



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:22 PM UTC

PDB ID : 7UA4 / pdb_00007ua4
EMDB ID : EMD-26414
Title : Structure of PKA phosphorylated human RyR2-R2474S in the open state in the presence of Calmodulin
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 2.93 Å(reported)
Based on initial model : 7UA3

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:

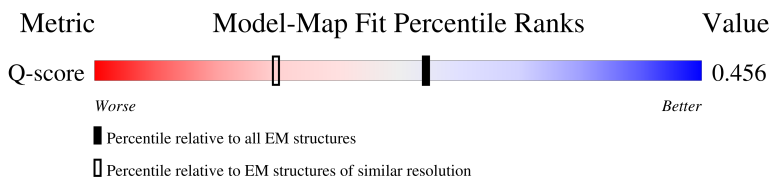
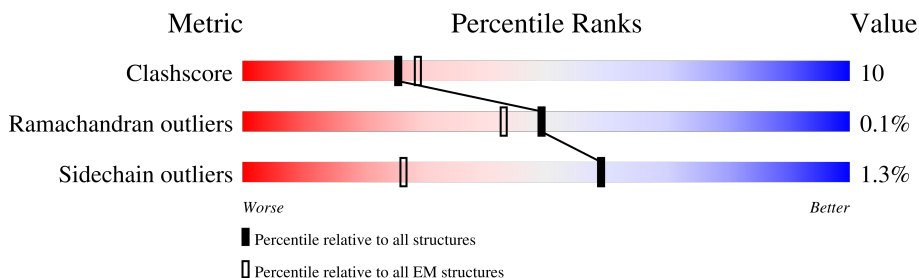
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.93 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.



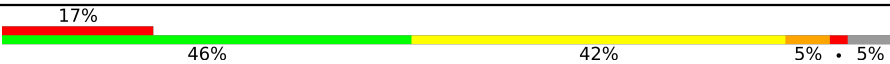
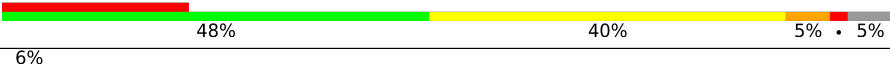
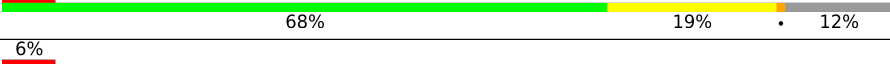
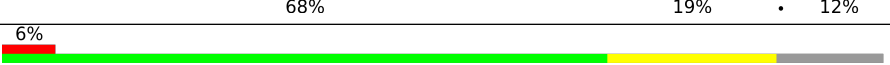
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13037 (2.43 - 3.43)

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	E	108	 76% 21% ...
1	F	108	 77% 20% ...
1	G	108	 75% 22% ...
1	H	108	 77% 20% ...

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Mol	Chain	Length	Quality of chain
2	I	149	
2	J	149	
2	K	149	
2	L	149	
3	A	4967	
3	B	4967	
3	C	4967	
3	D	4967	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 147868 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
2	J	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
2	K	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
2	L	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		

- Molecule 3 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
3	B	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
3	C	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
3	D	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		

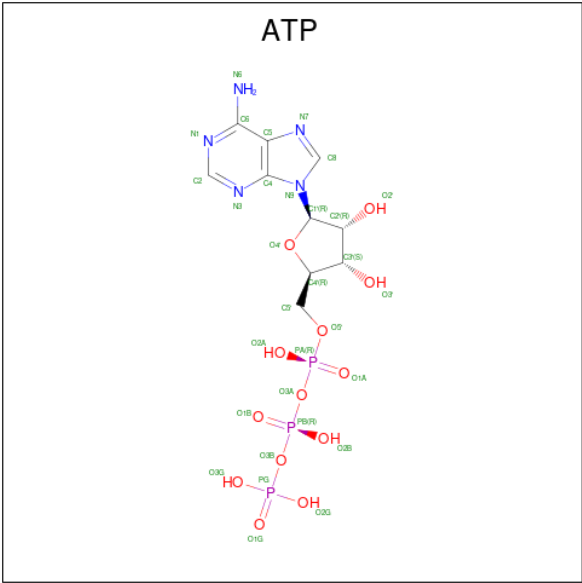
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



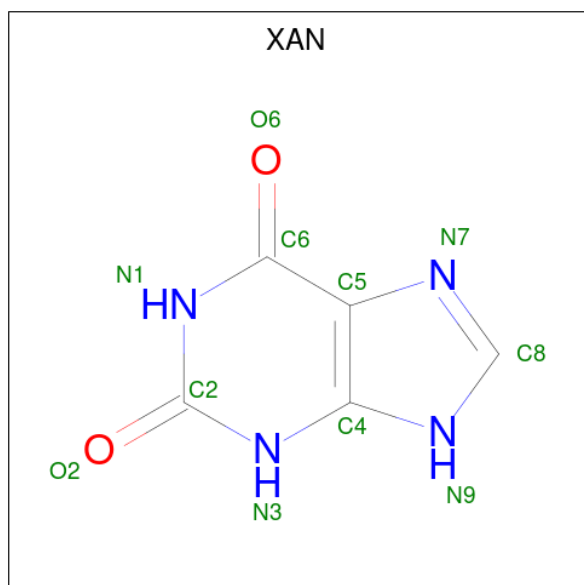
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Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is XANTHINE (CCD ID: XAN) (formula: C₅H₄N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			11	5	4	2	
7	B	1	Total	C	N	O	0
			11	5	4	2	
7	C	1	Total	C	N	O	0
			11	5	4	2	
7	D	1	Total	C	N	O	0
			11	5	4	2	

- Molecule 8 is water.

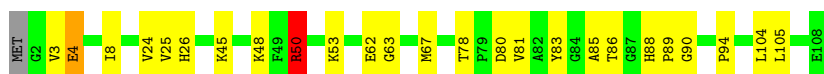
Mol	Chain	Residues	Atoms		AltConf
8	A	3	Total	O	0
			3	3	
8	B	3	Total	O	0
			3	3	
8	C	3	Total	O	0
			3	3	
8	D	3	Total	O	0
			3	3	

3 Residue-property plots [i](#)

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: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



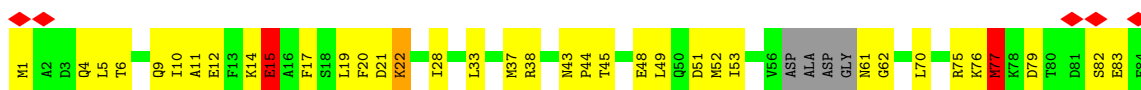
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

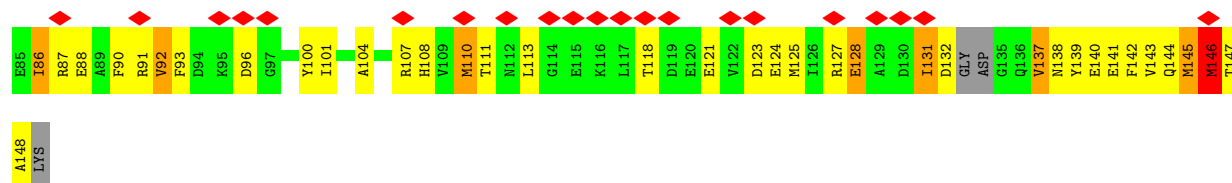
Chain H: 



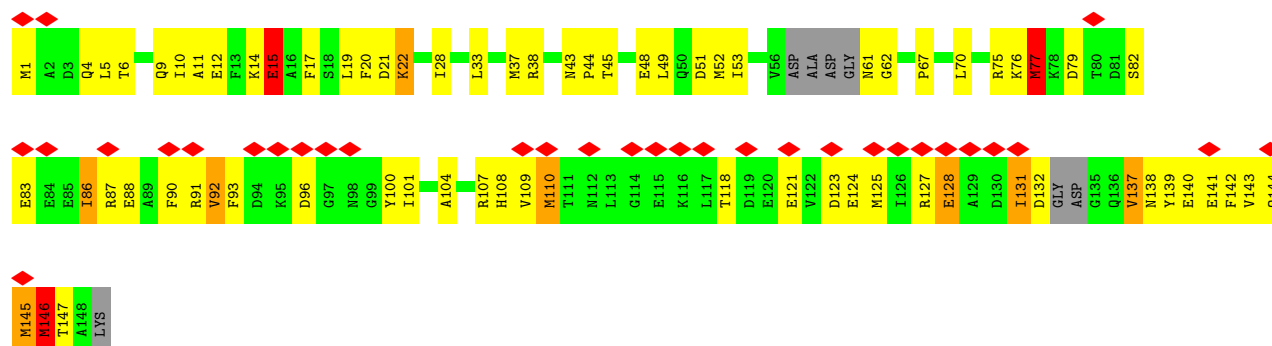
- Molecule 2: Calmodulin-1

Chain I: 

