:S:1561:SER:HG	1.56	0.48
5:S:1649:LEU:HA	5:S:1652:ILE:HD12	1.96	0.48
5:S:2414:GLN:O	5:S:2417:SER:OG	2.28	0.48
5:S:2522:ARG:NH1	5:S:2564:GLU:HG2	2.29	0.48
5:S:3182:ILE:HA	5:S:3185:ASN:HD21	1.79	0.48
5:S:3452:LYS:HA	5:S:3455:LYS:HG2	1.96	0.48
6:T:247:ARG:NH1	6:T:487:PHE:HB2	2.29	0.48
2:L:263:ALA:HA	2:L:364:VAL:HA	1.96	0.48
4:P:188:LYS:O	4:P:192:ARG:N	2.35	0.48
5:S:792:ILE:HG13	5:S:793:LEU:HD12	1.95	0.48
5:S:974:CYS:HA	5:S:981:ARG:HH12	1.79	0.48
5:S:2129:LEU:HA	5:S:2132:LYS:HG2	1.94	0.48
5:S:2318:ALA:HA	5:S:2321:GLU:HG2	1.96	0.48
5:S:2428:ASP:OD1	5:S:2428:ASP:N	2.45	0.48
5:S:2539:LEU:O	5:S:2542:LEU:HG	2.13	0.48
5:S:3240:MET:HE3	5:S:3272:TRP:CH2	2.49	0.48
1:E:731:LYS:HG3	1:E:732:THR:HG23	1.95	0.48
2:L:360:GLN:HE22	2:L:362:LEU:HB2	1.79	0.48
5:S:1083:ASN:O	5:S:1087:ARG:NH1	2.47	0.48
5:S:1184:ARG:NH2	5:S:1265:GLU:OE1	2.47	0.48
5:S:4004:VAL:HG23	5:S:4005:PHE:H	1.78	0.48
6:T:190:ALA:O	6:T:193:LEU:HG	2.14	0.48
7:i:28:DT:H1'	7:i:29:DA:H5'	1.95	0.48
7:i:37:DT:H5''	7:i:37:DT:C6	2.49	0.48
1:E:677:ASP:N	1:E:677:ASP:OD1	2.47	0.47
2:L:311:ILE:HD11	6:T:290:ARG:HD3	1.95	0.47
2:L:312:GLN:NE2	2:L:324:SER:O	2.46	0.47
2:L:541:GLU:HG2	6:T:268:VAL:HB	1.96	0.47
5:S:1115:HIS:NE2	5:S:1182:GLU:HB3	2.28	0.47
5:S:1115:HIS:CD2	5:S:1119:LYS:HE3	2.49	0.47
5:S:2234:ASN:O	5:S:2238:ILE:HD12	2.14	0.47
5:S:3621:LYS:HB2	5:S:3630:ARG:HH12	1.79	0.47
2:L:306:LEU:HG	2:L:308:GLU:H	1.79	0.47
5:S:80:GLU:HA	5:S:83:GLU:OE1	2.13	0.47
5:S:724:GLU:HB2	5:S:2599:SER:HA	1.95	0.47
5:S:1157:PHE:CE1	5:S:1159:PRO:HG2	2.49	0.47
6:T:247:ARG:NH1	6:T:488:ARG:HG3	2.28	0.47
1:E:656:SER:HA	1:E:733:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:343:LEU:HD11	2:L:394:ARG:HB2	1.96	0.47
5:S:1105:VAL:O	5:S:1108:MET:HG3	2.14	0.47
5:S:1740:VAL:HA	5:S:1743:MET:HG2	1.97	0.47
5:S:1793:THR:O	5:S:1797:LEU:HG	2.13	0.47
5:S:672:ILE:O	5:S:676:ASN:ND2	2.48	0.47
5:S:3455:LYS:HZ1	5:S:3489:SER:C	2.22	0.47
5:S:3860:LYS:HG2	5:S:4073:ALA:HB2	1.95	0.47
6:T:39:ILE:O	6:T:167:MET:N	2.44	0.47
5:S:1423:ILE:HD11	5:S:1428:ILE:HB	1.95	0.47
2:L:426:PHE:HB3	6:T:479:GLU:HA	1.97	0.47
5:S:2190:VAL:HA	5:S:2193:ILE:HG22	1.97	0.47
5:S:2205:VAL:HG13	5:S:2208:ASP:H	1.78	0.47
5:S:2826:LEU:HA	5:S:2829:LYS:HE2	1.97	0.47
5:S:3008:TRP:HA	5:S:3011:LEU:HD12	1.97	0.47
5:S:3048:LYS:HA	5:S:3051:LEU:HD12	1.97	0.47
5:S:3312:VAL:O	5:S:3316:LEU:N	2.40	0.47
2:L:18:PHE:HA	2:L:21:SER:HB2	1.96	0.47
2:L:188:HIS:HD1	2:L:519:PRO:HD3	1.80	0.47
5:S:67:VAL:HA	5:S:71:LYS:HB2	1.97	0.47
5:S:364:ARG:HA	5:S:415:GLN:NE2	2.29	0.47
5:S:367:GLY:HA3	5:S:416:SER:HB2	1.97	0.47
5:S:763:THR:O	5:S:766:ALA:N	2.47	0.47
5:S:1342:MET:O	5:S:1345:THR:OG1	2.32	0.47
5:S:2393:LEU:HD12	5:S:2393:LEU:H	1.79	0.47
5:S:3189:PHE:O	5:S:3193:ILE:HD12	2.15	0.47
5:S:3285:HIS:HE2	5:S:3333:THR:HB	1.80	0.47
5:S:3720:ALA:HB3	5:S:3743:HIS:HA	1.95	0.47
5:S:4111:ALA:O	5:S:4115:ASN:ND2	2.41	0.47
6:T:353:LEU:HD23	6:T:395:ALA:HB2	1.96	0.47
5:S:1751:GLU:HA	5:S:1785:ILE:HG22	1.97	0.47
5:S:2825:THR:HG23	5:S:2828:GLU:H	1.80	0.47
1:E:800:GLU:O	1:E:804:SER:N	2.48	0.47
4:P:183:VAL:HA	4:P:186:GLU:HG2	1.96	0.47
5:S:204:LEU:O	5:S:208:MET:HG3	2.15	0.47
5:S:1212:LEU:HD12	5:S:1215:GLU:HB2	1.97	0.47
5:S:2044:ASP:O	5:S:2048:GLY:N	2.47	0.47
5:S:2723:THR:HG23	5:S:2727:ARG:HH21	1.80	0.47
7:i:21:DA:P	8:j:37:DG:H21	2.38	0.47
4:P:191:ILE:HG22	4:P:195:HIS:CE1	2.50	0.47
5:S:1226:GLY:HA3	5:S:1263:ALA:HB2	1.97	0.47
5:S:1452:VAL:HG22	5:S:1517:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:1593:VAL:HA	5:S:1596:VAL:HG22	1.96	0.47
5:S:2196:TRP:NE1	5:S:2200:ALA:HB3	2.30	0.47
5:S:3069:MET:HE1	5:S:3078:LEU:HD11	1.96	0.47
5:S:3692:VAL:HG22	5:S:3696:ARG:HD3	1.96	0.47
2:L:496:HIS:CG	2:L:506:PRO:HD3	2.50	0.46
5:S:781:ASP:OD2	5:S:783:HIS:ND1	2.48	0.46
5:S:784:VAL:O	5:S:787:PRO:HD2	2.15	0.46
5:S:1046:PRO:O	5:S:1049:GLN:HG2	2.15	0.46
5:S:2330:VAL:HG12	5:S:2333:ARG:NH2	2.30	0.46
5:S:3758:LEU:O	5:S:3762:GLN:HG2	2.15	0.46
2:L:276:TRP:HB3	6:T:318:ARG:HB3	1.97	0.46
2:L:524:THR:HA	2:L:527:GLN:HG2	1.96	0.46
5:S:723:ASP:C	5:S:725:LEU:H	2.24	0.46
5:S:1406:LEU:HA	5:S:1409:SER:HB3	1.97	0.46
5:S:1824:LEU:HD13	5:S:1827:LEU:HD21	1.97	0.46
5:S:3085:GLU:OE1	5:S:3085:GLU:N	2.41	0.46
5:S:4099:SER:HB3	5:S:4102:THR:OG1	2.15	0.46
6:T:59:PRO:HA	6:T:62:MET:HG2	1.97	0.46
6:T:262:LYS:HA	6:T:267:ILE:O	2.14	0.46
2:L:357:MET:HG3	2:L:425:PRO:HB3	1.96	0.46
5:S:179:GLY:HA3	5:S:230:LEU:HB2	1.98	0.46
5:S:234:PHE:CD2	5:S:235:THR:HG23	2.51	0.46
5:S:782:ARG:HB3	5:S:3164:TRP:CZ2	2.49	0.46
5:S:935:HIS:CE1	5:S:984:TYR:HE1	2.33	0.46
5:S:1268:ASN:ND2	5:S:1343:GLU:OE2	2.49	0.46
5:S:1453:SER:HA	5:S:1456:LYS:HG2	1.97	0.46
5:S:3713:PRO:HB3	5:S:3715:TYR:CZ	2.51	0.46
5:S:4085:LYS:HB3	5:S:4087:HIS:CE1	2.50	0.46
9:A:42:SER:O	9:A:45:ARG:NH2	2.48	0.46
1:E:774:LEU:HD21	4:P:180:PHE:HB2	1.97	0.46
2:L:162:GLN:NE2	2:L:235:CYS:O	2.47	0.46
5:S:12:LEU:HD21	5:S:44:LEU:HD22	1.97	0.46
5:S:16:GLN:NE2	5:S:62:ASP:OD2	2.48	0.46
5:S:429:GLU:O	5:S:432:THR:OG1	2.34	0.46
5:S:1023:SER:HA	5:S:1026:ARG:HG3	1.98	0.46
5:S:2388:LYS:NZ	6:T:155:SER:O	2.39	0.46
5:S:3163:THR:O	5:S:3167:ARG:NH2	2.48	0.46
5:S:3964:THR:HG22	5:S:3967:PHE:HD2	1.80	0.46
8:j:32:DT:H2"	8:j:33:DA:C8	2.50	0.46
2:L:463:LEU:HD13	2:L:477:PHE:CD2	2.51	0.46
2:L:636:ILE:HA	2:L:639:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:176:LEU:HD13	4:Q:176:LEU:HD12	1.98	0.46
5:S:151:GLU:O	5:S:154:SER:OG	2.30	0.46
5:S:1015:ASP:OD1	5:S:1016:GLY:N	2.46	0.46
5:S:1740:VAL:HA	5:S:1743:MET:HE3	1.98	0.46
5:S:1767:CYS:HB3	5:S:1818:SER:OG	2.16	0.46
5:S:2402:LEU:HD13	5:S:2434:VAL:HG23	1.97	0.46
5:S:2414:GLN:OE1	5:S:2414:GLN:N	2.45	0.46
5:S:3133:GLN:O	5:S:3136:THR:HG22	2.14	0.46
5:S:3592:VAL:HB	5:S:3609:MET:HE1	1.98	0.46
5:S:3832:PRO:HB2	5:S:3877:LYS:HG2	1.98	0.46
5:S:4045:CYS:HA	5:S:4048:LYS:HG2	1.98	0.46
9:A:117:LEU:HD12	9:A:120:GLN:HE22	1.81	0.46
2:L:255:SER:OG	6:T:515:ASN:ND2	2.43	0.46
2:L:457:LEU:HD13	2:L:529:PRO:HB2	1.97	0.46
4:P:150:ARG:O	4:P:154:ASP:N	2.41	0.46
5:S:3176:MET:HA	5:S:3179:TRP:CD1	2.50	0.46
5:S:3328:ILE:O	5:S:3332:THR:OG1	2.27	0.46
5:S:4113:ASP:O	5:S:4117:LEU:HG	2.16	0.46
6:T:44:ALA:HB1	6:T:137:HIS:HA	1.98	0.46
9:A:65:ILE:HG13	9:A:70:GLY:HA3	1.98	0.46
1:E:656:SER:HB3	1:E:685:PHE:CD2	2.50	0.46
1:E:832:LYS:HD3	1:E:834:GLU:H	1.80	0.46
5:S:901:MET:SD	5:S:901:MET:N	2.89	0.46
5:S:913:ARG:NH1	5:S:917:LEU:HD11	2.31	0.46
5:S:1261:LEU:HD21	5:S:1337:VAL:HA	1.97	0.46
5:S:3324:ARG:HB3	5:S:3391:ALA:HB3	1.98	0.46
5:S:3493:TRP:CE2	5:S:3524:ASN:HB2	2.50	0.46
6:T:275:ASN:HD21	6:T:278:GLN:HB2	1.81	0.46
1:E:769:THR:HG21	4:P:184:LEU:HD13	1.98	0.46
2:L:252:THR:HB	2:L:341:SER:HA	1.97	0.46
2:L:511:HIS:ND1	2:L:515:MET:HE1	2.31	0.46
4:P:190:LYS:HD3	4:Q:191:ILE:HG21	1.97	0.46
5:S:113:SER:O	5:S:117:LYS:N	2.49	0.46
5:S:1712:ARG:O	5:S:1715:GLU:HG3	2.15	0.46
5:S:3547:THR:HA	5:S:3550:LYS:HZ2	1.80	0.46
5:S:3658:ASP:N	5:S:3658:ASP:OD1	2.48	0.46
5:S:3912:CYS:HB2	5:S:3961:PHE:HB2	1.96	0.46
6:T:102:ILE:HD12	6:T:146:VAL:HG12	1.97	0.46
5:S:31:GLY:HA3	5:S:77:GLU:HB2	1.97	0.46
5:S:996:THR:HG21	5:S:1039:TRP:HB3	1.98	0.46
5:S:2297:SER:OG	5:S:2298:GLU:OE1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3927:ASN:HA	5:S:3940:ILE:HB	1.96	0.46
6:T:372:GLU:OE2	6:T:379:SER:N	2.36	0.46
7:i:37:DT:H5"	7:i:37:DT:H6	1.80	0.46
1:E:725:TRP:NE1	1:E:736:VAL:O	2.43	0.46
5:S:901:MET:SD	5:S:2820:MET:HE1	2.56	0.46
5:S:907:LEU:HA	5:S:910:PHE:CD2	2.51	0.46
5:S:1105:VAL:HA	5:S:1108:MET:HG3	1.98	0.46
5:S:1406:LEU:HD13	5:S:1415:LEU:HD13	1.97	0.46
5:S:1626:TRP:CH2	5:S:1632:TRP:HB2	2.51	0.46
5:S:1770:GLN:NE2	5:S:1775:GLU:OE1	2.49	0.46
5:S:2328:ARG:NE	5:S:2370:SER:O	2.44	0.46
5:S:2375:ALA:O	5:S:2378:PHE:N	2.37	0.46
5:S:2891:ARG:HH22	5:S:3894:PRO:HB2	1.81	0.46
6:T:206:LYS:N	6:T:235:GLU:HB3	2.30	0.46
1:E:711:ASN:OD1	2:L:330:GLN:NE2	2.46	0.45
2:L:21:SER:HB3	2:L:100:PRO:HB3	1.98	0.45
2:L:368:ARG:HD2	2:L:368:ARG:HA	1.86	0.45
2:L:436:SER:O	6:T:369:TYR:OH	2.34	0.45
5:S:166:ILE:N	5:S:167:PRO:HD2	2.31	0.45
5:S:291:VAL:HA	5:S:294:PHE:CD2	2.51	0.45
5:S:861:SER:N	5:S:3136:THR:HG21	2.31	0.45
5:S:891:ARG:HH22	5:S:960:GLN:H	1.65	0.45
5:S:1115:HIS:O	5:S:1119:LYS:NZ	2.36	0.45
5:S:1626:TRP:CZ2	5:S:1630:ASP:HA	2.51	0.45
5:S:2386:LEU:HD12	5:S:2418:LYS:HG3	1.99	0.45
5:S:3247:ARG:NE	5:S:3282:ARG:HE	2.14	0.45
5:S:3837:CYS:SG	5:S:3873:LYS:HB3	2.56	0.45
5:S:3860:LYS:HE3	5:S:4072:PRO:HB2	1.97	0.45
6:T:348:MET:HG3	6:T:410:PHE:CE1	2.50	0.45
1:E:665:CYS:HB3	1:E:700:VAL:HG13	1.98	0.45
1:E:702:ALA:HB3	1:E:720:VAL:HG13	1.98	0.45
1:E:713:ILE:HA	1:E:745:HIS:CE1	2.51	0.45
2:L:65:ASP:N	2:L:77:ILE:O	2.41	0.45
5:S:436:GLU:HA	5:S:439:VAL:HG22	1.98	0.45
5:S:675:ARG:HA	5:S:678:LYS:HG2	1.97	0.45
5:S:1057:LYS:HB3	5:S:1061:LYS:NZ	2.30	0.45
5:S:1651:LYS:O	5:S:1654:GLN:HG2	2.16	0.45
5:S:3177:ASN:OD1	5:S:3178:ILE:N	2.49	0.45
5:S:3689:ASP:N	5:S:3689:ASP:OD1	2.47	0.45
5:S:3767:LEU:HD21	5:S:4002:MET:HA	1.98	0.45
2:L:262:ALA:N	2:L:365:PHE:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:81:CYS:O	5:S:85:ILE:HG12	2.17	0.45
5:S:87:LYS:HD3	5:S:831:LEU:HD13	1.98	0.45
5:S:1034:ARG:HH21	5:S:1087:ARG:HB2	1.81	0.45
5:S:1308:ALA:HB3	5:S:1310:GLU:HG2	1.98	0.45
5:S:2227:LYS:HB2	5:S:2230:VAL:HG22	1.98	0.45
5:S:2425:ARG:NH1	5:S:2460:GLU:OE2	2.49	0.45
5:S:3901:ARG:HH21	5:S:3970:LEU:HG	1.81	0.45
5:S:4040:PRO:O	5:S:4044:ILE:HD12	2.17	0.45
2:L:496:HIS:CD2	2:L:505:LEU:HD13	2.52	0.45
2:L:665:LYS:O	2:L:668:ILE:HG12	2.15	0.45
5:S:240:GLU:HB2	5:S:242:PRO:HD2	1.98	0.45
5:S:759:GLY:HA2	5:S:762:TYR:O	2.17	0.45
5:S:771:ASN:O	5:S:774:GLU:HG3	2.14	0.45
5:S:1844:VAL:HG23	5:S:1845:VAL:H	1.80	0.45
5:S:1849:ASP:OD1	5:S:1850:VAL:N	2.49	0.45
5:S:1864:ASP:OD1	5:S:1864:ASP:N	2.46	0.45
5:S:2360:PHE:O	5:S:2364:LEU:HD23	2.17	0.45
5:S:2387:PRO:O	6:T:158:GLN:NE2	2.30	0.45
5:S:2873:PRO:HB2	5:S:2925:GLU:OE1	2.17	0.45
5:S:3000:ASP:O	5:S:3004:HIS:ND1	2.32	0.45
5:S:4055:ASN:HD21	5:S:4057:ALA:HB3	1.80	0.45
1:E:720:VAL:HG23	1:E:745:HIS:HB3	1.98	0.45
2:L:327:ASP:O	2:L:331:MET:HG2	2.16	0.45
5:S:15:LEU:O	5:S:19:LEU:HG	2.16	0.45
5:S:213:ARG:O	6:T:404:ARG:NH2	2.50	0.45
5:S:559:SER:OG	5:S:560:LEU:N	2.38	0.45
5:S:3251:ASN:O	5:S:3254:LEU:HD22	2.16	0.45
6:T:102:ILE:HG21	6:T:149:VAL:HG21	1.98	0.45
9:A:68:HIS:CD2	9:A:122:ARG:HH22	2.35	0.45
1:E:835:GLY:HA2	4:P:150:ARG:HD2	1.98	0.45
2:L:315:ARG:HA	2:L:320:ILE:HA	1.98	0.45
5:S:452:LYS:HE3	5:S:453:MET:HE1	1.98	0.45
5:S:458:CYS:O	5:S:462:VAL:HG23	2.17	0.45
5:S:968:VAL:HA	5:S:971:ARG:HG2	1.98	0.45
5:S:1424:THR:HG23	5:S:1426:GLN:H	1.82	0.45
5:S:1633:TRP:CD2	5:S:1674:THR:HG21	2.51	0.45
5:S:3107:ILE:HG22	5:S:3135:LEU:HD13	1.98	0.45
5:S:3585:PHE:CG	5:S:3667:LEU:HD23	2.52	0.45
6:T:32:TYR:HE2	7:i:34:DC:H4'	1.80	0.45
6:T:200:LEU:HD23	6:T:200:LEU:H	1.82	0.45
6:T:400:TYR:N	6:T:409:TYR:O	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:61:THR:OG1	2:L:63:GLY:O	2.33	0.45
2:L:264:TYR:O	2:L:363:LYS:N	2.43	0.45
5:S:144:MET:HE3	5:S:144:MET:HA	1.99	0.45
5:S:476:ARG:NH2	5:S:1558:TYR:O	2.50	0.45
5:S:1397:ASP:OD1	5:S:1398:VAL:N	2.50	0.45
5:S:1952:ILE:HD12	5:S:1961:PHE:HD1	1.79	0.45
5:S:3568:ILE:HA	5:S:3571:PHE:HD2	1.82	0.45
5:S:3589:SER:HA	5:S:3592:VAL:HG12	1.98	0.45
6:T:86:VAL:HG23	6:T:104:VAL:HA	1.99	0.45
9:A:50:ARG:NH1	9:A:50:ARG:O	2.39	0.45
9:A:60:LEU:HA	9:A:63:LYS:HE3	1.98	0.45
9:A:114:TRP:HB2	9:A:130:PHE:CD2	2.51	0.45
4:P:158:VAL:HG22	4:P:161:ARG:HH22	1.81	0.45
5:S:442:GLN:O	5:S:445:SER:OG	2.31	0.45
5:S:978:GLN:OE1	5:S:2598:ARG:N	2.50	0.45
5:S:1297:PHE:HA	5:S:1301:ILE:HG12	1.99	0.45
5:S:1342:MET:O	5:S:1346:THR:HG23	2.17	0.45
6:T:340:PHE:HD2	6:T:408:PRO:HD2	1.82	0.45
8:j:19:DA:H1'	8:j:20:DT:H5'	1.99	0.45
9:A:117:LEU:HD23	9:A:125:VAL:HG21	1.97	0.45
2:L:161:LEU:HD12	2:L:163:PHE:CE1	2.51	0.45
5:S:745:VAL:HA	5:S:748:TYR:CD2	2.51	0.45
5:S:890:LYS:HA	5:S:890:LYS:HD3	1.74	0.45
5:S:994:TRP:CD2	5:S:2581:LEU:HD21	2.52	0.45
5:S:1387:GLY:O	5:S:1389:VAL:HG13	2.17	0.45
5:S:2584:CYS:SG	5:S:2585:GLU:N	2.89	0.45
1:E:825:VAL:HA	1:E:878:PHE:HZ	1.81	0.45
2:L:438:LEU:HD12	2:L:441:SER:HB3	1.99	0.45
