



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:33 AM UTC

PDB ID : 9Q9F / pdb_00009q9f
EMDB ID : EMD-52958
Title : DNA-PK bound to a 153 bp H2AX nucleosome model 1
Authors : Hall, C.; Chaplin, A.K.
Deposited on : 2025-02-26
Resolution : 4.54 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

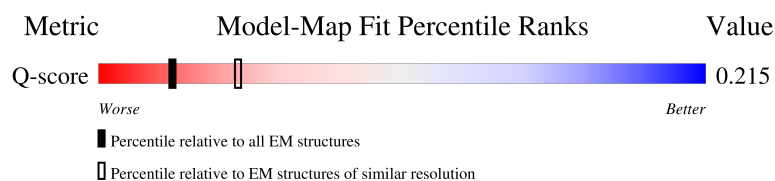
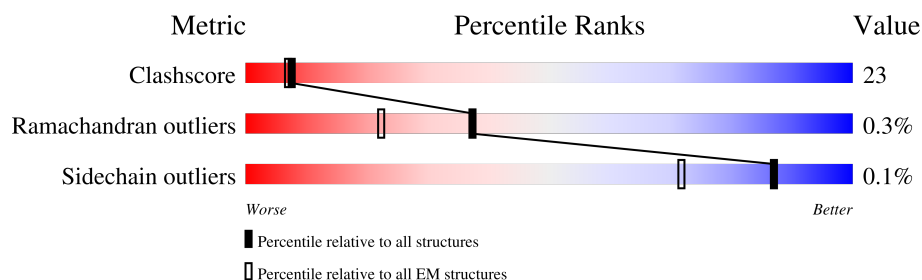
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2475 (4.04 - 5.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	K	609	
2	L	732	
3	I	153	
4	J	153	

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Mol	Chain	Length	Quality of chain
5	O	4128	
6	C	143	
6	G	143	
7	D	126	
7	H	126	
8	A	136	
8	E	136	
9	B	103	
9	F	103	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 46624 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	495	Total	C	N	O	S	0	0
			3926	2511	662	736	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	527	Total	C	N	O	S	0	0
			4165	2667	697	779	22		

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	129	Total	C	N	O	P	0	0
			2630	1247	481	773	129		

- Molecule 4 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	131	Total	C	N	O	P	0	0
			2697	1275	504	787	131		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	3527	Total	C	N	O	S	0	0
			27830	17852	4683	5123	172		

- Molecule 6 is a protein called Histone H2AX.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	95	Total	C	N	O	0	0
			690	432	133	125		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	94	Total	C	N	O	0	0
			692	438	132	122		

- Molecule 7 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	93	Total	C	N	O	S	0	0
			719	450	130	137	2		
7	H	92	Total	C	N	O	S	0	0
			718	453	127	136	2		

- Molecule 8 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	88	Total	C	N	O	S	0	0
			697	442	128	123	4		
8	E	88	Total	C	N	O	S	0	0
			711	450	131	126	4		

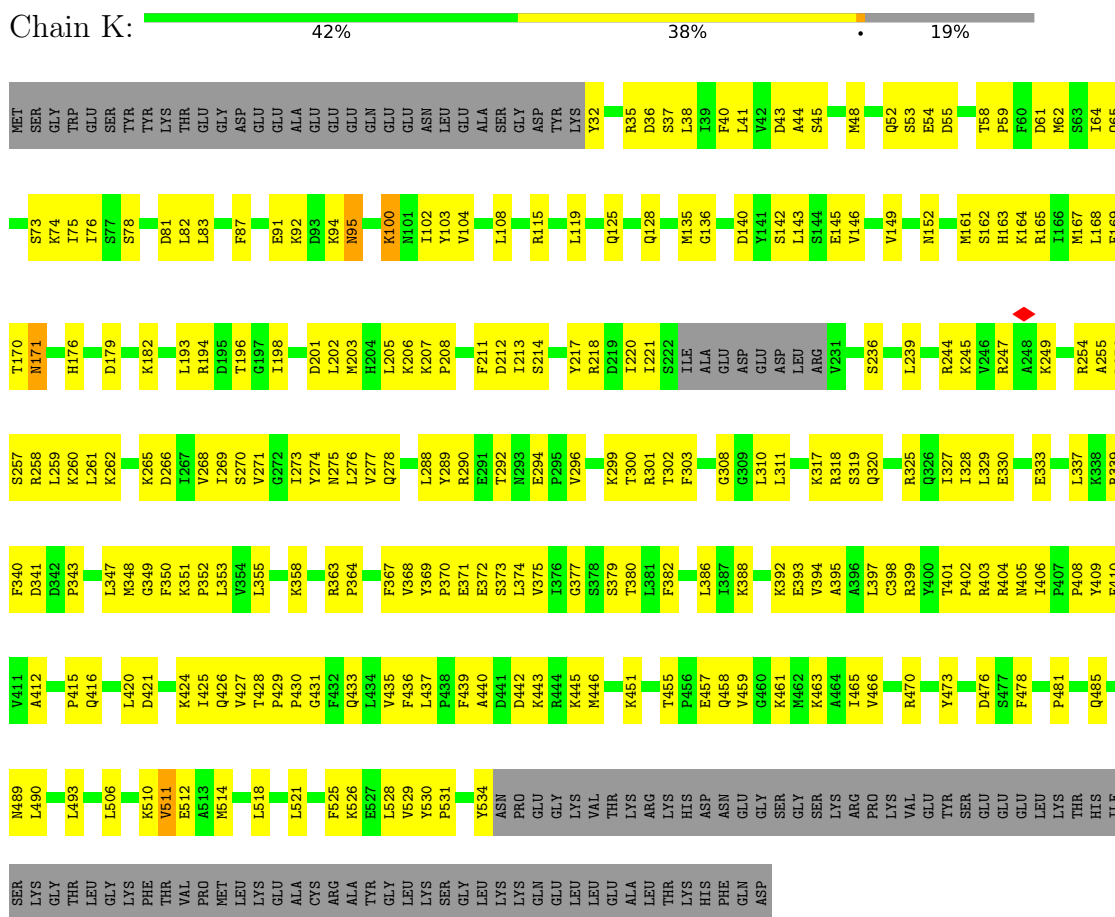
- Molecule 9 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	71	Total	C	N	O	S	0	0
			568	357	113	97	1		
9	F	72	Total	C	N	O	S	0	0
			581	370	112	98	1		

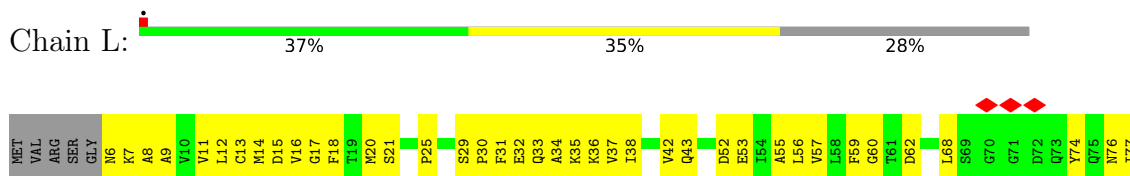
3 Residue-property plots

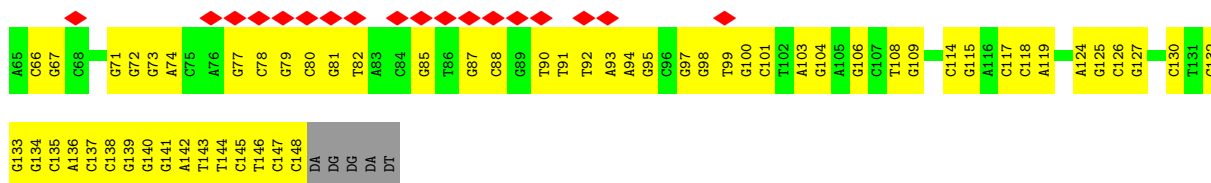
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: X-ray repair cross-complementing protein 6



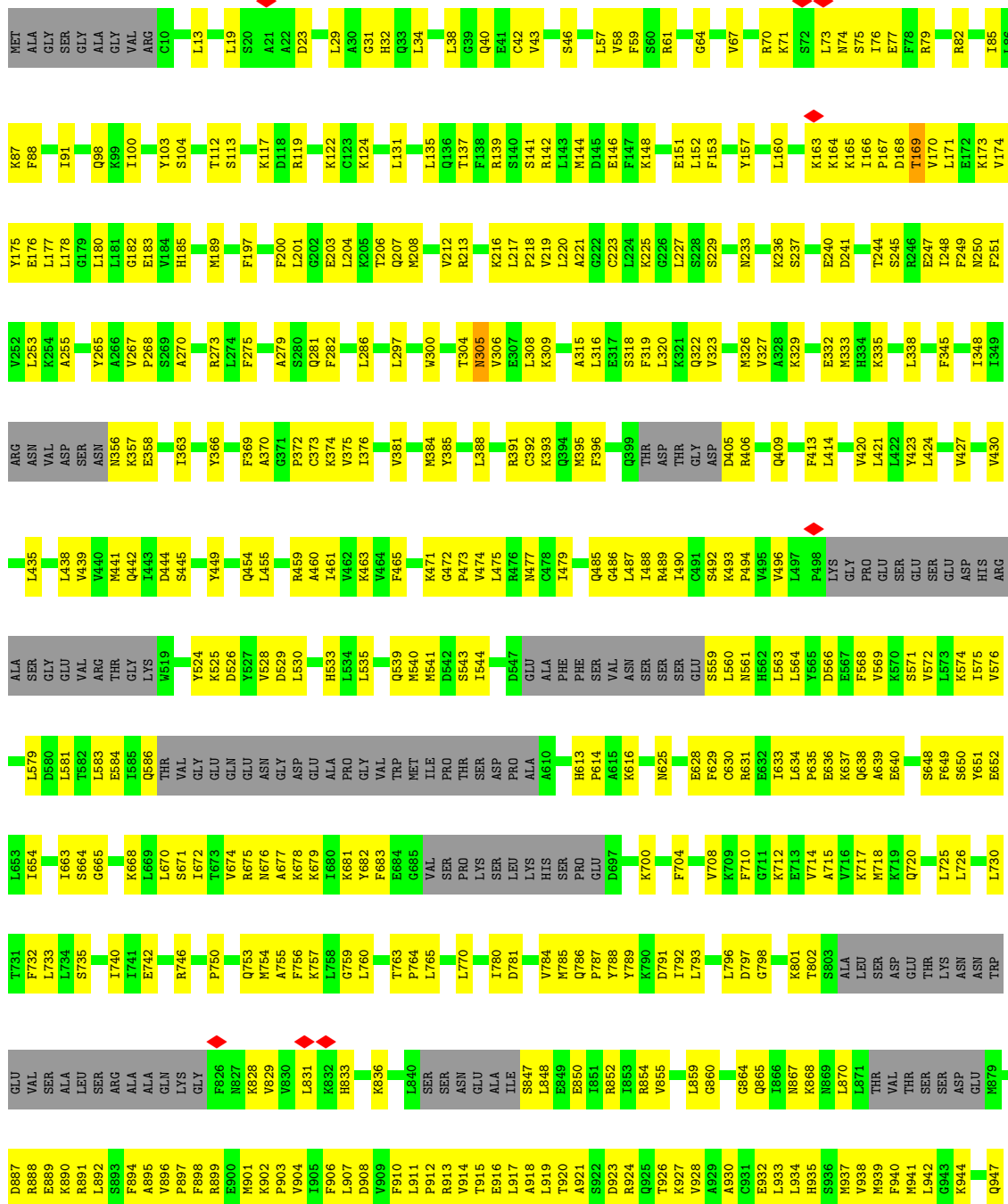
• Molecule 2: X-ray repair cross-complementing protein 5





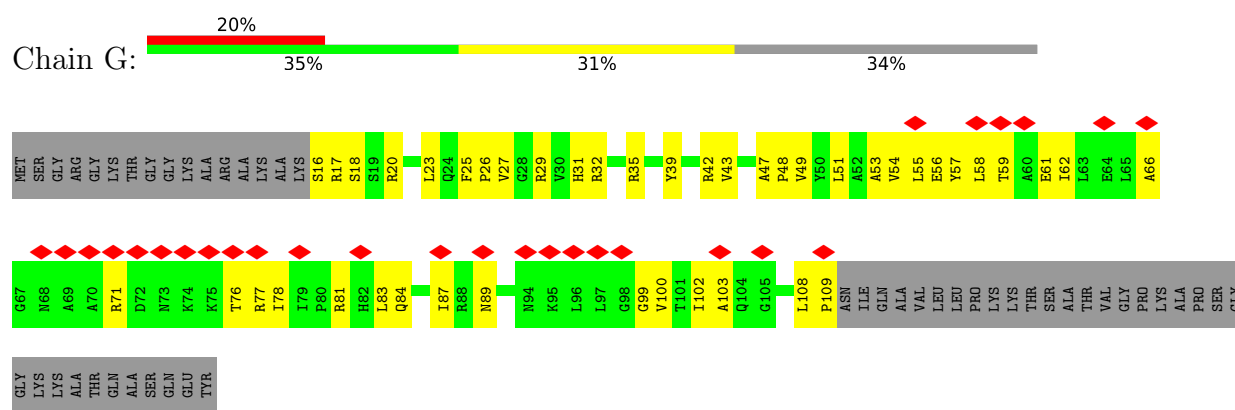
• Molecule 5: DNA-dependent protein kinase catalytic subunit

Chain O: 46% 39% 15%

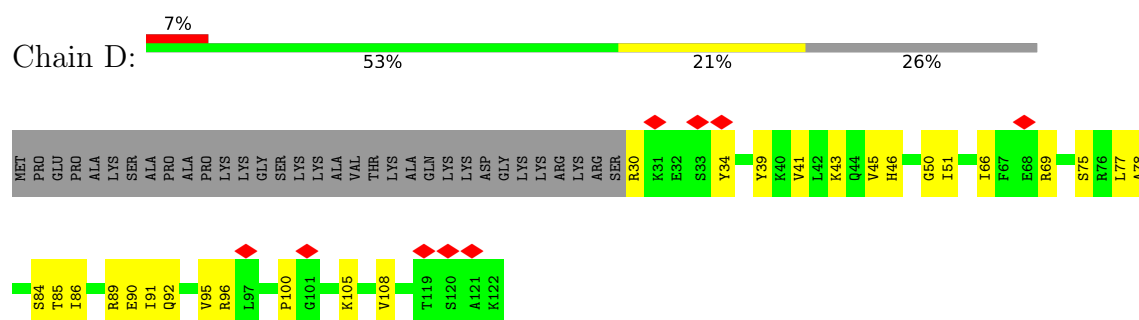




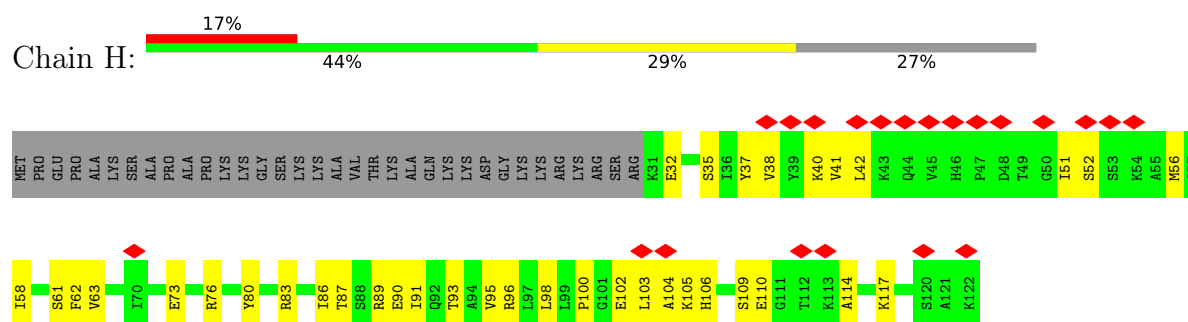
T3268	K3269	L3092	D3020	PRO	L2808	GLU	THR	T2535	C2435	N3365	P2284	D2208	P2136
D3270	D3271	A3099	S3021	P2918	G2815	LYS	LEU	L2536	I2438	K2366	L2285	L2211	I2137
W3272	W3273	K3100	ASN	D2919	E2819	LEU	GLN	R2537	P2367	P2138	C2292	R2214	V2138
L3273	L3274	Y3101	PRO	W2923	Q2834	LEU	ARG	L2542	N2442	L2140	Q2295	R2215	L2140
W3275	W3276	Y3102	ASP	W2924	K2835	THR	GLN	N2543	L2446	N2141	E2298	L2216	N2141
S3277	S3278	I3103	LEU	E2925	L2836	GLY	GLY	S2544	P2457	L2142	Y2299	P2218	L2142
Q3279	Q3280	Q3104	ASN	K2928	L2837	ARG	SER	L2545	P2457	R2143	F2300	L2219	L2146
		I3107	K3029	L2929	Q2838	GLY	LEU	P2548	E2460		Q2301		
		F3110	I3030	W2936	Q2839	VAL	SER	E2551	D2461		L2302	V2223	L2149
		Y3114	W3031	D2937	F2840	ALA	ALA	E2552	V2462		L2303	P2224	P2250
		Y3118	E3033	W2938	N2841	GLU	ARG	H2553	S2463		L2304	H2225	L2151
		D3118	P3034	L2939	R2842	GLN	THR	P2554	H2464		N2305	P2226	L2152
		W3119	F3035	PRO	L2847	LYS	PRO	H2555	P2465		N2306	K2227	T2153
		V3125	Q3036	I2942	T2848	ARG	ALA	S2556	S2466		F2309	R2228	E2154
		R3126	Q3037	K2950	F2848	GLY	ALA	L2557	T2467		V2310	A2229	E2155
		K3128	E3038	K2950	F2851	LYS	GLY	A2558			V2311	V2230	V2156
		L3129	T3039	L2957	P2852	GLU	GLN	T2559	R2470		R2311	F2231	F2157
		Q3133	M3044	L2957	P2853	ILE	ILE	N2560	E2471		R2158	R2232	
		L3135	I3045	A2961	F2854	VAL	ARG	E2564	Q2472		A2317	H2233	P2159
		T3136	K3046	D2973	V2855	GLY	ALA	M2565	N2473		G2391	N2234	V2160
		E3137	S3047	L2978	I2858	LEU	THR	T2566	T2476		A2318	L2235	A2161
		L3138	K3048	K2978	C2863	GLN	GLN	S2567	L2477		A2319	I2237	K2162
		W3139	L3049	Q2979	Q2864	LYS	HIS	D2571	I2480		L2323	K2238	W2164
		T3140	K3050	D2980	Q2864	ASP	ASP	Y2572			G2324	K2239	L2165
		Q3141	L3051	G2984	L2868	THR	PHE	T2573	Y2484		R2328	P2167	S2166
		F3142	L3052	E2985	L2869	LEU	THR	N2574	D2486		V2329	L2168	L2169
		L3143	L3053	E2986	L2869	GLY	LEU	S2582	PRO		M2331	S2250	Q2170
		Q3144	Q3054	P2986	L2869	LEU	GLN	F2586	GLY		E2332	I2251	L2171
		S3145	Q3059	T2987	P2873	PRO	GLY	E2587	S2500		K2334	P2252	A2172
		K3147	L3061	E2988	R2891	THR	ALA	E2588	GLY		N2335	Y2253	R2254
		V3155	L3062	K2991	E2894	GLY	ASP	Y2589	T2491		T2336	I2255	L2256
		F3156	T3063	D2992	E2895	VAL	GLY	T2590	E2497		L2337	K2259	
		L3157	F3064	F2993	A2896	ASP	ARG	L2591	L2411		E2338	P2260	L2182
		K3158	K3067	W2994	L2897	LYS	SER	D2592	Y2412		S2340	S2261	H2183
		R3159	E3072	L2996	L2898	LYS	ASP	D2593	F2413		C2342	D2264	V2186
		L3160	L3073	L2999	L2899	GLY	THR	D2594	Q2414		L2341	P2265	E2187
		L3161	Q3074	D3000	L2901	ALA	LEU	R2595	L2510		E2343	N2266	L2188
		N3162	Q3075	C3001	PRO	ALA	THR	F2597	I2511		L2344	S2267	L2189
		S3245	A3076	Y3002	ALA	R2721	GLY	R2598	D2420		V2345		V2190
		R3246	L3077	N3003	LEU	T2722	SER		F2421		A2346		
		W3164	L3078	H3004	GLY	T2723	SER	T2603	Q2422		L2349	N2270	K2191
		T3165	L3078	L3004	VAL	D2724	THR	PRO	V2423		Q2350		L2192
		P3169	H3081	W3008	ALA	D2725	ASP	MET	H2424		K2350		L2193
		F3252	Y3082	L3008	LYS	T2726	PRO	PHE	R2425		Q2351		L2194
		S3263	S3083	L3011	ARG	L2727	LEU	VAL	H2426		H2352		L2195
		M3176	Q3084	L3011	VAL	L2728	VAL	GLU	R2427		Q2353		L2276
		W3179	E3085	C3014	ARG	P2802	ASP	THR	D2428		T2529		V2196
		L3259	L3088	S3015	GLY	P2803	HIS	GLN	D2429		D2358		L2279
		H3263	L3089	S3018	LYS	T2804	THR	ALA	D2430		K2359		V2280
		L3254	Y3090	S3018	ALA	A2805	SER	SER	R2431		F2360		M2281
		L3254	Y3090	S3018	ARG	K2806	PRO	GLN	Q2432		I2361		V2205
		L3254	L3091	L3019	LEU	Q2807	SER	GLY	N2534		V2362		N2283



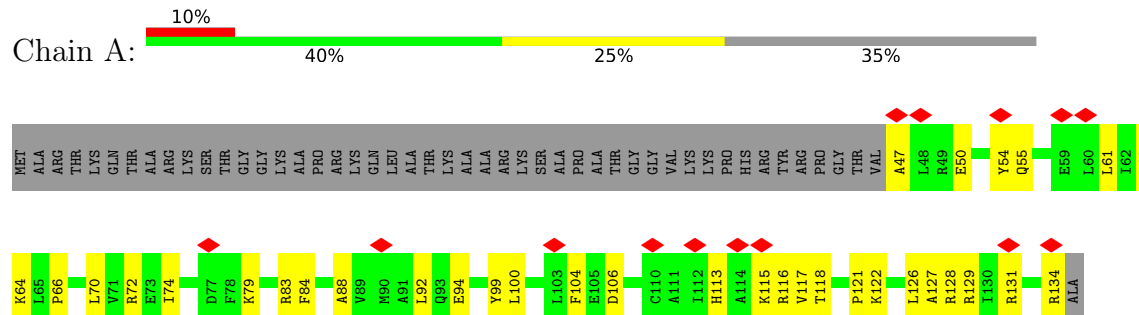
- Molecule 7: Histone H2B type 1-J



- Molecule 7: Histone H2B type 1-J

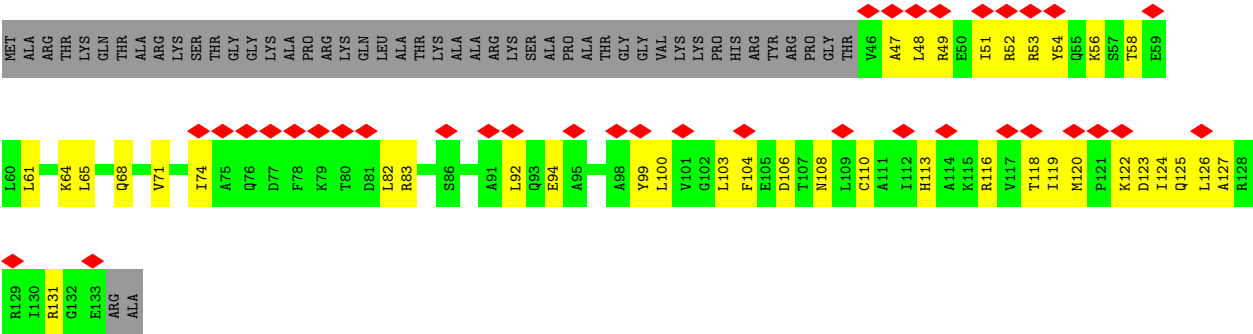


- Molecule 8: Histone H3.1

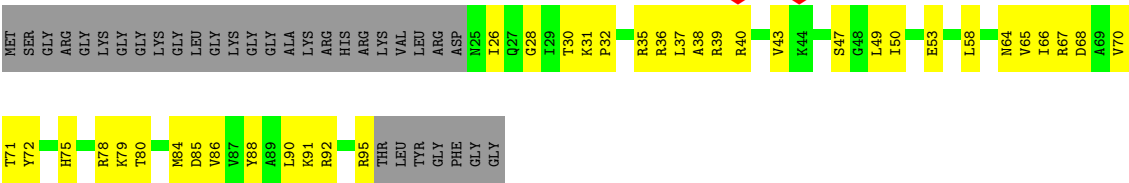


- Molecule 8: Histone H3.1

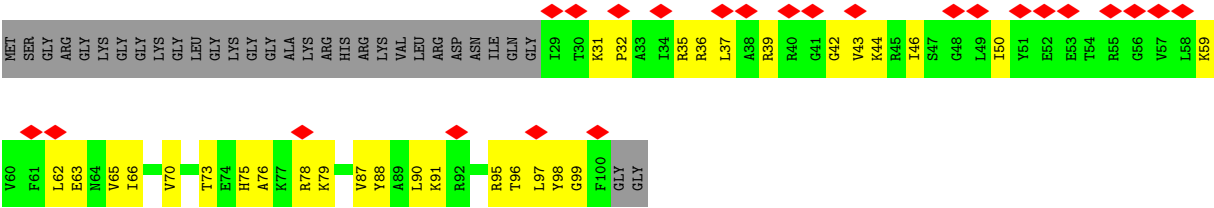




● Molecule 9: Histone H4



● Molecule 9: Histone H4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14174	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.59	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.839	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	692.16, 692.16, 692.16	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6479999, 1.6479999, 1.6479999	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	K	0.10	0/4004	0.32	0/5409
2	L	0.12	0/4249	0.34	0/5742
3	I	0.18	0/2947	0.37	0/4542
4	J	0.17	0/3027	0.36	0/4673
5	O	0.14	0/28381	0.37	0/38396
6	C	0.12	0/700	0.33	0/951
6	G	0.14	0/702	0.42	0/951
7	D	0.11	0/729	0.31	0/980
7	H	0.13	0/729	0.38	0/979
8	A	0.10	0/705	0.31	0/948
8	E	0.18	0/719	0.41	0/966
9	B	0.11	0/573	0.28	0/767
9	F	0.14	0/588	0.38	0/788
All	All	0.14	0/48053	0.36	0/66092

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	K	3926	0	3920	239	0
2	L	4165	0	4165	229	0
3	I	2630	0	1446	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	2697	0	1469	118	0
5	O	27830	0	27756	1243	0
6	C	690	0	676	42	0
6	G	692	0	704	57	0
7	D	719	0	735	23	0
7	H	718	0	740	42	0
8	A	697	0	710	46	0
8	E	711	0	737	44	0
9	B	568	0	614	39	0
9	F	581	0	625	40	0
All	All	46624	0	44297	2033	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 23.