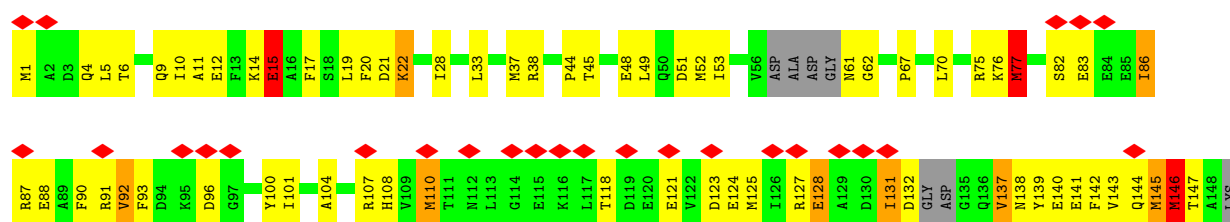




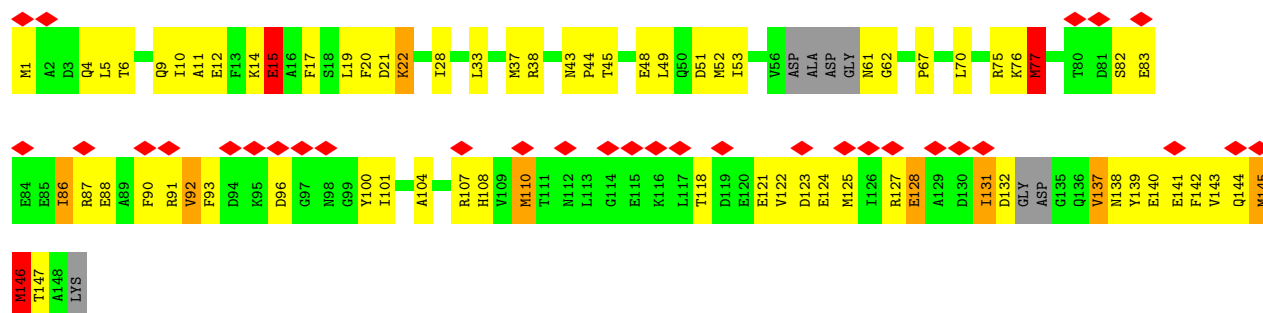
- Molecule 2: Calmodulin-1



- Molecule 2: Calmodulin-1

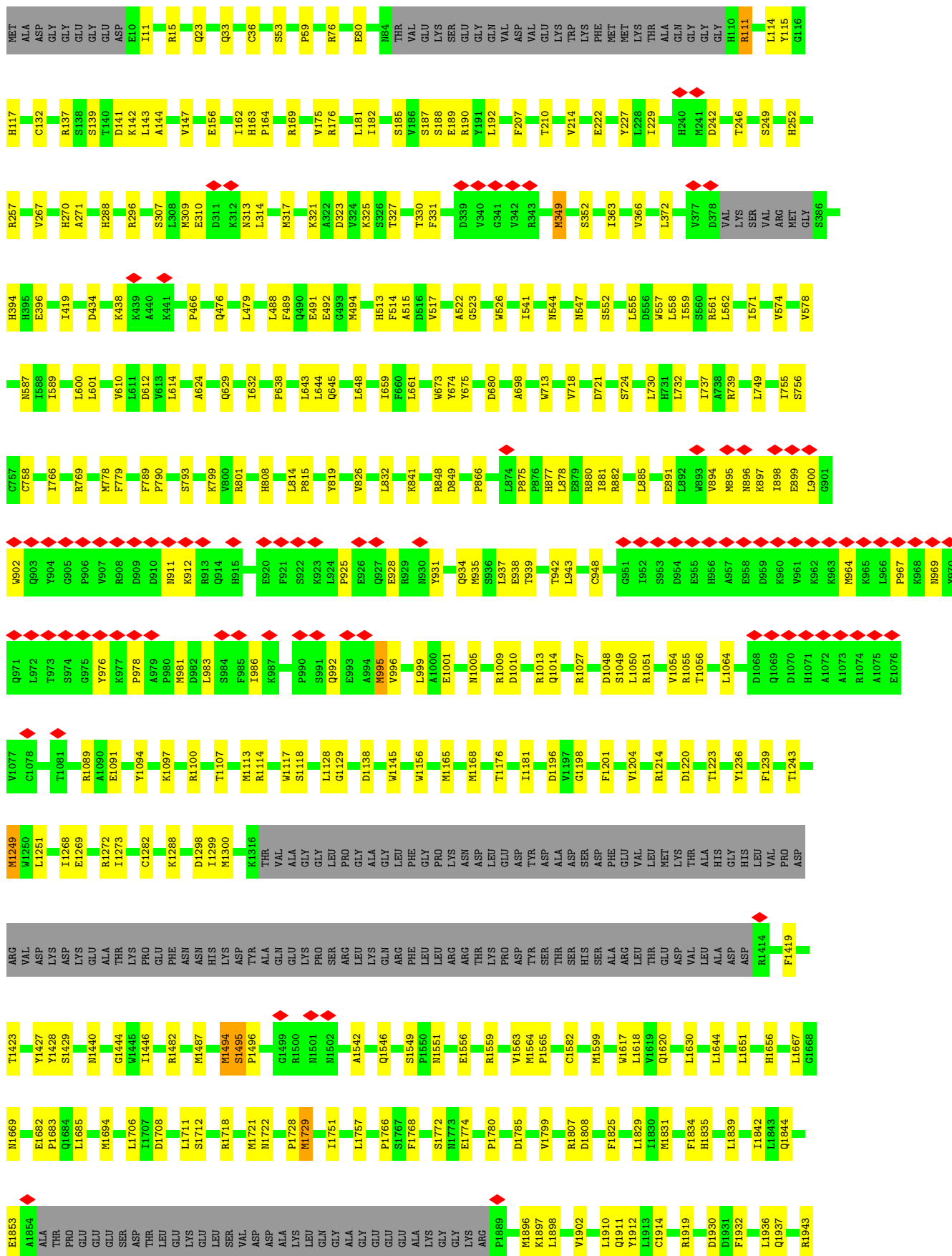


- Molecule 2: Calmodulin-1



- Molecule 3: Ryanodine receptor 2





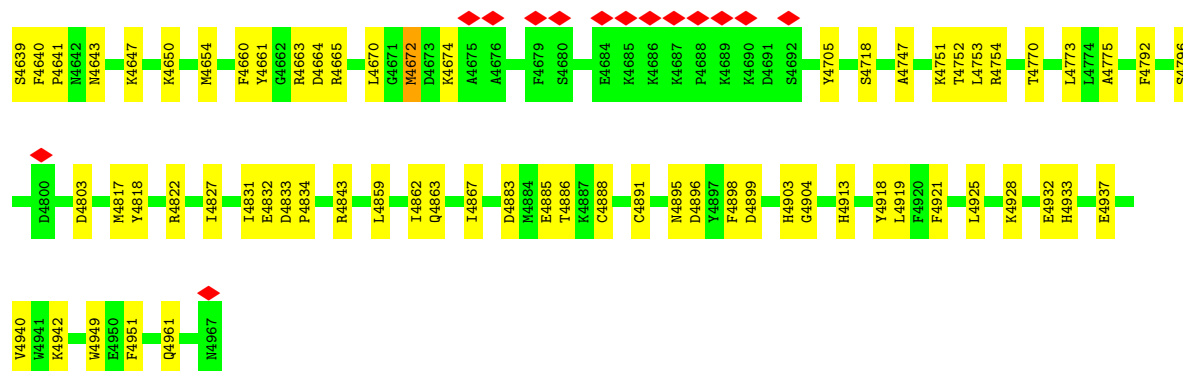




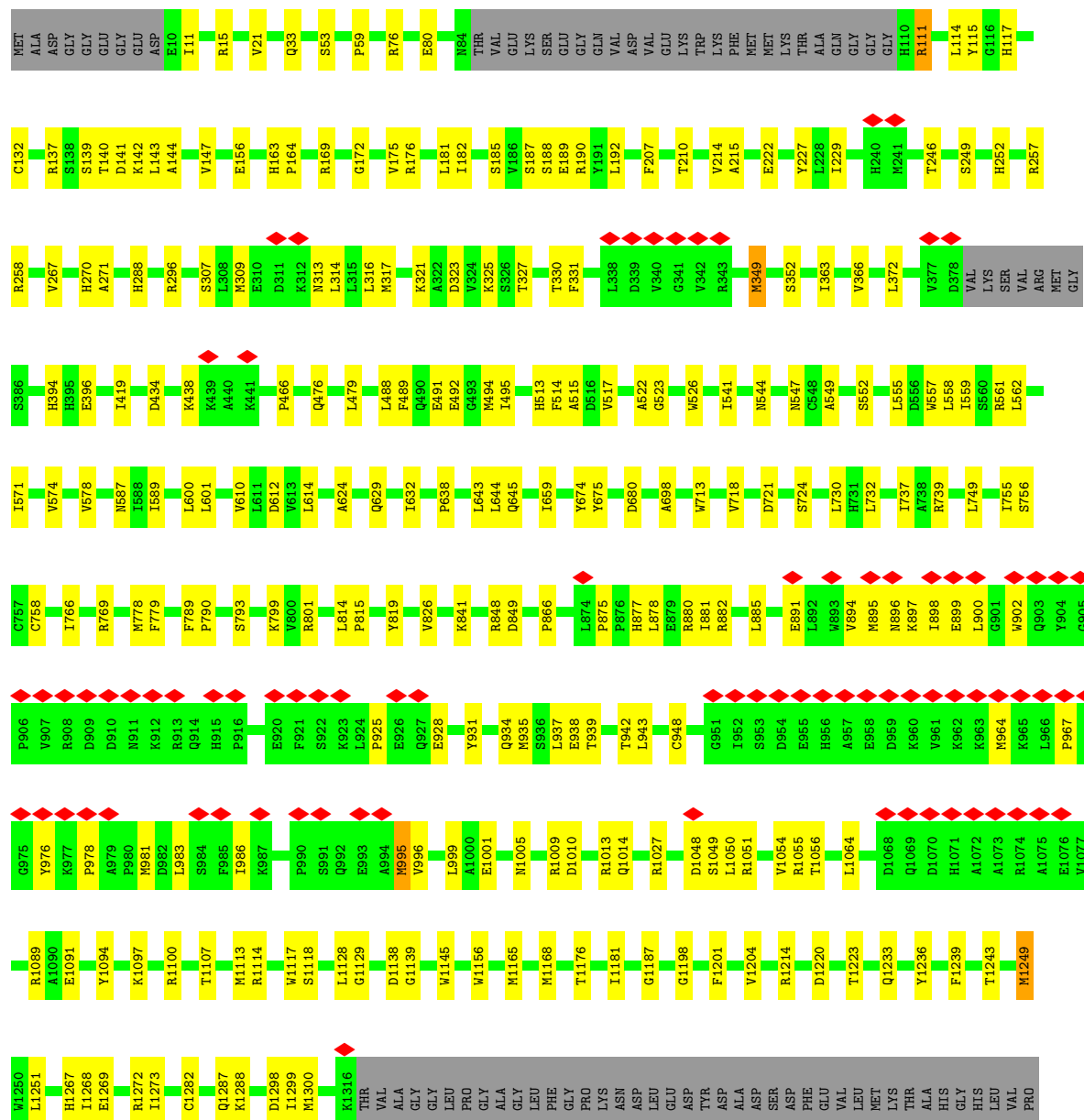


E3223	F3109	I2971	G2866	M2782	K2716	I2569	THR	Y2202	ALA	A1959	ASP	M1694
R3227	I3121	R2979	V2872	W2785	L2717	L2580	LEU	I2206	GLU	R1960	THR	L1706
M3231	I3122	R2981	G2786	W2787	F2720	P2581	ASP	Y2220	PRO	L1961	GLU	I1707
P3232	L3123	Y2981	R2787	R2788	L2721	R2582	GLU	L2221	VAL	D1708	LYS	D1708
H3233	E3124	R2988	L2877	I2789	W2722	S2583	GLU	L2222	GLU	F1965	GLU	L1711
V3234		P2989	K2884	I2789	K2723	M2584	SER	L2223	SER	R1966	LEU	L1966
M3235		L2990	E2887	T2792	K2724	R2590	ASP	M2224	ASP	S1967	SER	S1712
E3236	L3134	H2995	E2887	E2794	A2725	V2593	GLU			Q1972	VAL	R1718
V3237	A3139	V3015	E2887	E2794	E2726	V2593	GLU			I1973	ASP	M1721
I3238	L3140	F3022	V2802	E2794	D2730	V2593	GLU			M1974	ASP	M1722
L3242	S3145		ARG		D2730	V2593	GLU			L1975	LYS	M1722
M3246	V3148	D3025	THR		M2734	V2593	GLU			L1976	LEU	
R3247	E3149	D3025	ARG		D2735	V2593	GLU			F1979	GLN	M1729
W3249	R3150	Y3029	ARG		K2736	A2603	GLY			C1986	ALA	I1761
W3250	Q3151	I3029	ILE		L2737	M2605	GLY			P1987	GLY	I1761
N3256	Q3152	L3033	SER		A2738	P2606	GLU			P1987	GLU	P1766
L3268	R3153	L3033	GLN		K2739	L2607	GLU			C1988	GLU	S1767
N3269	H3034	V2903	THR		Y2743	L2610	GLU			P1989	GLU	F1768
S3270	S3153	R2903	SER		G2744	C2617	VAL			R1993	LYS	S1772
E3271	R2904	S2904	GLN		E2745	S2641	VAL			L1996	LYS	E1774
H3272	A3154	R2905	VAL		I2746	L2644	ALA			E2010	ARG	P1780
M3273	L3155	G2906	ASP		Y2747	F2645	ALA			LEU	ASP	P1889
N3274	G3037	K2908	ALA		D2749	L2655	ALA			GLU	ASP	I1792
T3275	Q3038	L2910	HIS		S2750	E2658	ALA			ASP	GLY	V1799
L3276	T3039	L2912			K2751	L2661	ALA			K1897	LEU	R1807
G3278	S2916	L2912			K2752	E2658	ALA			D1808	LEU	D1808
I3280	R2920	L2912			L2753	L2661	ALA			V1902	GLY	F1825
L3281	S2923	L2912			Q2754	A2665	ALA			L1910	GLY	L1829
I3284	L2929	L2912			P2755	V2672	ALA			Q1911	LYS	Q1911
I3290	L2934	L2912			L2756	L2676	ALA			Y1912	GLY	I1830
W3295	H2937	L2934			K2757	A2681	ALA			C1914	THR	M1831
M3296	Q2938	L2934			W2757	V2682	ALA			ILE	ILE	F1834
K3297	Y2939	L2934			K2758	F2682	ALA			ARG	ARG	H1835
L3299	I2940	L2934			P2759	S2683	ALA			D1930	ARG	D1838
I3307	G2945	L2934			Y2760	Y2685	ALA			F1932	LEU	L1839
N3308	G2946	L2934			L2761	M2688	ALA			L1936	SER	I1842
K3309	S2947	L2934			L2762	M2689	ALA			Q1937	VAL	L1843
P3312	R2949	L2934			L2763	E2690	ALA			R1943	GLY	Q1844
Q3313	G2949	L2934			S2764	K2691	ALA			E1946	THR	E1853
L3314	K2950	L2934			E2765	S2693	ALA			L1951	THR	A1854
L3315	G2951	L2934			K2766	S2697	ALA			N1952	GLU	PRO
K3316	E2952	L2934			L2767	E2698	ALA			A1955	GLU	GLU
F3319	E3220	L2934			L2768	G2699	ALA			T1958	GLN	SER
L3320	A3222	L2934			Y2769	T2708	ALA					
					L2781							

ALA	ILE	ASP	SER	SER	SER	HIS	ARG	ILE	14555	14565	14569	P4570	H4579	F4584	14587	G4588	Y4590	L4593	F4600	R4601	R4602	V4606	R4608	K4609	L4610	L4615	Y4616	14617	T4618	E4619	Q4620	P4621	S4622	E4623	D4624	D4625	T4626	R4627	R4632	L4633	V4634	14635	R4636	T4637	Q4638															