5:S:175:TYR:HB2	5:S:223:CYS:HB3	1.98	0.45
5:S:181:LEU:HD23	5:S:181:LEU:HA	1.83	0.45
5:S:1067:ALA:HB1	5:S:1110:SER:HB3	1.98	0.45
5:S:1770:GLN:O	5:S:1771:GLN:HG3	2.16	0.45
5:S:3100:LYS:HA	5:S:3103:ILE:HG22	1.99	0.45
5:S:3311:ASN:HB2	5:S:3314:SER:HA	1.98	0.45
5:S:3326:GLN:HA	5:S:3329:LEU:HD12	1.98	0.45
5:S:2210:VAL:O	5:S:2214:ARG:HG2	2.16	0.44
5:S:2434:VAL:O	5:S:2438:ILE:HG12	2.17	0.44
5:S:3075:LYS:HA	5:S:3078:LEU:HG	1.99	0.44
5:S:3700:GLU:HG3	5:S:3718:ARG:HH11	1.82	0.44
6:T:218:ARG:H	6:T:221:ILE:HG12	1.81	0.44
2:L:45:GLN:NE2	2:L:50:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:56:LEU:HD12	2:L:80:HIS:HB3	1.98	0.44
2:L:484:ASN:ND2	2:L:486:ARG:HB3	2.32	0.44
2:L:530:LEU:HD13	6:T:264:ASN:HD22	1.82	0.44
5:S:865:GLN:HB2	5:S:3168:TYR:CE2	2.51	0.44
5:S:1227:GLY:HA2	5:S:1260:LEU:HD23	1.97	0.44
5:S:2154:GLU:HA	5:S:2157:PHE:CE1	2.53	0.44
5:S:2254:ARG:CZ	5:S:2292:CYS:HA	2.47	0.44
5:S:2492:ASP:OD2	5:S:2495:SER:N	2.36	0.44
5:S:2832:ILE:N	5:S:2835:LYS:HZ2	2.15	0.44
5:S:3665:MET:HA	5:S:3668:LEU:HG	1.97	0.44
5:S:4085:LYS:O	5:S:4089:ILE:HG12	2.16	0.44
6:T:303:PHE:HA	6:T:311:LEU:H	1.81	0.44
1:E:725:TRP:HA	1:E:741:ARG:HH22	1.82	0.44
5:S:1034:ARG:NH1	5:S:1088:GLU:OE2	2.51	0.44
5:S:2751:GLN:HA	5:S:2754:GLU:CD	2.42	0.44
5:S:3820:MET:HG2	5:S:3824:GLU:HB3	1.99	0.44
5:S:3887:PHE:HA	5:S:3890:MET:HG3	1.99	0.44
5:S:3923:ARG:HD2	5:S:4121:TRP:CD1	2.51	0.44
2:L:71:GLY:O	2:L:73:GLN:N	2.51	0.44
2:L:523:THR:O	2:L:527:GLN:HG2	2.17	0.44
5:S:1071:ASN:ND2	5:S:1074:LYS:HG3	2.33	0.44
5:S:1215:GLU:OE1	5:S:1222:ASN:ND2	2.49	0.44
5:S:1220:LEU:O	5:S:1224:PHE:HB2	2.18	0.44
5:S:1874:TYR:HB3	5:S:1947:CYS:SG	2.57	0.44
5:S:2886:GLN:HB3	5:S:2929:LEU:HD12	1.99	0.44
5:S:3320:ILE:HD11	5:S:3394:GLU:HB2	1.99	0.44
5:S:3327:ASN:HB2	5:S:3388:ALA:HB2	2.00	0.44
5:S:3868:VAL:HG22	5:S:3872:ARG:HH11	1.83	0.44
1:E:702:ALA:N	1:E:721:VAL:O	2.47	0.44
5:S:1597:LEU:HD11	5:S:1648:LEU:HD22	1.99	0.44
5:S:2105:HIS:HB2	5:S:2156:VAL:HG13	2.00	0.44
5:S:2293:GLY:O	5:S:2295:GLN:N	2.50	0.44
5:S:3241:LYS:HE3	5:S:3241:LYS:HB2	1.75	0.44
5:S:3425:ARG:NH2	5:S:3428:GLU:HG2	2.31	0.44
6:T:403:ARG:HD3	6:T:404:ARG:O	2.16	0.44
1:E:668:SER:HG	1:E:708:ARG:HH21	1.63	0.44
5:S:655:LEU:O	5:S:659:ARG:HG2	2.17	0.44
5:S:746:ARG:HH22	5:S:788:TYR:HD2	1.66	0.44
5:S:981:ARG:HA	5:S:984:TYR:HB2	1.99	0.44
5:S:3234:CYS:O	5:S:3238:MET:HG2	2.17	0.44
1:E:864:ILE:HG13	1:E:889:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:653:GLN:O	2:L:657:ASN:ND2	2.51	0.44
5:S:465:PHE:CE1	5:S:479:ILE:HG22	2.53	0.44
5:S:733:LEU:HA	5:S:736:LEU:HD23	2.00	0.44
5:S:953:GLN:H	5:S:956:PRO:HD3	1.82	0.44
5:S:1633:TRP:CD1	5:S:1674:THR:HG21	2.53	0.44
5:S:675:ARG:NH1	5:S:676:ASN:OD1	2.50	0.44
5:S:1207:TRP:HE3	5:S:1208:LEU:HD12	1.82	0.44
5:S:1834:ASP:HA	5:S:1837:ARG:HD2	2.00	0.44
5:S:1850:VAL:HG21	5:S:1873:TYR:CZ	2.53	0.44
5:S:2328:ARG:HH21	5:S:2372:PRO:HD2	1.83	0.44
5:S:2791:ILE:HG13	5:S:2792:THR:N	2.33	0.44
5:S:3877:LYS:HZ2	5:S:4127:TRP:CG	2.36	0.44
5:S:4012:ASP:C	5:S:4014:LYS:N	2.76	0.44
6:T:115:ARG:HA	6:T:118:GLU:HG2	1.99	0.44
7:i:38:DT:N3	8:j:19:DA:N1	2.66	0.44
9:A:114:TRP:HB2	9:A:130:PHE:CG	2.53	0.44
1:E:722:LYS:HB2	1:E:742:PHE:HB2	1.99	0.44
2:L:56:LEU:HG	2:L:81:ARG:HB3	1.99	0.44
2:L:366:ALA:HB2	2:L:377:LEU:HD12	2.00	0.44
2:L:513:TRP:O	2:L:517:ASN:N	2.35	0.44
5:S:188:GLU:HG2	5:S:189:MET:H	1.83	0.44
5:S:374:LYS:HE2	5:S:381:VAL:HG21	2.00	0.44
5:S:1082:PHE:HZ	5:S:1134:LEU:HD21	1.83	0.44
5:S:1136:ARG:O	5:S:1139:GLU:HG2	2.18	0.44
5:S:1146:ASN:ND2	5:S:1199:PRO:HG3	2.33	0.44
5:S:3443:PRO:HA	5:S:3446:VAL:HG22	1.99	0.44
5:S:3447:VAL:HA	5:S:3450:MET:HE2	2.00	0.44
5:S:4064:LEU:HB3	5:S:4074:PHE:HE1	1.83	0.44
6:T:466:VAL:O	6:T:470:ARG:HG3	2.17	0.44
6:T:481:PRO:HA	6:T:484:GLN:HG2	1.99	0.44
6:T:483:LEU:HA	6:T:486:HIS:HD1	1.83	0.44
5:S:12:LEU:HA	5:S:15:LEU:HD12	2.00	0.43
5:S:380:ASP:HA	5:S:383:PHE:HB2	2.00	0.43
5:S:581:LEU:HB3	5:S:660:LEU:HD12	1.99	0.43
5:S:1000:LYS:HB2	5:S:1004:GLN:NE2	2.33	0.43
5:S:1019:ASP:OD1	5:S:1019:ASP:N	2.48	0.43
5:S:1204:PRO:HG2	5:S:1206:LEU:HG	2.00	0.43
5:S:1367:HIS:HB2	5:S:1370:ARG:CZ	2.48	0.43
5:S:1963:GLN:HB2	5:S:2125:TRP:CZ2	2.53	0.43
5:S:2430:GLU:HG2	5:S:2431:ARG:N	2.33	0.43
9:A:64:GLN:O	9:A:68:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:289:ILE:HA	6:T:311:LEU:HD11	2.00	0.43
2:L:402:ASN:N	7:i:25:DA:OP1	2.51	0.43
5:S:754:MET:HE3	5:S:1021:VAL:HG11	2.00	0.43
5:S:1102:GLU:HA	5:S:1154:PRO:HB3	2.00	0.43
5:S:2410:GLU:OE2	5:S:2412:TYR:N	2.51	0.43
1:E:682:ILE:HG13	1:E:730:PHE:CZ	2.50	0.43
2:L:205:LEU:HG	2:L:209:LYS:HD2	1.99	0.43
2:L:413:LYS:N	2:L:416:TYR:O	2.50	0.43
5:S:57:LEU:HB3	5:S:103:TYR:HE2	1.83	0.43
5:S:174:VAL:O	5:S:178:LEU:HG	2.19	0.43
5:S:708:VAL:C	5:S:712:LYS:HZ2	2.26	0.43
5:S:727:ALA:O	5:S:731:THR:OG1	2.30	0.43
5:S:781:ASP:O	5:S:785:MET:HG2	2.18	0.43
5:S:960:GLN:HA	5:S:963:LYS:HZ3	1.84	0.43
5:S:1390:GLN:HA	5:S:1393:ALA:HB3	1.99	0.43
5:S:1794:GLN:O	5:S:1798:LEU:HG	2.18	0.43
5:S:3247:ARG:HE	5:S:3282:ARG:HE	1.65	0.43
5:S:3289:ARG:H	5:S:3292:GLY:HA3	1.83	0.43
5:S:3772:ASN:HD21	5:S:3787:GLN:HE21	1.66	0.43
5:S:196:LEU:HB3	5:S:200:PHE:CE2	2.53	0.43
5:S:896:VAL:O	5:S:902:LYS:HB3	2.17	0.43
5:S:2311:ARG:HG2	5:S:2312:TYR:HD1	1.84	0.43
5:S:2805:ALA:HA	5:S:2808:LEU:HG	2.00	0.43
5:S:3257:LYS:HA	5:S:3257:LYS:HD3	1.71	0.43
5:S:3270:ASP:N	5:S:3270:ASP:OD1	2.50	0.43
5:S:3584:LEU:HD12	5:S:3799:ARG:HH21	1.84	0.43
5:S:3633:ILE:HG13	5:S:3634:GLN:N	2.33	0.43
5:S:3700:GLU:HA	5:S:3718:ARG:HA	2.00	0.43
5:S:3800:LEU:HD12	5:S:3800:LEU:HA	1.93	0.43
5:S:3901:ARG:NH2	5:S:3970:LEU:HG	2.32	0.43
6:T:420:LEU:HB3	6:T:424:LYS:HA	2.00	0.43
5:S:321:LYS:HD2	5:S:321:LYS:HA	1.71	0.43
5:S:417:VAL:O	5:S:421:LEU:HD23	2.18	0.43
5:S:1405:ALA:HA	5:S:1408:MET:HE2	2.00	0.43
5:S:1632:TRP:HD1	5:S:1645:VAL:HB	1.84	0.43
5:S:1948:ALA:O	5:S:1952:ILE:HG12	2.19	0.43
5:S:2254:ARG:HH11	5:S:2294:ILE:HG13	1.83	0.43
5:S:2271:SER:HA	5:S:2274:ILE:HD13	2.01	0.43
5:S:3718:ARG:H	5:S:3743:HIS:HB3	1.84	0.43
6:T:77:SER:HA	6:T:248:ALA:O	2.18	0.43
9:A:89:MET:HE2	9:A:89:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:513:TRP:HB3	2:L:517:ASN:ND2	2.33	0.43
4:Q:194:LEU:HA	4:Q:197:LYS:HE2	2.01	0.43
5:S:207:GLN:C	5:S:217:LEU:HD11	2.44	0.43
5:S:682:TYR:CZ	5:S:700:LYS:HG2	2.54	0.43
5:S:935:HIS:HA	5:S:938:VAL:HG12	2.00	0.43
5:S:1056:THR:HG21	5:S:1095:LEU:HD13	2.00	0.43
5:S:1475:LEU:HB2	5:S:1477:HIS:CE1	2.53	0.43
5:S:3075:LYS:O	5:S:3078:LEU:HG	2.18	0.43
5:S:3287:ARG:HA	5:S:3289:ARG:HH21	1.82	0.43
8:j:27:DT:H2"	8:j:28:DA:C8	2.53	0.43
2:L:662:LEU:HA	2:L:665:LYS:HE2	2.01	0.43
4:Q:161:ARG:HA	4:Q:164:LYS:HE3	2.01	0.43
5:S:290:TYR:OH	5:S:339:GLN:OE1	2.28	0.43
5:S:293:LEU:HA	5:S:296:VAL:HG12	2.01	0.43
5:S:1425:ALA:HA	5:S:1428:ILE:HG22	2.00	0.43
5:S:1504:ASP:O	5:S:1508:LYS:N	2.48	0.43
5:S:2300:PHE:HD2	5:S:2341:LEU:HD13	1.84	0.43
5:S:2467:THR:HB	5:S:2517:LEU:HD11	2.00	0.43
5:S:2497:GLU:HA	5:S:2500:LYS:HD2	2.00	0.43
5:S:2869:LEU:HB2	5:S:2899:ARG:HE	1.83	0.43
5:S:3739:ILE:HG23	5:S:3747:GLU:CD	2.44	0.43
5:S:4080:VAL:HG21	5:S:4119:ARG:HD2	2.01	0.43
1:E:806:ASP:HB3	1:E:816:HIS:CD2	2.53	0.43
2:L:604:GLN:HG3	2:L:605:LYS:HG3	2.01	0.43
4:Q:178:LYS:HA	4:Q:181:ILE:HG22	2.01	0.43
5:S:450:SER:N	5:S:453:MET:SD	2.92	0.43
5:S:864:GLY:N	5:S:3170:ASP:OD1	2.40	0.43
5:S:898:PHE:H	5:S:902:LYS:HE3	1.83	0.43
5:S:1287:GLN:OE1	5:S:1289:SER:N	2.48	0.43
5:S:2431:ARG:HA	5:S:2434:VAL:HG12	2.01	0.43
5:S:2816:ILE:O	5:S:2820:MET:HG2	2.18	0.43
5:S:3078:LEU:HD13	5:S:3086:LEU:HD11	1.99	0.43
5:S:3165:THR:O	5:S:3238:MET:HE1	2.19	0.43
5:S:3828:TYR:OH	5:S:4127:TRP:NE1	2.51	0.43
2:L:6:ASN:HA	2:L:51:LYS:HD2	2.01	0.43
2:L:675:TRP:O	2:L:679:VAL:N	2.48	0.43
4:P:183:VAL:HG11	4:Q:184:LEU:HD13	2.01	0.43
5:S:57:LEU:O	5:S:60:SER:OG	2.33	0.43
5:S:2752:LYS:HD2	5:S:2755:LYS:HZ1	1.84	0.43
5:S:3761:ASP:OD1	5:S:3762:GLN:N	2.51	0.43
5:S:3767:LEU:HA	5:S:3770:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3923:ARG:HH11	5:S:4121:TRP:HE1	1.66	0.43
6:T:99:PHE:CD2	6:T:145:GLU:HB2	2.54	0.43
6:T:357:LYS:HE2	6:T:359:HIS:NE2	2.33	0.43
2:L:154:LEU:HD23	2:L:154:LEU:HA	1.88	0.43
2:L:243:HIS:HD2	2:L:264:TYR:HE2	1.66	0.43
2:L:250:ARG:HA	2:L:260:ARG:HA	2.01	0.43
2:L:291:LYS:HA	6:T:302:THR:HA	2.00	0.43
2:L:463:LEU:C	6:T:351:LYS:HZ3	2.27	0.43
4:P:185:ASN:O	4:P:189:THR:HG23	2.19	0.43
5:S:1011:GLU:HA	5:S:1014:LEU:HG	2.01	0.43
5:S:1304:HIS:CD2	5:S:1307:ILE:HG23	2.54	0.43
5:S:1934:LEU:HA	5:S:1937:ARG:HH12	1.84	0.43
5:S:2150:VAL:HG23	5:S:2157:PHE:CZ	2.54	0.43
5:S:3972:LEU:HB3	5:S:3973:PRO:HD3	2.00	0.43
1:E:787:GLN:HE22	4:Q:178:LYS:NZ	2.17	0.42
1:E:812:MET:HE1	1:E:844:GLU:HB3	2.01	0.42
2:L:88:PHE:HD1	2:L:91:LEU:HD12	1.84	0.42
2:L:163:PHE:HB2	2:L:224:ILE:HG12	2.00	0.42
2:L:311:ILE:HA	2:L:325:LYS:NZ	2.34	0.42
5:S:23:ASP:OD1	5:S:23:ASP:N	2.52	0.42
5:S:247:GLU:OE1	5:S:285:CYS:HB2	2.19	0.42
5:S:851:ILE:O	5:S:855:VAL:HG23	2.19	0.42
5:S:977:ASP:HB3	5:S:980:THR:OG1	2.19	0.42
5:S:2331:MET:HE1	5:S:2338:GLU:OE1	2.18	0.42
5:S:3923:ARG:HD2	5:S:4121:TRP:HD1	1.84	0.42
5:S:3971:MET:SD	5:S:3974:MET:HB2	2.59	0.42
2:L:92:GLU:HA	2:L:95:GLU:HG3	2.01	0.42
5:S:721:TYR:HB2	5:S:726:LEU:HB3	2.00	0.42
5:S:785:MET:HB3	5:S:789:TYR:CZ	2.54	0.42
5:S:933:LEU:HD22	5:S:2797:VAL:HG21	2.00	0.42
5:S:1082:PHE:CZ	5:S:1134:LEU:HD21	2.55	0.42
5:S:2170:GLN:HA	5:S:2211:LEU:HD22	2.01	0.42
5:S:2183:HIS:O	5:S:2187:VAL:HG13	2.18	0.42
5:S:2317:ALA:O	5:S:2366:LYS:HD3	2.20	0.42
5:S:2452:ARG:CZ	5:S:2494:ASP:HB3	2.49	0.42
5:S:3172:LYS:HD2	5:S:3172:LYS:HA	1.77	0.42
5:S:3193:ILE:HA	5:S:3196:LYS:HG2	2.01	0.42
6:T:262:LYS:O	6:T:346:MET:HA	2.19	0.42
1:E:883:LYS:HD3	1:E:883:LYS:HA	1.81	0.42
5:S:1268:ASN:HD21	5:S:1344:PHE:HB2	1.84	0.42
5:S:1569:THR:O	5:S:1573:LYS:NZ	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2421:VAL:HA	5:S:2424:MET:HG3	2.01	0.42
5:S:2548:PRO:HB2	5:S:2848:PHE:CD1	2.55	0.42
5:S:3835:PRO:HB2	5:S:3836:PRO:HD3	2.00	0.42
6:T:301:ARG:NH1	9:A:57:ARG:HH21	2.17	0.42
9:A:41:LEU:HB2	9:A:68:HIS:HB2	2.00	0.42
2:L:61:THR:N	2:L:76:ASN:O	2.52	0.42
2:L:251:LEU:HD23	2:L:259:ILE:HD13	2.02	0.42
5:S:891:ARG:HH12	5:S:959:TYR:H	1.67	0.42
5:S:1256:TRP:CE2	5:S:1260:LEU:HD11	2.54	0.42
5:S:1614:GLN:HA	5:S:1617:LYS:HE2	2.01	0.42
6:T:301:ARG:HH12	9:A:57:ARG:HH21	1.65	0.42
2:L:250:ARG:NH2	6:T:536:PRO:HB2	2.35	0.42
5:S:130:LEU:HD12	5:S:130:LEU:HA	1.79	0.42
5:S:479:ILE:HA	5:S:482:VAL:HG22	2.01	0.42
5:S:858:MET:HE2	5:S:858:MET:HB2	1.94	0.42
5:S:943:GLY:HA3	5:S:2783:ILE:HG21	2.00	0.42
5:S:978:GLN:NE2	5:S:2597:PHE:HA	2.35	0.42
5:S:1017:ILE:HG13	5:S:1018:VAL:N	2.34	0.42
5:S:1658:SER:O	5:S:1662:ASN:HB3	2.19	0.42
5:S:1713:VAL:O	5:S:1716:GLN:HG2	2.20	0.42
5:S:1936:ARG:HH21	5:S:1937:ARG:NH2	2.17	0.42
5:S:2364:LEU:HA	5:S:2367:VAL:HG22	2.02	0.42
5:S:3416:LEU:HB3	5:S:3449:LYS:NZ	2.35	0.42
6:T:465:ILE:HG13	6:T:525:PHE:HE2	1.84	0.42
8:j:32:DT:H2"	8:j:33:DA:N7	2.34	0.42
2:L:298:ASN:HB3	6:T:297:LYS:HG2	2.01	0.42
2:L:327:ASP:OD1	2:L:328:GLU:N	2.51	0.42
2:L:497:ARG:NH2	2:L:500:HIS:O	2.53	0.42
2:L:596:GLU:HA	2:L:599:ARG:HD2	2.01	0.42
4:P:155:TRP:HD1	4:Q:155:TRP:HA	1.85	0.42
5:S:1834:ASP:N	5:S:1834:ASP:OD1	2.51	0.42
5:S:3588:TRP:CZ3	5:S:3609:MET:HG3	2.55	0.42
5:S:3700:GLU:OE2	5:S:3704:GLN:NE2	2.38	0.42
6:T:339:ARG:HA	6:T:405:ASN:HA	2.01	0.42
6:T:363:ARG:HG3	6:T:364:PRO:HD2	2.02	0.42
2:L:223:GLU:OE2	2:L:238:LYS:NZ	2.53	0.42
5:S:993:HIS:O	5:S:996:THR:OG1	2.37	0.42
5:S:1018:VAL:HG22	5:S:1074:LYS:HG2	2.01	0.42
5:S:1031:ARG:NH2	5:S:1034:ARG:HH11	2.14	0.42
5:S:2184:TYR:O	5:S:2187:VAL:HG22	2.19	0.42
5:S:2890:ILE:HD11	5:S:2929:LEU:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2953:THR:OG1	5:S:2994:TRP:NE1	2.52	0.42
6:T:32:TYR:HB2	6:T:252:ARG:HH22	1.83	0.42
6:T:403:ARG:NE	7:i:32:DA:OP1	2.43	0.42
1:E:778:PHE:CG	4:Q:176:LEU:HD22	2.54	0.42
2:L:677:ILE:HA	2:L:680:GLN:HG2	2.01	0.42
5:S:30:ALA:O	5:S:34:LEU:HG	2.20	0.42
5:S:73:LEU:O	5:S:82:ARG:NH2	2.53	0.42
5:S:520:LYS:HA	5:S:520:LYS:HD2	1.90	0.42
5:S:774:GLU:O	5:S:778:ILE:HG12	2.20	0.42
5:S:1258:ASP:HA	5:S:1261:LEU:HD12	2.02	0.42