All (2033) 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:O:965:THR:HG22	5:O:969:LEU:CD1	1.97	0.94
5:O:1633:TRP:HB2	5:O:1678:LEU:HD21	1.51	0.93
5:O:965:THR:HG22	5:O:969:LEU:HG	1.52	0.91
6:G:26:PRO:HB2	6:G:29:ARG:HB3	1.53	0.91
5:O:965:THR:HG22	5:O:969:LEU:CG	2.01	0.90
5:O:1452:VAL:HG22	5:O:1517:LEU:HD11	1.56	0.87
5:O:1840:PHE:HB2	5:O:1880:MET:HE1	1.55	0.87
2:L:118:ILE:HD11	2:L:132:ILE:HD11	1.59	0.84
1:K:421:ASP:HB3	1:K:427:VAL:HB	1.60	0.84
5:O:2256:ILE:HA	5:O:2259:LYS:HB2	1.59	0.82
5:O:1775:GLU:HA	5:O:1778:PHE:HD2	1.45	0.82
5:O:897:PRO:HB3	5:O:2571:ASP:HB3	1.62	0.81
5:O:1574:ASN:HD21	5:O:1577:LEU:HB2	1.47	0.80
5:O:965:THR:HG22	5:O:969:LEU:HD11	1.64	0.80
1:K:442:ASP:H	2:L:270:GLU:HG2	1.45	0.80
5:O:2165:LEU:HD11	5:O:2200:ALA:HB1	1.64	0.80
5:O:3811:THR:HG22	5:O:3929:MET:HE1	1.65	0.78
2:L:62:ASP:HA	2:L:103:GLN:HB2	1.67	0.77
3:I:94:DA:H4'	8:A:63:ARG:HH11	1.49	0.77
2:L:134:ILE:HG13	2:L:161:LEU:HD11	1.66	0.76
2:L:13:CYS:HB3	2:L:134:ILE:HA	1.67	0.76
9:B:38:ALA:HB1	9:B:43:VAL:HB	1.66	0.75
2:L:308:GLU:HG3	2:L:309:ASP:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1716:GLN:HA	5:O:1719:VAL:HB	1.70	0.74
6:G:102:ILE:HD12	7:H:58:ILE:HD13	1.69	0.74
1:K:299:LYS:HB2	2:L:297:LEU:HD21	1.68	0.73
5:O:2317:ALA:HA	5:O:2366:LYS:HE3	1.70	0.73
5:O:3737:ARG:HH11	5:O:3751:LEU:HB3	1.51	0.73
1:K:59:PRO:HB3	1:K:205:LEU:HD23	1.70	0.73
2:L:115:MET:HA	2:L:118:ILE:HD12	1.71	0.73
1:K:256:LEU:O	1:K:258:ARG:NH1	2.21	0.72
8:E:49:ARG:HB2	8:E:53:ARG:HH12	1.53	0.72
5:O:2254:ARG:NH1	5:O:2292:CYS:SG	2.63	0.72
5:O:3450:MET:HG2	5:O:3468:LEU:HD22	1.71	0.72
5:O:3483:MET:O	5:O:3486:GLU:HB3	1.89	0.72
5:O:3725:ARG:HB2	5:O:3739:ILE:HB	1.71	0.72
1:K:352:PRO:HA	1:K:394:VAL:HA	1.71	0.71
5:O:3263:HIS:O	5:O:3267:LYS:NZ	2.23	0.71
6:G:89:ASN:HA	6:G:108:LEU:HD22	1.71	0.71
5:O:726:LEU:HG	5:O:730:LEU:HD23	1.71	0.71
3:I:94:DA:H5'	3:I:94:DA:C8	2.26	0.71
5:O:965:THR:CG2	5:O:969:LEU:HD11	2.20	0.71
5:O:1326:GLU:HG3	5:O:1329:ARG:HG2	1.74	0.70
5:O:2372:PRO:HB3	5:O:2403:CYS:HB3	1.73	0.70
5:O:2461:PHE:HB2	5:O:2473:MET:HE3	1.73	0.70
6:G:43:VAL:HG13	7:H:86:ILE:HB	1.73	0.70
5:O:535:LEU:HB3	5:O:637:LYS:HE2	1.73	0.70
2:L:381:ILE:HG23	2:L:410:PRO:HB2	1.73	0.70
5:O:912:PRO:O	5:O:915:THR:HB	1.91	0.70
5:O:420:VAL:O	5:O:424:LEU:N	2.23	0.70
1:K:300:THR:HA	2:L:293:THR:HA	1.73	0.70
1:K:476:ASP:HA	2:L:427:MET:HG2	1.72	0.70
5:O:3716:HIS:CE1	5:O:3717:VAL:HG12	2.27	0.70
4:J:52:DC:H2'	4:J:53:DT:C6	2.26	0.70
5:O:1926:ASN:HD21	5:O:1967:PHE:HZ	1.39	0.70
6:G:81:ARG:HH22	6:G:109:PRO:HD3	1.57	0.70
2:L:165:LEU:HD21	2:L:224:ILE:HG23	1.73	0.70
2:L:364:VAL:HB	2:L:419:LEU:HB3	1.74	0.70
2:L:154:LEU:HD23	2:L:159:ILE:HG23	1.74	0.69
4:J:90:DT:H2''	4:J:91:DT:H2'	1.73	0.69
5:O:2591:ILE:HD11	5:O:2775:TYR:HB2	1.73	0.69
3:I:65:DC:N4	4:J:90:DT:O2	2.26	0.69
2:L:74:TYR:HB3	2:L:77:ILE:HD12	1.74	0.69
2:L:184:ARG:HH22	2:L:521:GLU:HG2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:497:ARG:NH2	2:L:503:GLU:O	2.26	0.69
5:O:3107:ILE:HD13	5:O:3135:LEU:HD13	1.75	0.69
1:K:294:GLU:OE2	2:L:298:ASN:ND2	2.26	0.69
1:K:529:VAL:HG13	1:K:530:TYR:H	1.58	0.69
5:O:663:ILE:HG22	5:O:665:GLY:H	1.57	0.69
5:O:2151:ILE:HG12	5:O:2192:THR:HG21	1.75	0.68
3:I:112:DC:H5'	4:J:43:DA:H2	1.57	0.68
5:O:306:VAL:HG23	5:O:309:LYS:HD2	1.74	0.68
5:O:793:LEU:HB3	5:O:870:LEU:HA	1.74	0.68
5:O:3961:PHE:HE1	5:O:4107:LEU:HD22	1.57	0.68
5:O:3142:ILE:O	5:O:3147:LYS:NZ	2.26	0.68
3:I:103:DG:H21	8:A:83:ARG:HH22	1.38	0.68
2:L:342:VAL:HA	2:L:393:VAL:HG12	1.74	0.68
1:K:277:VAL:HG21	2:L:425:PRO:HB3	1.76	0.68
5:O:216:LYS:HG2	5:O:218:PRO:HD3	1.75	0.67
5:O:1685:ASP:HB3	5:O:1688:LEU:HG	1.75	0.67
5:O:3015:SER:HA	5:O:3044:MET:HE1	1.75	0.67
5:O:1149:LYS:O	5:O:1163:LEU:N	2.27	0.67
3:I:14:DC:N3	4:J:140:DG:N2	2.41	0.67
5:O:1933:LEU:HG	5:O:1934:LEU:H	1.59	0.67
5:O:2791:ILE:HA	5:O:2794:LEU:HD12	1.77	0.67
8:A:61:LEU:HA	8:A:63:ARG:HH21	1.57	0.67
1:K:164:LYS:NZ	1:K:196:THR:O	2.28	0.67
1:K:439:PHE:O	1:K:443:LYS:NZ	2.27	0.67
1:K:534:TYR:HB3	2:L:260:ARG:HH12	1.58	0.67
1:K:455:THR:HG22	1:K:457:GLU:H	1.59	0.67
5:O:1820:VAL:HG23	5:O:1824:LEU:HB2	1.76	0.67
5:O:802:THR:OG1	5:O:852:ARG:NH2	2.28	0.67
5:O:1003:SER:OG	5:O:1004:GLN:OE1	2.12	0.67
5:O:1180:GLN:HB3	5:O:1183:CYS:HB3	1.75	0.67
1:K:48:MET:HE1	1:K:171:ASN:H	1.59	0.67
5:O:1373:VAL:HG21	5:O:1422:LYS:HE2	1.77	0.67
6:C:26:PRO:HD2	7:D:34:TYR:HE1	1.59	0.66
9:F:39:ARG:NH1	9:F:43:VAL:O	2.27	0.66
4:J:64:DA:H3'	9:B:30:THR:HG21	1.77	0.66
5:O:207:GLN:HG3	5:O:217:LEU:HD13	1.76	0.66
5:O:2330:VAL:HG13	5:O:2338:GLU:HB2	1.76	0.66
5:O:471:LYS:HD2	5:O:474:VAL:H	1.59	0.66
5:O:664:SER:HB2	5:O:725:LEU:HG	1.78	0.66
5:O:899:ARG:O	5:O:902:LYS:NZ	2.25	0.66
5:O:1180:GLN:O	5:O:1184:ARG:N	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3269:ARG:HB2	5:O:3272:TRP:CD1	2.29	0.66
5:O:3492:CYS:SG	5:O:3708:ARG:NH1	2.69	0.66
5:O:3670:MET:SD	5:O:3671:ASN:N	2.68	0.66
5:O:3680:LEU:HD13	5:O:3722:PHE:HB3	1.78	0.66
5:O:1141:LYS:NZ	5:O:1144:SER:OG	2.27	0.66
2:L:497:ARG:HG2	2:L:505:LEU:HD21	1.78	0.66
3:I:117:DG:H1	4:J:38:DT:H3	1.43	0.66
5:O:1550:VAL:HG23	5:O:1551:ILE:HG22	1.78	0.66
5:O:4014:LYS:HG2	5:O:4015:ASN:H	1.61	0.66
5:O:789:TYR:HA	5:O:792:ILE:HG22	1.78	0.66
1:K:353:LEU:HD21	1:K:415:PRO:HD2	1.77	0.65
3:I:57:DC:O2	4:J:98:DG:N1	2.22	0.65
5:O:487:LEU:HD13	5:O:575:ILE:HD13	1.77	0.65
5:O:892:LEU:HB3	5:O:908:ASP:HB3	1.78	0.65
5:O:3840:LYS:HG2	5:O:3842:TRP:HE1	1.61	0.65
5:O:374:LYS:NZ	5:O:423:TYR:O	2.30	0.65
6:C:78:ILE:HB	7:D:51:ILE:HA	1.77	0.65
1:K:91:GLU:HG2	1:K:136:GLY:HA3	1.79	0.65
5:O:1400:VAL:HG21	5:O:1460:ARG:HE	1.61	0.65
5:O:3768:PHE:HA	5:O:3771:MET:SD	2.37	0.65
1:K:44:ALA:HB2	1:K:87:PHE:HE2	1.61	0.65
5:O:225:LYS:HD2	5:O:270:ALA:HB1	1.79	0.65
5:O:3717:VAL:HG23	5:O:3743:HIS:HB3	1.79	0.65
1:K:404:ARG:HD2	5:O:213:ARG:HG3	1.79	0.65
5:O:635:PRO:HG3	5:O:672:ILE:HG23	1.77	0.65
5:O:1837:ARG:NH2	5:O:1884:LEU:O	2.29	0.65
5:O:2837:LEU:HD21	5:O:2868:LEU:HA	1.78	0.65
2:L:81:ARG:NH2	2:L:85:LEU:O	2.28	0.65
2:L:431:ARG:NH2	3:I:15:DC:OP2	2.29	0.65
5:O:229:SER:O	5:O:233:ASN:ND2	2.30	0.65
6:G:25:PHE:CD2	6:G:56:GLU:HG2	2.31	0.65
2:L:343:LEU:HD21	2:L:394:ARG:HB2	1.79	0.65
5:O:2303:LEU:HB3	5:O:2323:LEU:HD21	1.77	0.65
7:D:78:ALA:HB2	7:D:90:GLU:HG2	1.79	0.65
1:K:254:ARG:HG2	1:K:255:ALA:H	1.62	0.64
5:O:356:ASN:OD1	5:O:357:LYS:N	2.28	0.64
5:O:2589:TYR:HB2	5:O:2777:HIS:HB2	1.77	0.64
5:O:3737:ARG:HD2	5:O:3751:LEU:HD13	1.79	0.64
5:O:3353:GLU:HA	5:O:3357:ARG:HH21	1.62	0.64
2:L:14:MET:HA	2:L:135:PHE:HB2	1.79	0.64
2:L:249:CYS:SG	2:L:250:ARG:N	2.69	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:46:DA:N6	4:J:109:DG:H1	1.96	0.64
5:O:3859:TYR:O	5:O:4119:ARG:NH2	2.30	0.64
6:G:55:LEU:HD23	6:G:58:LEU:HD21	1.80	0.64
5:O:357:LYS:NZ	5:O:1731:PRO:O	2.31	0.64
5:O:2159:PRO:O	5:O:2162:LYS:NZ	2.31	0.64
2:L:20:MET:HB2	2:L:30:PRO:HB2	1.80	0.64
5:O:1768:ARG:O	5:O:1822:ARG:NH1	2.31	0.64
2:L:265:LYS:HD3	2:L:268:LEU:HD22	1.79	0.64
5:O:1519:PHE:HE2	5:O:1566:THR:HG22	1.63	0.64
5:O:1646:LEU:HD12	5:O:1678:LEU:HD12	1.80	0.64
5:O:3289:ARG:NH2	5:O:3295:GLU:OE2	2.31	0.64
5:O:3481:SER:O	5:O:3484:THR:HB	1.97	0.64
5:O:1693:VAL:HG22	5:O:1696:LEU:HD23	1.79	0.63
1:K:289:TYR:HD2	1:K:292:THR:H	1.44	0.63
5:O:848:LEU:HD12	5:O:852:ARG:HH22	1.62	0.63
5:O:1075:ARG:NH2	5:O:1117:ASP:OD2	2.31	0.63
5:O:3348:LEU:O	5:O:3352:GLU:N	2.29	0.63
6:G:83:LEU:HB2	6:G:102:ILE:HD13	1.81	0.63
5:O:924:ARG:HH21	5:O:2769:VAL:HG22	1.63	0.63
5:O:1488:TYR:HA	5:O:1559:PHE:HZ	1.64	0.63
5:O:112:THR:HG21	5:O:152:LEU:HD22	1.81	0.63
5:O:1754:GLN:HB3	5:O:1785:ILE:HD11	1.79	0.63
5:O:3720:ALA:HB3	5:O:3743:HIS:HA	1.81	0.63
5:O:3762:GLN:HG2	5:O:3795:PRO:HB3	1.80	0.63
3:I:53:DG:H21	8:E:83:ARG:HH22	1.45	0.63
4:J:44:DG:H4'	4:J:45:DT:H5'	1.80	0.63
5:O:887:ASP:OD1	5:O:891:ARG:NH1	2.32	0.63
5:O:1169:VAL:HG21	5:O:1198:LEU:HD21	1.80	0.63
5:O:1808:ASP:O	5:O:1816:ARG:NH1	2.32	0.63
5:O:3514:VAL:O	5:O:3518:VAL:N	2.27	0.63
1:K:364:PRO:HG3	2:L:357:MET:HB2	1.80	0.63
5:O:3923:ARG:O	5:O:3962:ARG:NH1	2.32	0.63
2:L:198:THR:H	2:L:201:GLN:HB2	1.64	0.63
5:O:3161:LEU:HD21	5:O:3186:ARG:HD2	1.81	0.63
6:G:29:ARG:NH2	7:H:32:GLU:OE1	2.32	0.63
1:K:260:LYS:HA	1:K:270:SER:HA	1.81	0.62
5:O:1233:SER:OG	5:O:1292:LYS:NZ	2.32	0.62
5:O:1686:LEU:HD22	5:O:1738:ASN:HB3	1.81	0.62
5:O:1751:GLU:O	5:O:1788:ARG:NH1	2.32	0.62
5:O:2586:PHE:HB3	5:O:2776:ARG:HH12	1.64	0.62
8:E:49:ARG:HB2	8:E:53:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:421:LEU:HA	5:O:424:LEU:HB3	1.80	0.62
6:C:42:ARG:HB2	7:D:85:THR:HA	1.81	0.62
5:O:2332:GLU:O	5:O:2334:LYS:NZ	2.27	0.62
5:O:4045:CYS:SG	5:O:4049:ARG:NH1	2.72	0.62
1:K:301:ARG:NH2	1:K:308:GLY:O	2.32	0.62
1:K:325:ARG:NH2	2:L:89:ASP:OD1	2.26	0.62
1:K:402:PRO:HD2	1:K:406:ILE:HG21	1.80	0.62
3:I:34:DT:H2'	3:I:35:DT:H71	1.80	0.62
1:K:367:PHE:HA	1:K:433:GLN:HA	1.82	0.62
5:O:933:LEU:HD13	5:O:2793:PRO:HB2	1.81	0.62
5:O:3114:TYR:OH	5:O:3125:ARG:NH1	2.32	0.62
5:O:913:ARG:NH1	5:O:916:GLU:OE2	2.29	0.62
6:C:88:ARG:HA	6:C:94:ASN:HD21	1.64	0.62
9:B:84:MET:SD	9:B:85:ASP:N	2.72	0.62
5:O:3860:LYS:HE3	5:O:4073:ALA:HB3	1.82	0.62
5:O:270:ALA:HA	5:O:273:ARG:HE	1.64	0.62
5:O:439:VAL:O	5:O:442:GLN:HB3	2.00	0.62
5:O:1727:ARG:NH1	5:O:1772:HIS:O	2.32	0.62
6:G:108:LEU:HD12	6:G:109:PRO:HD2	1.81	0.62
5:O:2168:LEU:HA	5:O:2171:LEU:HD12	1.82	0.62
5:O:3352:GLU:O	5:O:3357:ARG:NE	2.32	0.62
1:K:245:LYS:O	1:K:247:ARG:NH1	2.33	0.62
5:O:899:ARG:HH12	5:O:2566:THR:HA	1.62	0.62
5:O:965:THR:CG2	5:O:969:LEU:HG	2.28	0.62
5:O:1096:VAL:O	5:O:1100:VAL:HG13	2.00	0.62
1:K:259:LEU:HD22	1:K:273:ILE:HD11	1.81	0.61
3:I:55:DA:N6	4:J:101:DC:O2	2.33	0.61
5:O:3572:ILE:HG21	5:O:3800:LEU:HA	1.82	0.61
8:A:66:PRO:HB3	9:B:28:GLY:HA3	1.81	0.61
1:K:301:ARG:HE	1:K:310:LEU:HG	1.64	0.61
5:O:953:GLN:O	5:O:956:PRO:HD3	2.00	0.61
5:O:2136:PRO:O	5:O:2143:ARG:NH2	2.33	0.61
5:O:3806:LEU:HD23	5:O:3809:THR:HB	1.83	0.61
6:G:77:ARG:HH21	7:H:52:SER:HA	1.65	0.61
5:O:275:PHE:HZ	5:O:319:PHE:HB2	1.65	0.61
5:O:1196:PRO:HG3	5:O:1203:SER:HB2	1.82	0.61
6:G:81:ARG:HD3	8:E:58:THR:HB	1.82	0.61
5:O:286:LEU:HD23	5:O:319:PHE:HD1	1.65	0.61
5:O:1881:TYR:HB2	5:O:1950:SER:HB2	1.81	0.61
1:K:351:LYS:O	1:K:395:ALA:N	2.33	0.61
2:L:423:GLN:NE2	2:L:424:LEU:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1538:LEU:N	5:O:1553:PHE:O	2.32	0.61
5:O:3818:ASN:O	5:O:3822:GLN:NE2	2.33	0.61
6:C:91:GLU:O	6:C:95:LYS:N	2.32	0.61
5:O:395:MET:HB2	5:O:406:ARG:HD3	1.82	0.61
5:O:3795:PRO:O	5:O:3796:MET:HE2	2.01	0.61
8:A:121:PRO:HB3	9:B:53:GLU:HG3	1.83	0.61
5:O:895:ALA:HA	5:O:904:VAL:HA	1.82	0.61
5:O:1099:PHE:HE1	5:O:1152:ARG:HE	1.48	0.61
5:O:1458:LEU:O	5:O:1463:LEU:N	2.32	0.61
5:O:1610:ASN:OD1	5:O:1611:GLN:N	2.34	0.61
5:O:3034:PRO:HD2	5:O:3037:GLN:HB2	1.83	0.61
5:O:3269:ARG:HB2	5:O:3272:TRP:HD1	1.66	0.61
5:O:3471:ILE:HD13	5:O:3474:ARG:HD3	1.83	0.61
3:I:87:DC:N3	4:J:67:DG:N2	2.49	0.61
5:O:3592:VAL:HG23	5:O:3606:ILE:HD12	1.82	0.61
5:O:2228:ARG:O	5:O:2230:VAL:N	2.33	0.61
5:O:3296:GLN:HE21	5:O:3301:LEU:N	1.99	0.61
5:O:898:PHE:CE2	5:O:2535:THR:HB	2.35	0.60
5:O:2957:LEU:HD21	5:O:2993:PHE:HZ	1.66	0.60
8:E:64:LYS:HG3	8:E:65:LEU:HD12	1.82	0.60
1:K:330:GLU:N	1:K:333:GLU:OE1	2.35	0.60
4:J:23:DC:H2"	4:J:24:DA:N7	2.15	0.60
5:O:864:GLY:HA2	5:O:867:ASN:HB2	1.84	0.60
9:B:72:TYR:HB3	9:B:85:ASP:HB2	1.83	0.60
1:K:290:ARG:HH21	2:L:310:ILE:H	1.47	0.60
6:G:17:ARG:HA	6:G:20:ARG:HB2	1.82	0.60
1:K:392:LYS:NZ	2:L:459:ASP:OD1	2.35	0.60
5:O:385:TYR:HB2	5:O:420:VAL:HG11	1.84	0.60
5:O:718:MET:HB2	5:O:726:LEU:HD11	1.84	0.60
5:O:3608:LYS:HB2	5:O:3612:ARG:HH21	1.67	0.60
5:O:3948:SER:HA	5:O:3951:GLN:HE22	1.65	0.60
1:K:164:LYS:HB3	1:K:198:ILE:HG23	1.84	0.60
5:O:2266:ASN:O	5:O:2311:ARG:NH1	2.34	0.60
5:O:3244:ASP:HB2	5:O:3247:ARG:HH21	1.66	0.60
2:L:60:GLY:N	2:L:76:ASN:O	2.24	0.60
3:I:19:DG:H22	4:J:136:DA:H2	1.50	0.60
8:E:108:ASN:HB2	9:F:43:VAL:HG22	1.82	0.60
1:K:37:SER:HB3	1:K:108:LEU:HD11	1.83	0.60
2:L:35:LYS:NZ	2:L:94:ILE:O	2.34	0.60
5:O:2837:LEU:O	5:O:2841:ASN:ND2	2.33	0.60
6:C:81:ARG:NH2	8:A:55:GLN:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:216:GLU:HG3	2:L:219:ASP:HB3	1.83	0.59
5:O:908:ASP:HA	5:O:911:LEU:HD23	1.83	0.59
5:O:1396:PRO:HB3	5:O:1457:GLN:HE21	1.67	0.59
5:O:2485:ARG:HH12	5:O:2530:ARG:HA	1.66	0.59
1:K:165:ARG:NH1	1:K:201:ASP:OD2	2.30	0.59
2:L:11:VAL:HG22	2:L:55:ALA:HB3	1.83	0.59
5:O:2988:GLU:HA	5:O:2991:LYS:HE2	1.84	0.59
6:G:61:GLU:HG2	7:H:103:LEU:HD11	1.83	0.59
1:K:45:SER:HB3	1:K:48:MET:HG2	1.85	0.59
1:K:265:LYS:HB2	2:L:530:LEU:HD13	1.85	0.59
2:L:408:ALA:HB1	2:L:419:LEU:HD21	1.84	0.59
3:I:41:DT:O3'	6:C:42:ARG:NH2	2.35	0.59
3:I:88:DG:H2''	3:I:89:DT:H5''	1.84	0.59
5:O:742:GLU:HB3	5:O:780:ILE:HD12	1.84	0.59
5:O:1046:PRO:HA	5:O:1049:GLN:HB2	1.83	0.59
5:O:1709:GLU:HB3	5:O:1712:ARG:HH21	1.68	0.59
5:O:2104:MET:HE1	5:O:2122:LEU:HD13	1.84	0.59
5:O:2223:VAL:HG11	5:O:2238:ILE:HD11	1.85	0.59
7:D:89:ARG:NH1	9:F:75:HIS:O	2.35	0.59
5:O:1066:LEU:HD23	5:O:1078:ALA:HB2	1.84	0.59
5:O:3446:VAL:HA	5:O:3449:LYS:HG2	1.85	0.59
5:O:2543:ASN:ND2	5:O:2839:ASP:OD2	2.36	0.59
1:K:143:LEU:H	1:K:176:HIS:HE1	1.50	0.59
2:L:25:PRO:HA	2:L:185:LEU:HD23	1.84	0.59
5:O:3737:ARG:NH1	5:O:3751:LEU:HB3	2.18	0.59
4:J:44:DG:OP1	7:H:83:ARG:NH1	2.36	0.59
5:O:3243:ILE:HD12	5:O:3254:LEU:HD21	1.85	0.59
6:C:91:GLU:HA	6:C:94:ASN:HB2	1.85	0.59
1:K:372:GLU:OE1	1:K:379:SER:N	2.36	0.59
2:L:146:GLN:HB3	2:L:149:ILE:HB	1.85	0.59
4:J:63:DA:H3'	9:B:36:ARG:HH22	1.68	0.59
5:O:1111:LEU:HD11	5:O:1186:LYS:HZ2	1.68	0.59
5:O:3965:ARG:HA	5:O:3968:ILE:HD12	1.84	0.59
5:O:170:VAL:HA	5:O:219:VAL:HG21	1.83	0.58
5:O:1369:MET:SD	5:O:1370:ARG:NH1	2.76	0.58
5:O:1369:MET:HA	5:O:1372:LEU:HG	1.85	0.58
5:O:1936:ARG:O	5:O:1940:TYR:N	2.30	0.58
5:O:2723:THR:HA	5:O:2726:LEU:HD13	1.85	0.58
8:E:116:ARG:NH2	8:E:123:ASP:OD1	2.27	0.58
5:O:1350:ASN:OD1	5:O:1351:THR:N	2.35	0.58
5:O:2407:GLY:HA3	5:O:2411:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:277:VAL:HA	2:L:430:LEU:HA	1.85	0.58
5:O:1445:ARG:HB3	5:O:1510:LEU:HD11	1.85	0.58
1:K:526:LYS:O	1:K:530:TYR:HB2	2.03	0.58
5:O:67:VAL:HA	5:O:70:ARG:HB2	1.85	0.58
1:K:40:PHE:HE1	1:K:83:LEU:HD13	1.69	0.58
2:L:267:ILE:HB	2:L:361:VAL:HB	1.84	0.58
5:O:449:TYR:O	5:O:454:GLN:NE2	2.35	0.58
5:O:833:HIS:O	5:O:833:HIS:ND1	2.36	0.58
5:O:914:VAL:HA	5:O:917:LEU:HB2	1.85	0.58
5:O:1181:THR:HA	5:O:1184:ARG:HE	1.69	0.58
5:O:1793:THR:O	5:O:1797:LEU:HG	2.03	0.58
5:O:3604:LYS:N	5:O:3607:GLU:OE2	2.37	0.58
5:O:3723:ASP:HB3	5:O:3741:ARG:HD2	1.85	0.58
6:G:103:ALA:HA	9:F:97:LEU:HD11	1.84	0.58
7:H:37:TYR:O	7:H:41:VAL:HG23	2.04	0.58
5:O:1184:ARG:O	5:O:1188:ILE:HD12	2.03	0.58
5:O:3617:LEU:HB3	5:O:3632:PHE:HZ	1.67	0.58
5:O:19:LEU:HD22	5:O:34:LEU:HA	1.84	0.58
5:O:487:LEU:HD11	5:O:575:ILE:HG21	1.86	0.58
5:O:914:VAL:O	5:O:918:ALA:N	2.31	0.58
5:O:1128:CYS:HA	5:O:1131:ILE:HG12	1.86	0.58
5:O:2480:ILE:O	5:O:2484:TYR:HB2	2.03	0.58
2:L:461:MET:HB2	2:L:522:VAL:HG13	1.84	0.58
5:O:3502:MET:O	5:O:3506:LEU:HG	2.03	0.58
5:O:3907:SER:HB2	5:O:3937:VAL:HG22	1.86	0.58
5:O:3951:GLN:HB2	5:O:4067:GLY:HA3	1.85	0.58
5:O:3969:ASN:HA	5:O:3972:LEU:HG	1.85	0.58
2:L:512:ILE:HA	2:L:515:MET:HE3	1.85	0.58
5:O:1082:PHE:HA	5:O:1085:ILE:HG12	1.86	0.58
6:C:40:ALA:HA	7:D:86:ILE:HG13	1.86	0.58
1:K:59:PRO:HA	1:K:62:MET:HG2	1.86	0.58
1:K:318:ARG:HA	2:L:278:VAL:HA	1.85	0.58
1:K:481:PRO:HG2	2:L:403:PRO:HG2	1.86	0.58
5:O:828:LYS:HG2	5:O:829:VAL:H	1.67	0.58
5:O:3615:ALA:O	5:O:3621:LYS:NZ	2.36	0.58
5:O:144:MET:N	5:O:144:MET:SD	2.77	0.57
5:O:164:LYS:HB2	5:O:166:ILE:HG12	1.86	0.57
5:O:1044:ILE:HG22	5:O:1049:GLN:HG3	1.86	0.57
5:O:3793:VAL:HA	5:O:3803:ILE:HG13	1.86	0.57
1:K:341:ASP:OD2	1:K:399:ARG:NH1	2.36	0.57
2:L:361:VAL:HG22	2:L:422:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:455:LEU:O	5:O:459:ARG:HG3	2.04	0.57
5:O:1477:HIS:HB3	5:O:1481:THR:HG23	1.87	0.57
5:O:2351:GLN:O	5:O:2352:HIS:ND1	2.37	0.57
5:O:3837:CYS:O	5:O:3840:LYS:NZ	2.34	0.57
5:O:4074:PHE:HA	5:O:4077:TYR:HD2	1.68	0.57
5:O:348:ILE:HB	5:O:391:ARG:HH22	1.70	0.57
5:O:1279:LEU:HD23	5:O:1359:LEU:HD11	1.85	0.57
5:O:1607:GLU:OE2	5:O:1614:GLN:NE2	2.37	0.57
5:O:2595:TRP:O	5:O:2596:ARG:NE	2.37	0.57
5:O:2776:ARG:NH2	5:O:2782:ASP:OD2	2.38	0.57
5:O:4010:SER:HA	5:O:4014:LYS:HE3	1.86	0.57
1:K:53:SER:OG	1:K:54:GLU:N	2.37	0.57
5:O:42:CYS:O	5:O:46:SER:N	2.38	0.57
5:O:208:MET:HE3	5:O:208:MET:O	2.04	0.57
5:O:3554:PHE:HA	5:O:3557:ARG:HE	1.69	0.57
5:O:3588:TRP:CG	5:O:3609:MET:HE2	2.39	0.57
8:E:61:LEU:O	9:F:36:ARG:NH2	2.36	0.57
1:K:38:LEU:HD11	1:K:167:MET:HB2	1.86	0.57
1:K:458:GLN:HG3	1:K:528:LEU:HD13	1.84	0.57
5:O:71:LYS:HZ1	5:O:82:ARG:HG3	1.67	0.57
5:O:3965:ARG:HD2	5:O:3969:ASN:HD21	1.70	0.57
5:O:2225:HIS:CD2	5:O:2226:PRO:HD2	2.40	0.57
6:C:32:ARG:HA	6:C:35:ARG:HD2	1.86	0.57
8:E:108:ASN:ND2	9:F:42:GLY:O	2.37	0.57
1:K:61:ASP:OD2	1:K:65:GLN:NE2	2.38	0.57
1:K:372:GLU:OE2	1:K:377:GLY:N	2.38	0.57
2:L:496:HIS:CG	2:L:506:PRO:HD3	2.40	0.57
4:J:133:DG:H2'	4:J:134:DG:C8	2.39	0.57
5:O:300:TRP:HE3	5:O:308:LEU:HD21	1.69	0.57
5:O:755:ALA:HB1	5:O:765:LEU:HD11	1.86	0.57
5:O:1769:GLU:O	5:O:1772:HIS:ND1	2.38	0.57
5:O:2586:PHE:HB3	5:O:2776:ARG:HH22	1.70	0.57
5:O:3490:VAL:HG23	5:O:3494:GLN:HB2	1.85	0.57
2:L:57:VAL:HG22	2:L:79:VAL:HG13	1.86	0.57
4:J:92:DT:H1'	4:J:93:DA:H5'	1.86	0.57
4:J:94:DA:H2''	4:J:95:DG:C8	2.39	0.57
5:O:2329:TYR:HB3	5:O:2332:GLU:HA	1.87	0.57
1:K:244:ARG:NH1	1:K:245:LYS:O	2.37	0.57
2:L:450:GLN:HB3	2:L:537:PHE:CZ	2.40	0.57
5:O:441:MET:O	5:O:445:SER:N	2.37	0.57
5:O:1304:HIS:O	5:O:1334:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3445:LEU:O	5:O:3449:LYS:NZ	2.38	0.57
5:O:3796:MET:HG3	5:O:3802:LEU:H	1.68	0.57
5:O:4088:ASN:ND2	5:O:4109:ASP:OD1	2.33	0.57
2:L:184:ARG:HE	2:L:520:ALA:H	1.53	0.57
5:O:2167:PRO:O	5:O:2170:GLN:HB3	2.05	0.57
8:A:129:ARG:NH1	8:E:106:ASP:OD1	2.38	0.57
7:H:102:GLU:HG2	7:H:103:LEU:H	1.69	0.57
3:I:25:DG:N2	4:J:130:DC:N3	2.53	0.56
5:O:683:PHE:HD1	5:O:704:PHE:HE1	1.52	0.56
5:O:1491:ILE:HG13	5:O:1492:ALA:N	2.19	0.56
5:O:2391:GLY:O	5:O:2431:ARG:NH2	2.38	0.56
5:O:3370:SER:OG	5:O:3371:GLU:N	2.37	0.56
5:O:135:LEU:HD22	5:O:139:ARG:HH12	1.68	0.56
5:O:524:TYR:OH	5:O:625:ASN:O	2.20	0.56
5:O:1282:LEU:HD22	5:O:1359:LEU:HD22	1.86	0.56
5:O:1508:LYS:NZ	5:O:1562:LEU:O	2.38	0.56
5:O:3479:THR:O	5:O:3481:SER:N	2.38	0.56
5:O:911:LEU:O	5:O:915:THR:OG1	2.21	0.56
5:O:1369:MET:SD	5:O:1369:MET:N	2.78	0.56
5:O:3048:LYS:HB3	5:O:3061:LEU:HB2	1.86	0.56
5:O:3717:VAL:HG23	5:O:3743:HIS:H	1.71	0.56
5:O:3806:LEU:HG	5:O:3808:ASN:H	1.70	0.56
1:K:212:ASP:O	1:K:214:SER:N	2.38	0.56
2:L:395:TYR:HB3	2:L:404:GLN:HB3	1.87	0.56
5:O:1198:LEU:O	5:O:1202:ARG:NH2	2.38	0.56
5:O:1923:PHE:HD1	5:O:1941:HIS:HB3	1.70	0.56
5:O:2205:VAL:HG23	5:O:2208:ASP:H	1.71	0.56
5:O:3480:LEU:O	5:O:3484:THR:N	2.38	0.56
2:L:76:ASN:ND2	2:L:104:GLN:O	2.32	0.56
2:L:312:GLN:NE2	2:L:323:PHE:O	2.29	0.56
7:H:102:GLU:HG2	7:H:103:LEU:N	2.20	0.56
1:K:428:THR:HB	2:L:354:ARG:HH12	1.70	0.56
5:O:1009:LEU:HD11	5:O:1036:PHE:CE2	2.40	0.56
5:O:2275:GLN:O	5:O:2279:ILE:HG12	2.05	0.56
5:O:3064:PHE:HA	5:O:3067:LYS:HE3	1.87	0.56
5:O:3155:VAL:HG13	5:O:3157:LEU:HG	1.86	0.56
5:O:2533:SER:HA	5:O:2538:ARG:HB2	1.87	0.56
5:O:3516:HIS:O	5:O:3519:GLU:HB3	2.06	0.56
5:O:3634:GLN:HG2	5:O:3635:THR:HG23	1.86	0.56
5:O:3840:LYS:HG2	5:O:3842:TRP:NE1	2.20	0.56
6:G:71:ARG:HH21	6:G:76:THR:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:303:PHE:HA	1:K:311:LEU:H	1.71	0.56
5:O:297:LEU:HD13	5:O:316:LEU:HB2	1.85	0.56
5:O:1583:MET:HE3	5:O:1628:LYS:HB2	1.86	0.56
5:O:3724:GLU:O	5:O:3725:ARG:NH1	2.34	0.56
5:O:3991:PHE:O	5:O:3992:ARG:NE	2.39	0.56
9:F:63:GLU:O	9:F:66:ILE:HG12	2.06	0.56
1:K:416:GLN:NE2	1:K:429:PRO:O	2.38	0.56
3:I:41:DT:H2"	3:I:42:DA:C8	2.41	0.56
5:O:163:LYS:C	5:O:164:LYS:HD3	2.31	0.56
5:O:384:MET:O	5:O:388:LEU:HG	2.06	0.56
5:O:933:LEU:HG	5:O:937:MET:HE2	1.86	0.56
5:O:3784:ARG:HB2	5:O:3786:LEU:HD23	1.87	0.56
8:A:88:ALA:HB1	9:B:86:VAL:HG21	1.87	0.56
6:G:55:LEU:HD22	7:H:63:VAL:HG13	1.88	0.56
1:K:214:SER:HA	1:K:218:ARG:HB2	1.87	0.56
5:O:1768:ARG:HG2	5:O:1769:GLU:OE1	2.05	0.56
5:O:1917:LYS:NZ	5:O:1921:ASP:OD2	2.38	0.56
5:O:2138:VAL:O	5:O:2143:ARG:NH2	2.39	0.56
5:O:4006:VAL:HG23	5:O:4009:PRO:HD3	1.87	0.56
5:O:76:ILE:HA	5:O:79:ARG:HG2	1.88	0.55
5:O:332:GLU:O	5:O:335:LYS:NZ	2.39	0.55
5:O:990:GLN:HB3	5:O:2781:PRO:HD3	1.88	0.55
5:O:1249:SER:OG	5:O:1312:CYS:O	2.22	0.55
5:O:3356:ALA:HA	5:O:3359:ILE:HG12	1.87	0.55
1:K:455:THR:HB	1:K:458:GLN:NE2	2.21	0.55
2:L:448:GLU:HA	2:L:451:LEU:HD12	1.87	0.55
2:L:478:PRO:HB2	2:L:481:LYS:HB3	1.88	0.55
3:I:26:DC:N4	4:J:127:DG:O6	2.39	0.55
5:O:584:GLU:HB2	5:O:613:HIS:HB3	1.89	0.55
5:O:714:VAL:HB	5:O:733:LEU:HD21	1.87	0.55
5:O:2464:HIS:CE1	5:O:2466:SER:HB3	2.41	0.55
5:O:3546:SER:O	5:O:3549:HIS:NE2	2.39	0.55
9:B:68:ASP:OD2	9:B:92:ARG:NH2	2.38	0.55
2:L:20:MET:HG3	2:L:31:PHE:HB2	1.88	0.55
5:O:944:LYS:O	5:O:947:GLN:NE2	2.35	0.55
5:O:1091:GLU:OE1	5:O:1091:GLU:N	2.39	0.55
5:O:1098:GLN:OE1	5:O:1152:ARG:N	2.36	0.55
5:O:1418:HIS:O	5:O:1422:LYS:NZ	2.39	0.55
5:O:2346:ALA:HA	5:O:2349:LEU:HD12	1.86	0.55
5:O:3159:ARG:O	5:O:3163:THR:HG23	2.07	0.55
5:O:3506:LEU:HD21	5:O:3514:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:71:DG:H2''	4:J:72:DG:C8	2.42	0.55
5:O:225:LYS:HE3	5:O:270:ALA:O	2.06	0.55
5:O:850:GLU:HG2	5:O:854:ARG:HH22	1.71	0.55
5:O:2380:ASN:OD1	5:O:2381:ALA:N	2.38	0.55
5:O:2587:GLN:O	5:O:2777:HIS:N	2.38	0.55
2:L:253:ILE:HD13	2:L:257:LEU:HG	1.87	0.55
4:J:78:DC:H1'	4:J:79:DG:C8	2.42	0.55
5:O:327:VAL:HG22	5:O:333:MET:HB3	1.88	0.55
5:O:2264:ASP:HB2	5:O:2267:SER:HB3	1.88	0.55
5:O:3033:GLU:HG3	5:O:3034:PRO:HD3	1.87	0.55
5:O:3048:LYS:HZ1	5:O:3060:SER:HG	1.53	0.55
5:O:3285:HIS:HE1	5:O:3329:LEU:HB2	1.70	0.55
5:O:3531:TYR:O	5:O:3535:ILE:HG12	2.06	0.55
3:I:14:DC:N3	4:J:141:DG:N2	2.53	0.55
4:J:42:DG:H2''	4:J:43:DA:C8	2.42	0.55
5:O:435:LEU:HA	5:O:438:LEU:HD12	1.87	0.55
5:O:896:VAL:HG13	5:O:898:PHE:HB2	1.89	0.55
5:O:1436:LEU:O	5:O:1445:ARG:NH2	2.39	0.55
5:O:1833:LEU:HG	5:O:1835:ALA:H	1.71	0.55
5:O:3083:SER:OG	5:O:3102:TYR:O	2.24	0.55
5:O:3299:THR:HG22	5:O:3302:LYS:H	1.71	0.55
6:C:61:GLU:O	6:C:64:GLU:HG3	2.06	0.55
3:I:103:DG:N2	4:J:52:DC:O2	2.40	0.55
5:O:471:LYS:HB3	5:O:474:VAL:HG12	1.87	0.55
5:O:1742:CYS:HA	5:O:1745:LYS:HD2	1.88	0.55
5:O:1766:LEU:HD23	5:O:1822:ARG:HD2	1.87	0.55
5:O:2936:TYR:HA	5:O:2939:LEU:HD12	1.89	0.55
5:O:3227:ILE:HA	5:O:3230:LEU:HD12	1.89	0.55
2:L:345:PHE:HB2	2:L:389:MET:SD	2.47	0.55
4:J:35:DG:H2''	4:J:36:DA:H5''	1.88	0.55
5:O:2261:SER:O	5:O:2270:ASN:ND2	2.40	0.55
5:O:3493:TRP:HB2	5:O:3709:GLY:HA3	1.88	0.55
5:O:3772:ASN:O	5:O:3787:GLN:NE2	2.39	0.55
1:K:288:LEU:HG	2:L:313:GLY:HA3	1.89	0.55
2:L:6:ASN:HA	2:L:128:GLU:HG3	1.87	0.55