GLY	LYS	ASP	GLY	LYS	LYS	LYS	ASP	LYS	GLY	GLY	GLN	LYS	LEU	ARG	GLN	HIS	THR	ARG	GLY	PRO	GLY	VAL	PRO	SER	ALA	F4490	I4484	V4509	T4524	SER	VAL	VAL	GLY	LYS	GLY	GLY	GLY	PRO	THR	THR	ARG	SER	SER	SER	ASN															
LEU	LYS	ARG	GLY	GLY	GLY	GLY	GLN	VAL	LEU	SER	ASP	GLY	LEU	SER	ASP	LEU	ASN	VAL	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY															
LYS	ILE	LYS	VAL	ALA	LYS	ILE	PRO	ASP	PRO	THR	ASP	VAL	THR	ARG	GLY	GLY	GLY	ILE	PRO	PRO	THR	GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA														
LEU	LYS	ARG	GLY	GLY	GLY	ILE	PRO	HIS	ASN	PRO	ASN	ALA	GLY	SER	LEU	SER	GLY	VAL	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY															
L4066	E4074	L4078	D4079	E4082	A4091	T3874	K4092	D4093	E4107	H4108	M4109	T4113	Q4116	L4119	A4122	F4129	E4137	R4144	Y4149	S4155	Q4159	R4162	K4166	K4169	R4170	Q4171	F4172	V4176	Q4180	Q4181	E4182	M4186	E4187	L4188	F4189	V4190	N4191	T4196																						
Q3855	Q3861	T3867	V3868	T3872	S3873	T3874	V3875	S3884	W3890	Y3891	Y3892	D3899	L3920	I3924	Q3925	R3939	K3957	Q3975	V3979	K3997	L4014	M4019	L4023	L4026	T4027	S4028	K4033	K4040	K4045	M4052	E4053	Q4060	S4061	E4062	T4063	A4064	F4065																							
K3697	H3700	D3701	E3702	GLU	ASP	ASP	GLY	GLU	E3710	E3715	K3719	A3729	R3730	L3731	H3732	V3740	T3758	I3763	Q3774	L3778	A3794	L3803	D3804	R3810	G3818	M3819	V3820	T3821	E3822	E3823	G3824	S3825	V3829	D3832	F3835	D3838	L3839	F3840	F3854																					
PRO	GLN	ARG	SER	LYS	ALA	VAL	TRP	HIS	LYS	LEU	SER	LYS	Q3594	R3595	K3596	R3597	F3603	R3604	M3605	A3606	P3607	L3608	F3620	D3638	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	G3657	T3658	K3659	R3660	V3661	Q3666	E3678	E3684	D3685	F3686	L3687	Y3688	M3689	A3690	Y3691	M3695	A3696											
L3519	E3520	D3521	P3522	A3523	I3524	R3525	K3526	Q3527	M3528	A3529	L3530	Y3531	K3532	D3533	L3534	P3535	N3536	R3537	T3538	D3539	D3540	T3541	S3542	D3543	P3544	E3545	K3546	T3547	V3548	E3549	R3550	V3551	L3552	D3553	I3554	A3555	N3556	V3557	L3558	F3559	H3560	L3561	E3562	Q3563	K3564	SER	LYS	ARG	VAL	GLY	ARG	L3510	S3511	K3512	I3513	H3514	L3515	Q3516	G3517	K3518
Y3459	S3460	R3461	Q3462	T3463	S3464	L3465	V3466	V3467	A3468	A3469	L3470	K3471	R3472	L3473	L3474	P3475	I3476	Q3477	N3478	R3479	I3480	C3481	A3482	P3483	G3484	D3485	Q3486	E3487	L3488	I3489	A3490	L3491	A3492	K3493	N3494	R3495	F3496	S3497	L3498	K3499	D3500	T3501	E3502	D3503	E3504	V3505	R3506	D3507	I3508	I3509	K3510	S3511	K3512	I3513	H3514	L3515	Q3516	G3517	K3518	
V3399	A3400	E3401	V3402	F3403	I3404	Y3405	W3406	S3407	K3408	S3409	H3410	N3411	F3412	K3413	L3414	E3415	E3416	Q3417	N3418	F3419	V3420	V3421	Q3422	N3423	E3424	I3425	N3426	N3427	M3428	S3429	F3430	L3431	I3432	T3433	D3434	T3435	K3436	S3437	K3438	M3439	S3440	LYS	ALA	ALA	VAL	SER	GLN	GLU	ARG	LYS	LYS	MET	LYS	R3454	K3455	G3456	D3457	R3458		
P3321	L3322	M3323	E3324	K3325	L3326	K3327	A3331	T3332	V3333	S3334	E3335	E3336	E3337	D3338	H3339	L3340	K3341	A3342	E3343	F3344	R3345	G3346	H3347	N3348	S3349	E3350	A3351	E3352	L3353	I3354	L3366	V3370	F3371	L3372	L3373	L3374	R3375	F3376	V3377	D3378	Y3379	R3380	R3381	K3386	E3387	P3388	N3389	E3393	E3394	L3395	F3396	R3397	K3398							