5:S:2261:SER:O	5:S:2270:ASN:ND2	2.48	0.42
5:S:2584:CYS:HB3	5:S:2586:PHE:CZ	2.55	0.42
5:S:2820:MET:HA	5:S:2823:PHE:HE1	1.85	0.42
5:S:3156:PRO:O	5:S:3160:LEU:N	2.53	0.42
5:S:3741:ARG:HA	5:S:3747:GLU:HA	2.02	0.42
9:A:83:ILE:HG13	9:A:107:ALA:HB1	2.01	0.42
2:L:16:VAL:HG21	2:L:61:THR:HG22	2.02	0.42
2:L:154:LEU:HD13	2:L:215:LEU:HD13	2.02	0.42
2:L:155:LYS:HA	2:L:155:LYS:HD3	1.68	0.42
2:L:453:ALA:O	2:L:533:ILE:HD11	2.20	0.42
5:S:194:GLU:O	5:S:198:ARG:HG2	2.20	0.42
5:S:294:PHE:HE1	5:S:319:PHE:HE2	1.68	0.42
5:S:992:ILE:HG23	5:S:1036:PHE:CD1	2.49	0.42
5:S:2468:THR:HA	5:S:2471:GLU:CD	2.45	0.42
5:S:3295:GLU:O	5:S:3298:LEU:HG	2.20	0.42
5:S:3700:GLU:HG3	5:S:3718:ARG:HD3	2.01	0.42
5:S:3828:TYR:CD2	5:S:3829:LEU:HD22	2.54	0.42
6:T:82:LEU:C	6:T:83:LEU:HD12	2.44	0.42
6:T:488:ARG:CZ	6:T:503:ALA:HA	2.50	0.42
1:E:720:VAL:HG11	1:E:744:ILE:HB	2.02	0.42
1:E:811:SER:O	1:E:900:LYS:HG2	2.18	0.42
5:S:1588:ASP:OD1	5:S:1588:ASP:N	2.52	0.42
5:S:3580:ASN:OD1	5:S:3580:ASN:N	2.53	0.42
5:S:4010:SER:O	5:S:4011:PHE:C	2.62	0.42
6:T:33:SER:HB3	6:T:162:SER:HB2	2.02	0.42
6:T:64:ILE:O	6:T:68:GLN:HG2	2.20	0.42
7:i:20:DT:O2	8:j:38:DG:N1	2.50	0.42
8:j:15:DA:N3	8:j:16:DA:N6	2.67	0.42
1:E:675:LYS:HD2	1:E:675:LYS:HA	1.74	0.41
1:E:815:ARG:O	1:E:816:HIS:ND1	2.53	0.41
2:L:166:PRO:HA	2:L:227:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:366:TYR:HA	5:S:369:PHE:CD1	2.55	0.41
5:S:465:PHE:HE1	5:S:479:ILE:HG22	1.85	0.41
5:S:975:ASP:O	5:S:981:ARG:NH2	2.53	0.41
5:S:1135:CYS:HA	5:S:1138:ILE:HG12	2.01	0.41
5:S:2162:LYS:HZ3	5:S:2200:ALA:HA	1.83	0.41
5:S:2327:LEU:HG	5:S:2371:PHE:CG	2.55	0.41
5:S:2331:MET:O	5:S:2334:LYS:HG2	2.20	0.41
5:S:3110:PHE:HB3	5:S:3128:LYS:HE2	2.02	0.41
5:S:3353:GLU:HG3	5:S:3358:ARG:HH12	1.85	0.41
5:S:3449:LYS:HA	5:S:3452:LYS:HG2	2.02	0.41
5:S:3480:LEU:HD23	5:S:3480:LEU:HA	1.94	0.41
5:S:3765:GLU:OE2	5:S:3769:GLN:NE2	2.53	0.41
5:S:3872:ARG:HA	5:S:3875:GLU:HG2	2.01	0.41
5:S:4106:CYS:SG	5:S:4110:GLN:NE2	2.93	0.41
8;j:24:DT:H1'	8;j:25:DT:H5'	2.02	0.41
2:L:279:VAL:HG23	6:T:317:LYS:HB2	2.02	0.41
4:P:175:ASP:O	4:P:179:ARG:HG2	2.20	0.41
5:S:1607:GLU:OE1	5:S:1610:ASN:ND2	2.52	0.41
5:S:1952:ILE:HG23	5:S:1961:PHE:CE1	2.54	0.41
5:S:2208:ASP:OD1	5:S:2209:GLU:N	2.53	0.41
5:S:3090:TYR:HB3	5:S:3095:ASP:HB2	2.02	0.41
5:S:3171:ALA:HA	5:S:3179:TRP:CZ2	2.56	0.41
5:S:3639:GLU:HA	5:S:3642:LYS:HE2	2.02	0.41
6:T:269:ILE:HG23	6:T:378:SER:HB3	2.02	0.41
6:T:276:LEU:H	6:T:276:LEU:HD23	1.84	0.41
6:T:288:LEU:HA	6:T:295:PRO:HA	2.02	0.41
6:T:418:GLU:HA	6:T:428:THR:O	2.19	0.41
2:L:54:ILE:HG22	2:L:86:PRO:HD3	2.02	0.41
2:L:512:ILE:HA	2:L:515:MET:SD	2.61	0.41
5:S:337:LYS:HA	5:S:341:PHE:CD1	2.55	0.41
5:S:428:PRO:HB2	5:S:431:TYR:CD2	2.55	0.41
5:S:475:LEU:O	5:S:479:ILE:HG12	2.20	0.41
5:S:1506:SER:O	5:S:1509:GLN:NE2	2.53	0.41
5:S:1632:TRP:CD1	5:S:1645:VAL:HB	2.55	0.41
5:S:1713:VAL:HA	5:S:1716:GLN:NE2	2.35	0.41
5:S:1779:GLN:O	5:S:1783:ARG:HG2	2.20	0.41
5:S:3114:TYR:HB2	5:S:3128:LYS:HZ2	1.85	0.41
5:S:3761:ASP:HA	5:S:3764:VAL:HG12	2.02	0.41
5:S:3814:ASP:OD1	5:S:3814:ASP:N	2.54	0.41
5:S:3967:PHE:O	5:S:3970:LEU:HD22	2.20	0.41
2:L:291:LYS:HE2	6:T:300:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:618:ASN:HA	2:L:621:GLU:CD	2.45	0.41
5:S:275:PHE:CE2	5:S:319:PHE:HB2	2.55	0.41
5:S:446:PHE:CE1	5:S:454:GLN:HG2	2.55	0.41
5:S:993:HIS:HE2	5:S:1035:GLU:CD	2.27	0.41
5:S:1693:VAL:HG11	5:S:1746:PHE:CE1	2.55	0.41
5:S:2300:PHE:CD2	5:S:2341:LEU:HD13	2.55	0.41
5:S:2364:LEU:O	5:S:2368:THR:HG22	2.20	0.41
5:S:2514:ASN:HB3	5:S:2517:LEU:HG	2.02	0.41
5:S:2773:ARG:HH21	5:S:2785:ILE:HD13	1.85	0.41
5:S:3778:ASP:HB3	5:S:3781:CYS:HB2	2.02	0.41
5:S:4099:SER:HB3	5:S:4102:THR:HG1	1.86	0.41
6:T:67:ILE:HA	6:T:70:VAL:HG22	2.02	0.41
6:T:510:LYS:NZ	6:T:517:ARG:HH22	2.18	0.41
1:E:706:ASN:HB3	1:E:708:ARG:HH11	1.85	0.41
1:E:815:ARG:HA	1:E:851:LYS:HA	2.03	0.41
2:L:111:LEU:HD21	2:L:134:ILE:HG12	2.03	0.41
2:L:309:ASP:HA	6:T:290:ARG:HE	1.85	0.41
2:L:381:ILE:HG23	2:L:410:PRO:HB2	2.02	0.41
5:S:460:ALA:O	5:S:464:VAL:HG13	2.21	0.41
5:S:1489:LYS:HA	5:S:1489:LYS:HD3	1.82	0.41
5:S:1526:GLU:OE2	5:S:1527:ARG:NE	2.54	0.41
5:S:2840:PHE:HB2	5:S:2871:LEU:HD11	2.03	0.41
5:S:2935:GLU:OE1	5:S:2937:ASP:N	2.53	0.41
5:S:3011:LEU:HB3	5:S:3047:SER:CB	2.50	0.41
5:S:3033:GLU:HG2	5:S:3034:PRO:HD3	2.01	0.41
5:S:3459:ASN:O	5:S:3463:LEU:HG	2.21	0.41
5:S:3460:GLU:O	5:S:3464:LYS:NZ	2.48	0.41
5:S:3498:TRP:O	5:S:3502:MET:HG2	2.20	0.41
5:S:4061:CYS:O	5:S:4065:LEU:HG	2.20	0.41
6:T:512:GLU:H	6:T:512:GLU:CD	2.29	0.41
1:E:797:ALA:HB1	1:E:801:TYR:CZ	2.55	0.41
1:E:876:LYS:HD3	1:E:876:LYS:HA	1.90	0.41
2:L:468:GLU:O	2:L:469:LYS:HG2	2.20	0.41
2:L:529:PRO:HA	2:L:532:LYS:HE2	2.03	0.41
5:S:225:LYS:HD2	5:S:270:ALA:HB1	2.02	0.41
5:S:651:TYR:HD1	5:S:706:LEU:HD11	1.85	0.41
5:S:789:TYR:HA	5:S:792:ILE:HG12	2.02	0.41
5:S:833:HIS:HB2	5:S:835:LYS:NZ	2.36	0.41
5:S:1065:SER:O	5:S:1068:LEU:HG	2.20	0.41
5:S:3330:LEU:HD23	5:S:3384:HIS:CD2	2.56	0.41
5:S:3351:ILE:O	5:S:3357:ARG:NH1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:3585:PHE:CD2	5:S:3667:LEU:HD23	2.56	0.41
5:S:3713:PRO:HB2	5:S:3716:HIS:CE1	2.55	0.41
6:T:130:ARG:O	6:T:134:MET:HG3	2.21	0.41
6:T:369:TYR:CG	6:T:370:PRO:HD2	2.56	0.41
2:L:59:PHE:HA	2:L:77:ILE:HA	2.02	0.41
2:L:250:ARG:HG2	2:L:260:ARG:HG2	2.03	0.41
5:S:654:ILE:HD13	5:S:706:LEU:HD22	2.02	0.41
5:S:1205:ASN:OD1	5:S:1206:LEU:N	2.54	0.41
5:S:1753:SER:O	5:S:1754:GLN:HG2	2.20	0.41
5:S:2185:MET:O	5:S:2189:ILE:HG12	2.20	0.41
5:S:2253:TYR:CE1	5:S:2288:TYR:HA	2.55	0.41
5:S:2333:ARG:NH1	5:S:2336:ILE:HD11	2.36	0.41
5:S:3096:VAL:HG12	5:S:3100:LYS:NZ	2.35	0.41
5:S:3246:ALA:HA	5:S:3249:GLN:HB2	2.03	0.41
5:S:3753:LYS:HE3	5:S:3753:LYS:HB3	1.92	0.41
5:S:3780:ALA:HB3	5:S:3989:ARG:HH22	1.86	0.41
5:S:3815:LEU:HA	5:S:3818:ASN:HD21	1.86	0.41
5:S:3894:PRO:O	5:S:3897:PHE:HB3	2.20	0.41
6:T:94:LYS:HD3	6:T:103:TYR:CE1	2.55	0.41
1:E:816:HIS:H	1:E:851:LYS:N	2.19	0.41
4:P:154:ASP:HB3	4:Q:155:TRP:NE1	2.35	0.41
5:S:635:PRO:HA	5:S:675:ARG:HH12	1.86	0.41
5:S:672:ILE:HG23	5:S:675:ARG:NH2	2.36	0.41
5:S:714:VAL:HG13	5:S:733:LEU:HD21	2.03	0.41
5:S:1014:LEU:HA	5:S:1017:ILE:HG12	2.03	0.41
5:S:1047:GLN:C	5:S:1051:LYS:HZ2	2.29	0.41
5:S:1754:GLN:CD	5:S:1788:ARG:HH21	2.29	0.41
5:S:2187:VAL:HA	5:S:2190:VAL:HG22	2.02	0.41
5:S:2825:THR:O	5:S:2829:LYS:HG3	2.20	0.41
5:S:3075:LYS:HG3	5:S:3076:ALA:N	2.36	0.41
5:S:3281:CYS:O	5:S:3285:HIS:ND1	2.54	0.41
5:S:3471:ILE:HD12	5:S:3471:ILE:HA	1.97	0.41
5:S:3487:ILE:HD13	5:S:3487:ILE:HA	1.94	0.41
5:S:3626:GLY:O	5:S:3630:ARG:HD3	2.20	0.41
5:S:4069:GLU:HA	5:S:4074:PHE:CG	2.55	0.41
7:i:24:DA:H1'	7:i:25:DA:O4'	2.21	0.41
9:A:109:LEU:HD23	9:A:132:ILE:HB	2.03	0.41
1:E:768:ASP:OD1	1:E:768:ASP:N	2.54	0.41
2:L:395:TYR:N	2:L:404:GLN:O	2.37	0.41
2:L:528:ILE:O	2:L:531:SER:OG	2.30	0.41
5:S:87:LYS:O	5:S:90:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:135:LEU:HB2	5:S:177:LEU:HD11	2.02	0.41
5:S:418:ALA:HB2	5:S:464:VAL:HG12	2.03	0.41
5:S:832:LYS:NZ	5:S:836:LYS:HG3	2.36	0.41
5:S:931:CYS:O	5:S:934:LEU:HG	2.21	0.41
5:S:993:HIS:ND1	5:S:2779:ASP:HB2	2.36	0.41
5:S:1848:ILE:O	5:S:1852:LYS:NZ	2.43	0.41
5:S:2433:LYS:HG3	5:S:2472:GLN:HE22	1.86	0.41
5:S:2438:ILE:O	5:S:2442:MET:HG3	2.21	0.41
5:S:2575:PRO:HA	5:S:2785:ILE:O	2.20	0.41
5:S:2722:ARG:HA	5:S:2722:ARG:HD3	1.90	0.41
5:S:2869:LEU:HD13	5:S:2895:GLU:HG3	2.02	0.41
5:S:2957:LEU:HA	5:S:2960:GLU:HG3	2.03	0.41
5:S:2960:GLU:HB3	5:S:2968:ALA:HB2	2.03	0.41
5:S:3074:GLN:O	5:S:3077:ILE:HG12	2.20	0.41
5:S:3314:SER:HB3	5:S:3318:LYS:HD2	2.03	0.41
5:S:3563:ASP:O	5:S:3564:GLN:HG3	2.20	0.41
5:S:3686:TRP:CZ3	5:S:3691:LYS:HA	2.56	0.41
5:S:3757:ASP:O	5:S:3760:GLN:NE2	2.49	0.41
5:S:4055:ASN:ND2	5:S:4057:ALA:HB3	2.36	0.41
6:T:335:GLU:O	6:T:339:ARG:N	2.54	0.41
6:T:403:ARG:HE	7:i:32:DA:P	2.42	0.41
8:j:22:DG:H2"	8:j:23:DT:H71	2.03	0.41
9:A:50:ARG:HD3	9:A:55:ARG:NH1	2.36	0.41
2:L:443:LYS:H	2:L:443:LYS:HG2	1.73	0.41
2:L:667:GLU:HG2	2:L:675:TRP:NE1	2.36	0.41
3:M:194:LYS:HD2	3:M:195:PRO:O	2.20	0.41
5:S:326:MET:O	5:S:330:ASN:N	2.54	0.41
5:S:386:VAL:O	5:S:390:GLN:HG2	2.21	0.41
5:S:1176:CYS:HB3	5:S:1188:ILE:HD11	2.03	0.41
5:S:3048:LYS:HZ3	5:S:3061:LEU:HB2	1.85	0.41
5:S:3151:LEU:HA	5:S:3197:LEU:HG	2.03	0.41
5:S:3294:SER:HA	5:S:3297:VAL:HG22	2.02	0.41
5:S:3565:GLY:HA2	5:S:3568:ILE:HD13	2.03	0.41
5:S:3864:ARG:NH2	5:S:4085:LYS:HA	2.36	0.41
9:A:91:TYR:CD2	9:A:135:PRO:HD2	2.56	0.41
2:L:443:LYS:HG3	2:L:444:TYR:CD2	2.56	0.40
5:S:103:TYR:HA	5:S:106:GLU:CD	2.46	0.40
5:S:458:CYS:O	5:S:461:ILE:HG22	2.22	0.40
5:S:1087:ARG:HG3	5:S:1090:ARG:HH21	1.85	0.40
5:S:1164:CYS:N	5:S:1167:ASP:OD2	2.53	0.40
5:S:1947:CYS:O	5:S:1951:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2848:PHE:HD2	5:S:3077:ILE:HG22	1.87	0.40
5:S:3489:SER:OG	5:S:3490:VAL:N	2.53	0.40
6:T:275:ASN:ND2	6:T:278:GLN:HB2	2.37	0.40
6:T:308:GLY:HA3	9:A:61:PHE:HE1	1.87	0.40
2:L:40:MET:HA	2:L:43:GLN:HE21	1.86	0.40
2:L:277:THR:HB	2:L:286:LYS:HD2	2.03	0.40
2:L:466:LYS:HA	2:L:466:LYS:HD2	1.89	0.40
5:S:671:SER:HA	5:S:674:VAL:HG12	2.02	0.40
5:S:1065:SER:O	5:S:1069:HIS:ND1	2.55	0.40
5:S:2233:HIS:O	5:S:2237:ILE:HG13	2.21	0.40
5:S:3462:ARG:HG2	5:S:3498:TRP:HH2	1.85	0.40
6:T:74:LYS:HZ1	6:T:81:ASP:N	2.19	0.40
1:E:669:GLY:H	1:E:675:LYS:HD3	1.85	0.40
2:L:247:TRP:HB3	2:L:263:ALA:HB3	2.03	0.40
4:Q:149:GLU:OE2	4:Q:153:ARG:NH2	2.55	0.40
4:Q:181:ILE:HD12	4:Q:184:LEU:HD23	2.04	0.40
5:S:237:SER:C	5:S:238:MET:HE2	2.47	0.40
5:S:533:HIS:O	5:S:537:SER:HB2	2.21	0.40
5:S:639:ALA:HB2	5:S:676:ASN:HB3	2.03	0.40
5:S:889:GLU:OE2	5:S:891:ARG:HG2	2.21	0.40
5:S:1184:ARG:O	5:S:1188:ILE:HG12	2.21	0.40
5:S:1424:THR:C	5:S:1426:GLN:H	2.30	0.40
5:S:1775:GLU:HA	5:S:1778:PHE:HD2	1.84	0.40
5:S:1921:ASP:O	5:S:1924:THR:OG1	2.32	0.40
5:S:2220:MET:HE3	5:S:2255:LEU:HD21	2.04	0.40
5:S:3037:GLN:HA	5:S:3040:TYR:CD2	2.57	0.40
5:S:3259:LEU:O	5:S:3276:TRP:NE1	2.54	0.40
5:S:3576:ASP:O	5:S:3579:SER:OG	2.36	0.40
6:T:193:LEU:HB2	6:T:198:ILE:HB	2.04	0.40
6:T:278:GLN:OE1	6:T:279:LYS:N	2.55	0.40
9:A:117:LEU:HD12	9:A:120:GLN:NE2	2.36	0.40
2:L:310:ILE:H	6:T:290:ARG:HH21	1.68	0.40
2:L:439:LYS:HB2	2:L:439:LYS:HE2	1.89	0.40
5:S:356:ASN:N	5:S:358:GLU:OE2	2.55	0.40
5:S:1168:LEU:HA	5:S:1171:TRP:HB3	2.02	0.40
5:S:1574:ASN:HD21	5:S:1577:LEU:HB2	1.86	0.40
5:S:2851:PHE:CG	5:S:2853:PRO:HD2	2.57	0.40
5:S:2930:TYR:CE2	5:S:2938:VAL:HG11	2.56	0.40
5:S:3796:MET:HE1	5:S:3802:LEU:HB2	2.03	0.40
5:S:4087:HIS:O	5:S:4090:ARG:HD2	2.22	0.40
2:L:297:LEU:N	2:L:303:THR:O	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:339:CYS:HB2	2:L:394:ARG:HH22	1.85	0.40
5:S:111:CYS:HB2	5:S:130:LEU:CD1	2.44	0.40
5:S:124:LYS:HA	5:S:124:LYS:HD3	1.81	0.40
5:S:145:ASP:HA	5:S:147:PHE:CE2	2.56	0.40
5:S:246:ARG:NH1	5:S:247:GLU:HB2	2.36	0.40
5:S:374:LYS:HD3	5:S:374:LYS:HA	1.89	0.40
5:S:2218:PHE:O	5:S:2221:LYS:HG2	2.21	0.40
5:S:2408:MET:HA	5:S:2411:LEU:HD23	2.04	0.40
5:S:2886:GLN:H	5:S:2886:GLN:CD	2.29	0.40
5:S:2950:LYS:HB3	5:S:2952:ILE:HG22	2.03	0.40
5:S:3262:LEU:O	5:S:3266:SER:CB	2.70	0.40
5:S:3308:ASP:OD1	5:S:3308:ASP:N	2.52	0.40
5:S:3486:GLU:OE2	5:S:3487:ILE:HG12	2.21	0.40
5:S:3701:ILE:HD13	5:S:3719:ILE:HG12	2.02	0.40
5:S:3886:ALA:O	5:S:3889:ARG:HG2	2.20	0.40
5:S:3950:THR:HG23	5:S:3957:GLU:H	1.87	0.40
5:S:3953:LEU:HD13	5:S:3954:PRO:HD2	2.02	0.40
6:T:289:TYR:HD2	6:T:292:THR:H	1.68	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	E	242/911 (27%)	208 (86%)	32 (13%)	2 (1%)	16	53
2	L	635/732 (87%)	598 (94%)	36 (6%)	1 (0%)	44	78
3	M	21/204 (10%)	21 (100%)	0	0	100	100
4	P	55/336 (16%)	55 (100%)	0	0	100	100
4	Q	55/336 (16%)	55 (100%)	0	0	100	100
5	S	3459/4128 (84%)	3188 (92%)	263 (8%)	8 (0%)	44	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	497/609 (82%)	461 (93%)	36 (7%)	0	100	100
9	A	96/575 (17%)	96 (100%)	0	0	100	100
All	All	5060/7831 (65%)	4682 (92%)	367 (7%)	11 (0%)	45	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	814	ARG
5	S	4012	ASP
5	S	4013	TRP
5	S	1231	GLN
5	S	4010	SER
5	S	4011	PHE
5	S	4100	GLU
2	L	72	ASP
1	E	662	VAL
5	S	3304	VAL
5	S	2294	ILE