5:O:167:PRO:HA	5:O:171:LEU:HD23	1.87	0.55
5:O:672:ILE:O	5:O:676:ASN:ND2	2.40	0.55
5:O:2367:VAL:HG22	5:O:2374:LEU:HD21	1.89	0.55
5:O:2464:HIS:O	5:O:2470:ARG:NH1	2.40	0.55
6:C:29:ARG:HG3	6:C:32:ARG:HH21	1.70	0.55
8:E:104:PHE:HE2	9:F:37:LEU:HB3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:459:ARG:HG2	5:O:540:MET:SD	2.47	0.55
5:O:3471:ILE:HA	5:O:3474:ARG:HB2	1.89	0.55
1:K:290:ARG:HB2	2:L:309:ASP:HA	1.90	0.54
2:L:198:THR:O	2:L:202:LYS:N	2.39	0.54
2:L:286:LYS:O	2:L:286:LYS:NZ	2.31	0.54
3:I:39:DC:H2"	3:I:40:DG:C8	2.41	0.54
3:I:46:DA:H61	4:J:109:DG:H1	1.55	0.54
5:O:1444:ASP:HA	5:O:1447:ARG:HE	1.72	0.54
5:O:1684:LEU:O	5:O:1689:LYS:NZ	2.39	0.54
5:O:2335:ASN:OD1	5:O:2336:ILE:N	2.40	0.54
5:O:3588:TRP:NE1	5:O:3609:MET:HG3	2.22	0.54
5:O:3700:GLU:HA	5:O:3718:ARG:HD3	1.89	0.54
1:K:35:ARG:H	1:K:161:MET:HA	1.72	0.54
1:K:203:MET:HE3	1:K:239:LEU:HD13	1.89	0.54
5:O:888:ARG:O	5:O:3889:ARG:NE	2.40	0.54
5:O:965:THR:CG2	5:O:969:LEU:CG	2.82	0.54
5:O:1273:GLU:HB3	5:O:1275:THR:HG23	1.88	0.54
5:O:3390:GLN:HA	5:O:3393:GLU:HG2	1.88	0.54
5:O:3913:ILE:HB	5:O:3984:MET:SD	2.47	0.54
1:K:374:LEU:HD12	2:L:543:LYS:H	1.71	0.54
2:L:133:GLU:HG2	2:L:164:PHE:HE2	1.72	0.54
5:O:2169:LEU:HB3	5:O:2211:LEU:HD13	1.89	0.54
5:O:3545:THR:OG1	5:O:3546:SER:N	2.39	0.54
6:G:49:VAL:HG12	7:H:114:ALA:HB1	1.89	0.54
1:K:347:LEU:HD12	1:K:398:CYS:HB2	1.90	0.54
5:O:1420:ARG:NH2	5:O:1466:ASN:O	2.39	0.54
5:O:2950:LYS:NZ	5:O:2984:GLY:O	2.40	0.54
5:O:3103:ILE:O	5:O:3107:ILE:HG12	2.07	0.54
5:O:3798:SER:OG	5:O:3799:ARG:N	2.41	0.54
1:K:143:LEU:H	1:K:176:HIS:CE1	2.25	0.54
1:K:374:LEU:HB2	2:L:542:ALA:HB3	1.88	0.54
5:O:1959:LEU:C	5:O:1961:PHE:H	2.16	0.54
5:O:950:GLU:HG2	5:O:957:PRO:HD3	1.90	0.54
5:O:1696:LEU:HD11	5:O:1749:ALA:HB1	1.89	0.54
5:O:1825:LEU:O	5:O:1829:TRP:N	2.36	0.54
2:L:405:VAL:O	2:L:423:GLN:NE2	2.41	0.54
5:O:2869:LEU:HB2	5:O:2899:ARG:HH21	1.72	0.54
2:L:362:LEU:HB2	2:L:421:TYR:HB3	1.89	0.54
2:L:397:TYR:HB3	2:L:401:ALA:HB2	1.90	0.54
5:O:236:LYS:HG3	5:O:281:GLN:HE21	1.73	0.54
5:O:1751:GLU:HA	5:O:1785:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3531:TYR:HA	5:O:3534:ILE:HD12	1.90	0.54
6:G:53:ALA:O	6:G:56:GLU:HB2	2.07	0.54
1:K:164:LYS:HD2	1:K:198:ILE:HG12	1.90	0.54
5:O:169:THR:OG1	5:O:170:VAL:N	2.35	0.54
5:O:1601:LEU:HD21	5:O:1652:ILE:HG22	1.88	0.54
5:O:1696:LEU:O	5:O:1698:PHE:N	2.41	0.54
5:O:3819:THR:HG21	5:O:3886:ALA:HA	1.90	0.54
6:C:103:ALA:HA	8:A:94:GLU:HG2	1.90	0.54
8:A:127:ALA:O	8:A:131:ARG:HB2	2.08	0.54
2:L:229:GLU:HG3	2:L:233:LYS:NZ	2.24	0.54
5:O:414:LEU:HB2	5:O:460:ALA:HB1	1.90	0.54
5:O:1404:LYS:NZ	5:O:1460:ARG:O	2.41	0.54
5:O:1583:MET:HE1	5:O:1629:CYS:N	2.23	0.54
5:O:1722:PHE:CE1	5:O:1743:MET:HE3	2.42	0.54
5:O:2161:ALA:HA	5:O:2164:TRP:HB2	1.90	0.54
5:O:3428:GLU:OE2	5:O:3475:TYR:OH	2.26	0.54
1:K:140:ASP:OD1	1:K:182:LYS:NZ	2.40	0.53
5:O:860:GLY:HA3	5:O:3136:THR:HG21	1.90	0.53
5:O:2336:ILE:HG13	5:O:2339:GLU:HB3	1.90	0.53
5:O:3000:ASP:O	5:O:3004:HIS:ND1	2.41	0.53
5:O:3591:ASP:OD2	5:O:3605:ASN:ND2	2.41	0.53
6:C:80:PRO:HB2	6:C:105:GLY:HA2	1.90	0.53
1:K:168:LEU:HD21	1:K:202:LEU:HD12	1.90	0.53
5:O:71:LYS:HA	5:O:75:SER:HB2	1.90	0.53
5:O:1935:GLU:HB3	5:O:1939:LEU:HB2	1.90	0.53
5:O:2169:LEU:HA	5:O:2172:ALA:HB3	1.89	0.53
5:O:2211:LEU:HA	5:O:2214:ARG:HG2	1.90	0.53
9:B:71:THR:HG22	7:H:93:THR:HG23	1.91	0.53
6:G:78:ILE:HB	7:H:51:ILE:HD12	1.91	0.53
6:G:81:ARG:HH21	8:E:56:LYS:HD2	1.73	0.53
1:K:466:VAL:HG11	2:L:387:LEU:HD13	1.90	0.53
3:I:62:DA:H61	4:J:93:DA:H2	1.56	0.53
5:O:1145:LEU:O	5:O:1149:LYS:NZ	2.41	0.53
5:O:1178:ARG:NH2	5:O:1183:CYS:SG	2.72	0.53
5:O:1430:GLU:N	5:O:1430:GLU:OE1	2.40	0.53
5:O:3759:ARG:HH22	5:O:4005:PHE:HB2	1.74	0.53
7:H:87:THR:HB	7:H:89:ARG:HG2	1.90	0.53
1:K:41:LEU:HB2	1:K:168:LEU:HA	1.90	0.53
2:L:286:LYS:NZ	2:L:289:ILE:O	2.41	0.53
5:O:1125:GLN:NE2	5:O:1129:ASP:OD2	2.41	0.53
5:O:1407:LYS:HA	5:O:1412:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1801:VAL:HB	5:O:1824:LEU:HD21	1.90	0.53
5:O:3467:ARG:HD2	5:O:3470:GLN:HE21	1.73	0.53
5:O:3979:LEU:HD22	5:O:3980:MET:HE3	1.90	0.53
9:F:87:VAL:O	9:F:91:LYS:HG3	2.09	0.53
4:J:114:DC:H2"	4:J:115:DG:C8	2.44	0.53
5:O:1297:PHE:HA	5:O:1300:SER:OG	2.08	0.53
5:O:2219:LEU:O	5:O:2223:VAL:HG13	2.08	0.53
5:O:4120:THR:HG23	5:O:4126:PRO:HG3	1.91	0.53
9:F:62:LEU:O	9:F:65:VAL:HG22	2.09	0.53
5:O:141:SER:OG	5:O:146:GLU:OE2	2.27	0.53
5:O:1349:LEU:HB3	5:O:1405:ALA:HB1	1.91	0.53
5:O:1665:HIS:H	5:O:1668:PHE:HB3	1.74	0.53
5:O:1935:GLU:O	5:O:1938:ARG:N	2.37	0.53
5:O:3572:ILE:HG21	5:O:3800:LEU:HG	1.91	0.53
5:O:3604:LYS:HG3	5:O:3606:ILE:HG12	1.91	0.53
6:C:88:ARG:NH2	6:C:94:ASN:OD1	2.42	0.53
2:L:163:PHE:CG	2:L:212:MET:HE1	2.43	0.53
3:I:114:DC:O2	6:G:42:ARG:NH2	2.42	0.53
5:O:1211:VAL:O	5:O:1215:GLU:N	2.41	0.53
5:O:2362:VAL:HG12	5:O:2366:LYS:NZ	2.23	0.53
5:O:3082:TYR:HB3	5:O:3085:GLU:HB2	1.91	0.53
5:O:3287:ARG:O	5:O:3289:ARG:NH1	2.42	0.53
5:O:3324:ARG:HD2	5:O:3392:ALA:HB2	1.91	0.53
1:K:317:LYS:HE3	1:K:328:ILE:HG12	1.90	0.53
3:I:59:DC:H2"	3:I:60:DT:C5	2.43	0.53
5:O:176:GLU:HG2	5:O:223:CYS:HA	1.91	0.53
5:O:649:PHE:HA	5:O:652:GLU:OE2	2.09	0.53
5:O:1452:VAL:HA	5:O:1517:LEU:HD21	1.90	0.53
5:O:2193:ILE:HA	5:O:2196:TRP:CD1	2.44	0.53
5:O:3157:LEU:HA	5:O:3160:LEU:HB2	1.90	0.53
5:O:3245:SER:HA	5:O:3248:LYS:HE2	1.90	0.53
5:O:3518:VAL:HA	5:O:3521:ILE:HG12	1.90	0.53
1:K:397:LEU:HD11	1:K:410:PHE:HD2	1.72	0.53
1:K:485:GLN:OE1	1:K:489:ASN:ND2	2.41	0.53
5:O:3179:TRP:CZ2	5:O:3245:SER:HB2	2.44	0.53
8:A:106:ASP:HB3	8:A:127:ALA:HB1	1.91	0.53
2:L:461:MET:HB3	2:L:526:SER:HB3	1.91	0.53
5:O:563:LEU:O	5:O:566:ASP:N	2.41	0.53
5:O:1224:PHE:HE1	5:O:1266:CYS:HB3	1.74	0.53
5:O:1714:LEU:HD23	5:O:1717:LEU:HD23	1.91	0.53
5:O:2274:ILE:HD13	5:O:2319:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3883:LEU:HD23	5:O:3970:LEU:HB2	1.91	0.53
2:L:280:ASP:HB2	2:L:289:ILE:HD11	1.91	0.52
3:I:89:DT:H2'	3:I:90:DT:C4	2.44	0.52
5:O:442:GLN:HG2	5:O:461:ILE:HD11	1.92	0.52
5:O:576:VAL:HA	5:O:579:LEU:HD12	1.91	0.52
5:O:1711:ARG:HA	5:O:1714:LEU:HD12	1.90	0.52
5:O:2556:SER:O	5:O:2559:THR:OG1	2.23	0.52
8:A:47:ALA:N	8:A:50:GLU:OE1	2.42	0.52
2:L:8:ALA:N	2:L:52:ASP:OD1	2.42	0.52
2:L:397:TYR:HE2	4:J:132:DC:H4'	1.73	0.52
5:O:1963:GLN:HA	5:O:2125:TRP:CZ2	2.44	0.52
5:O:1966:LEU:O	5:O:1967:PHE:C	2.52	0.52
5:O:2365:ASN:ND2	5:O:2399:GLU:OE2	2.34	0.52
9:B:67:ARG:NH1	9:B:68:ASP:OD1	2.42	0.52
2:L:346:CYS:SG	2:L:347:LYS:N	2.81	0.52
5:O:2140:LEU:HA	5:O:2143:ARG:HG2	1.91	0.52
8:E:82:LEU:HD11	9:F:73:THR:HG21	1.92	0.52
1:K:319:SER:O	2:L:277:THR:OG1	2.20	0.52
1:K:442:ASP:OD1	2:L:270:GLU:N	2.38	0.52
5:O:1583:MET:HE2	5:O:1625:HIS:O	2.09	0.52
3:I:48:DC:H2''	3:I:49:DT:C2	2.44	0.52
5:O:1420:ARG:HH11	5:O:1424:THR:HG23	1.74	0.52
5:O:3879:PRO:HG2	5:O:3882:LEU:HD21	1.92	0.52
8:A:74:ILE:HG22	9:B:66:ILE:HG21	1.91	0.52
9:B:35:ARG:O	9:B:39:ARG:HG2	2.10	0.52
3:I:40:DG:H1'	3:I:41:DT:H5'	1.92	0.52
3:I:133:DC:H2''	3:I:134:DA:C8	2.45	0.52
4:J:43:DA:H2''	4:J:44:DG:C8	2.45	0.52
5:O:1110:SER:HA	5:O:1113:LEU:HD12	1.91	0.52
5:O:2281:MET:HE2	5:O:2281:MET:HA	1.91	0.52
5:O:2531:LEU:O	5:O:2538:ARG:NH2	2.41	0.52
5:O:3971:MET:HE3	5:O:3974:MET:HB2	1.92	0.52
5:O:4125:GLU:HA	5:O:4127:TRP:CZ3	2.45	0.52
1:K:380:THR:HG23	2:L:444:TYR:HD1	1.75	0.52
5:O:13:LEU:HB2	5:O:59:PHE:CZ	2.45	0.52
5:O:859:LEU:O	5:O:867:ASN:ND2	2.42	0.52
5:O:939:MET:SD	5:O:2783:ILE:HG13	2.50	0.52
5:O:1034:ARG:NE	5:O:1088:GLU:OE2	2.37	0.52
5:O:1483:LEU:HD11	5:O:1514:LEU:HB3	1.92	0.52
5:O:2034:SER:O	5:O:2037:SER:N	2.43	0.52
5:O:2126:MET:HE1	5:O:2164:TRP:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3662:ILE:HA	5:O:3665:MET:HE2	1.92	0.52
5:O:3980:MET:O	5:O:3984:MET:HG2	2.10	0.52
1:K:278:GLN:HB3	2:L:431:ARG:HD2	1.90	0.52
5:O:23:ASP:HB3	5:O:34:LEU:HD21	1.90	0.52
5:O:345:PHE:CE2	5:O:369:PHE:HB2	2.45	0.52
5:O:636:GLU:OE1	5:O:636:GLU:N	2.41	0.52
5:O:1330:TYR:CZ	5:O:1334:LYS:HD2	2.44	0.52
5:O:2548:PRO:HB3	5:O:2847:THR:HA	1.91	0.52
5:O:3588:TRP:CD1	5:O:3609:MET:HE2	2.45	0.52
8:A:113:HIS:HB2	8:E:126:LEU:HD13	1.92	0.52
1:K:41:LEU:O	1:K:169:PHE:N	2.43	0.52
1:K:44:ALA:HB2	1:K:87:PHE:CE2	2.42	0.52
1:K:202:LEU:HB2	1:K:221:ILE:HG22	1.92	0.52
1:K:510:LYS:O	1:K:512:GLU:N	2.42	0.52
2:L:154:LEU:HD13	2:L:215:LEU:HD21	1.91	0.52
4:J:147:DC:H1'	4:J:148:DC:C2	2.45	0.52
5:O:2891:ARG:NH1	5:O:2894:GLU:OE2	2.38	0.52
5:O:3872:ARG:HH12	5:O:4117:LEU:HD22	1.75	0.52
6:C:18:SER:OG	6:C:27:VAL:N	2.42	0.52
1:K:349:GLY:HA3	2:L:463:LEU:HD11	1.92	0.51
5:O:370:ALA:HB1	5:O:423:TYR:HE2	1.75	0.51
5:O:1201:ASN:HB3	5:O:1207:TRP:HB2	1.92	0.51
5:O:2514:ASN:HB3	5:O:2517:LEU:HD13	1.92	0.51
5:O:3133:GLN:NE2	5:O:3137:GLU:OE2	2.36	0.51
5:O:3296:GLN:HA	5:O:3299:THR:HB	1.93	0.51
5:O:3515:GLN:O	5:O:3519:GLU:N	2.34	0.51
5:O:3818:ASN:OD1	5:O:3819:THR:N	2.44	0.51
2:L:18:PHE:O	2:L:21:SER:OG	2.28	0.51
5:O:3021:SER:HG	5:O:3031:TRP:CD1	2.28	0.51
5:O:3363:SER:HB2	5:O:3380:ARG:HD3	1.91	0.51
5:O:3748:HIS:HB3	5:O:3750:PHE:CZ	2.45	0.51
3:I:92:DT:H3	4:J:63:DA:H2	1.57	0.51
3:I:94:DA:H2''	3:I:95:DC:H5''	1.93	0.51
5:O:279:ALA:HB2	5:O:318:SER:HB2	1.92	0.51
5:O:395:MET:HE2	5:O:406:ARG:HD3	1.92	0.51
5:O:2142:ILE:O	5:O:2146:LEU:HG	2.11	0.51
5:O:2371:PHE:HB3	5:O:2374:LEU:HD23	1.92	0.51
8:A:92:LEU:HD11	9:B:65:VAL:HG11	1.91	0.51
1:K:74:LYS:O	1:K:78:SER:N	2.41	0.51
2:L:18:PHE:HB3	2:L:102:SER:HA	1.93	0.51
4:J:137:DC:H2'	4:J:138:DC:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:87:LYS:O	5:O:91:ILE:HG12	2.10	0.51
5:O:1267:TYR:CE2	5:O:1290:LEU:HD21	2.46	0.51
5:O:1284:THR:OG1	5:O:1285:GLU:OE1	2.24	0.51
5:O:1762:MET:HE2	5:O:1778:PHE:CE1	2.45	0.51
6:C:76:THR:O	7:D:50:GLY:N	2.40	0.51
2:L:259:ILE:HG23	2:L:373:ALA:HB1	1.93	0.51
2:L:363:LYS:HD2	2:L:418:CYS:SG	2.51	0.51
5:O:58:VAL:O	5:O:61:ARG:HG3	2.11	0.51
5:O:3515:GLN:OE1	5:O:3515:GLN:N	2.41	0.51
6:G:32:ARG:HA	6:G:35:ARG:HG2	1.91	0.51
9:F:59:LYS:O	9:F:62:LEU:HG	2.10	0.51
3:I:116:DA:H5'	3:I:116:DA:H8	1.76	0.51
5:O:2158:ARG:NH2	5:O:2722:ARG:HH21	2.08	0.51
1:K:318:ARG:HE	2:L:276:TRP:HB3	1.75	0.51
3:I:102:DG:H1	4:J:52:DC:H42	1.59	0.51
5:O:913:ARG:O	5:O:916:GLU:HG3	2.10	0.51
5:O:1482:GLU:OE1	5:O:1482:GLU:N	2.42	0.51
5:O:2093:CYS:O	5:O:2094:MET:HE2	2.11	0.51
5:O:2462:VAL:N	5:O:2473:MET:HE1	2.25	0.51
5:O:3263:HIS:HB2	5:O:3276:TRP:CZ2	2.46	0.51
5:O:4088:ASN:ND2	5:O:4109:ASP:O	2.44	0.51
1:K:370:PRO:HD3	1:K:382:PHE:CE2	2.46	0.51
3:I:52:DA:H2''	3:I:53:DG:C8	2.45	0.51
4:J:41:DG:H2''	4:J:42:DG:H8	1.75	0.51
4:J:126:DC:H2''	4:J:127:DG:C8	2.45	0.51
4:J:139:DG:OP2	5:O:165:LYS:NZ	2.30	0.51
5:O:200:PHE:HZ	5:O:227:LEU:HD13	1.76	0.51
5:O:924:ARG:HH22	5:O:2595:TRP:HB3	1.76	0.51
5:O:1014:LEU:HA	5:O:1018:VAL:HG22	1.93	0.51
5:O:1841:SER:HA	5:O:1844:VAL:HG23	1.91	0.51
5:O:2534:ASN:O	5:O:2536:LEU:N	2.44	0.51
7:D:89:ARG:HG2	9:F:75:HIS:CE1	2.46	0.51
1:K:289:TYR:N	1:K:294:GLU:O	2.44	0.51
4:J:49:DC:H2''	4:J:50:DC:O4'	2.11	0.51
5:O:61:ARG:HG2	5:O:103:TYR:HE2	1.76	0.51
5:O:1023:SER:HA	5:O:1026:ARG:HG3	1.92	0.51
5:O:1135:CYS:HA	5:O:1138:ILE:HG12	1.92	0.51
5:O:1518:ALA:HB1	5:O:1524:LEU:HD21	1.92	0.51
5:O:1696:LEU:HD13	5:O:1758:LEU:HD11	1.93	0.51
5:O:2430:GLU:N	5:O:2430:GLU:OE1	2.44	0.51
5:O:3980:MET:HA	5:O:3983:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:4083:GLY:O	5:O:4088:ASN:HB2	2.11	0.51
7:H:73:GLU:HB2	7:H:98:LEU:HD22	1.93	0.51
1:K:94:LYS:H	1:K:103:TYR:HA	1.76	0.51
1:K:478:PHE:HA	1:K:506:LEU:HD11	1.93	0.51
3:I:34:DT:O4	4:J:119:DA:N6	2.44	0.51
3:I:97:DG:N1	4:J:58:DG:O6	2.44	0.51
5:O:3242:MET:HE2	5:O:3242:MET:HA	1.93	0.51
5:O:3959:MET:HG2	5:O:4124:TRP:CE2	2.46	0.51
8:A:113:HIS:HD2	8:E:122:LYS:HB3	1.76	0.51
1:K:43:ASP:HB2	1:K:170:THR:HG22	1.92	0.50
1:K:355:LEU:HD11	2:L:473:LEU:HB3	1.93	0.50
5:O:792:ILE:HG23	5:O:793:LEU:HD12	1.94	0.50
5:O:3158:LYS:HG3	5:O:3159:ARG:H	1.76	0.50
3:I:97:DG:O6	4:J:57:DC:N4	2.44	0.50
4:J:141:DG:P	5:O:213:ARG:HH22	2.34	0.50
5:O:1514:LEU:HA	5:O:1517:LEU:HD12	1.93	0.50
5:O:2168:LEU:HD22	5:O:2193:ILE:HD11	1.93	0.50
5:O:3840:LYS:HG3	5:O:3841:ASP:H	1.76	0.50
5:O:4114:PRO:HA	5:O:4117:LEU:HG	1.94	0.50
6:G:23:LEU:HD23	6:G:56:GLU:OE2	2.11	0.50
4:J:74:DA:OP1	8:A:117:VAL:N	2.43	0.50
5:O:639:ALA:H	5:O:679:LYS:NZ	2.09	0.50
5:O:2898:LEU:HD13	5:O:3973:PRO:HA	1.93	0.50
5:O:3762:GLN:HG3	5:O:3793:VAL:HG11	1.93	0.50
1:K:211:PHE:HD1	1:K:213:ILE:HG13	1.77	0.50
1:K:445:LYS:NZ	1:K:446:MET:SD	2.74	0.50
3:I:95:DC:H2'	3:I:96:DC:C6	2.46	0.50
5:O:708:VAL:HB	5:O:712:LYS:NZ	2.27	0.50
5:O:746:ARG:HB2	5:O:788:TYR:HE2	1.76	0.50
5:O:1294:VAL:HG11	5:O:1363:LEU:HG	1.94	0.50
5:O:1923:PHE:CD1	5:O:1941:HIS:HB3	2.46	0.50
5:O:2187:VAL:HG23	5:O:2728:LEU:HD21	1.93	0.50
5:O:2249:LEU:H	5:O:2249:LEU:HD12	1.77	0.50
5:O:3287:ARG:HE	5:O:3289:ARG:NH1	2.10	0.50
5:O:3368:GLU:HA	5:O:3372:LYS:HE2	1.92	0.50
6:G:84:GLN:HG2	6:G:102:ILE:HG12	1.93	0.50
1:K:534:TYR:O	2:L:260:ARG:NH2	2.43	0.50
2:L:450:GLN:NE2	2:L:536:LEU:O	2.34	0.50
3:I:79:DG:C8	3:I:79:DG:H5'	2.46	0.50
5:O:496:VAL:HG21	5:O:525:LYS:HZ1	1.77	0.50
5:O:933:LEU:HD21	5:O:2794:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1815:THR:OG1	5:O:1816:ARG:N	2.44	0.50
5:O:3002:TYR:HB3	5:O:3011:LEU:HD23	1.94	0.50
1:K:386:LEU:HD23	2:L:439:LYS:HE3	1.94	0.50
4:J:91:DT:H2''	4:J:92:DT:C5	2.47	0.50
5:O:932:GLU:O	5:O:2773:ARG:NH2	2.43	0.50
5:O:3759:ARG:HA	5:O:3762:GLN:HE21	1.77	0.50
1:K:271:VAL:HB	1:K:368:VAL:HG13	1.93	0.50
2:L:496:HIS:CD2	2:L:497:ARG:HH21	2.29	0.50
3:I:9:DG:N2	4:J:147:DC:O2	2.44	0.50
5:O:894:PHE:HB3	5:O:907:LEU:HD23	1.93	0.50
5:O:1190:LEU:HA	5:O:1193:LYS:HE2	1.94	0.50
5:O:1249:SER:OG	5:O:1310:GLU:OE2	2.29	0.50
5:O:2379:MET:HA	5:O:2382:VAL:HG12	1.93	0.50
3:I:14:DC:H42	4:J:140:DG:H1	1.58	0.50
3:I:103:DG:H2''	3:I:104:DG:O5'	2.11	0.50
4:J:71:DG:H2''	4:J:72:DG:N7	2.26	0.50
5:O:142:ARG:N	5:O:144:MET:HE1	2.26	0.50
5:O:1624:GLN:O	5:O:1627:LYS:NZ	2.35	0.50
5:O:1772:HIS:CD2	5:O:1773:VAL:HG23	2.46	0.50
5:O:1817:GLN:HB3	5:O:1868:THR:HG22	1.93	0.50
2:L:37:VAL:HG21	2:L:227:PHE:HB3	1.92	0.50
5:O:780:ILE:HB	5:O:785:MET:HE1	1.94	0.50
5:O:1019:ASP:O	5:O:1026:ARG:NH2	2.43	0.50
5:O:1075:ARG:HD2	5:O:1110:SER:HB2	1.93	0.50
5:O:1179:PRO:HG3	5:O:1259:LEU:HD13	1.92	0.50
5:O:1601:LEU:HD22	5:O:1655:ILE:HD12	1.94	0.50
7:H:106:HIS:HA	7:H:109:SER:HB3	1.94	0.50
1:K:421:ASP:OD1	1:K:425:ILE:N	2.45	0.49
3:I:43:DG:OP1	7:D:84:SER:N	2.45	0.49
4:J:38:DT:H2''	4:J:39:DA:N7	2.27	0.49
5:O:369:PHE:CE2	5:O:373:CYS:HB3	2.47	0.49
5:O:889:GLU:HB2	5:O:891:ARG:HH11	1.77	0.49
5:O:1231:GLN:HA	5:O:1292:LYS:HE2	1.94	0.49
5:O:1445:ARG:NH2	5:O:1507:CYS:SG	2.71	0.49
5:O:2410:GLU:HB3	5:O:2413:PHE:HB3	1.93	0.49
5:O:2432:GLN:HE21	5:O:2461:PHE:HE1	1.60	0.49
5:O:3176:MET:HE1	5:O:3249:GLN:HG3	1.94	0.49
5:O:3750:PHE:HD1	5:O:3804:GLU:HA	1.77	0.49
5:O:3908:HIS:HA	5:O:3937:VAL:HG21	1.94	0.49
6:C:72:ASP:OD1	6:C:73:ASN:N	2.45	0.49
1:K:48:MET:HA	1:K:59:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:MET:SD	1:K:171:ASN:OD1	2.69	0.49
1:K:257:SER:HB3	1:K:273:ILE:HD12	1.94	0.49
3:I:16:DG:H2''	3:I:17:DG:N7	2.27	0.49
3:I:124:DG:N2	4:J:31:DT:O2	2.45	0.49
5:O:100:ILE:HG22	5:O:103:TYR:HB2	1.94	0.49
5:O:2385:LEU:HD13	5:O:2388:LYS:HG3	1.92	0.49
5:O:2980:ASP:N	5:O:2980:ASP:OD1	2.43	0.49
5:O:3091:LEU:O	5:O:3192:LYS:NZ	2.46	0.49
5:O:3179:TRP:HZ2	5:O:3245:SER:HB2	1.77	0.49
6:G:26:PRO:HD3	7:H:37:TYR:CD1	2.47	0.49
1:K:375:VAL:HA	2:L:541:GLU:HA	1.93	0.49
5:O:206:THR:HG22	5:O:212:VAL:HG21	1.94	0.49
5:O:1375:THR:HG22	5:O:1382:ILE:HD13	1.94	0.49
5:O:1763:THR:O	5:O:1767:CYS:N	2.46	0.49
2:L:151:ILE:HD11	2:L:211:VAL:HG13	1.93	0.49
2:L:197:ILE:HD12	2:L:201:GLN:HB3	1.94	0.49
3:I:27:DC:H2''	3:I:28:DG:H5'	1.95	0.49
3:I:105:DG:H22	4:J:49:DC:H1'	1.76	0.49
5:O:898:PHE:HB3	5:O:903:PRO:HD2	1.94	0.49
5:O:1373:VAL:O	5:O:1377:CYS:N	2.46	0.49
5:O:2533:SER:O	5:O:2538:ARG:N	2.45	0.49
5:O:3854:ALA:O	5:O:3856:MET:N	2.45	0.49
8:E:54:TYR:HD2	9:F:39:ARG:HB2	1.77	0.49
4:J:52:DC:O2	8:A:83:ARG:NH2	2.45	0.49
4:J:63:DA:H2''	4:J:64:DA:C8	2.47	0.49
5:O:708:VAL:HB	5:O:712:LYS:HZ1	1.76	0.49
5:O:910:PHE:HB3	5:O:2804:ILE:HD11	1.95	0.49
5:O:1413:ASP:OD1	5:O:1414:ILE:N	2.41	0.49
6:C:64:GLU:HA	7:D:46:HIS:CE1	2.47	0.49
8:A:100:LEU:HD11	9:B:58:LEU:HD12	1.93	0.49
5:O:98:GLN:O	5:O:100:ILE:HG12	2.12	0.49
5:O:489:ARG:O	5:O:492:SER:OG	2.28	0.49
5:O:1131:ILE:HD12	5:O:1190:LEU:HD11	1.95	0.49
5:O:1143:VAL:O	5:O:1147:LYS:N	2.44	0.49
5:O:1553:PHE:HB2	5:O:1558:TYR:OH	2.12	0.49
5:O:2394:LYS:HB2	5:O:2431:ARG:HH22	1.78	0.49
5:O:3259:LEU:HD11	5:O:3283:LEU:HD13	1.93	0.49
5:O:3531:TYR:CE1	5:O:3796:MET:HA	2.48	0.49
5:O:4056:PRO:HG2	5:O:4107:LEU:HG	1.94	0.49
1:K:142:SER:OG	1:K:145:GLU:OE1	2.24	0.49
2:L:59:PHE:HA	2:L:77:ILE:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:56:DC:H2''	3:I:57:DC:C2	2.48	0.49
4:J:103:DA:H2''	4:J:104:DG:C8	2.47	0.49
5:O:682:TYR:CZ	5:O:700:LYS:HD3	2.47	0.49
5:O:1645:VAL:HA	5:O:1648:LEU:HG	1.92	0.49
5:O:3588:TRP:HZ2	5:O:3610:TYR:HB2	1.77	0.49
1:K:318:ARG:NH2	2:L:276:TRP:O	2.46	0.49
3:I:67:DC:H2''	3:I:68:DA:C8	2.48	0.49
3:I:116:DA:H2''	3:I:117:DG:C8	2.47	0.49
5:O:170:VAL:HA	5:O:219:VAL:HG11	1.95	0.49
5:O:750:PRO:O	5:O:753:GLN:HB2	2.13	0.49
5:O:1585:SER:OG	5:O:1588:ASP:OD1	2.28	0.49
5:O:2264:ASP:OD1	5:O:2264:ASP:N	2.45	0.49
9:B:90:LEU:HB3	9:B:95:ARG:HB2	1.95	0.49
2:L:165:LEU:HB2	2:L:166:PRO:HD2	1.94	0.49
5:O:1206:LEU:HA	5:O:1209:LYS:HB2	1.94	0.49
5:O:1352:SER:HB3	5:O:1356:TRP:CG	2.48	0.49
5:O:1611:GLN:HB2	5:O:1613:HIS:ND1	2.28	0.49
5:O:1949:ILE:HG12	5:O:2100:LEU:HD13	1.94	0.49
5:O:2773:ARG:NH2	5:O:2775:TYR:OH	2.46	0.49
5:O:3515:GLN:HA	5:O:3518:VAL:HB	1.94	0.49
3:I:85:DC:OP1	9:B:39:ARG:NH2	2.46	0.49
5:O:1633:TRP:HB3	5:O:1645:VAL:HG21	1.95	0.49
5:O:1685:ASP:OD1	5:O:1686:LEU:N	2.46	0.49
5:O:2295:GLN:HE21	5:O:2299:TYR:N	2.10	0.49
5:O:2396:LEU:O	5:O:2400:VAL:HG23	2.12	0.49
5:O:2925:GLU:HA	5:O:2928:LYS:HD3	1.95	0.49
5:O:3332:THR:O	5:O:3335:ARG:HG3	2.13	0.49
5:O:3727:THR:HB	5:O:3737:ARG:HB3	1.94	0.49
6:C:59:THR:HA	6:C:62:ILE:HG22	1.95	0.49
9:B:64:ASN:O	9:B:67:ARG:HG3	2.13	0.49
1:K:525:PHE:HD1	1:K:528:LEU:HD12	1.78	0.48
2:L:190:PRO:HG2	2:L:192:PHE:HE1	1.78	0.48
5:O:576:VAL:HA	5:O:579:LEU:CD1	2.43	0.48
5:O:1836:LEU:HA	5:O:1839:PHE:HB3	1.95	0.48
5:O:2283:ASN:HB2	5:O:2285:LEU:HD23	1.95	0.48
5:O:2986:PRO:HG2	5:O:2991:LYS:HZ2	1.78	0.48
5:O:3330:LEU:HD23	5:O:3384:HIS:CE1	2.48	0.48
8:A:83:ARG:HD3	9:B:79:LYS:HZ1	1.78	0.48
1:K:320:GLN:HG3	2:L:276:TRP:HA	1.95	0.48
1:K:329:LEU:HD21	2:L:497:ARG:HD2	1.95	0.48
1:K:363:ARG:NH1	2:L:269:GLN:OE1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:384:LEU:CB	2:L:410:PRO:HG3	2.44	0.48
3:I:64:DA:H1'	3:I:65:DC:H5	1.78	0.48
5:O:67:VAL:HG21	5:O:82:ARG:NH1	2.27	0.48
5:O:475:LEU:HD23	5:O:479:ILE:HD13	1.94	0.48
5:O:561:ASN:HA	5:O:564:LEU:HD12	1.95	0.48
5:O:1019:ASP:OD1	5:O:1026:ARG:NE	2.45	0.48
5:O:1098:GLN:HE22	5:O:1151:ARG:HA	1.78	0.48
7:D:92:GLN:OE1	7:D:96:ARG:NH1	2.46	0.48
6:G:31:HIS:HA	6:G:48:PRO:HB3	1.95	0.48
1:K:55:ASP:N	1:K:55:ASP:OD1	2.45	0.48
2:L:29:SER:O	2:L:32:GLU:N	2.46	0.48
2:L:360:GLN:OE1	2:L:360:GLN:N	2.45	0.48
3:I:105:DG:H2''	3:I:106:DA:C8	2.48	0.48
5:O:1254:LEU:HD11	5:O:1329:ARG:NH1	2.28	0.48
5:O:1491:ILE:HG13	5:O:1492:ALA:H	1.78	0.48
5:O:3589:SER:HA	5:O:3592:VAL:HG12	1.95	0.48
9:F:39:ARG:HH12	9:F:46:ILE:HG23	1.79	0.48
1:K:382:PHE:CZ	1:K:431:GLY:HA2	2.48	0.48
1:K:461:LYS:O	1:K:465:ILE:HG12	2.12	0.48
2:L:198:THR:O	2:L:202:LYS:HG2	2.13	0.48
2:L:323:PHE:CZ	2:L:328:GLU:HA	2.47	0.48
4:J:139:DG:H2''	4:J:140:DG:OP2	2.13	0.48
5:O:786:GLN:HB3	5:O:787:PRO:HD3	1.94	0.48
5:O:1220:LEU:HG	5:O:1287:GLN:HE21	1.78	0.48
5:O:2435:CYS:HA	5:O:2438:ILE:HD12	1.94	0.48
5:O:2535:THR:OG1	5:O:2536:LEU:N	2.46	0.48
5:O:3797:THR:HG23	5:O:3800:LEU:HD13	1.95	0.48
6:G:57:TYR:CE1	7:H:106:HIS:HB3	2.48	0.48
4:J:98:DG:H2''	4:J:99:DT:H71	1.96	0.48
4:J:140:DG:H3'	5:O:213:ARG:NH2	2.28	0.48
5:O:323:VAL:HA	5:O:326:MET:HG3	1.95	0.48
5:O:754:MET:O	5:O:757:LYS:HB2	2.13	0.48
5:O:1838:GLU:O	5:O:1841:SER:OG	2.22	0.48
5:O:1960:LYS:O	5:O:1961:PHE:C	2.55	0.48
5:O:2301:GLN:HA	5:O:2304:VAL:HG22	1.96	0.48
5:O:3745:GLU:H	5:O:3745:GLU:CD	2.20	0.48
5:O:3805:TRP:HD1	5:O:3807:GLU:HG2	1.78	0.48
1:K:193:LEU:HD22	1:K:198:ILE:HD12	1.94	0.48
1:K:451:LYS:HG2	2:L:417:GLU:H	1.78	0.48
5:O:29:LEU:HA	5:O:32:HIS:CE1	2.48	0.48
5:O:797:ASP:O	5:O:801:LYS:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:847:SER:OG	5:O:848:LEU:N	2.47	0.48
5:O:1380:ALA:HA	5:O:1384:PHE:HA	1.94	0.48
5:O:1468:LEU:HD21	5:O:1476:HIS:CG	2.49	0.48
5:O:3050:LYS:HG2	5:O:3054:GLN:HE22	1.78	0.48
5:O:3244:ASP:OD1	5:O:3245:SER:N	2.47	0.48
5:O:3665:MET:O	5:O:3669:LYS:NZ	2.42	0.48
5:O:3759:ARG:HA	5:O:3762:GLN:NE2	2.28	0.48
5:O:3909:ALA:HB1	5:O:3984:MET:HE3	1.95	0.48
6:C:104:GLN:H	8:A:94:GLU:HG2	1.77	0.48
2:L:384:LEU:HB2	2:L:410:PRO:HG3	1.96	0.48
5:O:322:GLN:O	5:O:322:GLN:NE2	2.47	0.48
5:O:529:ASP:OD1	5:O:530:LEU:N	2.47	0.48
5:O:760:LEU:HD21	5:O:798:GLY:HA3	1.95	0.48
5:O:965:THR:CG2	5:O:969:LEU:CD1	2.79	0.48
5:O:1762:MET:HE2	5:O:1778:PHE:HE1	1.78	0.48
5:O:2168:LEU:O	5:O:2172:ALA:N	2.45	0.48
1:K:142:SER:HA	1:K:176:HIS:CE1	2.49	0.48
1:K:455:THR:HB	1:K:458:GLN:HE22	1.79	0.48
2:L:223:GLU:OE2	2:L:238:LYS:NZ	2.35	0.48
5:O:73:LEU:HG	5:O:74:ASN:H	1.78	0.48
8:A:122:LYS:NZ	8:E:113:HIS:O	2.47	0.48
6:G:54:VAL:HG11	7:H:95:VAL:HG21	1.95	0.48
2:L:96:SER:O	2:L:99:GLN:NE2	2.43	0.48
3:I:126:DC:H2'	3:I:127:DA:C5	2.48	0.48
5:O:1479:VAL:HG22	5:O:1521:PHE:CE2	2.49	0.48
5:O:1964:GLY:H	5:O:2125:TRP:NE1	2.12	0.48
5:O:2239:LYS:HG3	5:O:2279:ILE:HD12	1.96	0.48
5:O:2553:HIS:O	5:O:2556:SER:OG	2.23	0.48
3:I:103:DG:H4'	3:I:104:DG:OP1	2.13	0.48
5:O:237:SER:OG	5:O:240:GLU:OE1	2.32	0.48
5:O:345:PHE:HA	5:O:366:TYR:HE1	1.79	0.48
5:O:639:ALA:H	5:O:679:LYS:HZ3	1.62	0.48
5:O:1298:LEU:HB2	5:O:1367:HIS:CD2	2.48	0.48
5:O:2542:LEU:HA	5:O:2545:LEU:HD13	1.95	0.48
5:O:2873:PRO:HB2	5:O:2925:GLU:HG3	1.95	0.48
5:O:3074:GLN:O	5:O:3078:LEU:HG	2.14	0.48
5:O:3077:ILE:O	5:O:3081:HIS:ND1	2.43	0.48
5:O:3091:LEU:HD13	5:O:3141:PHE:CE2	2.49	0.48
8:E:92:LEU:HD11	9:F:65:VAL:HG21	1.95	0.48
1:K:36:ASP:H	1:K:81:ASP:CG	2.22	0.47
2:L:296:CYS:HB2	2:L:299:ASP:CG	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:304:THR:OG1	5:O:305:ASN:N	2.47	0.47
5:O:916:GLU:O	5:O:920:THR:N	2.35	0.47
5:O:1020:PRO:HA	5:O:1073:PHE:HE2	1.79	0.47
5:O:1102:GLU:H	5:O:1102:GLU:CD	2.22	0.47
5:O:1878:ASP:OD1	5:O:1879:VAL:N	2.46	0.47
5:O:2544:SER:HA	5:O:2842:ARG:HH22	1.79	0.47
5:O:3385:LEU:HB3	5:O:3416:LEU:CD1	2.44	0.47
7:D:77:LEU:HB3	9:F:75:HIS:CD2	2.49	0.47
7:D:92:GLN:HA	7:D:95:VAL:HG22	1.96	0.47
7:H:62:PHE:HD1	9:F:98:TYR:CE2	2.31	0.47
1:K:92:LYS:HD3	1:K:135:MET:HA	1.95	0.47
1:K:348:MET:HB2	1:K:397:LEU:HG	1.95	0.47
1:K:352:PRO:HG3	2:L:464:ALA:HB2	1.95	0.47