• Molecule 3: Ryanodine receptor 2



G2946	H2849	L2770	L2527	S2358	G2182	LYS	Q1844	H1856	F1419	ASP
S2947	K2856	Y2771	H2541	P2364	E2183	VAL	E1853	L1867	T1423	ARG
R2948	K2857	W2772	I2545	ASN	I2187	THR	A1854	G1868	Y1427	ASP
G2949	K2858	W2773	I2545	GLY	M2192	LEU	ALA	N1669	Y1428	LYS
K2950	E2859	L2774	L2548	SER	M2193	LYS	THR	E1882	S1429	GLY
G2951	L2860	K2776	L2548	SER	V2199	LYS	GLU	P1683	G1435	ALA
E2952	E2777	S2777	S2556	LYS	F2199	GLN	GLU	L1685	N1440	THR
Q2958	K2863	S2778	S2560	THR	Y2202	ALA	SER	L1706	G1444	PRO
L2968	G2864	L2779	L2561	LEU	I2206	LYS	ASP	I1707	W1445	GLU
P2969	G2865	K2781	L2561	ASP	Y2220	VAL	THR	D1708	I1446	PHE
L2970	G2866	M2782	Q2565	THR	F1961	GLU	GLU	L1711	R1482	ASN
I2971	V2872	K2716	R2566	GLU	T1962	SER	LYS	S1712	M1487	LYS
R2979	P2873	L2717	I2569	E2377	F1865	ASP	LEU	R1718	M1494	TYR
L2980	L2877	F2720	L2580	E2378	R1966	SER	SER	M1721	S1495	ALA
Y2981	K2884	N2721	R2581	D2380	S1967	VAL	ASP	N1722	P1496	GLN
R2988	E2887	K2723	S2583	I2388	Q1972	ASP	ALA	M1729	G1499	LYS
P2989	L2893	Y2724	M2584	M2389	I1973	LYS	LYS	I1751	R1500	PRO
L2990	E2794	A2725	R2590	T2390	M1975	LEU	LEU	P1766	ARG	SER
H2995	W2802	E2730	V2593	E2405	L1976	GLY	GLY	F1767	LEU	LEU
K2999	THR	K2734	V2596	H2407	F1979	ALA	ALA	F1768	GLN	GLN
V3015	ARG	K2735	V2596	L2408	C1986	GLY	GLY	S1772	ARG	ARG
F3022	SER	L2737	A2603	E2415	D2077	GLU	GLU	E1774	P1550	ARG
A2902	GLN	A2738	K2604	I2422	R2082	GLU	GLU	P1780	N1551	THR
V2903	THR	N2739	M2605	L2426	L2087	ALA	ALA	D1785	E1586	LYS
S2904	SER	Y2743	P2606	S2425	R2090	LYS	LYS	I1792	R1559	PRO
R2905	GLN	G2744	L2607	L2435	Q2091	ARG	ARG	V1799	V1563	ASP
G2906	VAL	Z2745	L2610	V2436	R2133	GLY	GLY	R1807	M1564	THR
F2907	SER	E2746	C2617	I2436	E2139	GLY	M1896	D1808	P1585	HIS
K2908	ASP	Y2747	S2641	I2478	M2142	GLY	K1897	F1825	C1582	SER
L2910	ALA	S2748	L2644	D2482	M2150	ASP	L1898	L1829	M1599	ALA
E2911	HIS	D2749	K2655	F2483	K2153	ASP	V1902	I1830	W1617	LEU
L2912	G2890	S2750	E2658	H2486	R2154	THR	L1910	M1831	L1618	GLU
S2916	P2893	K2751	L2658	L2487	ILE	ILE	Q1911	F1834	Q1620	ASP
I2917	R2894	Q2754	L2661	L2488	M2158	ARG	Y1912	H1835	ALA	ALA
R2920	A2895	P2755	A2685	E2489	V2171	LEU	L1913	D1838	L1630	ARG
Y2923	L2826	L2756	L2676	V2490	V2174	LEU	C1914	L1839	L1644	THR
L2929	M2828	K2757	M2681	G2491	M2175	GLY	R1919	I1842	L1651	GLU
E3073	S2829	P2759	F2681	L2496	V2176	SER	D1930	L1936		
K3070	N2830	Y2760	S2508	S2508	G2332	LEU	F1932	Q1937		
T3071	S2834	K2761	L2762	S2512	R2336	LEU	L1936			
K3072	L2837	L2763	S2683	M2512	L2344	LEU				
E3073	H2838	S2764	R2684	L2520		VAL				
K3076	Y2939	E2765	Y2685			GLU				
Q3077	I2940	K2766	E2767							
F3080	F3081	HIS	THR							
T3081										
THR										







LEU	L2969	L3094	V3204	K3309	K3386	GLU	I3508	P3685	D3832	F4065	A4203	LEU
LYS	L2970	A3100	L3214	P3312	E3387	ARG	I3509	F3686	F3832	L4066	A4206	VAL
GLN	I2971	A3101	M3215	Q3313	P3388	LYS	R3510	L3687	F3835	F4074	I4206	ASN
MET	R2979	L3102	M3215	L3314	N3389	LYS	S3511	M3689	D3838	L4078	S4209	LEU
LYS	L2980	P3103	M3215	L3315	K3316		R3512	A3690	L3839	D4079	ASP	LEU
VAL	Y2981	M3104	V3219	K3316		R3454	I3513	Y3691	F3840		ASP	LEU
VAL	S2984	F3109	E3220	L3320	E3393	K3455	H3514	M3695	F3854	E4082	ASN	ASN
LYS	R2988	L3121	A3222	P3321	E3394	G3456	L3515	A3696	F3854	A4091	GLU	ASN
THR	L2876	L3122	A3222	M3323	F3396	D3457	L3616	K3697	Q3861	K4092	ARG	ARG
VAL	L2877	L3123	A3223	R3397	F3397	R3458	G3517	M3398		D4093	SER	SER
LYS	K2884	E3124	R3227	E3324	V3399	R3459	K3518	V3399			ALA	ALA
ASP			M3231	K3325	A3400	Y3460	K3518	A3400	T3867	E4107	ASN	ASN
LYS	H2995	Q3127	P3232	L3326	A3401	S3461	L3519	E3702	V3868	E4107	LYS	LYS
MET	K2999	L3134	P3232	K3327	E3401	Q3462	E3520	GLU		H4108	GLU	GLU
THR	E3000	L3134	H3233	K3328	V3402	ASP	E3520	ASP	I3872	M4109	SER	SER
ALA	K3001	L3139	V3234	K3329	F3403	T3463	D3521	ASP	T3873		GLU	GLU
PHE	L2896	L3140	M3235	A3330	F3404	S3464	P3522	ASP	T3874	T4113	GLU	GLU
ALA	L2897	L3140	E3236	A3331	Y3405	G3465	A3523	GLY	V3875		LYS	LYS
SER	L2898	S3145	V3237	T3332	H3406	I3466	I3524	GLU		Q4116	GLU	GLU
THR			I3238	V3333	S3407	F3467	R3525	GLU	S3884	L4119	ARG	ARG
TRP			L3242	V3334	K3408	A3468	W3526	LEU	Y3892		GLU	GLU
SER			M3246	S3335	S3409	A3469	Q3527	SER		A4122	GLU	GLU
ILE			E3337	E3336	H3410	L3470	M3528	LYS	D3899	F4129	GLN	GLN
PHE			S3247	D3338	F3411	K3471	R3529	GLY	L3920		GLY	GLY
THR			R3248	H3339	F3412	R3472	A3596	PRO		E4137	PRO	PRO
THR			W3250	H3339	K3413	L3473	L3530	ARG	I3924		ARG	ARG
LEU			N3256	K3341	R3414	L3474	Y3531	MET		R4144	MET	MET
LEU			L3268	A3342	E3415	P3475	K3532	ALA	K3957		ALA	ALA
HIS			N3269	E3343	E3416	I3476	D3533	PHE	K3997	Y4149	PHE	PHE
PHE			E3157	A3344	Q3417	G3477	L3534	ILE		S4155	SER	SER
VAL			E3270	E3345	N3418	L3478	P3535	ALA	L4014		LEU	LEU
SER			K3271	R3345	F3419	N3479	R3536	THR	M4019	Q4159	THR	THR
VAL			H3272	G3346	V3420	I3480	R3537	VAL		K4162	VAL	VAL
PHE			N3273	D3347	V3421	C3481	T3538	ARG	L4023	K4166	ARG	ARG
GLY			N3274	M3348	Q3422	A3482	D3539	GLY	L4026		ALA	ALA
PHE			T3275	S3349	E3424	P3483	D3540	LEU	T4027	L4026	LEU	LEU
ARG			L3276	E3350	E3425	G3484	T3541	PHE	S4028	A4169	PHE	PHE
ILE			G3278	A3351	N3426	D3485	S3542	ALA		R4170	ALA	ALA
ILE			N3279	E3352	Q3427	Q3486	S3542	LEU	K4033	Q4171	LEU	LEU
CYS			L3280	L3353	M3428	E3487	D3543	ARG		F4172	ARG	ARG
SER			L3281	L3354	N3428	L3488	F3544	E3653	G4039	V4176	TYR	TYR
LEU			I3284	I3355	S3429	I3489	E3545	E3654	K4040		ASN	ASN
LEU			I3290	L3366	F3430	A3490	K3546	D3655	K4045		LEU	LEU
GLY			W3295	Y3370	L3431	L3491	T3547	E3656		G4181	LEU	LEU
SER			M3296	P3371	I3432	A3492	V3548	C3657	K3819	E4182	GLY	GLY
LEU			K3297	L3372	T3433	K3493	E3549	T3658	M4052	K4183	MET	MET
VAL			E3298	L3373	D3434	K3493	R3550	R3659	E4053	M4186	ARG	ARG
GLU			L3299	I3374	T3435	N3494	V3551	K3660	Q4060	E4187	LEU	LEU
GLY			I3307	K3375	K3436	R3495	L3552	V3661	S4061	L4188	LEU	LEU
ALA			N3308	F3376	S3437	F3496	D3553	Q3666	F4189	F4189	SER	SER
				V3377	K3438	S3497	I3554		V4190	V4190	LYS	LYS
				D3378	M3439	L3498	A3555	E3678	T4196			
				Y3379	K3499	K3499	N3556	E3684				
				R3381	S3440	D3500	V3557					
				ALA	ALA	T3501	L3558					
				VAL	VAL	E3502	F3559					
				SER	SER	D3503	H3560					
				ASP	ASP	E3504	H3561					
				GLN	GLN	R3505	E3562					
						R3506	Q3563					
						D3507	K3564					
							SER					
							LYS					
							ARG					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102257	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.728	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.16	0/834	0.46	2/1123 (0.2%)
1	F	0.16	0/834	0.46	2/1123 (0.2%)
1	G	0.16	0/834	0.46	2/1123 (0.2%)
1	H	0.16	0/834	0.46	2/1123 (0.2%)
2	I	0.31	0/1122	0.79	4/1504 (0.3%)
2	J	0.31	0/1122	0.79	4/1504 (0.3%)
2	K	0.31	0/1122	0.79	4/1504 (0.3%)
2	L	0.32	0/1122	0.79	4/1504 (0.3%)
3	A	0.16	0/35720	0.37	7/48254 (0.0%)
3	B	0.16	0/35720	0.37	5/48254 (0.0%)
3	C	0.16	0/35720	0.37	7/48254 (0.0%)
3	D	0.16	0/35720	0.37	5/48254 (0.0%)
All	All	0.17	0/150704	0.39	48/203524 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	2
3	B	0	2
3	C	0	2
3	D	0	2
All	All	0	8