### 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	E	217/808 (27%)	217 (100%)	0	100	100
2	L	559/649 (86%)	559 (100%)	0	100	100
3	M	16/160 (10%)	16 (100%)	0	100	100
4	P	53/303 (18%)	53 (100%)	0	100	100
4	Q	51/303 (17%)	51 (100%)	0	100	100
5	S	2998/3671 (82%)	2998 (100%)	0	100	100
6	T	444/548 (81%)	444 (100%)	0	100	100
9	A	81/480 (17%)	81 (100%)	0	100	100
All	All	4419/6922 (64%)	4419 (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 (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	787	GLN
1	E	904	GLN
2	L	80	HIS
2	L	119	GLN
2	L	201	GLN
2	L	360	GLN
2	L	657	ASN
2	L	672	ASN
3	M	187	ASN
4	P	185	ASN
4	Q	145	GLN
4	Q	148	ASN
5	S	54	GLN
5	S	98	GLN
5	S	771	ASN
5	S	786	GLN
5	S	833	HIS
5	S	1049	GLN
5	S	1055	ASN
5	S	1071	ASN
5	S	1084	ASN
5	S	1125	GLN
5	S	1146	ASN
5	S	1350	ASN
5	S	1426	GLN
5	S	1471	GLN
5	S	1476	HIS
5	S	1509	GLN
5	S	1611	GLN
5	S	1737	ASN
5	S	1830	HIS
5	S	2213	ASN
5	S	2301	GLN
5	S	2306	ASN
5	S	2353	GLN
5	S	2493	ASN
5	S	2508	GLN
5	S	3154	GLN
5	S	3250	ASN