3:I:34:DT:P	6:C:17:ARG:HE	2.37	0.47
3:I:81:DC:H2''	3:I:82:DC:C5	2.48	0.47
4:J:59:DG:H1'	4:J:60:DT:C2	2.49	0.47
4:J:125:DG:H1'	4:J:126:DC:H5'	1.97	0.47
5:O:714:VAL:HG12	5:O:733:LEU:HD11	1.95	0.47
5:O:1279:LEU:HG	5:O:1356:TRP:NE1	2.29	0.47
5:O:1423:ILE:HD11	5:O:1426:GLN:O	2.14	0.47
5:O:2855:VAL:HA	5:O:2858:ILE:HD12	1.95	0.47
5:O:2897:LEU:HD21	5:O:2923:TRP:NE1	2.29	0.47
5:O:3580:ASN:HD21	5:O:3582:GLU:HB3	1.79	0.47
8:A:83:ARG:HD3	9:B:79:LYS:NZ	2.29	0.47
1:K:261:LEU:N	1:K:269:ILE:O	2.39	0.47
4:J:115:DG:H5''	6:C:42:ARG:HB3	1.95	0.47
5:O:137:THR:O	5:O:141:SER:OG	2.27	0.47
5:O:635:PRO:HG3	5:O:672:ILE:HD12	1.96	0.47
5:O:1872:GLY:HA2	5:O:1875:LYS:HG2	1.96	0.47
5:O:2254:ARG:C	5:O:2256:ILE:H	2.22	0.47
5:O:2806:LYS:HD2	5:O:2853:PRO:HB3	1.96	0.47
5:O:3573:ASN:OD1	5:O:3574:ALA:N	2.47	0.47
5:O:3579:SER:OG	5:O:3580:ASN:N	2.47	0.47
5:O:3951:GLN:HA	5:O:4068:HIS:CD2	2.49	0.47
6:C:78:ILE:HG23	6:C:82:HIS:HE1	1.78	0.47
1:K:36:ASP:OD1	1:K:162:SER:OG	2.26	0.47
1:K:339:ARG:HA	1:K:405:ASN:HA	1.95	0.47
1:K:426:GLN:OE1	2:L:435:PHE:O	2.32	0.47
1:K:473:TYR:O	2:L:350:GLN:NE2	2.45	0.47
5:O:320:LEU:HA	5:O:323:VAL:HG22	1.96	0.47
5:O:867:ASN:HB3	5:O:3129:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1111:LEU:HB2	5:O:1127:CYS:SG	2.54	0.47
5:O:1179:PRO:HB3	5:O:1258:ASP:OD1	2.14	0.47
5:O:1762:MET:HA	5:O:1765:VAL:HG12	1.95	0.47
5:O:3922:ASP:OD1	5:O:3927:ASN:ND2	2.47	0.47
7:H:76:ARG:HG3	7:H:80:TYR:CE2	2.50	0.47
1:K:257:SER:HB2	4:J:141:DG:H4'	1.96	0.47
5:O:672:ILE:HD13	5:O:675:ARG:HH12	1.79	0.47
5:O:717:LYS:NZ	5:O:1119:LYS:O	2.46	0.47
5:O:1389:VAL:HG13	5:O:1391:VAL:H	1.80	0.47
5:O:1538:LEU:HG	5:O:1555:HIS:CE1	2.49	0.47
5:O:3099:ALA:O	5:O:3103:ILE:HG13	2.14	0.47
5:O:3183:ILE:HG13	5:O:3242:MET:SD	2.54	0.47
5:O:3193:ILE:HA	5:O:3196:LYS:HG2	1.95	0.47
5:O:3824:GLU:HG2	5:O:3827:ALA:HB3	1.95	0.47
1:K:529:VAL:HG22	1:K:531:PRO:HD3	1.97	0.47
3:I:42:DA:H2''	3:I:43:DG:C8	2.49	0.47
5:O:526:ASP:OD1	5:O:526:ASP:N	2.47	0.47
5:O:1420:ARG:NH1	5:O:1424:THR:HG23	2.29	0.47
5:O:1477:HIS:HB3	5:O:1481:THR:H	1.79	0.47
5:O:4009:PRO:HA	5:O:4012:ASP:HB3	1.95	0.47
5:O:4094:PRO:HB2	5:O:4098:LEU:HD11	1.97	0.47
3:I:103:DG:N2	8:A:83:ARG:HH22	2.09	0.47
4:J:40:DG:H2''	4:J:41:DG:N7	2.30	0.47
5:O:251:PHE:O	5:O:255:ALA:N	2.42	0.47
5:O:326:MET:HA	5:O:329:LYS:HG2	1.97	0.47
5:O:373:CYS:HB2	5:O:381:VAL:HG22	1.96	0.47
5:O:486:GLY:O	5:O:490:ILE:HG12	2.15	0.47
5:O:901:MET:HG3	5:O:2819:GLU:HB3	1.95	0.47
5:O:1452:VAL:O	5:O:1456:LYS:HG2	2.14	0.47
5:O:1576:ASP:OD1	5:O:1576:ASP:N	2.46	0.47
5:O:2154:GLU:C	5:O:2156:VAL:H	2.23	0.47
5:O:2510:LEU:O	5:O:2518:GLN:NE2	2.36	0.47
5:O:3524:ASN:OD1	5:O:3525:TYR:N	2.48	0.47
5:O:4116:ILE:HG13	5:O:4126:PRO:HB2	1.97	0.47
9:B:75:HIS:HE1	7:H:90:GLU:HG2	1.79	0.47
2:L:165:LEU:H	2:L:165:LEU:HD23	1.79	0.47
3:I:122:DC:H2''	3:I:123:DA:C8	2.50	0.47
5:O:629:PHE:O	5:O:633:ILE:HG12	2.15	0.47
5:O:2324:GLY:HA3	5:O:2370:SER:OG	2.14	0.47
5:O:2361:ILE:HD11	5:O:2393:LEU:HB3	1.96	0.47
5:O:3052:LEU:HB3	5:O:3092:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:67:ARG:HH12	7:H:100:PRO:HG3	1.79	0.47
5:O:683:PHE:HD1	5:O:704:PHE:CE1	2.31	0.47
5:O:770:LEU:HD21	5:O:855:VAL:HG22	1.97	0.47
5:O:1346:THR:O	5:O:1350:ASN:ND2	2.48	0.47
5:O:1428:ILE:HG22	5:O:1448:LEU:HD22	1.97	0.47
5:O:3030:ILE:H	5:O:3067:LYS:NZ	2.12	0.47
1:K:369:TYR:OH	2:L:436:SER:O	2.30	0.47
2:L:17:GLY:O	2:L:20:MET:HE3	2.14	0.47
5:O:568:PHE:O	5:O:572:VAL:HG13	2.15	0.47
5:O:919:LEU:HA	5:O:972:LEU:HD11	1.96	0.47
5:O:1338:VAL:O	5:O:1341:ILE:HG12	2.15	0.47
5:O:1425:ALA:O	5:O:1429:GLU:HB2	2.15	0.47
5:O:1476:HIS:HE1	5:O:1522:GLY:H	1.63	0.47
5:O:3369:ASP:H	5:O:3372:LYS:HB2	1.79	0.47
1:K:412:ALA:HB3	1:K:435:VAL:HB	1.95	0.46
2:L:43:GLN:HE22	2:L:492:GLN:HA	1.79	0.46
4:J:60:DT:H2"	4:J:61:DT:C5	2.50	0.46
5:O:135:LEU:O	5:O:139:ARG:HG2	2.15	0.46
5:O:148:LYS:HG2	5:O:151:GLU:OE2	2.15	0.46
5:O:668:LYS:O	5:O:672:ILE:HG12	2.15	0.46
5:O:1267:TYR:CZ	5:O:1290:LEU:HD11	2.49	0.46
5:O:3738:ILE:O	5:O:3738:ILE:HG13	2.16	0.46
6:C:38:HIS:ND1	6:G:39:TYR:O	2.48	0.46
8:A:122:LYS:HG2	8:E:113:HIS:NE2	2.30	0.46
1:K:270:SER:OG	1:K:371:GLU:O	2.28	0.46
1:K:288:LEU:N	2:L:311:ILE:O	2.48	0.46
5:O:31:GLY:HA3	5:O:77:GLU:HB2	1.95	0.46
5:O:300:TRP:CE3	5:O:308:LEU:HD21	2.49	0.46
5:O:2589:TYR:H	5:O:2776:ARG:HA	1.80	0.46
5:O:4060:THR:O	5:O:4063:GLU:HG3	2.15	0.46
8:E:65:LEU:O	8:E:68:GLN:HG3	2.15	0.46
1:K:218:ARG:NE	1:K:218:ARG:O	2.47	0.46
2:L:16:VAL:HA	2:L:31:PHE:HE1	1.81	0.46
3:I:10:DA:H2	4:J:146:DT:H3	1.62	0.46
3:I:82:DC:O2	4:J:73:DG:N2	2.47	0.46
5:O:173:LYS:HA	5:O:173:LYS:HD2	1.78	0.46
5:O:335:LYS:HA	5:O:338:LEU:HG	1.98	0.46
5:O:934:LEU:HA	5:O:937:MET:HE3	1.97	0.46
5:O:1834:ASP:OD1	5:O:1834:ASP:N	2.46	0.46
5:O:1958:GLU:HB2	5:O:1961:PHE:CZ	2.51	0.46
5:O:2340:SER:O	5:O:2344:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3512:VAL:O	5:O:3515:GLN:HB2	2.16	0.46
5:O:3751:LEU:HD22	5:O:3805:TRP:HB2	1.96	0.46
5:O:3886:ALA:O	5:O:3890:MET:HG3	2.16	0.46
5:O:3965:ARG:NH1	5:O:3969:ASN:OD1	2.49	0.46
8:A:70:LEU:HD22	9:B:26:ILE:HA	1.96	0.46
6:G:53:ALA:HB1	7:H:110:GLU:HG3	1.97	0.46
8:E:51:ILE:HD11	9:F:43:VAL:C	2.40	0.46
1:K:379:SER:HB2	2:L:444:TYR:CG	2.50	0.46
4:J:145:DC:H2''	4:J:146:DT:C5	2.49	0.46
5:O:174:VAL:O	5:O:177:LEU:HB2	2.15	0.46
5:O:1062:ARG:NH1	5:O:1065:SER:OG	2.48	0.46
5:O:1411:TYR:O	5:O:1414:ILE:HG22	2.16	0.46
5:O:1668:PHE:HA	5:O:1671:VAL:HG22	1.96	0.46
5:O:3529:ILE:O	5:O:3532:PRO:HD2	2.16	0.46
1:K:301:ARG:O	2:L:292:GLU:N	2.39	0.46
4:J:79:DG:H2''	4:J:80:DC:H5'	1.97	0.46
5:O:559:SER:O	5:O:561:ASN:N	2.48	0.46
5:O:901:MET:HG2	5:O:903:PRO:HD3	1.97	0.46
5:O:1072:ALA:HA	5:O:1075:ARG:HB2	1.98	0.46
5:O:2295:GLN:HG3	5:O:2298:GLU:HB3	1.97	0.46
5:O:3059:GLN:HG2	5:O:3062:LEU:HD13	1.97	0.46
5:O:3758:LEU:O	5:O:3762:GLN:NE2	2.49	0.46
6:G:57:TYR:CZ	7:H:103:LEU:HD13	2.51	0.46
2:L:188:HIS:N	2:L:515:MET:HA	2.31	0.46
4:J:58:DG:C8	4:J:58:DG:H5'	2.50	0.46
4:J:100:DG:H1'	4:J:101:DC:H5'	1.98	0.46
5:O:1178:ARG:HG3	5:O:1180:GLN:HB2	1.96	0.46
6:G:16:SER:O	6:G:20:ARG:N	2.49	0.46
6:G:53:ALA:HA	6:G:56:GLU:HG3	1.97	0.46
3:I:49:DT:H2''	3:I:50:DC:N3	2.30	0.46
5:O:1696:LEU:HD12	5:O:1697:PRO:N	2.30	0.46
5:O:1755:SER:HB3	5:O:1758:LEU:HD12	1.98	0.46
5:O:4061:CYS:SG	5:O:4078:VAL:HG13	2.55	0.46
8:E:124:ILE:HD11	9:F:50:ILE:HG23	1.98	0.46
1:K:303:PHE:CE1	2:L:292:GLU:HB2	2.50	0.46
1:K:461:LYS:HZ2	1:K:521:LEU:HA	1.81	0.46
2:L:269:GLN:NE2	2:L:270:GLU:O	2.31	0.46
2:L:390:VAL:HG12	2:L:409:PHE:HA	1.98	0.46
4:J:81:DG:H1'	4:J:82:DT:C6	2.51	0.46
5:O:393:LYS:HD2	5:O:1687:HIS:CE1	2.51	0.46
5:O:541:MET:SD	5:O:560:LEU:HD23	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:956:PRO:N	5:O:957:PRO:HD2	2.31	0.46
5:O:1253:THR:HG21	5:O:1310:GLU:HG3	1.97	0.46
5:O:1713:VAL:HA	5:O:1716:GLN:NE2	2.30	0.46
5:O:2353:GLN:HB3	5:O:2360:PHE:HB2	1.97	0.46
5:O:2512:ASP:N	5:O:2518:GLN:OE1	2.49	0.46
5:O:2854:PHE:CZ	5:O:2858:ILE:HD11	2.51	0.46
5:O:3469:LEU:HA	5:O:3472:ILE:HD12	1.98	0.46
5:O:3809:THR:HA	5:O:3931:ALA:HA	1.98	0.46
9:F:35:ARG:O	9:F:39:ARG:HG2	2.16	0.46
1:K:94:LYS:HB2	1:K:103:TYR:CD1	2.50	0.46
1:K:102:ILE:HG12	1:K:146:VAL:HG12	1.98	0.46
1:K:262:LYS:HA	1:K:268:VAL:HG22	1.97	0.46
1:K:353:LEU:N	1:K:393:GLU:O	2.33	0.46
1:K:529:VAL:HG13	1:K:530:TYR:N	2.29	0.46
5:O:677:ALA:O	5:O:681:LYS:N	2.49	0.46
5:O:1301:ILE:O	5:O:1304:HIS:N	2.41	0.46
5:O:2228:ARG:HA	5:O:2231:PHE:HB3	1.96	0.46
5:O:2485:ARG:NH1	5:O:2530:ARG:HA	2.29	0.46
5:O:2511:ILE:HD11	5:O:2553:HIS:HB2	1.98	0.46
5:O:3034:PRO:O	5:O:3038:GLU:N	2.43	0.46
5:O:3880:ALA:O	5:O:3885:ARG:NH2	2.28	0.46
1:K:296:VAL:HG12	2:L:296:CYS:HA	1.97	0.46
2:L:59:PHE:HD2	2:L:105:ALA:HB3	1.81	0.46
2:L:285:LYS:HD3	2:L:285:LYS:HA	1.65	0.46
5:O:708:VAL:HG12	5:O:740:ILE:HG23	1.97	0.46
5:O:781:ASP:HB3	5:O:784:VAL:HG23	1.97	0.46
5:O:1015:ASP:N	5:O:1015:ASP:OD1	2.41	0.46
5:O:1323:SER:N	5:O:1328:GLU:OE2	2.49	0.46
5:O:1639:LEU:HA	5:O:1642:LYS:HD2	1.97	0.46
5:O:1744:LYS:HB2	5:O:1744:LYS:HE2	1.83	0.46
5:O:2802:PRO:O	5:O:2806:LYS:HG3	2.16	0.46
5:O:4008:GLU:HB2	5:O:4011:PHE:CE2	2.51	0.46
5:O:583:LEU:HB2	5:O:614:PRO:HA	1.98	0.45
5:O:650:SER:O	5:O:654:ILE:HG12	2.15	0.45
5:O:921:ALA:HB3	5:O:927:LYS:HB2	1.98	0.45
5:O:934:LEU:HD22	5:O:937:MET:HE3	1.98	0.45
5:O:1011:GLU:HA	5:O:1014:LEU:HG	1.98	0.45
5:O:1218:SER:O	5:O:1222:ASN:HB2	2.16	0.45
5:O:2182:ILE:HG13	5:O:2183:HIS:H	1.81	0.45
5:O:2804:ILE:HG13	5:O:2808:LEU:HD23	1.98	0.45
5:O:2978:LYS:HA	5:O:2978:LYS:HD2	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3118:ASP:OD1	5:O:3119:VAL:N	2.49	0.45
5:O:3244:ASP:HB3	5:O:3282:ARG:NH2	2.31	0.45
5:O:3625:LEU:HB2	5:O:3685:PRO:HD3	1.99	0.45
8:E:47:ALA:HB3	9:F:44:LYS:HD2	1.97	0.45
1:K:43:ASP:HB3	1:K:48:MET:HE3	1.99	0.45
2:L:531:SER:HA	2:L:534:LYS:HE3	1.97	0.45
3:I:90:DT:H1'	3:I:91:DT:C4	2.51	0.45
5:O:131:LEU:HG	5:O:177:LEU:HG	1.97	0.45
5:O:785:MET:HA	5:O:788:TYR:HD1	1.81	0.45
5:O:1479:VAL:H	5:O:1521:PHE:HE2	1.62	0.45
5:O:1963:GLN:HA	5:O:2125:TRP:CE2	2.51	0.45
5:O:2362:VAL:HG12	5:O:2366:LYS:HZ3	1.80	0.45
5:O:2395:THR:HA	5:O:2398:LEU:HD12	1.98	0.45
5:O:2724:ASP:OD1	5:O:2725:LEU:N	2.49	0.45
5:O:3737:ARG:CZ	5:O:3739:ILE:HG13	2.46	0.45
8:E:119:ILE:O	8:E:120:MET:HE2	2.16	0.45
2:L:12:LEU:HD13	2:L:38:ILE:HG12	1.97	0.45
2:L:33:GLN:O	2:L:37:VAL:HG23	2.16	0.45
3:I:10:DA:H2''	3:I:11:DA:H8	1.81	0.45
3:I:62:DA:H1'	3:I:63:DA:H5'	1.98	0.45
5:O:100:ILE:O	5:O:104:SER:N	2.50	0.45
5:O:275:PHE:CD2	5:O:315:ALA:HB1	2.51	0.45
5:O:1339:VAL:HA	5:O:1342:MET:HG3	1.99	0.45
5:O:2358:ASP:O	5:O:2362:VAL:HG23	2.16	0.45
5:O:3732:LEU:HG	5:O:3733:ARG:HH11	1.81	0.45
1:K:369:TYR:CG	1:K:370:PRO:HD2	2.51	0.45
1:K:403:ARG:HD2	4:J:140:DG:H4'	1.98	0.45
1:K:489:ASN:ND2	2:L:331:MET:HB3	2.32	0.45
2:L:9:ALA:HB2	2:L:127:PHE:CE2	2.51	0.45
3:I:74:DG:OP1	8:E:118:THR:OG1	2.25	0.45
5:O:178:LEU:HD22	5:O:227:LEU:HD11	1.98	0.45
5:O:487:LEU:CD1	5:O:575:ILE:HD13	2.45	0.45
5:O:923:ASP:O	5:O:926:THR:OG1	2.30	0.45
5:O:3321:LEU:O	5:O:3324:ARG:HG2	2.16	0.45
5:O:4080:VAL:HG11	5:O:4119:ARG:HH12	1.82	0.45
6:G:99:GLY:O	9:F:95:ARG:HA	2.17	0.45
1:K:374:LEU:HD23	1:K:374:LEU:H	1.82	0.45
2:L:14:MET:HE1	2:L:34:ALA:HB3	1.98	0.45
2:L:15:ASP:OD2	2:L:140:SER:OG	2.27	0.45
2:L:144:LYS:HE3	2:L:207:ILE:HD11	1.99	0.45
3:I:84:DC:H1'	3:I:85:DC:C2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:463:LYS:HB3	5:O:463:LYS:HE2	1.80	0.45
5:O:572:VAL:HA	5:O:575:ILE:HG12	1.98	0.45
5:O:938:VAL:HA	5:O:941:MET:HG3	1.98	0.45
5:O:1031:ARG:O	5:O:1034:ARG:HG2	2.16	0.45
5:O:1279:LEU:HG	5:O:1356:TRP:HE1	1.81	0.45
5:O:1403:MET:HA	5:O:1406:LEU:HD12	1.98	0.45
5:O:1415:LEU:HA	5:O:1418:HIS:ND1	2.31	0.45
5:O:1844:VAL:HG12	5:O:1845:VAL:HG23	1.98	0.45
5:O:2155:GLU:HG2	5:O:2158:ARG:HB2	1.99	0.45
5:O:3077:ILE:HG23	5:O:3081:HIS:CE1	2.52	0.45
5:O:3419:PHE:O	5:O:3423:GLN:HG2	2.17	0.45
5:O:3442:TYR:O	5:O:3445:LEU:HD22	2.17	0.45
5:O:3822:GLN:O	5:O:3825:LYS:NZ	2.32	0.45
5:O:4114:PRO:O	5:O:4118:GLY:N	2.50	0.45
8:A:99:TYR:OH	8:A:128:ARG:NH1	2.49	0.45
8:A:113:HIS:O	8:A:115:LYS:NZ	2.50	0.45
8:A:122:LYS:C	8:E:113:HIS:HE2	2.24	0.45
1:K:74:LYS:HZ1	1:K:81:ASP:HB2	1.81	0.45
2:L:154:LEU:HD23	2:L:159:ILE:CG2	2.46	0.45
2:L:229:GLU:HG3	2:L:233:LYS:HZ3	1.79	0.45
3:I:97:DG:N1	4:J:57:DC:N3	2.65	0.45
4:J:104:DG:H3'	9:F:79:LYS:HB2	1.98	0.45
5:O:175:TYR:HB2	5:O:223:CYS:HB2	1.97	0.45
5:O:183:GLU:O	5:O:185:HIS:ND1	2.42	0.45
5:O:529:ASP:O	5:O:533:HIS:ND1	2.42	0.45
5:O:1456:LYS:NZ	5:O:1516:GLU:OE1	2.46	0.45
5:O:1782:PHE:HA	5:O:1785:ILE:HG22	1.99	0.45
5:O:1836:LEU:O	5:O:1839:PHE:HB3	2.17	0.45
5:O:2235:LEU:HA	5:O:2238:ILE:HD12	1.99	0.45
5:O:2472:GLN:O	5:O:2476:ILE:HG12	2.17	0.45
5:O:2586:PHE:CE1	5:O:2782:ASP:HB3	2.52	0.45
5:O:2919:ASP:OD1	5:O:2919:ASP:N	2.49	0.45
5:O:3322:ALA:O	5:O:3326:GLN:HG2	2.17	0.45
5:O:3385:LEU:HB3	5:O:3416:LEU:HD11	1.98	0.45
5:O:3750:PHE:CD1	5:O:3804:GLU:HA	2.51	0.45
6:C:69:ALA:HB2	6:C:86:ALA:HB2	1.99	0.45
6:C:110:ASN:HB2	8:A:55:GLN:NE2	2.31	0.45
1:K:193:LEU:HB3	1:K:198:ILE:HB	1.98	0.45
2:L:33:GLN:OE1	2:L:227:PHE:HB2	2.17	0.45
2:L:68:LEU:HB3	2:L:74:TYR:CE2	2.52	0.45
2:L:132:ILE:HB	2:L:161:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:346:CYS:C	2:L:389:MET:HG2	2.42	0.45
5:O:275:PHE:CZ	5:O:319:PHE:HB2	2.49	0.45
5:O:372:PRO:O	5:O:376:ILE:HG13	2.17	0.45
5:O:979:VAL:HA	5:O:982:GLN:HG2	1.99	0.45
5:O:2158:ARG:N	5:O:2159:PRO:HD2	2.32	0.45
8:E:99:TYR:CZ	8:E:103:LEU:HD11	2.52	0.45
3:I:70:DG:H21	4:J:85:DG:H22	1.65	0.45
5:O:363:ILE:HG12	5:O:413:PHE:CD1	2.52	0.45
5:O:989:MET:SD	5:O:1035:GLU:HG2	2.57	0.45
5:O:2319:ALA:O	5:O:2323:LEU:HD23	2.17	0.45
5:O:2839:ASP:O	5:O:2842:ARG:HG2	2.17	0.45
5:O:3835:PRO:HB3	5:O:3839:TYR:CE2	2.52	0.45
9:F:62:LEU:O	9:F:66:ILE:HG23	2.17	0.45
1:K:73:SER:HB3	1:K:249:LYS:HZ1	1.81	0.45
1:K:207:LYS:HD3	1:K:208:PRO:HD2	1.99	0.45
2:L:7:LYS:HG3	2:L:127:PHE:CD1	2.51	0.45
2:L:68:LEU:HD12	2:L:113:VAL:HA	1.97	0.45
2:L:246:HIS:HB2	2:L:262:ALA:HB1	1.99	0.45
3:I:75:DC:H2''	3:I:76:DG:H5'	1.98	0.45
5:O:406:ARG:HA	5:O:409:GLN:HE22	1.81	0.45
5:O:2923:TRP:HE3	5:O:2942:ILE:HG23	1.81	0.45
5:O:4077:TYR:HA	5:O:4080:VAL:HG22	1.99	0.45
8:A:113:HIS:CE1	8:E:110:CYS:HB3	2.52	0.45
9:B:38:ALA:O	9:B:43:VAL:N	2.50	0.45
9:B:78:ARG:NH2	9:B:80:THR:OG1	2.48	0.45
6:G:103:ALA:HB2	9:F:98:TYR:O	2.17	0.45
7:H:38:VAL:HB	7:H:56:MET:HE1	1.98	0.45
7:H:42:LEU:HD22	7:H:51:ILE:HD13	1.99	0.45
1:K:75:ILE:HG21	2:L:316:TYR:CE2	2.52	0.45
1:K:278:GLN:O	2:L:431:ARG:NH1	2.50	0.45
1:K:398:CYS:SG	1:K:399:ARG:N	2.90	0.45
3:I:48:DC:O2	4:J:106:DG:N2	2.50	0.45
5:O:197:PHE:O	5:O:201:LEU:HG	2.17	0.45
5:O:204:LEU:HD23	5:O:217:LEU:HD11	1.99	0.45
5:O:793:LEU:HA	5:O:796:LEU:HD12	1.98	0.45
5:O:1200:GLY:H	5:O:1202:ARG:HH12	1.65	0.45
5:O:1412:LYS:O	5:O:1416:GLU:N	2.34	0.45
5:O:1697:PRO:HB3	5:O:1753:SER:HB3	1.99	0.45
5:O:3868:VAL:HG12	5:O:4117:LEU:HD13	1.99	0.45
1:K:94:LYS:N	1:K:103:TYR:HA	2.32	0.44
1:K:440:ALA:HA	2:L:480:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:490:LEU:HA	1:K:493:LEU:HD12	1.99	0.44
4:J:34:DA:P	6:G:17:ARG:H	2.40	0.44
4:J:95:DG:H2'	4:J:95:DG:OP2	2.17	0.44
4:J:124:DA:H2''	4:J:125:DG:C8	2.51	0.44
5:O:247:GLU:HG2	5:O:282:PHE:HD1	1.82	0.44
5:O:966:PHE:HD1	5:O:969:LEU:HD12	1.80	0.44
5:O:998:ASN:OD1	5:O:998:ASN:N	2.51	0.44
5:O:2427:ARG:HE	5:O:2465:PRO:HD2	1.82	0.44
5:O:2557:LEU:O	5:O:2560:ASN:HB2	2.18	0.44
5:O:3141:PHE:HA	5:O:3144:PHE:HD2	1.82	0.44
5:O:3738:ILE:HD11	5:O:3752:VAL:HG22	1.98	0.44
7:D:41:VAL:O	7:D:45:VAL:HG22	2.16	0.44
8:E:122:LYS:O	8:E:125:GLN:HG3	2.17	0.44
5:O:249:PHE:O	5:O:253:LEU:N	2.40	0.44
5:O:356:ASN:N	5:O:358:GLU:OE2	2.50	0.44
5:O:372:PRO:HA	5:O:375:VAL:HG22	1.97	0.44
5:O:1212:LEU:O	5:O:1216:GLY:N	2.50	0.44
5:O:1685:ASP:H	5:O:1688:LEU:HD12	1.82	0.44
5:O:1837:ARG:O	5:O:1840:PHE:HB3	2.16	0.44
5:O:2477:LEU:HD13	5:O:2505:VAL:HG23	2.00	0.44
5:O:2815:GLY:O	5:O:2819:GLU:HG2	2.17	0.44
5:O:3951:GLN:OE1	5:O:3951:GLN:N	2.50	0.44
8:E:49:ARG:HG3	8:E:53:ARG:HH22	1.82	0.44
8:E:119:ILE:HD11	9:F:46:ILE:HG22	1.99	0.44
9:F:87:VAL:HG22	9:F:97:LEU:HB3	1.99	0.44
3:I:80:DT:H2''	3:I:81:DC:OP2	2.17	0.44
4:J:58:DG:H5'	4:J:58:DG:H8	1.82	0.44
5:O:64:GLY:HA2	5:O:67:VAL:HG12	2.00	0.44
5:O:540:MET:O	5:O:544:ILE:HG12	2.17	0.44
5:O:1583:MET:SD	5:O:1586:SER:OG	2.67	0.44
5:O:2328:ARG:HA	5:O:2371:PHE:CD1	2.51	0.44
5:O:2333:ARG:HH22	5:O:2336:ILE:HD13	1.82	0.44
5:O:2374:LEU:O	5:O:2377:ARG:NH1	2.51	0.44
5:O:3270:ASP:HA	5:O:3273:LEU:HB3	1.99	0.44
5:O:3328:ILE:HD11	5:O:3415:THR:OG1	2.17	0.44
5:O:3493:TRP:CH2	5:O:3711:PRO:HD3	2.52	0.44
5:O:3617:LEU:HA	5:O:3629:ARG:HD2	1.99	0.44
1:K:74:LYS:NZ	1:K:81:ASP:HB2	2.32	0.44
1:K:340:PHE:CZ	2:L:486:ARG:HA	2.52	0.44
1:K:353:LEU:HD12	1:K:393:GLU:HA	1.99	0.44
2:L:121:GLU:OE2	2:L:125:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:122:DC:H2''	3:I:123:DA:N7	2.32	0.44
5:O:250:ASN:HA	5:O:253:LEU:HB2	1.99	0.44
5:O:579:LEU:HB3	5:O:581:LEU:HD23	1.99	0.44
5:O:1307:ILE:HG23	5:O:1311:LYS:H	1.81	0.44
5:O:2238:ILE:O	5:O:2242:VAL:HG12	2.18	0.44
1:K:58:THR:HG23	1:K:61:ASP:H	1.81	0.44
1:K:256:LEU:HD12	1:K:273:ILE:HG22	1.98	0.44
3:I:78:DT:O2	4:J:77:DG:N2	2.50	0.44
6:C:90:ASP:OD1	6:C:91:GLU:N	2.51	0.44
1:K:333:GLU:O	1:K:337:LEU:HG	2.18	0.44
2:L:7:LYS:HB2	2:L:52:ASP:HA	2.00	0.44
2:L:55:ALA:N	2:L:83:LEU:HD12	2.33	0.44
2:L:57:VAL:HG13	2:L:79:VAL:HG22	2.00	0.44
3:I:92:DT:H2''	3:I:93:DA:C8	2.52	0.44
4:J:20:DT:N3	4:J:21:DG:O6	2.51	0.44
5:O:40:GLN:HA	5:O:43:VAL:HG12	1.99	0.44
5:O:465:PHE:CD1	5:O:479:ILE:HG22	2.53	0.44
5:O:950:GLU:O	5:O:956:PRO:HG2	2.17	0.44
5:O:1105:VAL:HA	5:O:1108:MET:HG3	2.00	0.44
5:O:1601:LEU:HB3	5:O:2045:PHE:HZ	1.83	0.44
5:O:3588:TRP:HE1	5:O:3609:MET:C	2.25	0.44
5:O:3593:ARG:NE	5:O:3660:ASN:HD21	2.16	0.44
5:O:3809:THR:OG1	5:O:3930:VAL:O	2.36	0.44
6:C:47:ALA:HB3	6:C:48:PRO:HD3	1.99	0.44
7:D:66:ILE:HG22	7:D:69:ARG:HH12	1.83	0.44
6:G:103:ALA:HA	9:F:97:LEU:CD1	2.48	0.44
1:K:318:ARG:CZ	2:L:278:VAL:HB	2.46	0.44
1:K:412:ALA:HB2	1:K:437:LEU:HD21	1.98	0.44
2:L:348:SER:OG	2:L:390:VAL:HG13	2.18	0.44
3:I:116:DA:H5'	3:I:116:DA:C8	2.52	0.44
5:O:1368:LEU:HD12	5:O:1369:MET:N	2.32	0.44
5:O:1532:LEU:C	5:O:1592:MET:HE1	2.42	0.44
5:O:1773:VAL:HB	5:O:1778:PHE:HE2	1.82	0.44
5:O:3287:ARG:HE	5:O:3289:ARG:HH12	1.64	0.44
5:O:3294:SER:O	5:O:3298:LEU:N	2.41	0.44
5:O:3812:LEU:HB3	5:O:3925:LEU:HG	2.00	0.44
5:O:3819:THR:HA	5:O:3889:ARG:NH1	2.33	0.44
1:K:206:LYS:HD2	1:K:236:SER:HB3	1.99	0.44
1:K:459:VAL:O	1:K:463:LYS:HG2	2.18	0.44
2:L:295:TYR:H	2:L:307:LYS:HZ3	1.64	0.44
2:L:413:LYS:HB2	2:L:416:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:DA:H5''	4:J:63:DA:H4'	2.00	0.44
4:J:56:DG:H2''	4:J:57:DC:C5	2.52	0.44
5:O:42:CYS:HB3	5:O:88:PHE:CD1	2.52	0.44
5:O:265:TYR:HE1	5:O:308:LEU:HD22	1.82	0.44
5:O:525:LYS:O	5:O:528:VAL:HG22	2.17	0.44
5:O:894:PHE:HB2	5:O:940:PHE:CZ	2.53	0.44
5:O:1464:LEU:O	5:O:1468:LEU:N	2.50	0.44
5:O:2276:LEU:O	5:O:2280:VAL:HG23	2.18	0.44
5:O:3049:LEU:O	5:O:3053:LEU:HD23	2.18	0.44
5:O:3446:VAL:HG23	5:O:3468:LEU:HD21	2.00	0.44
5:O:3901:ARG:NH2	5:O:3970:LEU:O	2.47	0.44
7:D:89:ARG:O	7:D:92:GLN:HG3	2.18	0.44
8:A:104:PHE:HE2	9:B:37:LEU:HG	1.83	0.44
7:H:37:TYR:O	7:H:40:LYS:HG2	2.17	0.44
9:F:70:VAL:HA	9:F:73:THR:HG22	2.00	0.44
1:K:420:LEU:HB3	1:K:424:LYS:HA	2.00	0.44
2:L:327:ASP:HB2	2:L:331:MET:HE1	2.00	0.44
3:I:118:DT:H2''	3:I:119:DC:C6	2.53	0.44
4:J:81:DG:H2''	4:J:82:DT:O5'	2.16	0.44
4:J:115:DG:H3'	6:C:43:VAL:H	1.83	0.44
5:O:203:GLU:HB3	5:O:220:LEU:HD21	2.00	0.44
5:O:1428:ILE:HA	5:O:1431:LEU:HB2	1.99	0.44
5:O:1525:CYS:O	5:O:1529:VAL:HG23	2.18	0.44
5:O:2149:LEU:O	5:O:2153:THR:HG23	2.18	0.44
5:O:2528:GLU:H	5:O:2528:GLU:CD	2.21	0.44
5:O:2582:SER:HB2	5:O:2780:LEU:HD22	2.00	0.44
5:O:3135:LEU:O	5:O:3138:ILE:HG22	2.17	0.44
5:O:3580:ASN:ND2	5:O:3582:GLU:HB3	2.33	0.44
5:O:3767:LEU:HD23	5:O:3771:MET:CE	2.48	0.44
6:G:29:ARG:HA	6:G:32:ARG:HG2	2.00	0.44
8:E:71:VAL:HA	8:E:74:ILE:HG22	1.99	0.44
1:K:258:ARG:HG2	4:J:142:DA:H5'	2.00	0.43
1:K:265:LYS:HD2	1:K:265:LYS:HA	1.80	0.43
1:K:428:THR:HB	2:L:354:ARG:NH1	2.33	0.43
2:L:33:GLN:O	2:L:36:LYS:HG2	2.18	0.43
2:L:187:GLY:HA2	2:L:514:ASN:C	2.43	0.43
2:L:370:ASP:HB2	2:L:373:ALA:HB3	2.00	0.43
2:L:426:PHE:C	2:L:428:GLU:H	2.26	0.43
5:O:1477:HIS:ND1	5:O:1480:GLY:HA3	2.33	0.43
5:O:2133:LEU:HD12	5:O:2164:TRP:CZ3	2.53	0.43
5:O:2573:PRO:O	5:O:2786:LYS:NZ	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3072:GLU:HA	5:O:3075:LYS:HE2	1.99	0.43
5:O:3100:LYS:HG2	5:O:3104:GLN:HE22	1.83	0.43
5:O:3578:LEU:HD23	5:O:3677:PRO:HD2	2.00	0.43
1:K:95:ASN:N	1:K:95:ASN:HD22	2.16	0.43
2:L:381:ILE:HD13	2:L:417:GLU:HG2	2.00	0.43
2:L:431:ARG:NE	3:I:15:DC:OP1	2.47	0.43
3:I:132:DT:H6	3:I:132:DT:H2'	1.63	0.43
5:O:638:GLN:HB2	5:O:640:GLU:OE1	2.18	0.43
5:O:648:SER:O	5:O:651:TYR:N	2.51	0.43
5:O:1086:TYR:HA	5:O:1089:PHE:HB3	1.99	0.43
5:O:1205:ASN:O	5:O:1208:LEU:HG	2.19	0.43
5:O:1564:SER:O	5:O:1568:ASN:ND2	2.51	0.43
5:O:1675:TYR:CD1	5:O:1679:LEU:HD23	2.53	0.43
5:O:1743:MET:SD	5:O:1762:MET:HE1	2.57	0.43
5:O:1775:GLU:HA	5:O:1778:PHE:CD2	2.37	0.43
5:O:1963:GLN:HB2	5:O:2123:PRO:O	2.18	0.43
5:O:2869:LEU:HD13	5:O:2896:ALA:HA	1.99	0.43
5:O:2919:ASP:O	5:O:2923:TRP:HD1	2.01	0.43
6:G:18:SER:HA	6:G:27:VAL:H	1.83	0.43
7:H:37:TYR:HA	7:H:40:LYS:HE3	2.00	0.43
1:K:511:VAL:H	1:K:514:MET:HE2	1.82	0.43
3:I:15:DC:H2''	3:I:16:DG:C8	2.54	0.43
3:I:91:DT:H2'	3:I:92:DT:H72	2.00	0.43
3:I:95:DC:OP2	8:A:64:LYS:HB3	2.18	0.43
4:J:72:DG:H4'	4:J:73:DG:OP1	2.18	0.43
5:O:1105:VAL:HG21	5:O:1154:PRO:HB3	2.01	0.43
5:O:1300:SER:HA	5:O:1304:HIS:HB2	1.99	0.43
5:O:1825:LEU:HD21	5:O:1875:LYS:HG3	2.00	0.43
5:O:2442:MET:HE1	5:O:2446:LEU:HD22	2.01	0.43
5:O:3165:THR:O	5:O:3169:PRO:HD3	2.18	0.43
5:O:3291:GLN:O	5:O:3295:GLU:HG2	2.17	0.43
8:A:54:TYR:HB2	9:B:40:ARG:HA	2.00	0.43
1:K:149:VAL:HA	1:K:152:ASN:ND2	2.33	0.43
1:K:161:MET:CE	1:K:164:LYS:HG3	2.48	0.43
2:L:37:VAL:HG22	2:L:231:LEU:HG	2.00	0.43
2:L:151:ILE:O	2:L:155:LYS:HG2	2.18	0.43
3:I:50:DC:H1'	3:I:51:DT:C2	2.53	0.43
5:O:201:LEU:HD22	5:O:249:PHE:CD2	2.52	0.43
5:O:275:PHE:HA	5:O:282:PHE:CE2	2.53	0.43
5:O:405:ASP:OD1	5:O:405:ASP:N	2.50	0.43
5:O:430:VAL:HG11	5:O:1644:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:441:MET:HA	5:O:444:ASP:HB2	2.00	0.43
5:O:1205:ASN:CG	5:O:1275:THR:HA	2.43	0.43
5:O:1278:ALA:HB3	5:O:1356:TRP:CD1	2.53	0.43
5:O:1528:LEU:HD21	5:O:1567:ILE:HG23	2.00	0.43
5:O:1649:LEU:O	5:O:1652:ILE:HG12	2.18	0.43
5:O:2151:ILE:HD13	5:O:2188:GLU:HB3	2.01	0.43
5:O:2428:ASP:O	5:O:2432:GLN:HG2	2.17	0.43
5:O:2937:ASP:HB2	5:O:3982:SER:OG	2.19	0.43
5:O:3114:TYR:HB2	5:O:3128:LYS:HG2	2.00	0.43
5:O:3309:GLU:HA	5:O:3312:VAL:HG13	2.01	0.43
5:O:3617:LEU:HB3	5:O:3632:PHE:CZ	2.50	0.43
5:O:4088:ASN:HB3	5:O:4110:GLN:HB3	1.99	0.43
6:G:77:ARG:NE	7:H:51:ILE:O	2.50	0.43
8:E:48:LEU:HA	8:E:51:ILE:HD12	2.00	0.43
1:K:276:LEU:HD23	1:K:276:LEU:H	1.84	0.43
2:L:295:TYR:H	2:L:307:LYS:NZ	2.17	0.43
3:I:118:DT:H6	3:I:118:DT:H2'	1.63	0.43
5:O:142:ARG:HE	5:O:182:GLY:HA3	1.82	0.43
5:O:275:PHE:HD2	5:O:315:ALA:HB1	1.83	0.43
5:O:763:THR:OG1	5:O:764:PRO:HD3	2.18	0.43
5:O:1299:GLU:O	5:O:1304:HIS:ND1	2.52	0.43
5:O:1342:MET:O	5:O:1345:THR:OG1	2.29	0.43
5:O:1843:ILE:O	5:O:1843:ILE:HG22	2.18	0.43
5:O:1962:TYR:O	5:O:1963:GLN:C	2.61	0.43
5:O:2339:GLU:HA	5:O:2342:CYS:SG	2.58	0.43
5:O:3325:ASP:O	5:O:3328:ILE:HG22	2.18	0.43
5:O:4069:GLU:HA	5:O:4074:PHE:CG	2.53	0.43
8:A:126:LEU:HB2	8:E:113:HIS:CD2	2.53	0.43
1:K:300:THR:HG22	5:O:164:LYS:HD2	2.00	0.43
2:L:496:HIS:CD2	2:L:505:LEU:HD23	2.53	0.43
4:J:54:DT:P	8:A:72:ARG:HH21	2.41	0.43
5:O:670:LEU:HB3	5:O:732:PHE:CE1	2.53	0.43
5:O:2415:LEU:HD22	5:O:2420:PHE:HB2	2.01	0.43
5:O:2420:PHE:HA	5:O:2423:VAL:HG12	2.01	0.43
5:O:3463:LEU:O	5:O:3466:PRO:HD2	2.17	0.43
5:O:3660:ASN:OD1	5:O:3661:ASP:N	2.51	0.43