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	77	MET	CB-CG-SD	8.34	137.71	112.70
2	K	77	MET	CB-CG-SD	8.34	137.72	112.70
2	L	77	MET	CB-CG-SD	8.33	137.69	112.70
2	I	77	MET	CB-CG-SD	8.33	137.68	112.70
3	C	1729	MET	CB-CG-SD	-8.22	88.05	112.70
3	A	1729	MET	CB-CG-SD	-8.21	88.08	112.70
3	B	1729	MET	CB-CG-SD	-8.21	88.08	112.70
3	D	1729	MET	CB-CG-SD	-8.20	88.11	112.70
2	L	15	GLU	CA-CB-CG	7.60	129.30	114.10
2	I	15	GLU	CA-CB-CG	7.59	129.27	114.10
2	J	15	GLU	CA-CB-CG	7.58	129.25	114.10
2	K	15	GLU	CA-CB-CG	7.57	129.24	114.10
3	B	3461	MET	CB-CG-SD	6.54	132.32	112.70
3	A	3461	MET	CB-CG-SD	6.53	132.27	112.70
3	C	3461	MET	CB-CG-SD	6.53	132.28	112.70
3	D	3461	MET	CB-CG-SD	6.52	132.27	112.70
2	L	146	MET	CB-CG-SD	6.47	132.12	112.70
2	J	146	MET	CB-CG-SD	6.46	132.08	112.70
2	K	146	MET	CB-CG-SD	6.46	132.07	112.70
2	I	146	MET	CB-CG-SD	6.46	132.06	112.70
1	E	4	GLU	CA-CB-CG	6.20	126.50	114.10
1	H	4	GLU	CA-CB-CG	6.20	126.50	114.10
1	F	4	GLU	CA-CB-CG	6.19	126.49	114.10
1	G	4	GLU	CA-CB-CG	6.17	126.45	114.10
1	H	50	ARG	CG-CD-NE	5.84	124.85	112.00
1	F	50	ARG	CG-CD-NE	5.84	124.84	112.00
1	E	50	ARG	CG-CD-NE	5.83	124.82	112.00
1	G	50	ARG	CG-CD-NE	5.82	124.80	112.00
2	J	15	GLU	N-CA-CB	5.82	118.77	110.16
2	I	15	GLU	N-CA-CB	5.80	118.74	110.16
2	K	15	GLU	N-CA-CB	5.80	118.74	110.16
2	L	15	GLU	N-CA-CB	5.78	118.71	110.16
3	D	3231	MET	CB-CG-SD	5.45	129.05	112.70
3	A	3231	MET	CB-CG-SD	5.45	129.04	112.70
3	C	3231	MET	CB-CG-SD	5.44	129.03	112.70
3	B	3231	MET	CB-CG-SD	5.44	129.01	112.70
3	D	3231	MET	CA-CB-CG	5.29	124.68	114.10
3	B	3231	MET	CA-CB-CG	5.28	124.66	114.10
3	A	3231	MET	CA-CB-CG	5.28	124.65	114.10
3	C	3231	MET	CA-CB-CG	5.26	124.62	114.10
3	A	3461	MET	CA-CB-CG	5.24	124.58	114.10
3	C	3461	MET	CA-CB-CG	5.24	124.57	114.10
3	D	3461	MET	CA-CB-CG	5.23	124.56	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3461	MET	CA-CB-CG	5.22	124.54	114.10
3	C	3527	GLN	CA-C-N	-5.01	112.37	121.14
3	C	3527	GLN	C-N-CA	-5.01	112.37	121.14
3	A	3527	GLN	CA-C-N	-5.00	112.39	121.14
3	A	3527	GLN	C-N-CA	-5.00	112.39	121.14

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	3190	ARG	Sidechain
3	A	3381	ARG	Sidechain
3	B	3190	ARG	Sidechain
3	B	3381	ARG	Sidechain
3	C	3190	ARG	Sidechain
3	C	3381	ARG	Sidechain
3	D	3190	ARG	Sidechain
3	D	3381	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	818	0	821	17	0
1	F	818	0	821	15	0
1	G	818	0	821	18	0
1	H	818	0	821	15	0
2	I	1112	0	1053	92	0
2	J	1112	0	1053	78	0
2	K	1112	0	1053	79	0
2	L	1112	0	1053	80	0
3	A	34959	0	34588	673	0
3	B	34959	0	34588	667	0
3	C	34959	0	34588	682	0
3	D	34959	0	34588	669	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	62	0	24	4	0
5	B	62	0	24	4	0
5	C	62	0	24	4	0
5	D	62	0	24	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	11	0	4	0	0
7	B	11	0	4	0	0
7	C	11	0	4	0	0
7	D	11	0	4	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	3	0	0	0	0
All	All	147868	0	145960	3014	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 10.