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Mol	Chain	Res	Type
5	S	3278	GLN
5	S	3383	GLN
5	S	3510	GLN
5	S	3549	HIS
5	S	3577	GLN
5	S	3590	ASN
5	S	3787	GLN
5	S	3818	ASN
5	S	4000	ASN
5	S	4042	GLN
5	S	4055	ASN
5	S	4110	GLN
6	T	68	GLN
6	T	152	ASN
6	T	416	GLN
6	T	433	GLN
6	T	484	GLN
6	T	489	ASN
6	T	515	ASN
9	A	82	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

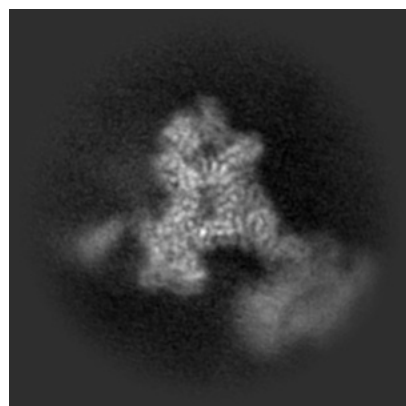
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51249. These allow visual inspection of the internal detail of the map and identification of artifacts.

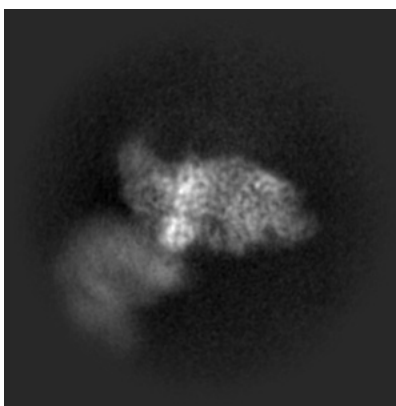
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