5:O:3682:GLU:HA	5:O:3688:SER:OG	2.18	0.43
5:O:3757:ASP:HA	5:O:3798:SER:H	1.84	0.43
6:C:26:PRO:O	6:C:29:ARG:N	2.51	0.43
7:D:105:LYS:HA	7:D:108:VAL:HG22	2.01	0.43
6:G:51:LEU:HD22	7:H:91:ILE:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:205:LEU:HB3	2:L:209:LYS:NZ	2.34	0.43
2:L:467:ASP:OD1	2:L:472:THR:OG1	2.37	0.43
3:I:11:DA:H3'	5:O:124:LYS:HE2	2.00	0.43
3:I:32:DA:H4'	7:D:30:ARG:NH2	2.34	0.43
4:J:43:DA:H2''	4:J:44:DG:C4	2.54	0.43
5:O:151:GLU:OE1	5:O:151:GLU:N	2.45	0.43
5:O:473:PRO:O	5:O:477:ASN:ND2	2.52	0.43
5:O:487:LEU:HD12	5:O:488:ILE:N	2.33	0.43
5:O:1374:GLN:O	5:O:1378:GLU:N	2.39	0.43
5:O:2166:SER:OG	5:O:2167:PRO:HD3	2.18	0.43
5:O:2186:VAL:O	5:O:2190:VAL:HG23	2.17	0.43
5:O:3091:LEU:HD13	5:O:3141:PHE:HE2	1.82	0.43
5:O:3460:GLU:H	5:O:3460:GLU:CD	2.24	0.43
5:O:3548:GLY:O	5:O:3552:LYS:HG2	2.18	0.43
6:C:34:LEU:HD12	6:C:48:PRO:HG3	2.00	0.43
9:B:49:LEU:HD23	9:B:49:LEU:H	1.84	0.43
1:K:363:ARG:HB2	1:K:436:PHE:CD2	2.54	0.43
2:L:184:ARG:NH2	2:L:521:GLU:HG2	2.31	0.43
5:O:474:VAL:HA	5:O:477:ASN:HD21	1.83	0.43
5:O:1193:LYS:O	5:O:1196:PRO:HD2	2.19	0.43
5:O:2457:PRO:HA	5:O:2460:GLU:CD	2.44	0.43
5:O:2961:ALA:O	5:O:3989:ARG:NH1	2.44	0.43
5:O:3708:ARG:NH2	5:O:3709:GLY:O	2.51	0.43
5:O:3948:SER:HA	5:O:3951:GLN:NE2	2.33	0.43
7:H:105:LYS:HD3	7:H:105:LYS:HA	1.90	0.43
8:E:52:ARG:HA	8:E:52:ARG:HD3	1.86	0.43
1:K:161:MET:HE2	1:K:164:LYS:HG3	2.01	0.43
5:O:267:VAL:HB	5:O:268:PRO:HD3	2.01	0.43
5:O:586:GLN:CD	5:O:586:GLN:H	2.27	0.43
5:O:958:MET:HB2	5:O:961:LEU:HB2	2.00	0.43
5:O:1391:VAL:O	5:O:1395:LEU:HG	2.19	0.43
5:O:1633:TRP:CE3	5:O:1674:THR:HG23	2.54	0.43
5:O:2371:PHE:HD2	5:O:2374:LEU:HD23	1.84	0.43
5:O:3002:TYR:CE2	5:O:3014:CYS:HB3	2.54	0.43
5:O:3059:GLN:HA	5:O:3062:LEU:HD13	2.01	0.43
5:O:3110:PHE:CD2	5:O:3135:LEU:HD11	2.53	0.43
5:O:3179:TRP:HE1	5:O:3242:MET:HE1	1.83	0.43
5:O:3767:LEU:HD23	5:O:3771:MET:HE1	2.00	0.43
9:F:90:LEU:HB3	9:F:95:ARG:HB3	1.99	0.43
1:K:382:PHE:HZ	1:K:431:GLY:HA2	1.83	0.43
3:I:134:DA:N6	4:J:21:DG:H1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:630:CYS:HB2	5:O:634:LEU:HD23	2.00	0.43
5:O:1444:ASP:OD1	5:O:1445:ARG:N	2.52	0.43
5:O:1920:TYR:O	5:O:1924:THR:N	2.47	0.43
5:O:3641:ASP:OD1	5:O:3642:LYS:NZ	2.52	0.43
5:O:3780:ALA:O	5:O:3783:GLN:HB2	2.19	0.43
5:O:3929:MET:O	5:O:3937:VAL:HA	2.18	0.43
6:C:51:LEU:HB2	7:D:91:ILE:HD13	2.01	0.43
9:F:76:ALA:HB3	9:F:78:ARG:HE	1.84	0.43
1:K:276:LEU:HD22	2:L:354:ARG:HH21	1.83	0.42
1:K:380:THR:HG23	2:L:444:TYR:CD1	2.53	0.42
2:L:457:LEU:HD13	2:L:529:PRO:HB2	2.01	0.42
4:J:87:DG:H4'	4:J:88:DC:OP1	2.19	0.42
5:O:157:TYR:O	5:O:160:LEU:HB3	2.19	0.42
5:O:493:LYS:HG3	5:O:494:PRO:HD2	2.01	0.42
5:O:755:ALA:O	5:O:759:GLY:N	2.51	0.42
5:O:1020:PRO:HA	5:O:1073:PHE:CE2	2.54	0.42
5:O:1284:THR:HG23	5:O:1286:ALA:H	1.84	0.42
5:O:1346:THR:HG22	5:O:1350:ASN:ND2	2.34	0.42
5:O:1854:ARG:HH12	5:O:1867:ILE:HG22	1.84	0.42
5:O:2301:GLN:O	5:O:2304:VAL:HG22	2.19	0.42
5:O:2335:ASN:OD1	5:O:2337:LEU:N	2.50	0.42
7:H:100:PRO:HA	7:H:104:ALA:HB2	1.99	0.42
1:K:36:ASP:HA	1:K:163:HIS:HB3	2.01	0.42
1:K:176:HIS:ND1	1:K:182:LYS:HB3	2.35	0.42
1:K:194:ARG:NH2	1:K:221:ILE:O	2.52	0.42
2:L:131:HIS:ND1	2:L:239:LYS:HG2	2.33	0.42
2:L:252:THR:HB	2:L:341:SER:HA	1.99	0.42
5:O:1707:LEU:N	5:O:1709:GLU:OE1	2.52	0.42
5:O:2233:HIS:O	5:O:2237:ILE:HG12	2.19	0.42
5:O:4108:MET:HE2	5:O:4108:MET:N	2.34	0.42
8:A:122:LYS:HG2	8:E:113:HIS:CD2	2.55	0.42
1:K:409:TYR:HE2	1:K:436:PHE:HA	1.83	0.42
1:K:440:ALA:HB2	2:L:481:LYS:O	2.19	0.42
1:K:528:LEU:HD23	1:K:528:LEU:HA	1.82	0.42
2:L:307:LYS:HD3	2:L:307:LYS:HA	1.67	0.42
3:I:113:DC:H6	3:I:113:DC:H2'	1.64	0.42
5:O:98:GLN:O	5:O:100:ILE:N	2.53	0.42
5:O:485:GLN:HA	5:O:488:ILE:HG22	2.02	0.42
5:O:1047:GLN:H	5:O:1047:GLN:CD	2.27	0.42
5:O:1267:TYR:HB3	5:O:1344:PHE:HE1	1.83	0.42
5:O:1621:THR:O	5:O:1625:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1661:PHE:H	5:O:1665:HIS:CD2	2.37	0.42
5:O:1791:CYS:SG	5:O:1792:VAL:N	2.91	0.42
5:O:2125:TRP:HB3	5:O:2128:PHE:HB3	2.01	0.42
5:O:2252:PRO:C	5:O:2254:ARG:H	2.26	0.42
5:O:2349:LEU:HB3	5:O:2360:PHE:HE1	1.84	0.42
5:O:2587:GLN:OE1	5:O:2587:GLN:N	2.52	0.42
5:O:2782:ASP:OD1	5:O:2782:ASP:N	2.48	0.42
5:O:2987:THR:HG22	5:O:2990:GLU:HG3	2.01	0.42
5:O:3008:TRP:HB2	5:O:3051:LEU:HD22	2.00	0.42
5:O:3591:ASP:HB3	5:O:3609:MET:HE1	2.00	0.42
5:O:3624:GLY:N	5:O:3685:PRO:HD2	2.34	0.42
5:O:3640:PHE:HB2	5:O:3667:LEU:HD21	2.02	0.42
5:O:3687:MET:HA	5:O:3722:PHE:HE2	1.84	0.42
5:O:3887:PHE:O	5:O:3891:SER:N	2.52	0.42
8:A:126:LEU:HD22	8:E:113:HIS:ND1	2.35	0.42
6:G:83:LEU:O	6:G:87:ILE:HG12	2.20	0.42
6:G:100:VAL:HG13	9:F:96:THR:OG1	2.18	0.42
1:K:94:LYS:HE2	1:K:104:VAL:HB	2.00	0.42
1:K:100:LYS:O	1:K:102:ILE:HD12	2.19	0.42
1:K:176:HIS:CE1	1:K:182:LYS:HB3	2.55	0.42
1:K:299:LYS:HG3	5:O:164:LYS:NZ	2.34	0.42
1:K:350:PHE:H	2:L:461:MET:HE1	1.84	0.42
2:L:397:TYR:CE2	4:J:132:DC:H4'	2.53	0.42
3:I:20:DC:N4	4:J:134:DG:O6	2.53	0.42
4:J:25:DC:H2''	4:J:26:DG:H8	1.85	0.42
5:O:950:GLU:OE1	5:O:950:GLU:N	2.52	0.42
5:O:955:ALA:CB	5:O:1004:GLN:HB3	2.48	0.42
5:O:1559:PHE:N	5:O:1559:PHE:CD1	2.85	0.42
5:O:1588:ASP:OD1	5:O:1589:ASN:N	2.52	0.42
5:O:3448:GLU:HB2	5:O:3449:LYS:HZ2	1.83	0.42
5:O:3669:LYS:HA	5:O:3669:LYS:HD3	1.74	0.42
8:A:113:HIS:ND1	8:E:126:LEU:HD22	2.34	0.42
1:K:64:ILE:HD11	1:K:119:LEU:HB3	2.01	0.42
1:K:115:ARG:O	1:K:119:LEU:HG	2.20	0.42
1:K:379:SER:HB2	2:L:444:TYR:CD1	2.54	0.42
2:L:38:ILE:O	2:L:42:VAL:HG23	2.18	0.42
5:O:153:PHE:CE2	5:O:189:MET:HG2	2.54	0.42
5:O:524:TYR:OH	5:O:629:PHE:HB2	2.19	0.42
5:O:2186:VAL:O	5:O:2189:ILE:HG12	2.19	0.42
5:O:3103:ILE:HD12	5:O:3142:ILE:HD13	2.02	0.42
5:O:3772:ASN:OD1	5:O:3788:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3901:ARG:HB2	5:O:3970:LEU:HD21	2.00	0.42
6:G:66:ALA:HB1	6:G:78:ILE:HD12	2.00	0.42
1:K:329:LEU:HD12	2:L:276:TRP:CH2	2.55	0.42
1:K:440:ALA:N	2:L:482:ILE:O	2.39	0.42
2:L:15:ASP:CG	2:L:20:MET:HE1	2.44	0.42
3:I:114:DC:H1'	3:I:115:DT:C2	2.55	0.42
4:J:44:DG:P	7:H:83:ARG:HH12	2.42	0.42
5:O:358:GLU:H	5:O:358:GLU:CD	2.26	0.42
5:O:1474:ASP:OD1	5:O:1474:ASP:N	2.52	0.42
5:O:2421:VAL:HG23	5:O:2457:PRO:HG3	2.02	0.42
5:O:3045:ILE:HG13	5:O:3046:ARG:N	2.35	0.42
5:O:3271:ASP:OD1	5:O:3272:TRP:N	2.50	0.42
5:O:3509:ASP:OD1	5:O:3509:ASP:N	2.53	0.42
5:O:3569:GLN:O	5:O:3573:ASN:ND2	2.53	0.42
5:O:3614:TYR:CE2	5:O:3618:GLY:HA3	2.55	0.42
5:O:3728:VAL:HG12	5:O:3736:LYS:HD2	2.02	0.42
5:O:3870:SER:O	5:O:3874:ARG:HG2	2.19	0.42
1:K:276:LEU:C	2:L:431:ARG:H	2.26	0.42
2:L:81:ARG:HH12	2:L:86:PRO:HA	1.84	0.42
3:I:42:DA:H2''	3:I:43:DG:H8	1.83	0.42
3:I:129:DG:H2''	3:I:130:DT:O5'	2.19	0.42
4:J:63:DA:H5''	8:A:63:ARG:CZ	2.49	0.42
4:J:140:DG:H2''	4:J:141:DG:C8	2.55	0.42
5:O:19:LEU:HD13	5:O:38:LEU:HG	2.02	0.42
5:O:87:LYS:HD2	5:O:831:LEU:HD22	2.02	0.42
5:O:994:TRP:CE3	5:O:997:ASN:ND2	2.87	0.42
5:O:2249:LEU:O	5:O:2251:ILE:HD12	2.20	0.42
5:O:2306:ASN:HA	5:O:2309:PHE:HB2	2.01	0.42
5:O:2564:GLU:O	5:O:2567:SER:OG	2.36	0.42
6:C:81:ARG:HD2	6:C:106:GLY:HA3	2.02	0.42
2:L:167:PHE:HA	2:L:226:SER:HB2	2.02	0.42
2:L:508:ILE:HD12	2:L:508:ILE:H	1.84	0.42
4:J:23:DC:C2	4:J:24:DA:C6	3.08	0.42
4:J:124:DA:H2''	4:J:125:DG:H8	1.85	0.42
5:O:539:GLN:OE1	5:O:539:GLN:N	2.50	0.42
5:O:1476:HIS:CE1	5:O:1522:GLY:H	2.38	0.42
5:O:1533:LEU:HD23	5:O:1592:MET:HE2	2.01	0.42
5:O:1853:SER:O	5:O:1870:LYS:NZ	2.53	0.42
5:O:1921:ASP:OD1	5:O:1922:ALA:N	2.51	0.42
5:O:2353:GLN:HB3	5:O:2360:PHE:CB	2.49	0.42
5:O:2863:CYS:SG	5:O:2864:GLN:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3114:TYR:CE2	5:O:3125:ARG:HD2	2.54	0.42
5:O:3175:PRO:O	5:O:3179:TRP:HB3	2.19	0.42
5:O:3459:ASN:O	5:O:3463:LEU:HG	2.20	0.42
5:O:3483:MET:O	5:O:3486:GLU:CB	2.64	0.42
5:O:3609:MET:O	5:O:3612:ARG:HG2	2.20	0.42
5:O:3700:GLU:HB2	5:O:3718:ARG:NH1	2.34	0.42
5:O:3877:LYS:HZ2	5:O:4127:TRP:CD1	2.37	0.42
5:O:3988:LEU:HD23	5:O:4100:GLU:HA	2.00	0.42
6:G:47:ALA:HB3	6:G:48:PRO:HD3	2.02	0.42
6:G:103:ALA:O	8:E:94:GLU:HG2	2.20	0.42
1:K:179:ASP:HB3	1:K:182:LYS:HB2	2.02	0.42
1:K:296:VAL:HG13	2:L:299:ASP:H	1.83	0.42
3:I:111:DT:H1'	4:J:44:DG:H22	1.84	0.42
4:J:143:DT:H6	4:J:143:DT:H2'	1.63	0.42
5:O:119:ARG:HA	5:O:122:LYS:HG2	2.02	0.42
5:O:217:LEU:HB2	5:O:220:LEU:HD23	2.00	0.42
5:O:1458:LEU:O	5:O:1462:GLY:N	2.53	0.42
5:O:1476:HIS:O	5:O:1476:HIS:ND1	2.52	0.42
5:O:2834:GLN:NE2	5:O:2838:GLN:OE1	2.43	0.42
5:O:3011:LEU:HB3	5:O:3047:SER:HB2	2.01	0.42
5:O:3018:SER:O	5:O:3020:ASP:N	2.46	0.42
9:B:32:PRO:O	9:B:36:ARG:HG3	2.19	0.42
6:G:20:ARG:HD2	6:G:20:ARG:HA	1.80	0.42
6:G:25:PHE:CZ	7:H:41:VAL:HG22	2.54	0.42
6:G:31:HIS:HA	6:G:48:PRO:CB	2.50	0.42
1:K:388:LYS:HE3	2:L:451:LEU:HB3	2.02	0.42
1:K:416:GLN:O	1:K:430:PRO:HA	2.20	0.42
4:J:48:DT:H2''	4:J:49:DC:H5'	2.00	0.42
5:O:569:VAL:O	5:O:572:VAL:HG22	2.20	0.42
5:O:631:ARG:HG3	5:O:668:LYS:HD3	2.02	0.42
5:O:753:GLN:NE2	5:O:791:ASP:O	2.52	0.42
5:O:1112:ALA:HB1	5:O:1180:GLN:HG2	2.02	0.42
5:O:1196:PRO:O	5:O:1202:ARG:NH2	2.43	0.42
5:O:1960:LYS:C	5:O:1962:TYR:N	2.76	0.42
5:O:2476:ILE:O	5:O:2480:ILE:HG12	2.20	0.42
5:O:2995:GLU:O	5:O:2999:LEU:HG	2.19	0.42
5:O:3236:PHE:HD2	5:O:3269:ARG:HH21	1.67	0.42
5:O:3797:THR:O	5:O:3800:LEU:HB2	2.20	0.42
7:D:39:TYR:O	7:D:43:LYS:HG2	2.19	0.42
6:G:100:VAL:HG12	6:G:100:VAL:O	2.20	0.42
2:L:7:LYS:HD2	2:L:53:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:489:ARG:NH1	2:L:508:ILE:HG13	2.35	0.41
2:L:497:ARG:NH2	2:L:501:PRO:O	2.52	0.41
2:L:538:PRO:C	2:L:539:LEU:HD12	2.45	0.41
3:I:19:DG:N2	4:J:136:DA:H2	2.16	0.41
3:I:85:DC:OP2	9:B:35:ARG:NE	2.53	0.41
4:J:77:DG:H2'	4:J:78:DC:C2	2.55	0.41
5:O:217:LEU:HG	5:O:221:ALA:HB2	2.00	0.41
5:O:756:PHE:HE2	5:O:792:ILE:HD11	1.85	0.41
5:O:1208:LEU:HD11	5:O:1275:THR:O	2.20	0.41
5:O:1630:ASP:HA	5:O:1633:TRP:NE1	2.35	0.41
5:O:2771:LEU:HD23	5:O:2771:LEU:H	1.85	0.41
5:O:2973:ASP:OD2	5:O:3002:TYR:OH	2.35	0.41
5:O:3247:ARG:HD3	5:O:3283:LEU:HA	2.00	0.41
5:O:3823:GLU:OE1	5:O:3823:GLU:N	2.36	0.41
8:A:126:LEU:HD22	8:E:113:HIS:CG	2.55	0.41
8:A:128:ARG:NE	8:A:134:ARG:HD2	2.35	0.41
2:L:16:VAL:HA	2:L:31:PHE:CE1	2.55	0.41
2:L:184:ARG:HH21	2:L:520:ALA:N	2.19	0.41
2:L:347:LYS:NZ	2:L:387:LEU:O	2.34	0.41
3:I:49:DT:H1'	3:I:50:DC:O2	2.21	0.41
4:J:108:DT:H2''	4:J:109:DG:N7	2.35	0.41
4:J:117:DC:H2''	4:J:118:DC:C5	2.55	0.41
5:O:245:SER:O	5:O:248:ILE:HG12	2.20	0.41
5:O:575:ILE:HG13	5:O:576:VAL:N	2.35	0.41
5:O:1256:TRP:O	5:O:1260:LEU:HG	2.20	0.41
5:O:1630:ASP:HA	5:O:1633:TRP:HE1	1.83	0.41
5:O:1780:SER:OG	5:O:1784:ARG:NH2	2.53	0.41
5:O:1948:ALA:HA	5:O:1951:VAL:HG22	2.02	0.41
5:O:2305:ASN:O	5:O:2309:PHE:N	2.51	0.41
5:O:2548:PRO:HB2	5:O:2848:PHE:CD1	2.56	0.41
5:O:3274:VAL:HG11	5:O:3312:VAL:HA	2.03	0.41
5:O:3348:LEU:HA	5:O:3351:ILE:HD12	2.02	0.41
5:O:3587:ASP:HA	5:O:3590:ASN:HD22	1.85	0.41
8:A:72:ARG:HG2	8:A:84:PHE:CE2	2.55	0.41
6:G:59:THR:HG23	7:H:41:VAL:HG11	2.01	0.41
6:G:71:ARG:NH2	6:G:76:THR:HA	2.35	0.41
8:E:51:ILE:HA	9:F:39:ARG:HB3	2.01	0.41
8:E:74:ILE:HG23	9:F:66:ILE:HD13	2.02	0.41
9:F:87:VAL:HG12	9:F:91:LYS:HE2	2.01	0.41
1:K:125:GLN:HA	1:K:128:GLN:HG2	2.00	0.41
5:O:151:GLU:H	5:O:151:GLU:CD	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:163:LYS:O	5:O:164:LYS:HD3	2.19	0.41
5:O:474:VAL:HA	5:O:477:ASN:ND2	2.36	0.41
5:O:930:ALA:O	5:O:934:LEU:HD23	2.20	0.41
5:O:1418:HIS:HA	5:O:1421:GLU:CD	2.46	0.41
5:O:2190:VAL:O	5:O:2194:LEU:HD23	2.21	0.41
5:O:2415:LEU:O	5:O:2419:ASP:N	2.53	0.41
5:O:3036:TYR:O	5:O:3039:THR:OG1	2.32	0.41
5:O:3277:VAL:HG13	5:O:3306:LEU:HB2	2.02	0.41
5:O:3626:GLY:C	5:O:3628:PHE:H	2.29	0.41
6:C:62:ILE:HD11	6:C:87:ILE:HD11	2.02	0.41
6:C:85:LEU:HG	6:C:108:LEU:HD23	2.03	0.41
8:A:116:ARG:HG3	8:A:118:THR:H	1.85	0.41
7:H:35:SER:HA	7:H:56:MET:HE2	2.02	0.41
1:K:52:GLN:HG3	1:K:206:LYS:HG2	2.02	0.41
1:K:161:MET:SD	1:K:163:HIS:N	2.93	0.41
2:L:299:ASP:HB2	2:L:305:VAL:N	2.36	0.41
2:L:407:VAL:HB	2:L:424:LEU:HD11	2.01	0.41
2:L:427:MET:HA	2:L:430:LEU:HD23	2.03	0.41
4:J:135:DC:H2'	4:J:136:DA:C8	2.55	0.41
4:J:144:DT:H1'	4:J:145:DC:C2	2.55	0.41
5:O:113:SER:O	5:O:117:LYS:HG2	2.20	0.41
5:O:924:ARG:O	5:O:928:VAL:HG22	2.20	0.41
5:O:1152:ARG:O	5:O:1163:LEU:HD11	2.20	0.41
5:O:1422:LYS:HA	5:O:1422:LYS:HD3	1.85	0.41
5:O:1949:ILE:HG23	5:O:2100:LEU:HD12	2.01	0.41
5:O:2470:ARG:HB2	5:O:2517:LEU:HD21	2.01	0.41
5:O:2551:GLU:OE2	5:O:2851:PHE:N	2.47	0.41
5:O:3771:MET:O	5:O:3775:LEU:HG	2.20	0.41
5:O:3959:MET:HG3	5:O:3960:PRO:O	2.20	0.41
5:O:4007:LYS:HD2	5:O:4038:TRP:HE3	1.85	0.41
8:A:79:LYS:HB2	9:B:70:VAL:HG11	2.03	0.41
9:B:66:ILE:O	9:B:70:VAL:HG23	2.20	0.41
9:B:88:TYR:HA	9:B:91:LYS:HE3	2.02	0.41
1:K:399:ARG:HD2	1:K:408:PRO:HB2	2.02	0.41
1:K:445:LYS:HD2	1:K:445:LYS:HA	1.83	0.41
3:I:63:DA:H2''	3:I:64:DA:C8	2.55	0.41
5:O:391:ARG:O	5:O:395:MET:HG3	2.19	0.41
5:O:671:SER:HA	5:O:674:VAL:HG12	2.02	0.41
5:O:865:GLN:O	5:O:868:LYS:NZ	2.54	0.41
5:O:1230:GLY:O	5:O:1233:SER:OG	2.33	0.41
5:O:1477:HIS:CB	5:O:1481:THR:HG23	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1690:GLY:HA2	5:O:1693:VAL:HG12	2.01	0.41
5:O:2310:VAL:HA	5:O:2316:TYR:CD2	2.55	0.41
5:O:2429:ASP:N	5:O:2429:ASP:OD1	2.54	0.41
5:O:3088:LEU:HG	5:O:3138:ILE:HD12	2.01	0.41
5:O:3136:THR:O	5:O:3140:GLU:OE1	2.38	0.41
5:O:3252:PHE:CE2	5:O:3289:ARG:HD3	2.55	0.41
5:O:3279:SER:O	5:O:3282:ARG:HG2	2.20	0.41
5:O:3296:GLN:HE21	5:O:3301:LEU:H	1.63	0.41
5:O:3420:CYS:O	5:O:3424:LEU:HG	2.20	0.41
5:O:3498:TRP:HD1	5:O:3501:HIS:CE1	2.39	0.41
5:O:3952:PHE:CE2	5:O:4038:TRP:HB3	2.56	0.41
6:C:92:GLU:HA	6:C:95:LYS:HE2	2.01	0.41
9:F:31:LYS:HB3	9:F:32:PRO:HD3	2.01	0.41
1:K:470:ARG:HH22	2:L:347:LYS:HB2	1.85	0.41
3:I:104:DG:H2''	3:I:105:DG:H5'	2.03	0.41
4:J:41:DG:H2''	4:J:42:DG:C8	2.53	0.41
4:J:66:DC:H41	9:B:31:LYS:HD2	1.86	0.41
5:O:82:ARG:HA	5:O:85:ILE:HG22	2.03	0.41
5:O:472:GLY:O	5:O:475:LEU:HB3	2.20	0.41
5:O:616:LYS:HZ1	5:O:2034:SER:H	1.69	0.41
5:O:891:ARG:NH2	5:O:956:PRO:O	2.53	0.41
5:O:941:MET:HE1	5:O:962:TYR:CE1	2.56	0.41
5:O:1396:PRO:HB3	5:O:1457:GLN:NE2	2.34	0.41
5:O:1909:ASN:HB3	5:O:1910:GLU:H	1.56	0.41
5:O:1959:LEU:C	5:O:1961:PHE:N	2.79	0.41
5:O:2531:LEU:HG	5:O:2538:ARG:NE	2.35	0.41
5:O:3283:LEU:O	5:O:3287:ARG:HG2	2.21	0.41
5:O:3460:GLU:OE1	5:O:3460:GLU:N	2.37	0.41
5:O:3579:SER:HB3	5:O:3736:LYS:NZ	2.36	0.41
5:O:3731:SER:OG	5:O:3732:LEU:N	2.52	0.41
5:O:3919:GLY:HA3	5:O:3946:PHE:HA	2.01	0.41
5:O:3929:MET:HE2	5:O:3929:MET:HA	2.02	0.41
9:B:47:SER:OG	9:B:50:ILE:HG12	2.20	0.41
1:K:276:LEU:HD11	2:L:355:PHE:CE1	2.56	0.41
1:K:302:THR:HA	2:L:291:LYS:HA	2.03	0.41
1:K:355:LEU:HD21	2:L:473:LEU:HB2	2.02	0.41
1:K:358:LYS:HE3	1:K:358:LYS:HB3	1.92	0.41
2:L:35:LYS:HZ2	2:L:98:ILE:HB	1.85	0.41
5:O:978:GLN:N	5:O:978:GLN:OE1	2.54	0.41
5:O:1333:SER:O	5:O:1337:VAL:HG23	2.21	0.41
5:O:1487:VAL:HG12	5:O:1559:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:2295:GLN:HG3	5:O:2298:GLU:H	1.86	0.41
5:O:2533:SER:OG	5:O:2534:ASN:N	2.54	0.41
5:O:2995:GLU:HG3	5:O:2996:LEU:HD12	2.01	0.41
5:O:3090:TYR:HE2	5:O:3102:TYR:CE2	2.38	0.41
5:O:3660:ASN:HB2	5:O:3664:ASN:OD1	2.21	0.41
5:O:3771:MET:HB2	5:O:3991:PHE:HE1	1.86	0.41
9:B:35:ARG:NH2	9:B:39:ARG:HH12	2.19	0.41
2:L:56:LEU:HD23	2:L:80:HIS:ND1	2.36	0.41
2:L:131:HIS:HB2	2:L:240:ILE:HD11	2.01	0.41
5:O:135:LEU:HD21	5:O:177:LEU:HA	2.03	0.41
5:O:241:ASP:OD1	5:O:244:THR:OG1	2.39	0.41
5:O:424:LEU:HD21	5:O:427:VAL:HG23	2.03	0.41
5:O:631:ARG:HE	5:O:668:LYS:NZ	2.19	0.41
5:O:654:ILE:HD12	5:O:710:PHE:CD1	2.56	0.41
5:O:679:LYS:HE3	5:O:679:LYS:HB3	1.91	0.41
5:O:1146:ASN:ND2	5:O:1165:LEU:HD23	2.36	0.41
5:O:1414:ILE:HD12	5:O:1414:ILE:HA	1.88	0.41
5:O:1531:LEU:HD11	5:O:1559:PHE:HE2	1.86	0.41
5:O:1589:ASN:CG	5:O:1592:MET:HG2	2.46	0.41
5:O:2214:ARG:HA	5:O:2217:ASN:ND2	2.35	0.41
5:O:2497:GLU:HA	5:O:2500:LYS:HE2	2.03	0.41
5:O:3552:LYS:HA	5:O:3555:VAL:HG22	2.03	0.41
5:O:3593:ARG:HE	5:O:3660:ASN:HD21	1.68	0.41
5:O:3692:VAL:HG21	5:O:3719:ILE:O	2.20	0.41
5:O:4040:PRO:HB2	5:O:4041:ARG:NH2	2.36	0.41
5:O:4064:LEU:O	5:O:4068:HIS:N	2.47	0.41
6:G:81:ARG:NH2	6:G:109:PRO:HD3	2.30	0.41
7:H:61:SER:OG	9:F:99:GLY:N	2.49	0.41
9:F:88:TYR:HA	9:F:91:LYS:HD2	2.03	0.41
1:K:32:TYR:HE2	4:J:143:DT:H4'	1.85	0.41
1:K:95:ASN:HD22	1:K:95:ASN:C	2.28	0.41
1:K:164:LYS:HE3	1:K:164:LYS:HB2	1.74	0.41
1:K:171:ASN:O	1:K:207:LYS:HB2	2.21	0.41
1:K:265:LYS:HG3	1:K:266:ASP:H	1.86	0.41
1:K:275:ASN:HD21	2:L:431:ARG:HD2	1.86	0.41
1:K:451:LYS:HB2	1:K:451:LYS:HE2	1.64	0.41
3:I:102:DG:H1'	3:I:103:DG:C8	2.56	0.41
3:I:105:DG:OP1	9:B:79:LYS:N	2.35	0.41
3:I:119:DC:N4	4:J:35:DG:O6	2.54	0.41
5:O:13:LEU:HD13	5:O:59:PHE:CD1	2.56	0.41
5:O:180:LEU:HG	5:O:185:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:236:LYS:HA	5:O:236:LYS:HD3	1.85	0.41
5:O:392:CYS:O	5:O:396:PHE:HB2	2.21	0.41
5:O:574:LYS:HD3	5:O:574:LYS:HA	1.89	0.41
5:O:678:LYS:HE3	5:O:735:SER:O	2.21	0.41
5:O:785:MET:HA	5:O:788:TYR:CD1	2.56	0.41
5:O:933:LEU:HG	5:O:937:MET:CE	2.50	0.41
5:O:938:VAL:O	5:O:942:LEU:HD23	2.21	0.41
5:O:941:MET:SD	5:O:942:LEU:HD22	2.60	0.41
5:O:965:THR:HG21	5:O:969:LEU:HD11	2.02	0.41
5:O:1323:SER:OG	5:O:1324:PRO:HD3	2.21	0.41
5:O:1565:GLU:HG2	5:O:1566:THR:N	2.35	0.41
5:O:1605:PHE:HB3	5:O:2042:GLN:OE1	2.21	0.41
5:O:1824:LEU:O	5:O:1828:LEU:N	2.40	0.41
5:O:2303:LEU:HA	5:O:2306:ASN:ND2	2.36	0.41
5:O:2421:VAL:O	5:O:2425:ARG:HG2	2.21	0.41
5:O:2835:LYS:O	5:O:2838:GLN:HG2	2.21	0.41
5:O:3110:PHE:HD2	5:O:3135:LEU:HD11	1.86	0.41
5:O:3681:LYS:NZ	5:O:3683:CYS:HB2	2.36	0.41
5:O:3758:LEU:C	5:O:3762:GLN:HE22	2.28	0.41
5:O:3930:VAL:HG12	5:O:3937:VAL:HG12	2.02	0.41
9:B:75:HIS:CE1	7:H:90:GLU:HA	2.56	0.41
1:K:37:SER:HA	1:K:82:LEU:O	2.21	0.41
1:K:217:TYR:HD1	1:K:220:ILE:HD12	1.86	0.41
1:K:463:LYS:HD3	2:L:383:ALA:HB1	2.03	0.41
3:I:104:DG:H2"	3:I:105:DG:H8	1.85	0.41
4:J:97:DG:C6	4:J:98:DG:C6	3.09	0.41
5:O:671:SER:HB2	5:O:675:ARG:HH22	1.86	0.41
5:O:720:GLN:OE1	5:O:720:GLN:N	2.44	0.41
5:O:1013:ILE:HG21	5:O:1062:ARG:HH21	1.85	0.41
5:O:1251:GLN:HA	5:O:1254:LEU:HD12	2.03	0.41
5:O:1421:GLU:HB2	5:O:1422:LYS:NZ	2.36	0.41
5:O:1554:SER:N	5:O:1557:GLU:OE2	2.52	0.41
5:O:2467:THR:HA	5:O:2470:ARG:HH11	1.86	0.41
5:O:3241:LYS:HA	5:O:3244:ASP:OD2	2.21	0.41
5:O:3882:LEU:HD22	5:O:3885:ARG:NH2	2.36	0.41
5:O:3912:CYS:HB3	5:O:3961:PHE:CD2	2.56	0.41
5:O:3979:LEU:HD23	5:O:3980:MET:N	2.36	0.41
5:O:4086:ASP:N	5:O:4086:ASP:OD1	2.54	0.41
6:G:58:LEU:O	6:G:62:ILE:HG12	2.21	0.41
8:E:127:ALA:O	8:E:131:ARG:HB2	2.21	0.41
1:K:343:PRO:HA	1:K:401:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:LEU:HA	1:K:398:CYS:HA	2.03	0.40
1:K:353:LEU:HD23	1:K:395:ALA:HB2	2.02	0.40
1:K:369:TYR:CD1	1:K:370:PRO:HD2	2.55	0.40
1:K:478:PHE:HA	1:K:506:LEU:CD1	2.51	0.40
2:L:299:ASP:HB2	2:L:305:VAL:H	1.85	0.40
3:I:130:DT:H2''	3:I:131:DG:C4	2.56	0.40
4:J:45:DT:H2''	4:J:46:DA:C8	2.56	0.40
4:J:77:DG:OP2	4:J:78:DC:N4	2.54	0.40
5:O:58:VAL:HG23	5:O:61:ARG:HE	1.86	0.40
5:O:487:LEU:HD21	5:O:571:SER:HB2	2.01	0.40
5:O:540:MET:HE3	5:O:543:SER:OG	2.21	0.40
5:O:1057:LYS:O	5:O:1061:LYS:HG2	2.20	0.40
5:O:3842:TRP:O	5:O:3843:LEU:HG	2.21	0.40
5:O:3864:ARG:O	5:O:3868:VAL:HG13	2.21	0.40
5:O:3946:PHE:HE1	5:O:4046:TYR:HB2	1.86	0.40
6:C:92:GLU:HG2	7:D:100:PRO:HG2	2.03	0.40
6:C:96:LEU:HG	6:C:97:LEU:HG	2.02	0.40
6:G:27:VAL:O	6:G:31:HIS:HB2	2.21	0.40
1:K:244:ARG:HD2	1:K:244:ARG:HA	1.81	0.40
1:K:274:TYR:HB2	1:K:367:PHE:HD2	1.86	0.40
1:K:340:PHE:HZ	2:L:486:ARG:HA	1.85	0.40
1:K:510:LYS:N	1:K:514:MET:HE1	2.35	0.40
3:I:134:DA:H2''	3:I:135:DG:C8	2.56	0.40
4:J:35:DG:C2	4:J:36:DA:C5	3.10	0.40
4:J:74:DA:P	8:A:116:ARG:HB2	2.62	0.40
5:O:168:ASP:H	5:O:171:LEU:HB3	1.86	0.40
5:O:270:ALA:HA	5:O:273:ARG:HH21	1.87	0.40
5:O:890:LYS:HD2	5:O:906:PHE:CG	2.56	0.40
5:O:1369:MET:O	5:O:1373:VAL:HG22	2.20	0.40
5:O:1570:GLU:HG3	5:O:1571:LEU:HD23	2.04	0.40
5:O:2395:THR:O	5:O:2399:GLU:OE1	2.39	0.40
5:O:2571:ASP:OD1	5:O:2574:ASN:HB2	2.21	0.40
5:O:3828:TYR:HE2	5:O:4128:MET:HE1	1.86	0.40
9:B:67:ARG:HD3	7:H:96:ARG:HH12	1.86	0.40
7:H:114:ALA:HA	7:H:117:LYS:HZ2	1.86	0.40
1:K:403:ARG:HB2	5:O:213:ARG:HH12	1.85	0.40
2:L:247:TRP:HB3	2:L:263:ALA:HB3	2.04	0.40
5:O:91:ILE:HD12	5:O:833:HIS:CE1	2.56	0.40
5:O:460:ALA:O	5:O:463:LYS:HG2	2.22	0.40
5:O:836:LYS:HD2	5:O:836:LYS:HA	1.84	0.40
5:O:1797:LEU:O	5:O:1800:SER:OG	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:2215:LEU:HD23	5:O:2218:PHE:HD2	1.87	0.40
5:O:2328:ARG:NE	5:O:2370:SER:O	2.55	0.40
5:O:2336:ILE:HD12	5:O:2336:ILE:HA	1.91	0.40
5:O:2395:THR:N	5:O:2431:ARG:HH12	2.19	0.40
5:O:2804:ILE:HD12	5:O:2804:ILE:HA	1.93	0.40
5:O:4084:SER:OG	5:O:4085:LYS:N	2.51	0.40
6:C:39:TYR:HB3	7:D:75:SER:HB2	2.02	0.40
6:C:88:ARG:NH1	6:C:98:GLY:O	2.47	0.40
1:K:76:ILE:HD12	1:K:76:ILE:HA	1.93	0.40
1:K:350:PHE:N	2:L:461:MET:HE1	2.36	0.40
1:K:493:LEU:HD21	2:L:323:PHE:HD1	1.85	0.40
1:K:510:LYS:H	1:K:514:MET:HE1	1.85	0.40
3:I:22:DG:H2''	3:I:23:DA:C5	2.57	0.40
3:I:80:DT:H6	3:I:80:DT:H2'	1.64	0.40
5:O:57:LEU:HD11	5:O:100:ILE:HG23	2.04	0.40
5:O:628:GLU:OE1	5:O:631:ARG:NH2	2.41	0.40
5:O:715:ALA:O	5:O:718:MET:HG3	2.21	0.40
5:O:899:ARG:NH2	5:O:2565:MET:O	2.51	0.40
5:O:914:VAL:HG13	5:O:934:LEU:HD21	2.04	0.40
5:O:1166:LEU:HD11	5:O:1207:TRP:CZ2	2.57	0.40
5:O:1619:ALA:HA	5:O:1622:ILE:HG22	2.03	0.40
5:O:1648:LEU:O	5:O:1652:ILE:HG23	2.21	0.40
5:O:3270:ASP:O	5:O:3273:LEU:HB3	2.22	0.40
5:O:3376:GLY:N	5:O:3379:GLN:OE1	2.51	0.40
5:O:3547:THR:HG23	5:O:3550:LYS:HE2	2.03	0.40
8:E:100:LEU:HD13	9:F:37:LEU:HD13	2.04	0.40
1:K:465:ILE:HD12	1:K:518:LEU:HD22	2.04	0.40
2:L:147:LEU:O	2:L:151:ILE:HG12	2.21	0.40
2:L:476:LEU:O	2:L:477:PHE:HD1	2.04	0.40
2:L:528:ILE:HB	2:L:529:PRO:HD3	2.03	0.40
3:I:87:DC:H2''	3:I:88:DG:H8	1.85	0.40
5:O:628:GLU:CD	5:O:631:ARG:HH12	2.28	0.40
5:O:672:ILE:HG22	5:O:676:ASN:HD21	1.87	0.40
5:O:935:HIS:CD2	5:O:2773:ARG:HH12	2.39	0.40
5:O:1961:PHE:C	5:O:1963:GLN:N	2.78	0.40
5:O:2376:ASP:O	5:O:2379:MET:HE1	2.22	0.40
5:O:2592:ASP:OD1	5:O:2593:SER:N	2.45	0.40
5:O:2925:GLU:O	5:O:2929:LEU:HG	2.21	0.40
5:O:3179:TRP:HH2	5:O:3246:ALA:HB2	1.85	0.40
5:O:3192:LYS:HG3	5:O:3196:LYS:HZ1	1.87	0.40
6:C:26:PRO:HD2	7:D:34:TYR:CE1	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:57:TYR:CZ	7:H:106:HIS:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	491/609 (81%)	438 (89%)	49 (10%)	4 (1%)	16	53
2	L	523/732 (71%)	471 (90%)	52 (10%)	0	100	100
5	O	3455/4128 (84%)	3065 (89%)	379 (11%)	11 (0%)	36	71
6	C	93/143 (65%)	83 (89%)	9 (10%)	1 (1%)	11	45
6	G	92/143 (64%)	81 (88%)	11 (12%)	0	100	100
7	D	91/126 (72%)	88 (97%)	3 (3%)	0	100	100
7	H	90/126 (71%)	83 (92%)	7 (8%)	0	100	100
8	A	86/136 (63%)	82 (95%)	4 (5%)	0	100	100
8	E	86/136 (63%)	82 (95%)	4 (5%)	0	100	100
9	B	69/103 (67%)	68 (99%)	1 (1%)	0	100	100
9	F	70/103 (68%)	66 (94%)	4 (6%)	0	100	100
All	All	5146/6485 (79%)	4607 (90%)	523 (10%)	16 (0%)	37	71