All (3014) 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)
2:L:128:GLU:CB	2:L:131:ILE:CD1	1.83	1.57
2:L:128:GLU:HB3	2:L:131:ILE:CD1	1.11	1.56
2:J:128:GLU:HB3	2:J:131:ILE:CD1	1.11	1.55
2:I:128:GLU:HB3	2:I:131:ILE:CD1	1.11	1.54
2:K:128:GLU:HB3	2:K:131:ILE:CD1	1.11	1.54
2:K:128:GLU:CB	2:K:131:ILE:CD1	1.83	1.54
2:I:128:GLU:CB	2:I:131:ILE:CD1	1.83	1.51
2:J:128:GLU:CB	2:J:131:ILE:CD1	1.83	1.50
3:C:3427:ASN:CB	3:C:3463:THR:HB	1.49	1.43
3:D:3427:ASN:CB	3:D:3463:THR:HB	1.48	1.43
3:A:3427:ASN:CB	3:A:3463:THR:HB	1.49	1.41
3:B:3427:ASN:CB	3:B:3463:THR:HB	1.48	1.41
3:B:3375:ARG:NH2	3:B:3437:SER:OG	1.56	1.37
3:B:3427:ASN:CG	3:B:3463:THR:O	1.68	1.37
3:D:3427:ASN:CG	3:D:3463:THR:O	1.68	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3427:ASN:CG	3:A:3463:THR:O	1.68	1.34
3:C:3427:ASN:CG	3:C:3463:THR:O	1.68	1.33
3:D:3375:ARG:NH2	3:D:3437:SER:OG	1.56	1.33
3:A:3375:ARG:NH2	3:A:3437:SER:OG	1.56	1.33
3:C:3375:ARG:NH2	3:C:3437:SER:OG	1.56	1.33
3:D:3427:ASN:CB	3:D:3463:THR:CB	2.22	1.18
3:C:3427:ASN:CB	3:C:3463:THR:CB	2.22	1.17
3:B:3427:ASN:ND2	3:B:3463:THR:O	1.77	1.16
3:C:3427:ASN:ND2	3:C:3463:THR:O	1.77	1.16
3:D:3427:ASN:ND2	3:D:3463:THR:O	1.77	1.16
3:A:3427:ASN:CB	3:A:3463:THR:CB	2.22	1.16
3:A:3427:ASN:ND2	3:A:3463:THR:O	1.77	1.15
3:B:3427:ASN:CB	3:B:3463:THR:CB	2.22	1.15
3:D:3427:ASN:HB2	3:D:3463:THR:CB	1.76	1.14
3:A:3427:ASN:HB2	3:A:3463:THR:CB	1.76	1.14
3:B:3427:ASN:HB2	3:B:3463:THR:CB	1.76	1.14
3:C:3427:ASN:HB2	3:C:3463:THR:CB	1.76	1.13
2:K:128:GLU:CB	2:K:131:ILE:HD12	1.63	1.09
3:B:3423:ASN:O	3:B:3425:ILE:HD12	1.55	1.07
3:C:3423:ASN:O	3:C:3425:ILE:HD12	1.55	1.07
2:L:128:GLU:CB	2:L:131:ILE:HD12	1.63	1.06
3:A:3423:ASN:O	3:A:3425:ILE:HD12	1.54	1.06
2:L:128:GLU:HB3	2:L:131:ILE:HD13	1.07	1.06
2:K:128:GLU:HB3	2:K:131:ILE:HD13	1.07	1.06
2:J:132:ASP:O	2:J:137:VAL:HG21	1.56	1.05
2:I:128:GLU:CB	2:I:131:ILE:HD12	1.63	1.05
3:D:3423:ASN:O	3:D:3425:ILE:HD12	1.54	1.05
2:J:128:GLU:HB3	2:J:131:ILE:HD13	1.07	1.04
2:I:128:GLU:HB3	2:I:131:ILE:HD13	1.07	1.04
2:I:132:ASP:O	2:I:137:VAL:HG21	1.56	1.04
2:J:128:GLU:CB	2:J:131:ILE:HD12	1.63	1.04
2:K:132:ASP:O	2:K:137:VAL:HG21	1.56	1.04
3:C:3375:ARG:CZ	3:C:3437:SER:OG	2.06	1.03
3:B:3375:ARG:CZ	3:B:3437:SER:OG	2.06	1.03
2:L:132:ASP:O	2:L:137:VAL:HG21	1.56	1.02
2:I:128:GLU:CG	2:I:131:ILE:CD1	2.37	1.02
2:J:128:GLU:CG	2:J:131:ILE:CD1	2.37	1.02
3:D:3375:ARG:CZ	3:D:3437:SER:OG	2.06	1.02
3:A:3375:ARG:CZ	3:A:3437:SER:OG	2.06	1.02
2:K:128:GLU:CB	2:K:131:ILE:HD11	1.90	1.01
3:D:3427:ASN:HB2	3:D:3463:THR:OG1	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:146:MET:CE	3:A:3596:LYS:HB2	1.91	1.01
2:L:128:GLU:CB	2:L:131:ILE:HD11	1.90	1.01
2:L:128:GLU:CG	2:L:131:ILE:CD1	2.37	1.01
3:C:3427:ASN:HB2	3:C:3463:THR:OG1	1.59	1.01
2:J:128:GLU:CB	2:J:131:ILE:HD11	1.90	1.01
2:K:128:GLU:CG	2:K:131:ILE:CD1	2.37	1.01
3:B:3427:ASN:HB2	3:B:3463:THR:OG1	1.59	1.00
3:B:3427:ASN:HB3	3:B:3463:THR:HB	1.01	1.00
3:A:3427:ASN:HB2	3:A:3463:THR:OG1	1.59	1.00
3:A:3427:ASN:HB3	3:A:3463:THR:HB	1.01	1.00
3:D:3427:ASN:HB3	3:D:3463:THR:HB	1.01	0.98
2:I:128:GLU:CB	2:I:131:ILE:HD11	1.90	0.98
2:I:146:MET:HE1	3:A:3596:LYS:HB2	1.41	0.98
3:C:3427:ASN:ND2	3:C:3463:THR:C	2.23	0.97
3:B:3427:ASN:ND2	3:B:3463:THR:C	2.23	0.97
3:A:3427:ASN:ND2	3:A:3463:THR:C	2.23	0.97
2:L:132:ASP:O	2:L:137:VAL:CG2	2.13	0.96
3:D:3427:ASN:ND2	3:D:3463:THR:C	2.23	0.96
2:K:132:ASP:O	2:K:137:VAL:CG2	2.13	0.96
3:C:3427:ASN:HB3	3:C:3463:THR:HB	1.01	0.96
2:J:132:ASP:O	2:J:137:VAL:CG2	2.13	0.95
2:I:132:ASP:O	2:I:137:VAL:CG2	2.13	0.95
3:C:3427:ASN:HB3	3:C:3463:THR:CB	1.93	0.94
2:I:108:HIS:HB3	3:A:1959:ALA:HB2	1.48	0.93
2:J:128:GLU:HB3	2:J:131:ILE:HD12	0.93	0.93
2:K:128:GLU:HB3	2:K:131:ILE:HD12	0.93	0.93
2:I:132:ASP:C	2:I:137:VAL:CG2	2.43	0.92
2:J:132:ASP:C	2:J:137:VAL:CG2	2.43	0.92
2:K:132:ASP:C	2:K:137:VAL:CG2	2.43	0.92
2:I:128:GLU:HB3	2:I:131:ILE:HD12	0.93	0.92
2:J:128:GLU:CA	2:J:131:ILE:HD12	2.00	0.91
2:L:132:ASP:C	2:L:137:VAL:CG2	2.43	0.91
2:I:128:GLU:CA	2:I:131:ILE:HD12	2.00	0.91
2:L:128:GLU:HB3	2:L:131:ILE:HD12	0.93	0.91
3:C:3650:GLU:HG2	3:C:3651:PRO:HD3	1.53	0.90
3:A:3650:GLU:HG2	3:A:3651:PRO:HD3	1.53	0.90
3:C:3509:ILE:HD12	3:C:3552:LEU:HD21	1.54	0.90
2:K:128:GLU:CA	2:K:131:ILE:HD12	2.01	0.90
2:L:128:GLU:CG	2:L:131:ILE:HD11	2.02	0.90
3:A:3509:ILE:HD12	3:A:3552:LEU:HD21	1.54	0.90
3:B:3650:GLU:HG2	3:B:3651:PRO:HD3	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3650:GLU:HG2	3:D:3651:PRO:HD3	1.53	0.90
2:J:128:GLU:CG	2:J:131:ILE:HD11	2.01	0.90
3:D:3509:ILE:HD12	3:D:3552:LEU:HD21	1.54	0.90
3:D:3427:ASN:HB3	3:D:3463:THR:CB	1.93	0.89
2:L:128:GLU:CA	2:L:131:ILE:HD12	2.00	0.89
3:B:3509:ILE:HD12	3:B:3552:LEU:HD21	1.54	0.89
2:K:128:GLU:CG	2:K:131:ILE:HD11	2.02	0.88
2:K:128:GLU:CA	2:K:131:ILE:CD1	2.52	0.88
2:I:128:GLU:CA	2:I:131:ILE:CD1	2.52	0.87
2:J:128:GLU:CA	2:J:131:ILE:CD1	2.52	0.87
2:L:128:GLU:CA	2:L:131:ILE:CD1	2.52	0.87
3:A:3427:ASN:HB3	3:A:3463:THR:CB	1.93	0.87
2:I:128:GLU:CG	2:I:131:ILE:HD13	2.05	0.85
3:B:3427:ASN:HB3	3:B:3463:THR:CB	1.93	0.85
2:I:128:GLU:CG	2:I:131:ILE:HD11	2.01	0.84
2:L:128:GLU:CG	2:L:131:ILE:HD13	2.05	0.84
2:L:128:GLU:CB	2:L:131:ILE:HD13	1.75	0.84
3:D:3378:ASP:OD2	3:D:3434:ASP:OD2	1.96	0.83
3:D:3427:ASN:HB2	3:D:3463:THR:HB	1.38	0.83
3:B:3378:ASP:OD2	3:B:3434:ASP:OD2	1.96	0.83