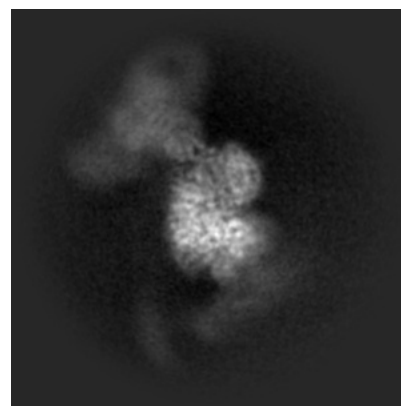
#### 6.1.1 Primary map



X

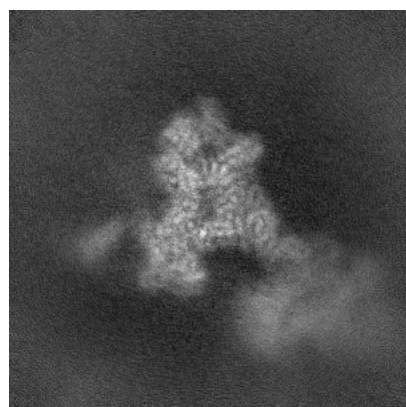


Y

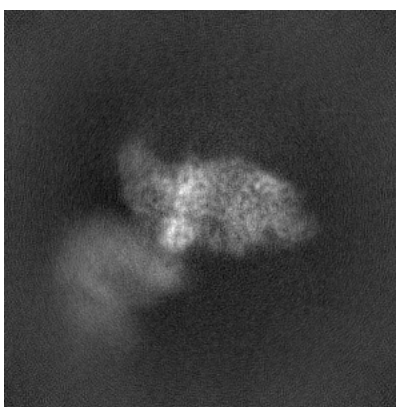


Z

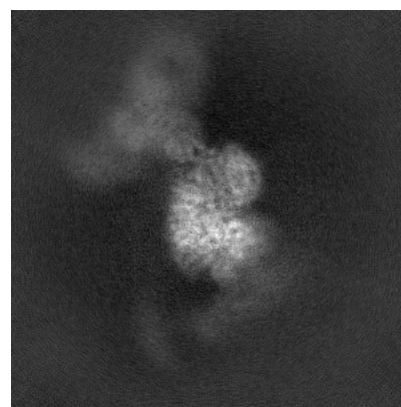
#### 6.1.2 Raw map



X



Y

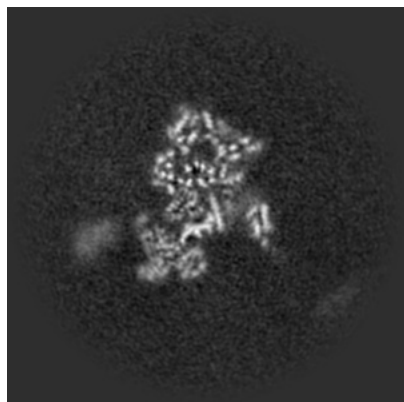


Z

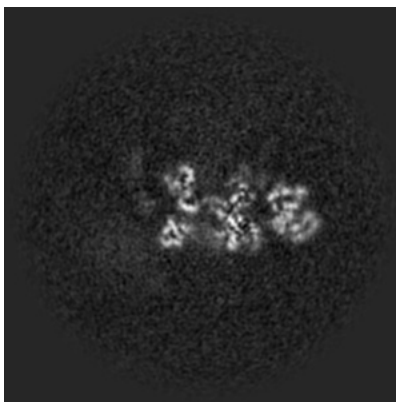
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

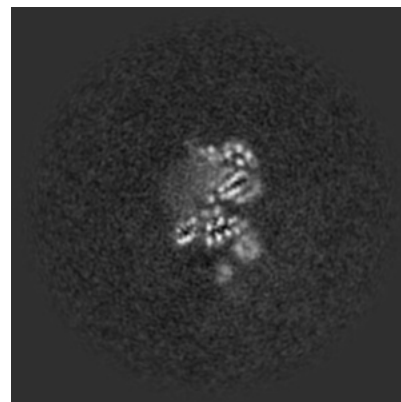
### 6.2.1 Primary map



X Index: 160

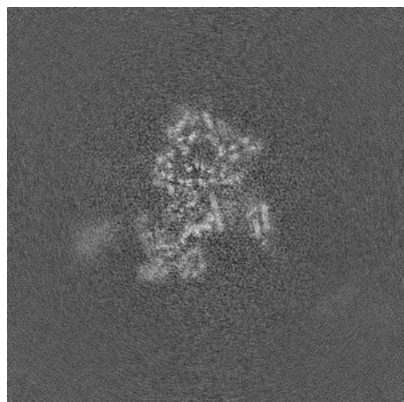


Y Index: 160

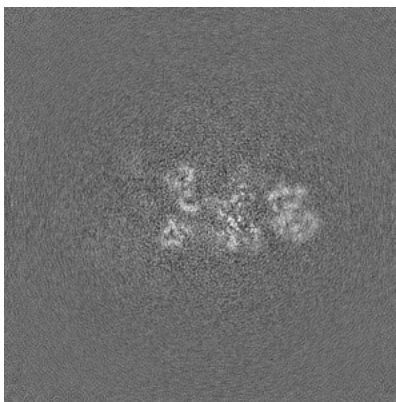


Z Index: 160

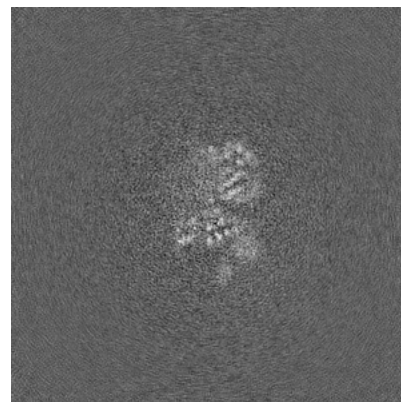
### 6.2.2 Raw map



X Index: 160



Y Index: 160

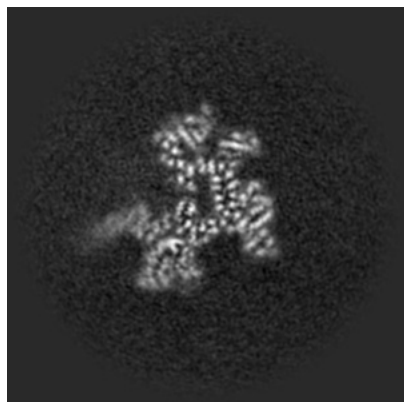


Z Index: 160

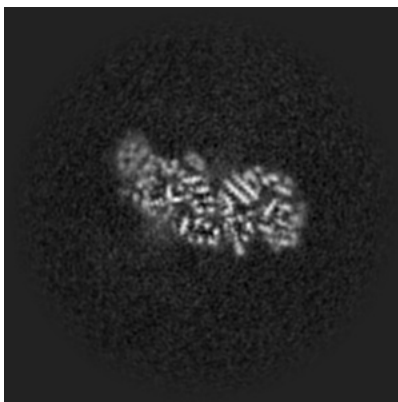
The images above show central slices of the map in three orthogonal directions.

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

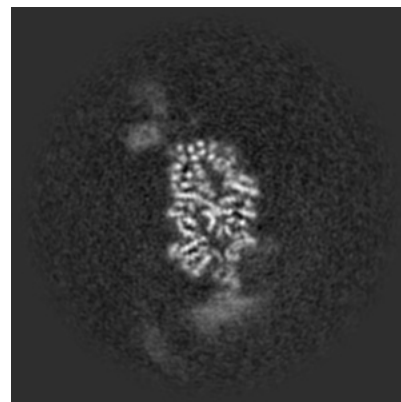
### 6.3.1 Primary map



X Index: 175

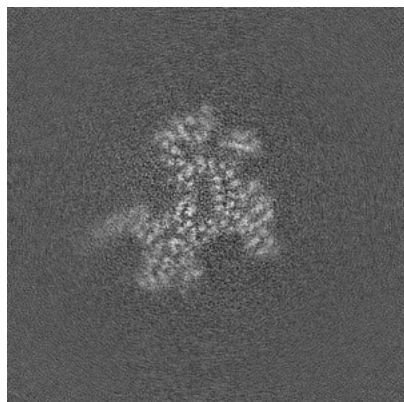


Y Index: 138

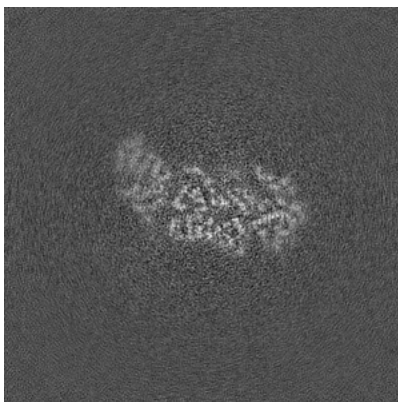


Z Index: 142

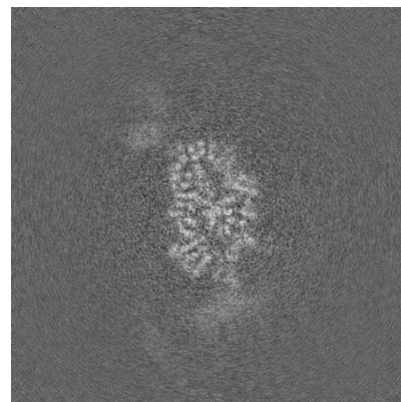
### 6.3.2 Raw map



X Index: 174



Y Index: 143



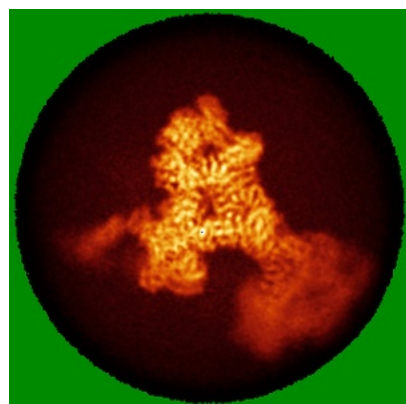
Z Index: 142

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

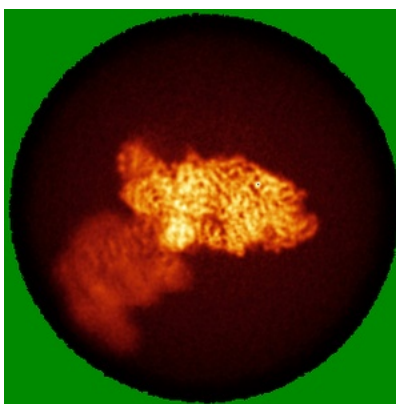


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

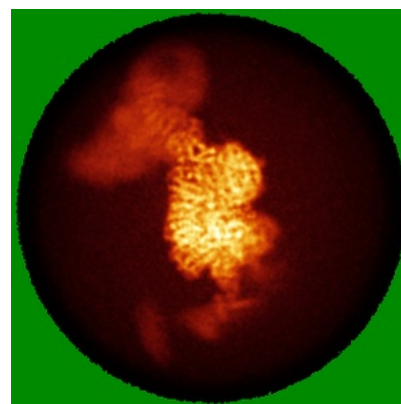
### 6.4.1 Primary map



X

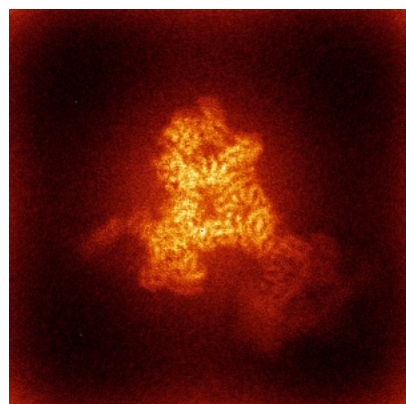


Y

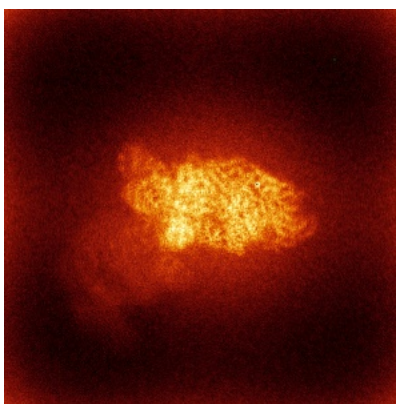


Z

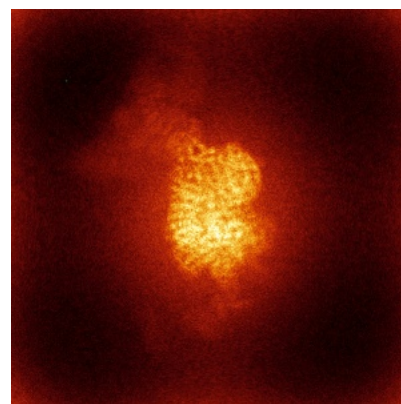
### 6.4.2 Raw map



X



Y

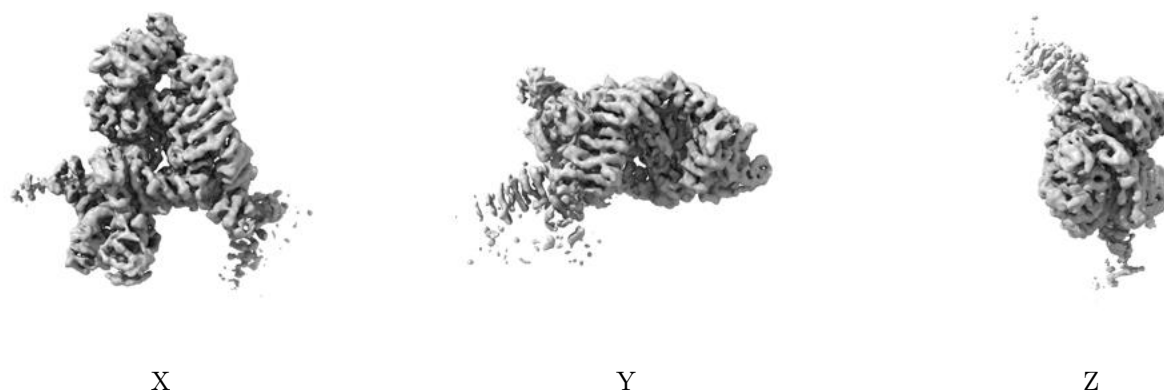


Z

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.