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	O	2229	ALA
5	O	2535	THR
5	O	3295	GLU
5	O	3480	LEU
5	O	3855	TYR

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Mol	Chain	Res	Type
1	K	373	SER
5	O	1936	ARG
5	O	1427	SER
1	K	327	ILE
5	O	169	THR
1	K	100	LYS
1	K	511	VAL
5	O	3304	VAL
6	C	102	ILE
5	O	1123	THR
5	O	3842	TRP

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	K	432/548 (79%)	430 (100%)	2 (0%)	81	81
2	L	462/649 (71%)	462 (100%)	0	100	100
5	O	3042/3671 (83%)	3040 (100%)	2 (0%)	88	88
6	C	63/106 (59%)	63 (100%)	0	100	100
6	G	65/106 (61%)	65 (100%)	0	100	100
7	D	77/105 (73%)	77 (100%)	0	100	100
7	H	78/105 (74%)	78 (100%)	0	100	100
8	A	71/111 (64%)	71 (100%)	0	100	100
8	E	75/111 (68%)	75 (100%)	0	100	100
9	B	59/79 (75%)	59 (100%)	0	100	100
9	F	60/79 (76%)	60 (100%)	0	100	100
All	All	4484/5670 (79%)	4480 (100%)	4 (0%)	87	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	95	ASN
1	K	171	ASN
5	O	305	ASN
5	O	1961	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	458	GLN
5	O	1385	ASN
5	O	1926	ASN
5	O	2217	ASN
5	O	3470	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