3:A:3378:ASP:OD2	3:A:3434:ASP:OD2	1.96	0.83
2:J:128:GLU:CG	2:J:131:ILE:HD13	2.05	0.83
2:K:128:GLU:CG	2:K:131:ILE:HD13	2.05	0.83
3:B:2830:ASN:HD22	3:C:1435:GLY:HA2	1.44	0.83
3:C:3378:ASP:OD2	3:C:3434:ASP:OD2	1.96	0.83
3:B:943:LEU:HD21	3:B:999:LEU:HD22	1.62	0.82
3:A:943:LEU:HD21	3:A:999:LEU:HD22	1.62	0.82
3:A:2688:MET:HE1	3:A:2907:PHE:HB3	1.61	0.82
2:I:108:HIS:HE1	3:A:1956:ALA:HA	1.45	0.82
3:C:4834:PRO:HB3	3:C:4843:ARG:HD3	1.62	0.82
3:A:4834:PRO:HB3	3:A:4843:ARG:HD3	1.62	0.81
3:C:2688:MET:HE1	3:C:2907:PHE:HB3	1.61	0.81
3:C:3427:ASN:HB2	3:C:3463:THR:HB	1.38	0.81
3:C:3595:ARG:HA	3:C:3818:GLY:HA3	1.62	0.81
2:K:128:GLU:CB	2:K:131:ILE:HD13	1.75	0.81
3:D:2688:MET:HE1	3:D:2907:PHE:HB3	1.61	0.81
3:B:4834:PRO:HB3	3:B:4843:ARG:HD3	1.62	0.81
3:C:943:LEU:HD21	3:C:999:LEU:HD22	1.62	0.81
2:I:128:GLU:CB	2:I:131:ILE:HD13	1.75	0.81
3:D:3595:ARG:HA	3:D:3818:GLY:HA3	1.62	0.81
3:D:4834:PRO:HB3	3:D:4843:ARG:HD3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:943:LEU:HD21	3:D:999:LEU:HD22	1.62	0.80
3:B:3397:ARG:HH21	3:B:3550:ARG:HD2	1.47	0.80
3:D:3397:ARG:HH21	3:D:3550:ARG:HD2	1.47	0.80
3:B:3595:ARG:HA	3:B:3818:GLY:HA3	1.62	0.80
3:B:2688:MET:HE1	3:B:2907:PHE:HB3	1.61	0.80
3:A:3397:ARG:HH21	3:A:3550:ARG:HD2	1.47	0.80
3:A:3595:ARG:HA	3:A:3818:GLY:HA3	1.62	0.80
3:A:996:VAL:HG13	3:A:1050:LEU:HD22	1.64	0.79
3:C:3397:ARG:HH21	3:C:3550:ARG:HD2	1.47	0.79
3:D:996:VAL:HG13	3:D:1050:LEU:HD22	1.64	0.79
3:C:996:VAL:HG13	3:C:1050:LEU:HD22	1.64	0.79
2:L:128:GLU:C	2:L:131:ILE:HD12	2.09	0.78
2:K:128:GLU:HG2	2:K:131:ILE:HD13	1.66	0.78
2:K:128:GLU:O	2:K:131:ILE:HD12	1.84	0.77
2:J:128:GLU:CB	2:J:131:ILE:HD13	1.75	0.77
2:K:128:GLU:C	2:K:131:ILE:HD12	2.09	0.77
3:B:996:VAL:HG13	3:B:1050:LEU:HD22	1.64	0.77
3:B:3499:LYS:HE3	3:B:3564:LYS:HZ2	1.49	0.77
2:J:128:GLU:C	2:J:131:ILE:HD12	2.09	0.77
2:I:128:GLU:C	2:I:131:ILE:HD12	2.09	0.77
3:D:3427:ASN:HB2	3:D:3463:THR:HG1	1.48	0.77
2:I:128:GLU:HG2	2:I:131:ILE:HD13	1.66	0.77
2:L:128:GLU:O	2:L:131:ILE:HD12	1.84	0.77
3:C:3227:ARG:HH12	3:C:3290:ILE:HD12	1.50	0.77
2:K:107:ARG:HG3	2:K:125:MET:HE1	1.67	0.77
3:B:3308:ASN:OD1	3:B:3437:SER:HB3	1.85	0.77
3:C:3308:ASN:OD1	3:C:3437:SER:HB3	1.84	0.77
3:D:3373:LEU:HD11	3:D:3395:LEU:HD21	1.67	0.77
3:B:1751:ILE:HG13	3:B:1839:LEU:HD23	1.66	0.76
2:I:128:GLU:O	2:I:131:ILE:HD12	1.84	0.76
3:A:1751:ILE:HG13	3:A:1839:LEU:HD23	1.66	0.76
2:J:128:GLU:HG2	2:J:131:ILE:HD13	1.66	0.76
3:A:3308:ASN:OD1	3:A:3437:SER:HB3	1.84	0.76
3:D:3227:ARG:HH12	3:D:3290:ILE:HD12	1.50	0.76
3:D:3509:ILE:CD1	3:D:3552:LEU:HD21	2.15	0.76
2:I:107:ARG:HG3	2:I:125:MET:HE1	1.67	0.76
2:J:128:GLU:O	2:J:131:ILE:HD12	1.84	0.76
3:A:3378:ASP:OD2	3:A:3434:ASP:CG	2.29	0.76
3:B:3227:ARG:HH12	3:B:3290:ILE:HD12	1.50	0.76
3:C:1751:ILE:HG13	3:C:1839:LEU:HD23	1.66	0.76
3:B:3509:ILE:CD1	3:B:3552:LEU:HD21	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3308:ASN:OD1	3:D:3437:SER:HB3	1.85	0.76
3:A:3509:ILE:CD1	3:A:3552:LEU:HD21	2.15	0.76
3:D:1751:ILE:HG13	3:D:1839:LEU:HD23	1.67	0.76
3:C:3509:ILE:CD1	3:C:3552:LEU:HD21	2.15	0.76
2:L:128:GLU:HG2	2:L:131:ILE:HD13	1.66	0.75
3:C:3378:ASP:OD2	3:C:3434:ASP:CG	2.29	0.75
2:L:107:ARG:HG3	2:L:125:MET:HE1	1.67	0.75
3:C:2425:SER:O	3:D:142:LYS:NZ	2.19	0.75
3:B:3378:ASP:OD2	3:B:3434:ASP:CG	2.29	0.75
3:B:3832:ASP:HB3	3:B:3835:PHE:HB3	1.69	0.75
3:C:3832:ASP:HB3	3:C:3835:PHE:HB3	1.69	0.75
3:A:3373:LEU:HD11	3:A:3395:LEU:HD21	1.67	0.75
3:D:3832:ASP:HB3	3:D:3835:PHE:HB3	1.69	0.75
3:B:3250:TRP:O	3:B:3256:ASN:ND2	2.20	0.75
3:D:3378:ASP:OD2	3:D:3434:ASP:CG	2.29	0.75
3:B:3373:LEU:HD11	3:B:3395:LEU:HD21	1.67	0.75
3:C:3373:LEU:HD11	3:C:3395:LEU:HD21	1.67	0.75
2:J:107:ARG:HG3	2:J:125:MET:HE1	1.67	0.75
3:A:3227:ARG:HH12	3:A:3290:ILE:HD12	1.50	0.74
2:I:108:HIS:CE1	3:A:1956:ALA:HA	2.22	0.74
3:A:3832:ASP:HB3	3:A:3835:PHE:HB3	1.69	0.74
3:D:3250:TRP:O	3:D:3256:ASN:ND2	2.20	0.74
3:A:2988:ARG:HH12	3:A:2995:HIS:HB2	1.52	0.74
3:D:2988:ARG:HH12	3:D:2995:HIS:HB2	1.52	0.74
3:C:3493:LYS:NZ	3:C:3558:LEU:HB3	2.03	0.74
3:A:3250:TRP:O	3:A:3256:ASN:ND2	2.20	0.74
3:B:2988:ARG:HH12	3:B:2995:HIS:HB2	1.52	0.74
3:C:3250:TRP:O	3:C:3256:ASN:ND2	2.20	0.74
3:B:3493:LYS:NZ	3:B:3558:LEU:HB3	2.03	0.73
3:C:2988:ARG:HH12	3:C:2995:HIS:HB2	1.52	0.73
2:J:87:ARG:HE	2:J:90:PHE:HE1	1.37	0.73
3:A:3148:VAL:HG12	3:A:3151:GLN:HE21	1.54	0.73
2:I:132:ASP:C	2:I:137:VAL:HG22	2.14	0.73
3:D:3493:LYS:NZ	3:D:3558:LEU:HB3	2.03	0.73
2:I:143:VAL:HA	2:I:146:MET:HG3	1.71	0.72
2:J:143:VAL:HA	2:J:146:MET:HG3	1.71	0.72
3:B:3148:VAL:HG12	3:B:3151:GLN:HE21	1.54	0.72
3:D:3022:PHE:HB3	3:D:3025:ASP:HB2	1.71	0.72
3:A:3493:LYS:NZ	3:A:3558:LEU:HB3	2.03	0.72
2:K:87:ARG:HE	2:K:90:PHE:HE1	1.37	0.72
3:C:3022:PHE:HB3	3:C:3025:ASP:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3378:ASP:OD2	3:D:3434:ASP:OD1	2.07	0.72
2:J:132:ASP:C	2:J:137:VAL:HG22	2.14	0.72
2:K:132:ASP:C	2:K:137:VAL:HG22	2.14	0.72
3:D:3148:VAL:HG12	3:D:3151:GLN:HE21	1.54	0.72
2:I:87:ARG:HE	2:I:90:PHE:HE1	1.37	0.72
3:A:3499:LYS:HE3	3:A:3564:LYS:HZ2	1.54	0.72
3:C:3378:ASP:OD2	3:C:3434:ASP:OD1	2.07	0.72
3:C:3499:LYS:HE3	3:C:3564:LYS:HZ2	1.53	0.72
2:K:143:VAL:HA	2:K:146:MET:HG3	1.71	0.72
3:B:3378:ASP:OD2	3:B:3434:ASP:OD1	2.07	0.72
3:B:3493:LYS:NZ	3:B:3558:LEU:CB	2.53	0.72
2:L:87:ARG:HE	2:L:90:PHE:HE1	1.37	0.71