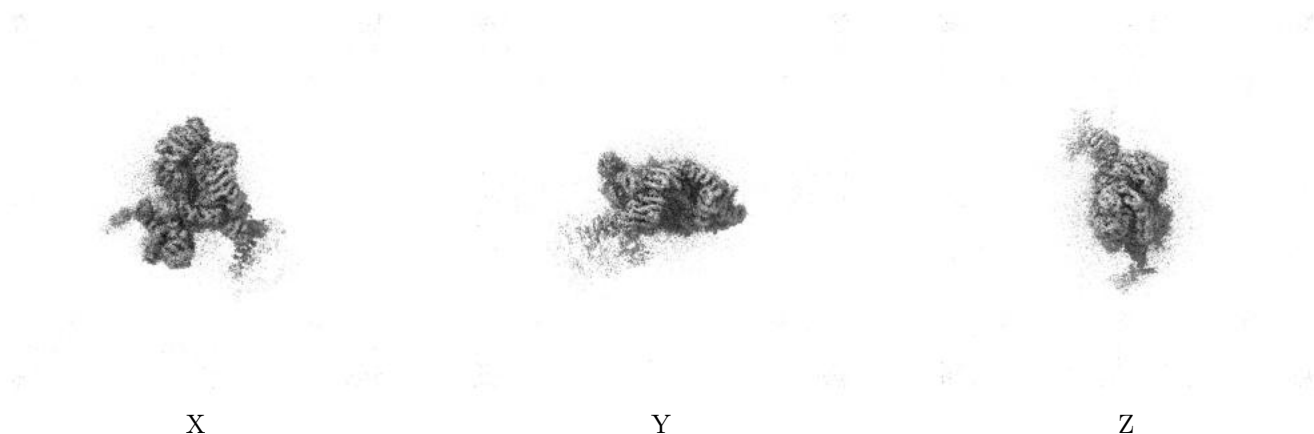
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.211. 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.



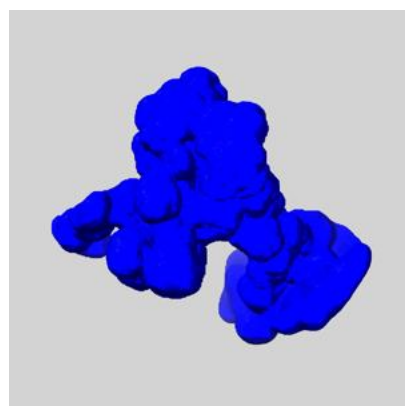
## 6.6 Mask visualisation [i](#)

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

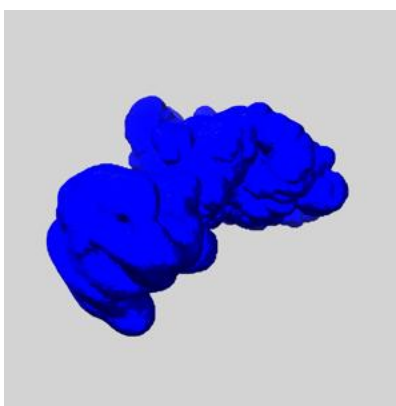
A mask typically either:

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

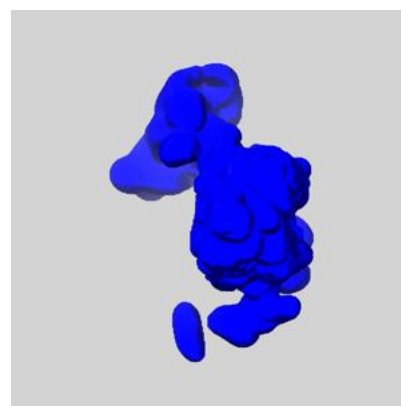
### 6.6.1 emd\_51249\_msk\_1.map [i](#)



X



Y

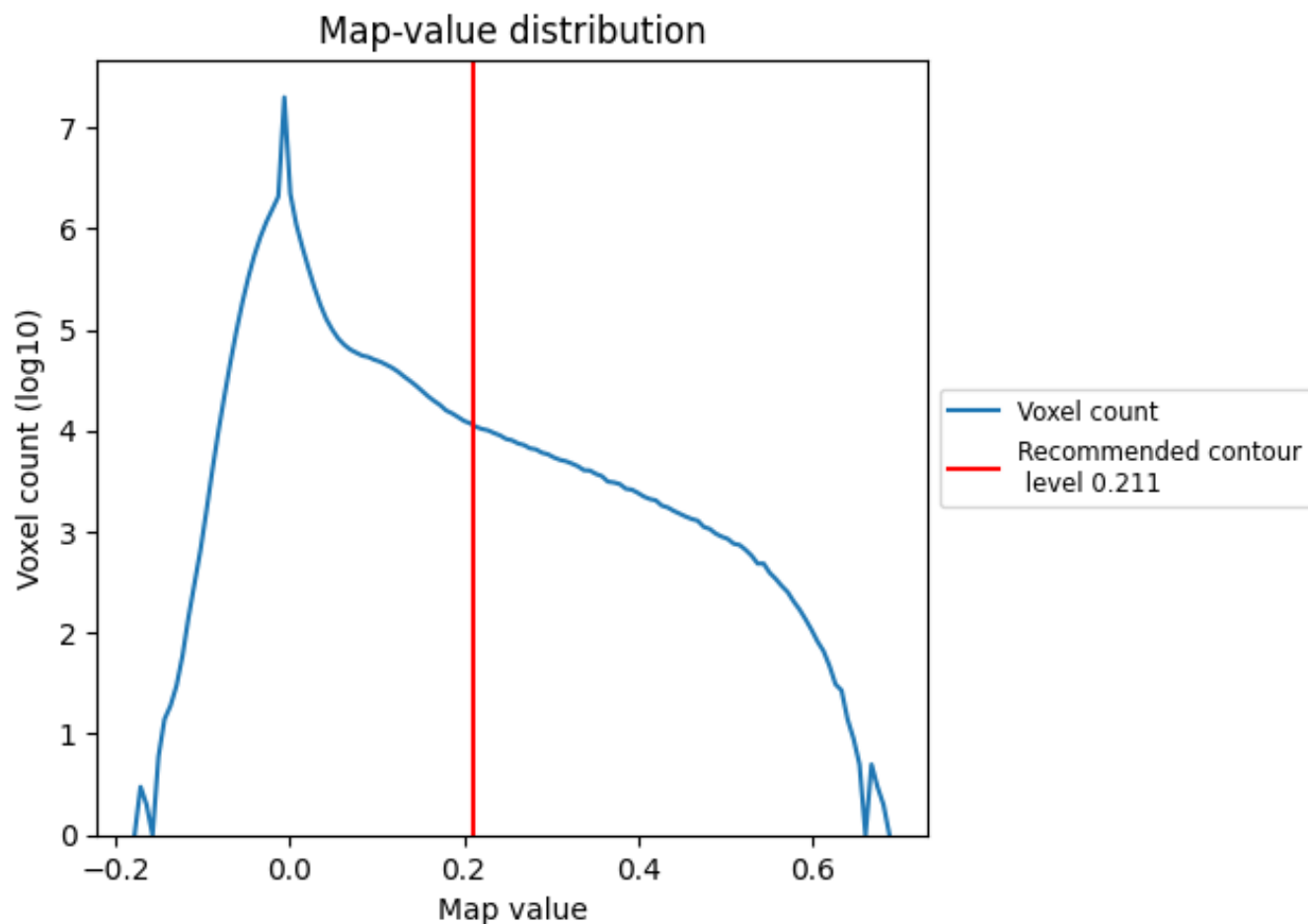


Z

## 7 Map analysis [i](#)

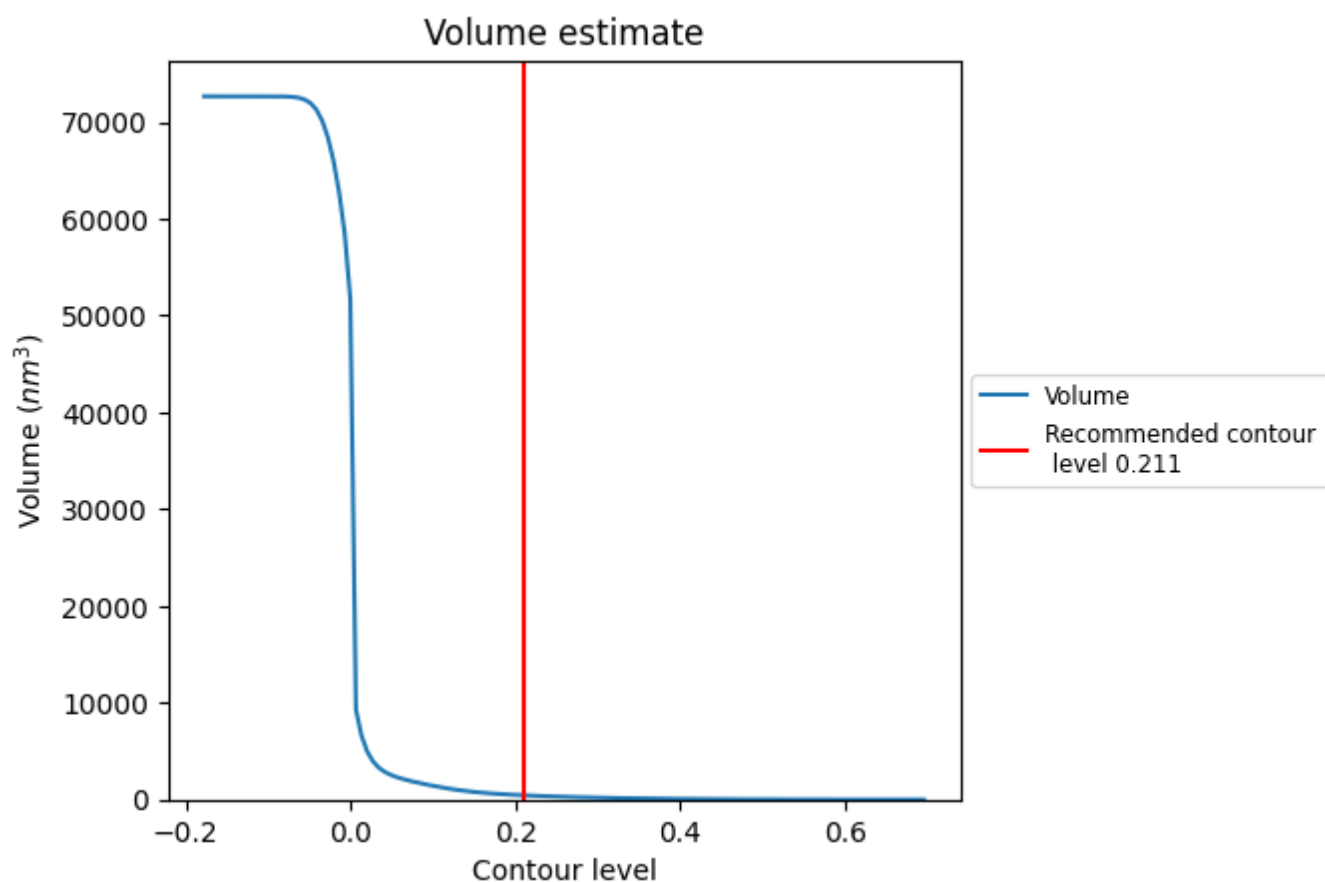
This section contains the results of statistical analysis of the map.

### 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.

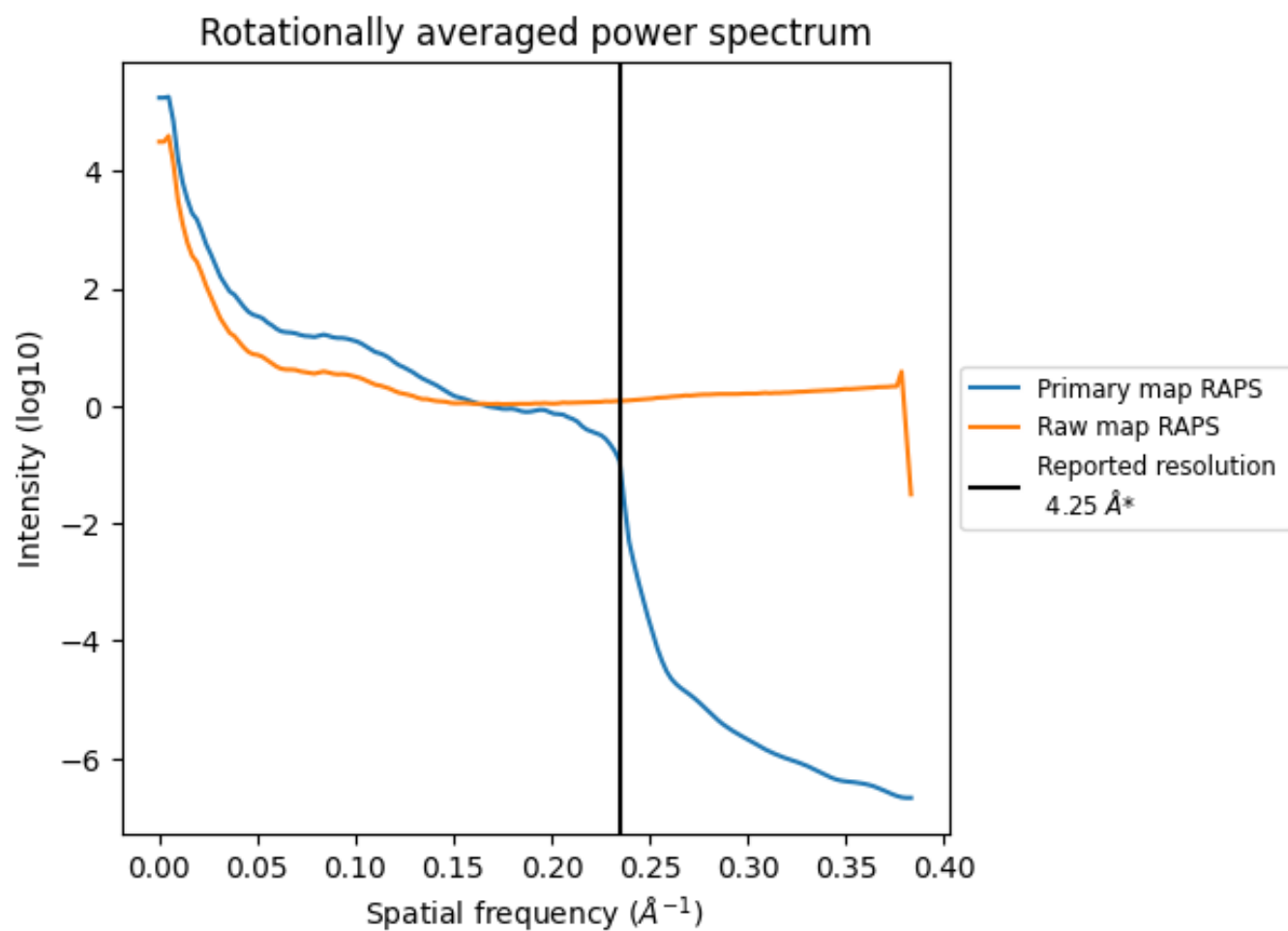
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 434 nm<sup>3</sup>; this corresponds to an approximate mass of 392 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 ⓘ