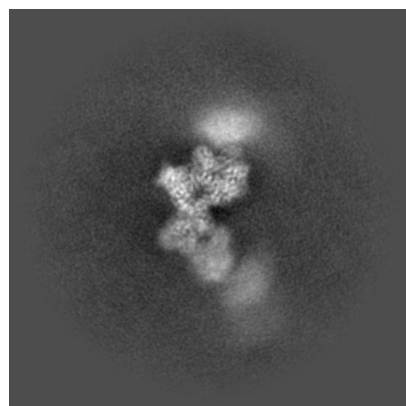
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52958. These allow visual inspection of the internal detail of the map and identification of artifacts.

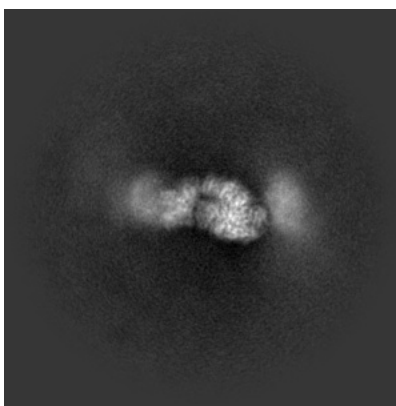
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

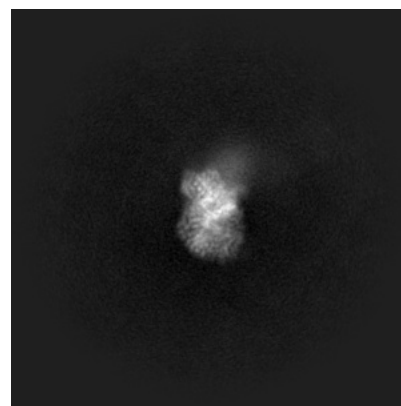
6.1.1 Primary map



X

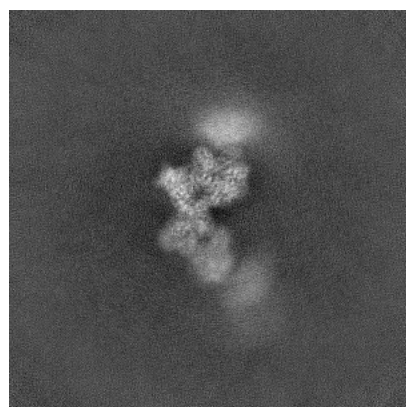


Y

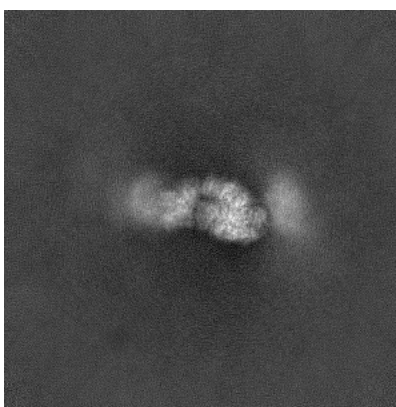


Z

6.1.2 Raw map



X



Y

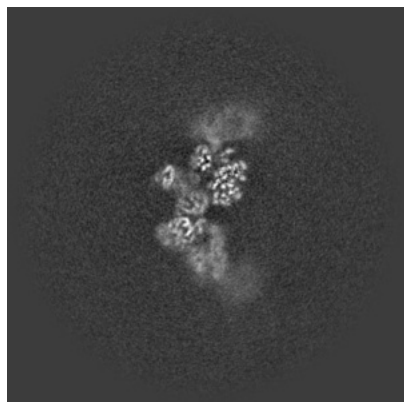


Z

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

6.2 Central slices [i](#)

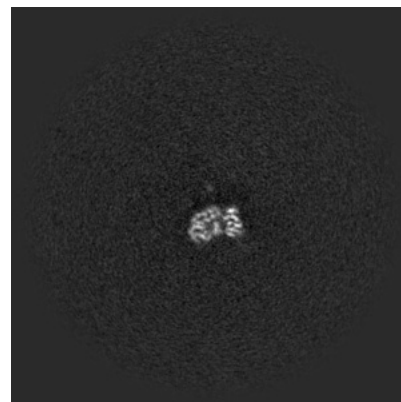
6.2.1 Primary map



X Index: 210

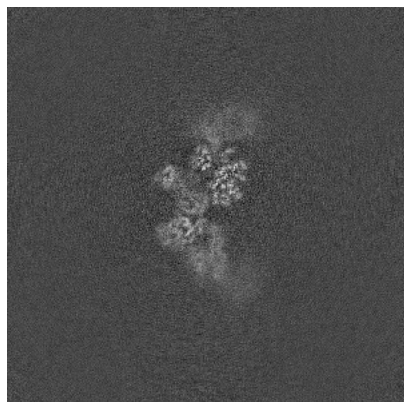


Y Index: 210



Z Index: 210

6.2.2 Raw map



X Index: 210



Y Index: 210

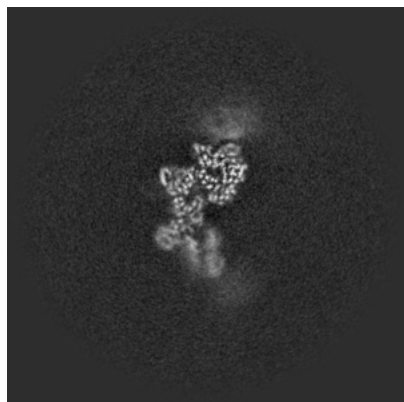


Z Index: 210

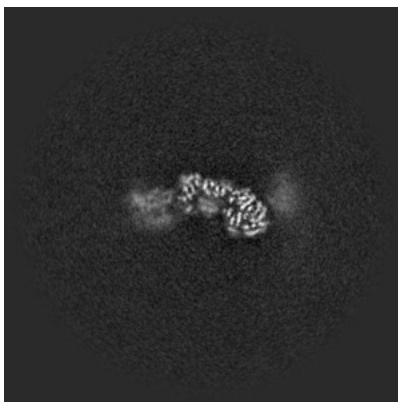
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

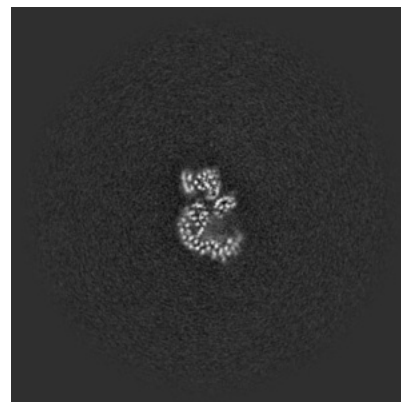
6.3.1 Primary map



X Index: 202



Y Index: 206



Z Index: 243

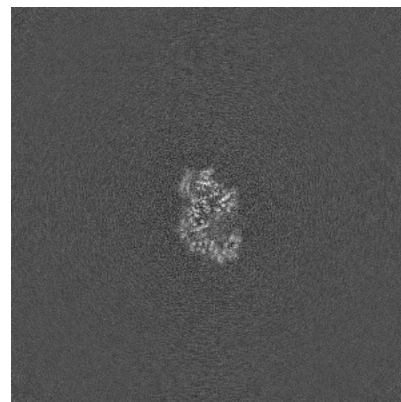
6.3.2 Raw map



X Index: 202



Y Index: 212

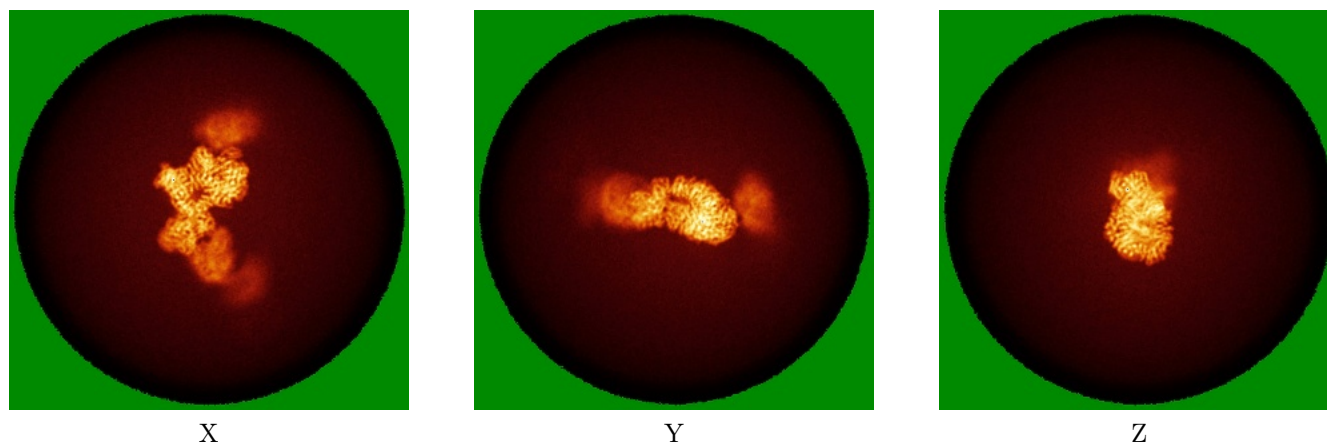


Z Index: 238

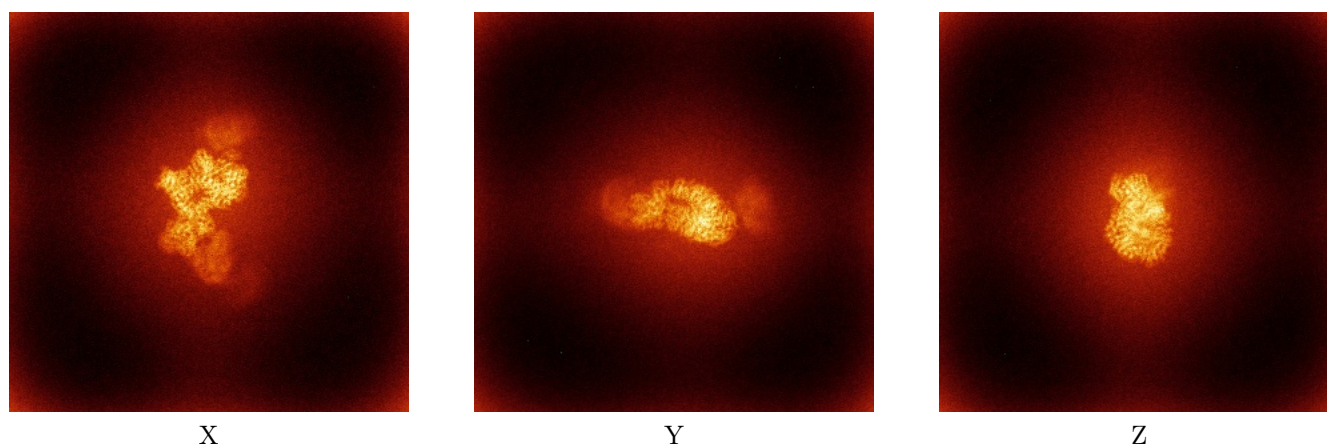
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

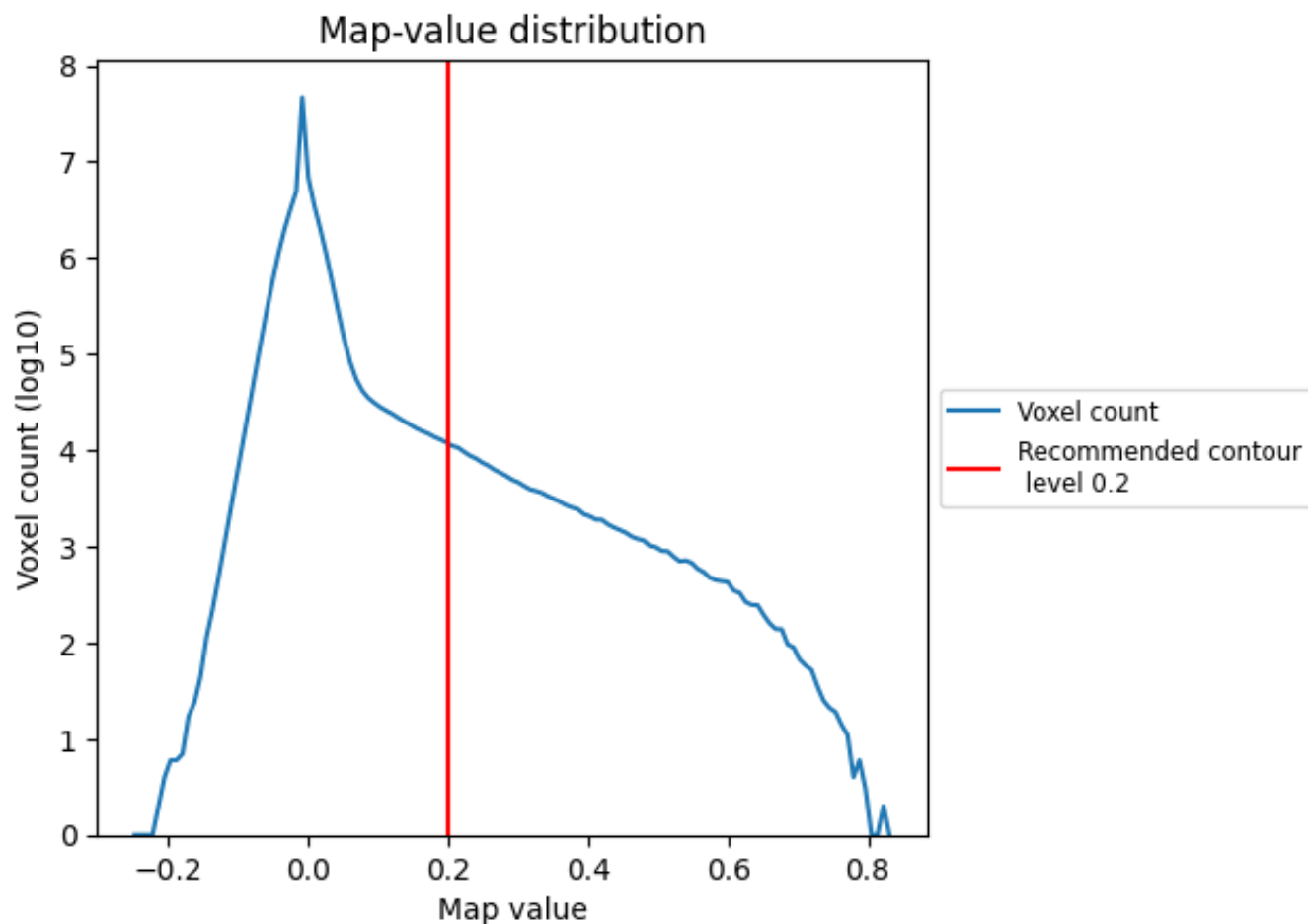
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

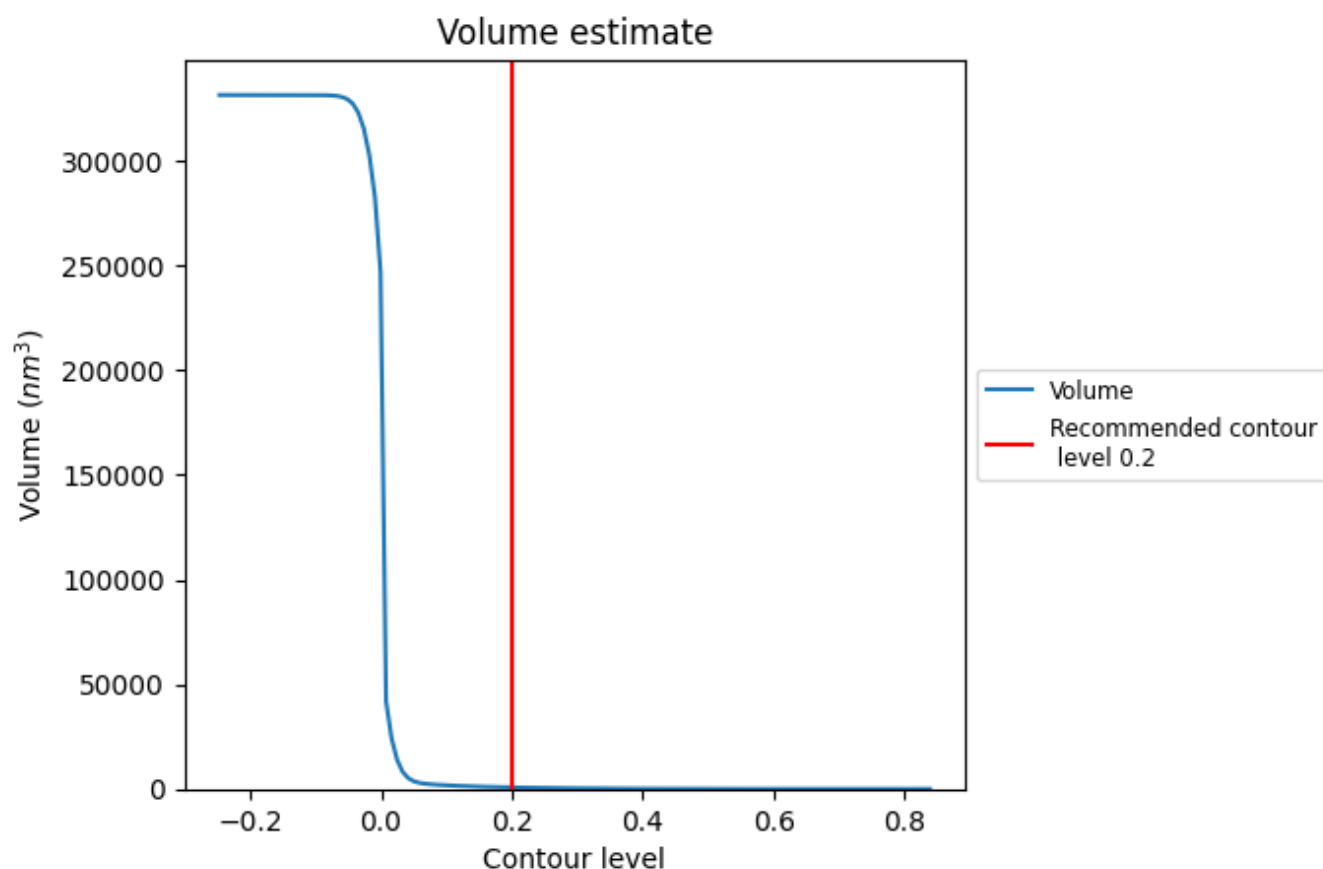
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

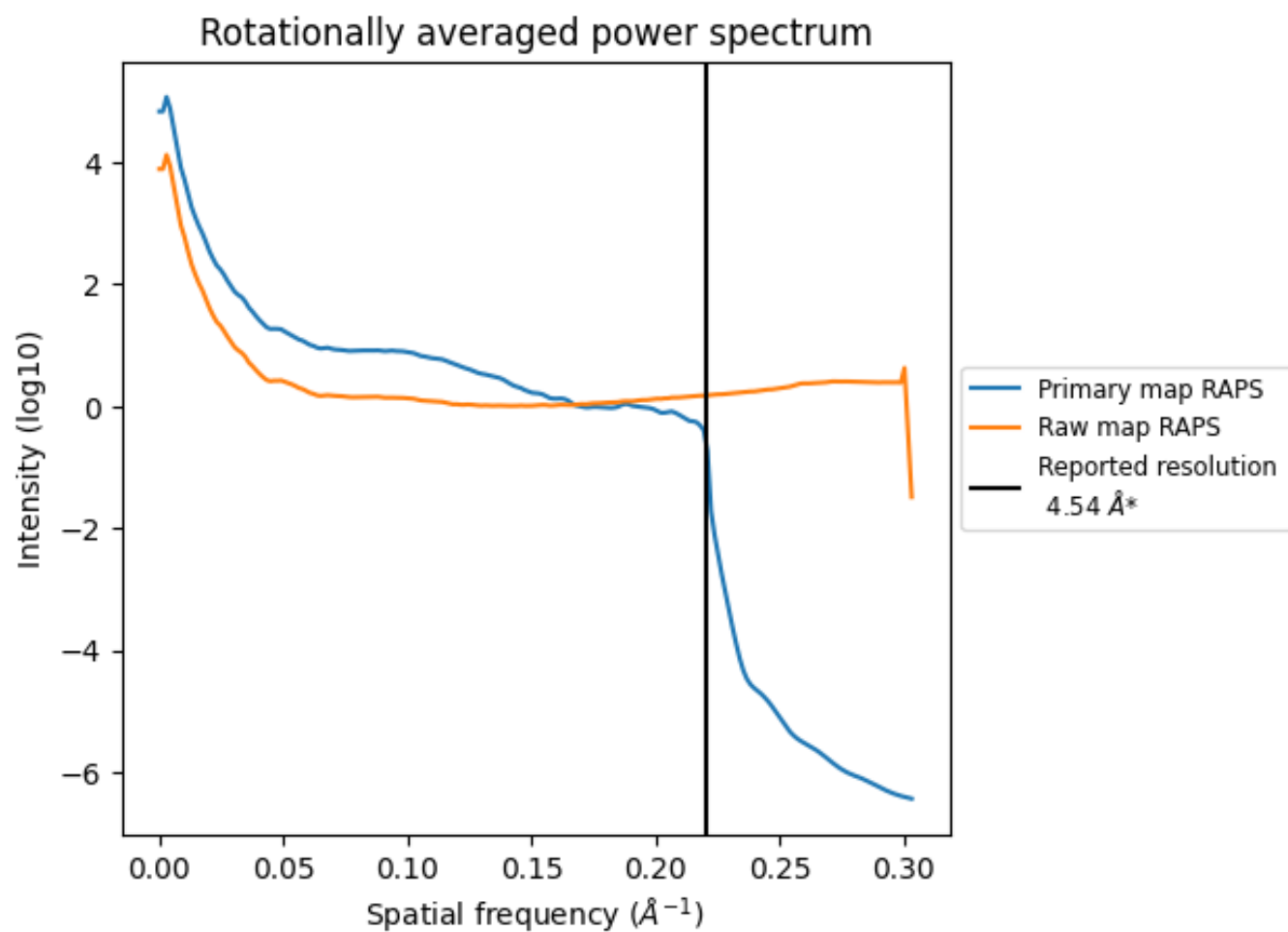
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm^3 ; this corresponds to an approximate mass of 654 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 ⓘ

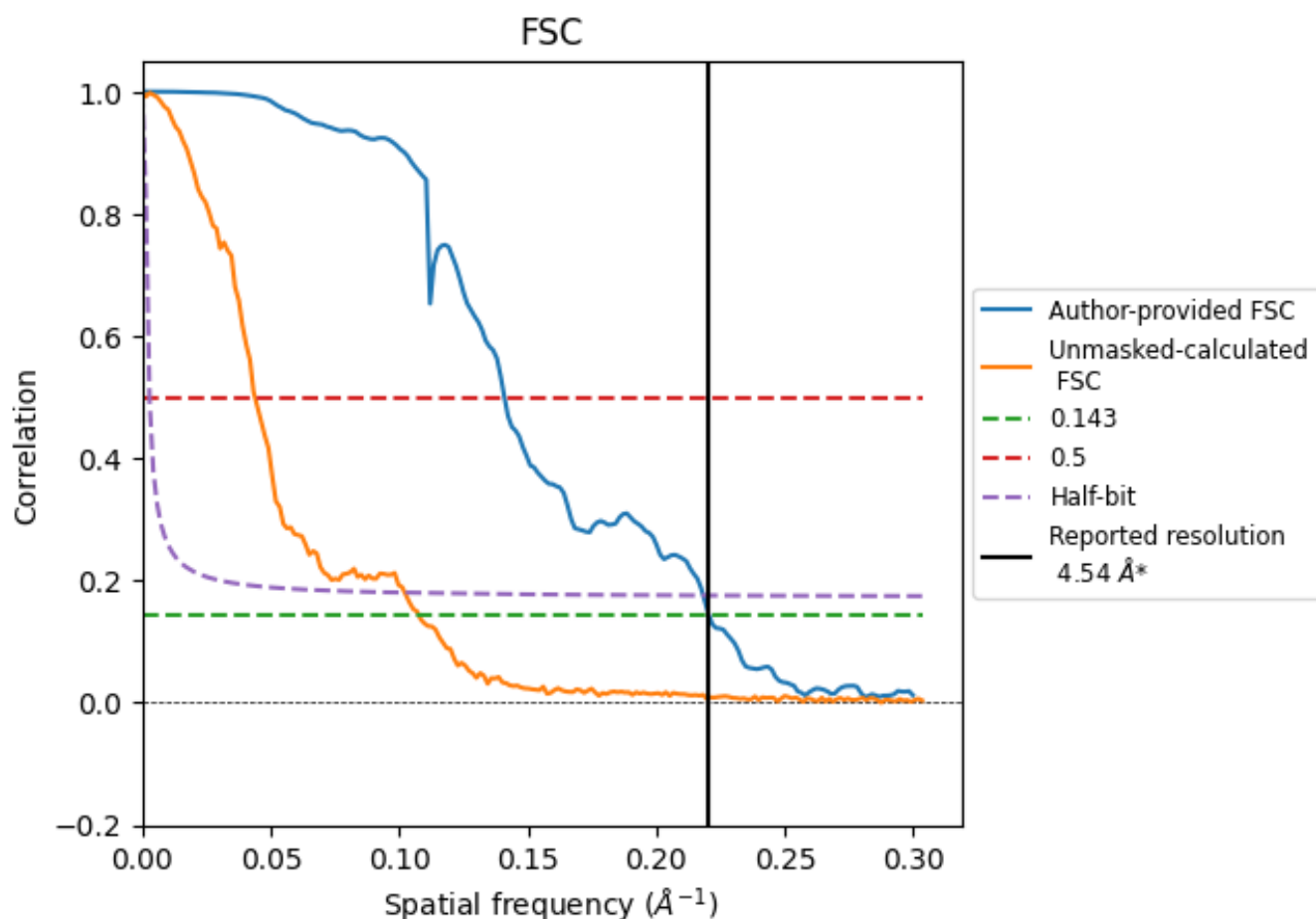


*Reported resolution corresponds to spatial frequency of 0.220 Å⁻¹

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 0.220 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

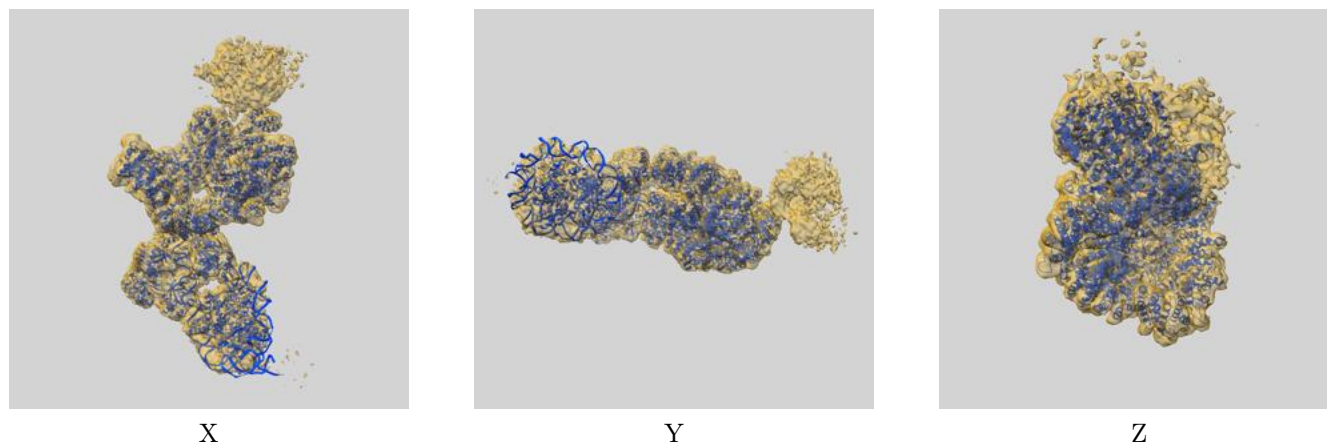
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.54	-	-
Author-provided FSC curve	4.54	7.10	4.58
Unmasked-calculated*	9.29	22.78	9.79

*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 9.29 differs from the reported value 4.54 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52958 and PDB model 9Q9F. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



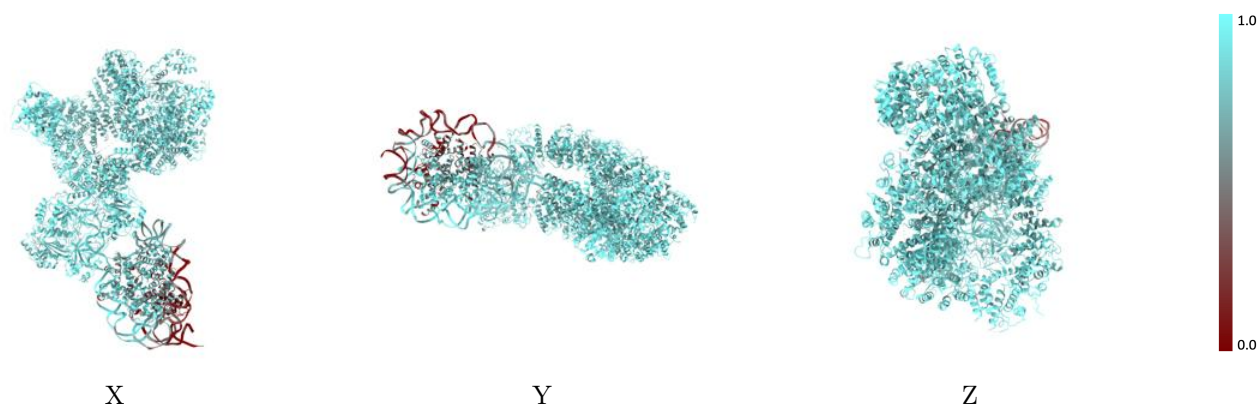
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



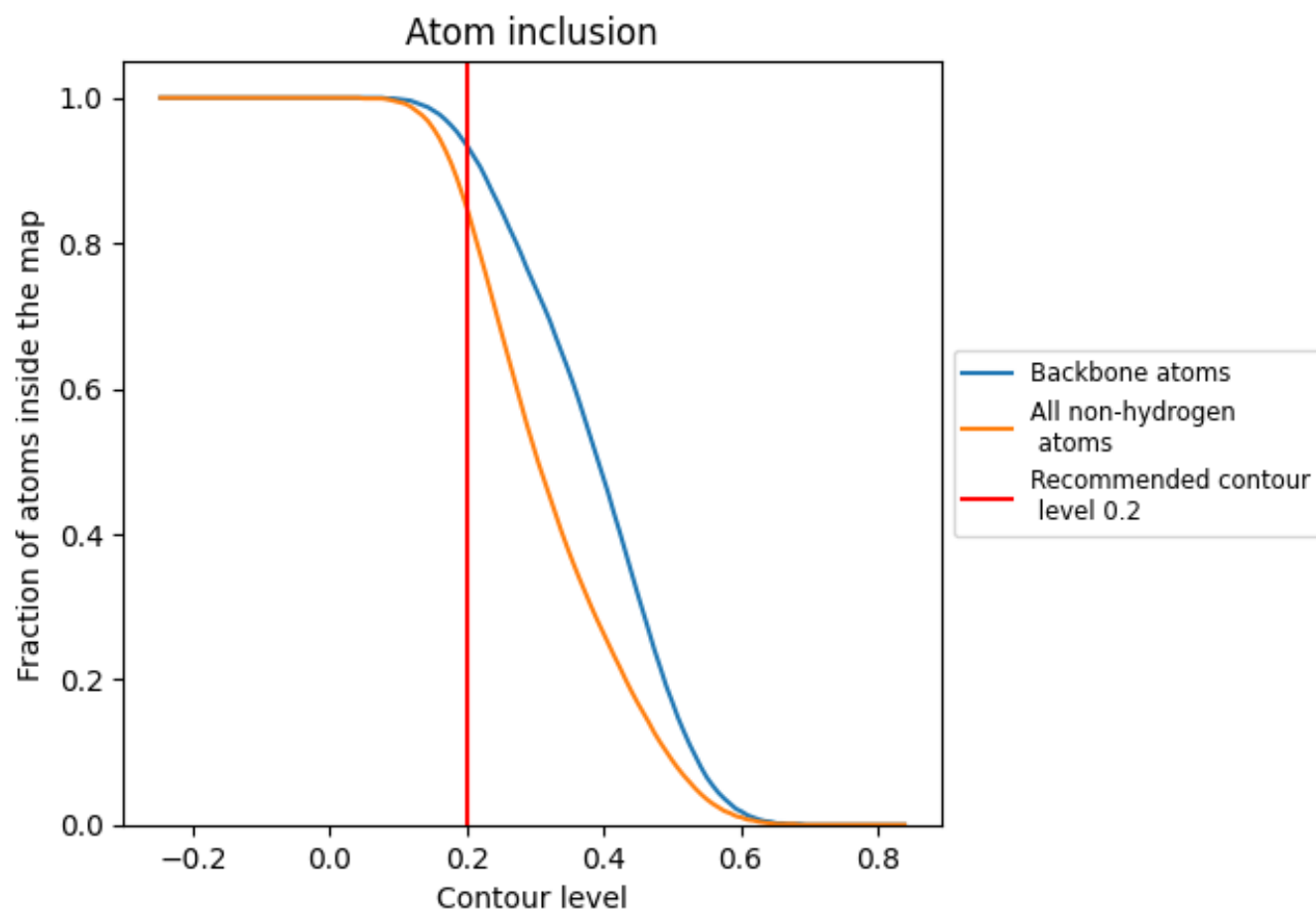
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.2150
A	 0.7080	 0.1420
B	 0.8730	 0.1350
C	 0.7110	 0.1680
D	 0.7520	 0.1730
E	 0.4830	 0.1280
F	 0.5730	 0.1700
G	 0.6360	 0.1440
H	 0.6560	 0.1340
I	 0.6720	 0.1590
J	 0.6990	 0.1710
K	 0.9250	 0.2250
L	 0.9060	 0.2030
O	 0.8960	 0.2380