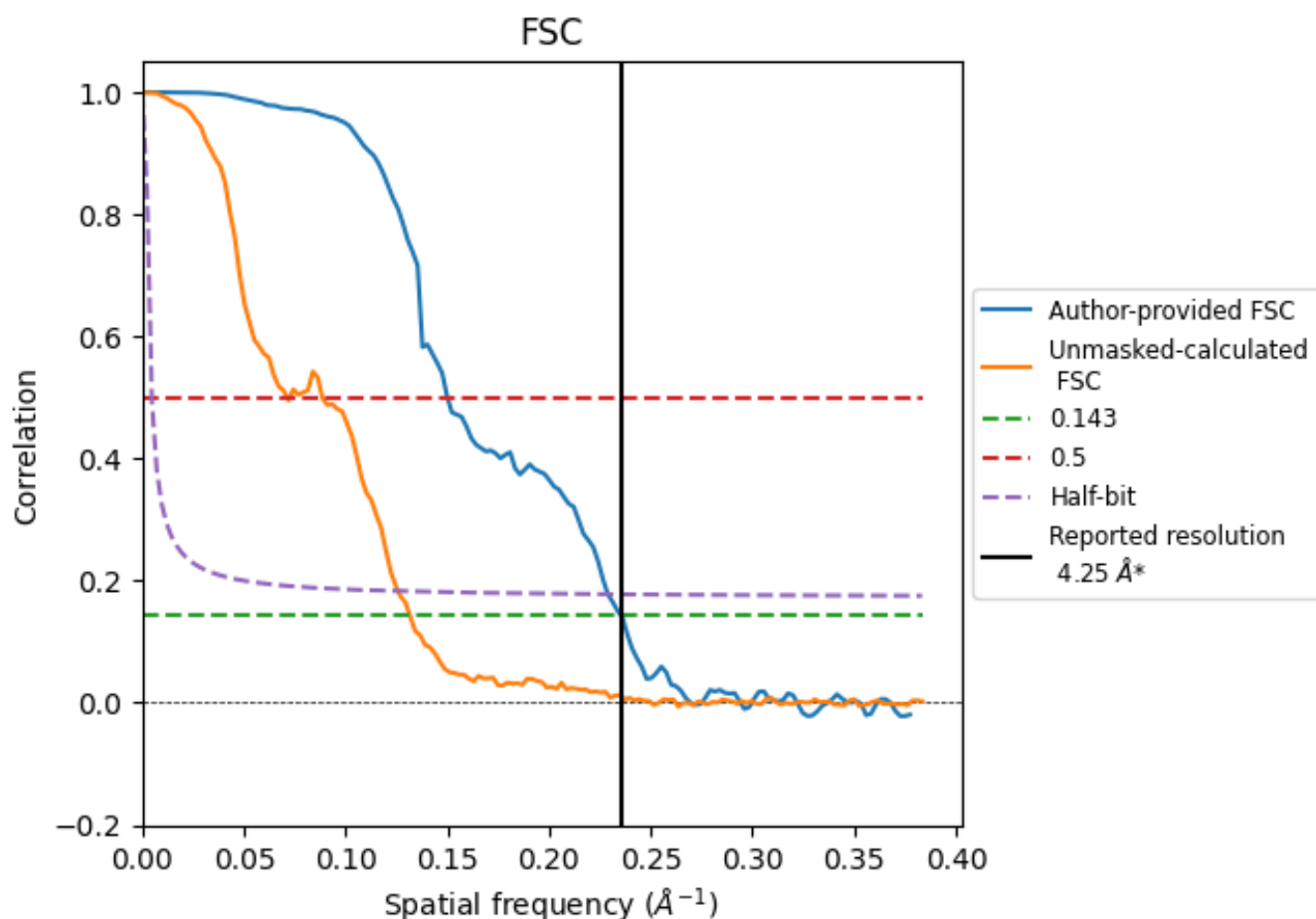


\*Reported resolution corresponds to spatial frequency of 0.235 Å<sup>-1</sup>

## 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 0.235  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

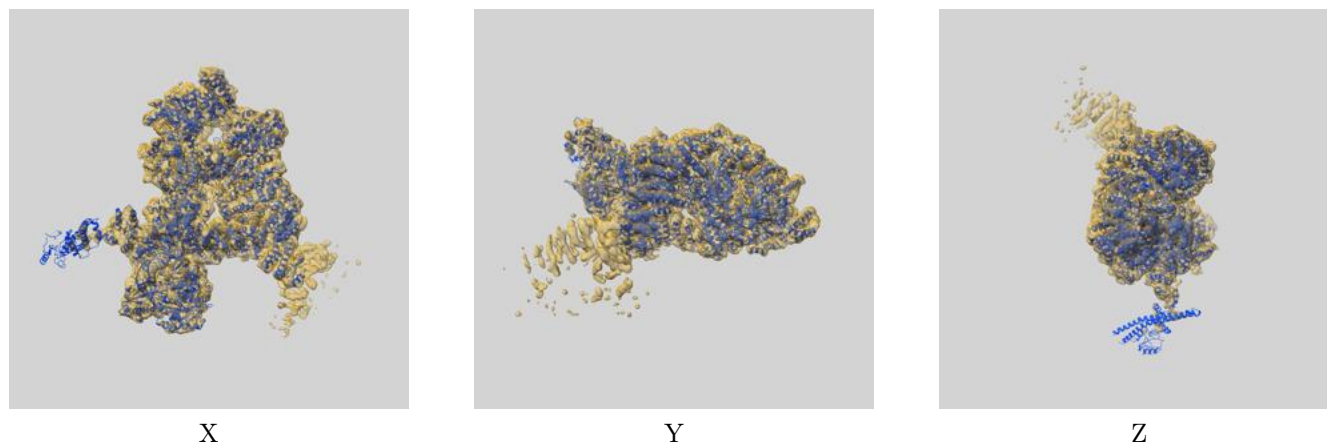
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.25	6.66	4.37
Unmasked-calculated*	7.60	14.04	7.95

\*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 7.60 differs from the reported value 4.25 by more than 10 %

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

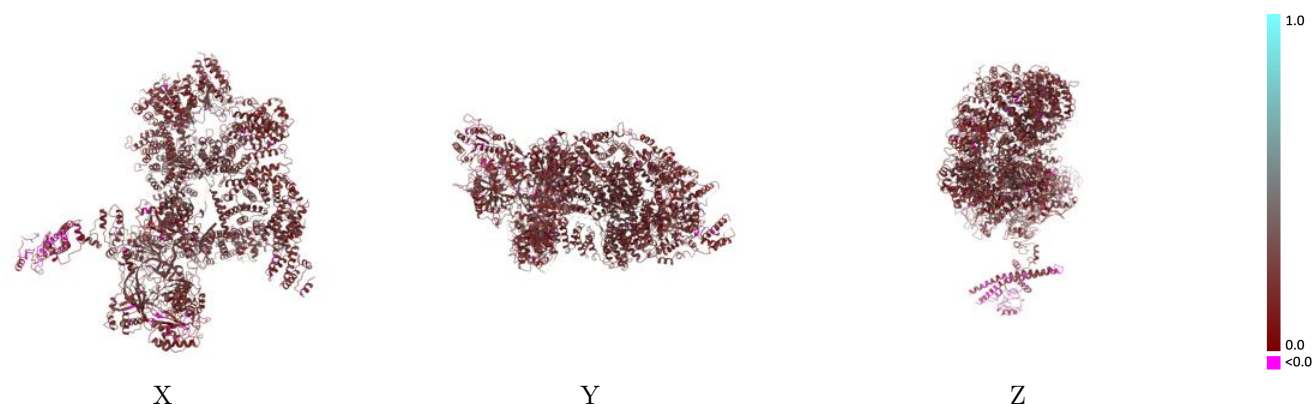
This section contains information regarding the fit between EMDB map EMD-51249 and PDB model 9GD7. Per-residue inclusion information can be found in section 3 on page 6.

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



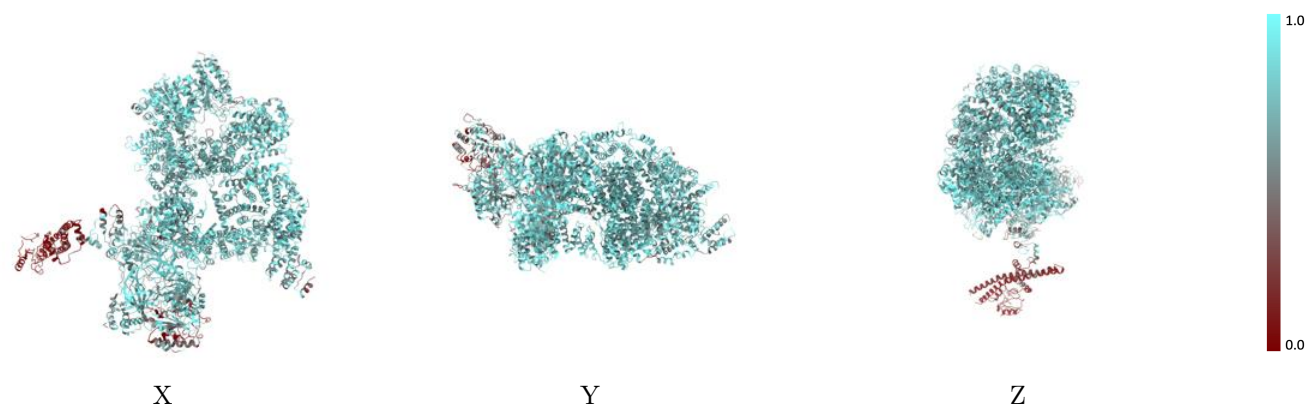
The images above show the 3D surface view of the map at the recommended contour level 0.211 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

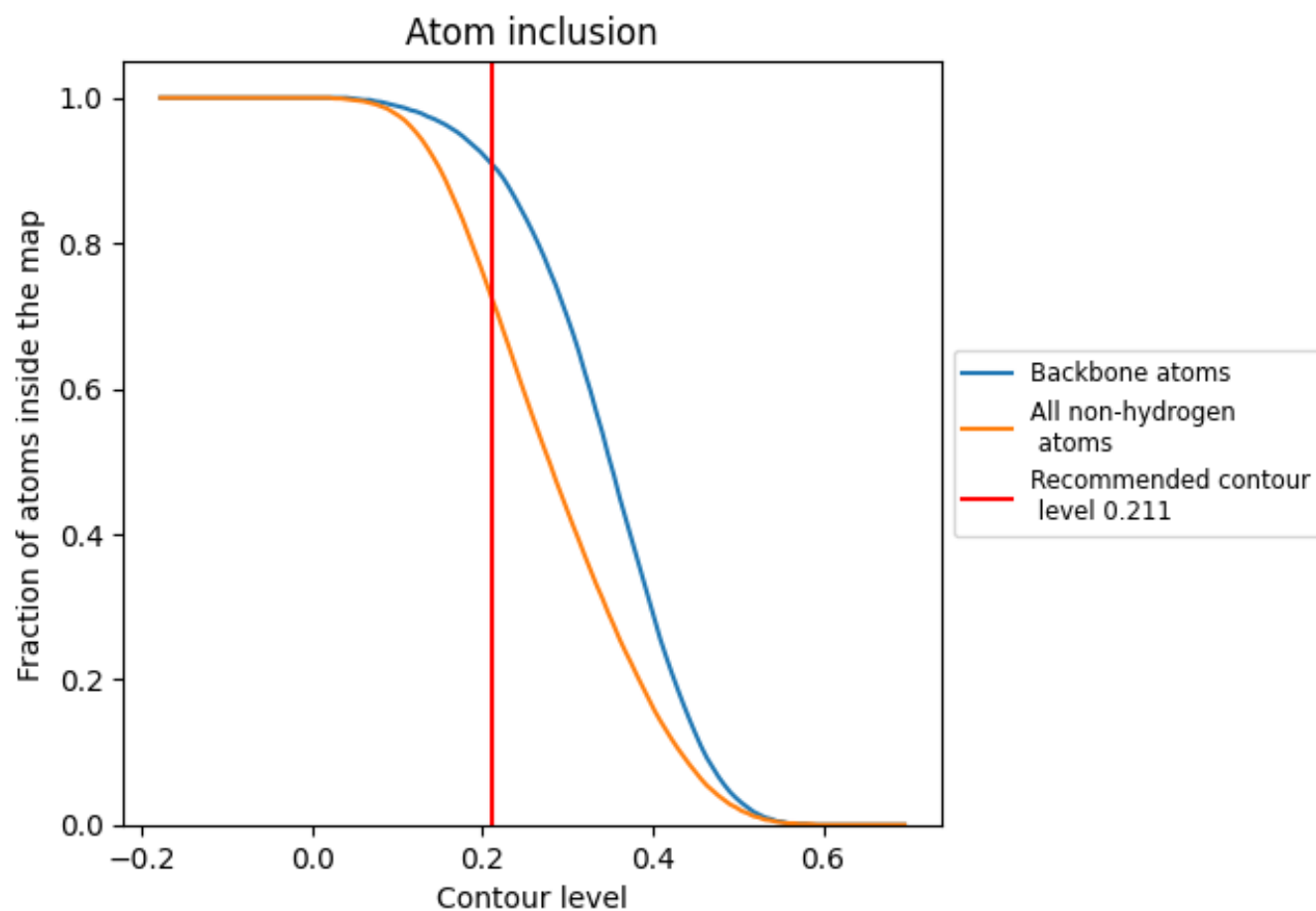
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.211).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 72% 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 (0.211) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7240	<div></div> 0.2280
A	<div></div> 0.7750	<div></div> 0.2160
E	<div></div> 0.2650	<div></div> 0.1390
L	<div></div> 0.6110	<div></div> 0.2070
M	<div></div> 0.6560	<div></div> 0.2950
P	<div></div> 0.0530	<div></div> 0.0970
Q	<div></div> 0.0970	<div></div> 0.0800
S	<div></div> 0.7870	<div></div> 0.2370
T	<div></div> 0.7420	<div></div> 0.2480
i	<div></div> 0.9770	<div></div> 0.3020
j	<div></div> 0.9810	<div></div> 0.2960

1.0

0.0

<0.0