2:L:143:VAL:HA	2:L:146:MET:HG3	1.71	0.71
3:A:3022:PHE:HB3	3:A:3025:ASP:HB2	1.71	0.71
3:B:3324:GLU:HG2	3:B:3327:LYS:HZ3	1.55	0.71
3:C:3148:VAL:HG12	3:C:3151:GLN:HE21	1.54	0.71
3:B:3022:PHE:HB3	3:B:3025:ASP:HB2	1.71	0.71
3:C:2235:ARG:HG2	3:C:2297:ARG:HH12	1.56	0.71
3:C:4903:HIS:H	3:D:4183:LYS:HD2	1.54	0.71
3:A:3493:LYS:NZ	3:A:3558:LEU:CB	2.53	0.71
3:B:2235:ARG:HG2	3:B:2297:ARG:HH12	1.55	0.71
3:D:2235:ARG:HG2	3:D:2297:ARG:HH12	1.55	0.71
3:A:2235:ARG:HG2	3:A:2297:ARG:HH12	1.55	0.71
3:A:3378:ASP:OD2	3:A:3434:ASP:OD1	2.07	0.71
3:C:3493:LYS:NZ	3:C:3558:LEU:CB	2.53	0.71
2:L:132:ASP:C	2:L:137:VAL:HG22	2.14	0.71
3:D:3493:LYS:NZ	3:D:3558:LEU:CB	2.53	0.71
3:A:2916:SER:OG	3:A:2920:ARG:NH2	2.24	0.71
3:B:2916:SER:OG	3:B:2920:ARG:NH2	2.24	0.70
3:A:4775:ALA:HA	3:A:4817:MET:HE1	1.74	0.70
3:D:2916:SER:OG	3:D:2920:ARG:NH2	2.24	0.70
2:K:14:LYS:HG2	3:C:2153:LYS:HD3	1.72	0.70
3:B:2752:LYS:HA	3:B:2754:GLN:HE22	1.56	0.70
3:C:2916:SER:OG	3:C:2920:ARG:NH2	2.24	0.70
2:I:77:MET:HE2	2:I:77:MET:O	1.92	0.70
3:D:894:VAL:O	3:D:898:ILE:HD12	1.92	0.70
3:D:3215:MET:HE2	3:D:3215:MET:HA	1.74	0.70
3:D:3184:TYR:HA	3:D:3192:ARG:HH12	1.57	0.70
3:C:2752:LYS:HA	3:C:2754:GLN:HE22	1.56	0.70
3:C:3184:TYR:HA	3:C:3192:ARG:HH12	1.57	0.70
3:A:3215:MET:HE2	3:A:3215:MET:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4609:LYS:HD2	3:B:4615:LEU:HD13	1.74	0.69
2:K:77:MET:O	2:K:77:MET:HE2	1.92	0.69
3:C:4609:LYS:HD2	3:C:4615:LEU:HD13	1.74	0.69
3:D:4775:ALA:HA	3:D:4817:MET:HE1	1.74	0.69
3:C:1685:LEU:HB3	3:C:1706:LEU:HD12	1.74	0.69
3:B:1685:LEU:HB3	3:B:1706:LEU:HD12	1.74	0.69
3:A:2752:LYS:HA	3:A:2754:GLN:HE22	1.56	0.69
3:D:2761:LYS:HE2	3:D:2761:LYS:HA	1.74	0.69
2:J:77:MET:HE2	2:J:77:MET:O	1.92	0.69
2:L:77:MET:HE2	2:L:77:MET:O	1.91	0.69
3:A:3184:TYR:HA	3:A:3192:ARG:HH12	1.57	0.69
3:A:894:VAL:O	3:A:898:ILE:HD12	1.92	0.69
3:C:894:VAL:O	3:C:898:ILE:HD12	1.92	0.69
3:D:1685:LEU:HB3	3:D:1706:LEU:HD12	1.74	0.69
3:D:4609:LYS:HD2	3:D:4615:LEU:HD13	1.74	0.69
2:I:148:ALA:HB3	3:A:3597:ARG:HH22	1.56	0.69
3:A:2761:LYS:HE2	3:A:2761:LYS:HA	1.74	0.69
3:B:3184:TYR:HA	3:B:3192:ARG:HH12	1.57	0.69
3:D:2752:LYS:HA	3:D:2754:GLN:HE22	1.56	0.69
3:A:1685:LEU:HB3	3:A:1706:LEU:HD12	1.74	0.69
3:C:4775:ALA:HA	3:C:4817:MET:HE1	1.74	0.69
3:B:2979:ARG:HG3	3:B:3039:THR:HG22	1.75	0.68
3:B:3215:MET:HE2	3:B:3215:MET:HA	1.74	0.68
3:C:3215:MET:HE2	3:C:3215:MET:HA	1.74	0.68
3:A:4609:LYS:HD2	3:A:4615:LEU:HD13	1.74	0.68
3:C:3525:ARG:HA	3:C:3528:MET:SD	2.34	0.68
3:A:3525:ARG:HA	3:A:3528:MET:SD	2.34	0.68
3:B:2761:LYS:HA	3:B:2761:LYS:HE2	1.74	0.68
3:B:3525:ARG:HA	3:B:3528:MET:SD	2.34	0.68
3:B:4775:ALA:HA	3:B:4817:MET:HE1	1.74	0.68
3:B:894:VAL:O	3:B:898:ILE:HD12	1.92	0.68
3:C:2761:LYS:HE2	3:C:2761:LYS:HA	1.74	0.68
3:D:3409:SER:HB3	3:D:3412:PHE:CE2	2.29	0.68
2:L:128:GLU:HG2	2:L:131:ILE:CD1	2.21	0.68
3:A:3409:SER:HB3	3:A:3412:PHE:CE2	2.29	0.67
2:J:128:GLU:HG2	2:J:131:ILE:CD1	2.21	0.67
3:A:2979:ARG:HG3	3:A:3039:THR:HG22	1.75	0.67
3:C:2764:SER:OG	3:C:2767:GLU:OE1	2.13	0.67
3:D:3525:ARG:HA	3:D:3528:MET:SD	2.34	0.67
3:B:3148:VAL:HA	3:B:3151:GLN:HG2	1.77	0.67
3:C:2979:ARG:HG3	3:C:3039:THR:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2979:ARG:HG3	3:D:3039:THR:HG22	1.75	0.67
3:A:4602:ARG:HH12	3:A:4627:LYS:HB3	1.59	0.67
3:C:114:LEU:HB2	3:C:117:HIS:CD2	2.30	0.67
3:D:114:LEU:HB2	3:D:117:HIS:CD2	2.30	0.67
3:A:3148:VAL:HA	3:A:3151:GLN:HG2	1.77	0.67
3:B:4818:TYR:OH	3:C:4847:ASP:OD2	2.10	0.67
3:B:3409:SER:HB3	3:B:3412:PHE:CE2	2.29	0.67
3:C:3409:SER:HB3	3:C:3412:PHE:CE2	2.29	0.67
2:I:6:THR:OG1	2:I:9:GLN:OE1	2.13	0.67
3:B:114:LEU:HB2	3:B:117:HIS:CD2	2.30	0.67
3:D:1239:PHE:O	3:D:1807:ARG:NH2	2.28	0.67
3:C:4602:ARG:HH12	3:C:4627:LYS:HB3	1.59	0.66
3:D:2764:SER:OG	3:D:2767:GLU:OE1	2.13	0.66
3:B:2425:SER:O	3:C:142:LYS:NZ	2.29	0.66
3:D:4602:ARG:HH12	3:D:4627:LYS:HB3	1.59	0.66
3:A:142:LYS:NZ	3:D:2425:SER:O	2.27	0.66
3:C:3148:VAL:HA	3:C:3151:GLN:HG2	1.77	0.66
2:K:6:THR:OG1	2:K:9:GLN:OE1	2.13	0.66
3:A:2764:SER:OG	3:A:2767:GLU:OE1	2.13	0.66
3:B:4602:ARG:HH12	3:B:4627:LYS:HB3	1.59	0.66
3:A:114:LEU:HB2	3:A:117:HIS:CD2	2.30	0.66
3:B:2764:SER:OG	3:B:2767:GLU:OE1	2.13	0.66
3:D:3148:VAL:HA	3:D:3151:GLN:HG2	1.77	0.66
2:L:146:MET:C	2:L:146:MET:HE2	2.21	0.65
2:J:6:THR:OG1	2:J:9:GLN:OE1	2.13	0.65
3:A:1239:PHE:O	3:A:1807:ARG:NH2	2.28	0.65
3:B:1239:PHE:O	3:B:1807:ARG:NH2	2.28	0.65
3:A:4052:MET:HE2	3:A:4063:THR:HG23	1.78	0.65
3:B:1729:MET:HE2	3:B:1930:ASP:HB2	1.78	0.65
3:C:3427:ASN:HB2	3:C:3463:THR:HG1	1.61	0.65
2:K:146:MET:C	2:K:146:MET:HE2	2.21	0.65
3:B:3412:PHE:O	3:B:3416:GLU:HB2	1.97	0.65
3:B:3427:ASN:HB2	3:B:3463:THR:HB	1.38	0.65
3:C:3412:PHE:O	3:C:3416:GLU:HB2	1.97	0.65
3:D:3412:PHE:O	3:D:3416:GLU:HB2	1.97	0.65
3:A:1729:MET:HE2	3:A:1930:ASP:HB2	1.78	0.65
3:D:3427:ASN:CB	3:D:3463:THR:O	2.45	0.65
3:D:3499:LYS:HE3	3:D:3564:LYS:HZ2	1.62	0.65
3:D:4052:MET:HE2	3:D:4063:THR:HG23	1.78	0.65
2:I:146:MET:C	2:I:146:MET:HE2	2.21	0.65
2:J:146:MET:HE2	2:J:146:MET:C	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3324:GLU:HG2	3:C:3327:LYS:HZ3	1.62	0.65
3:C:1239:PHE:O	3:C:1807:ARG:NH2	2.28	0.64
3:C:1729:MET:HE2	3:C:1930:ASP:HB2	1.78	0.64
2:I:108:HIS:HB3	3:A:1959:ALA:CB	2.26	0.64
3:D:1766:PRO:HG3	3:D:1780:PRO:HB3	1.80	0.64
3:C:4052:MET:HE2	3:C:4063:THR:HG23	1.78	0.64
2:I:128:GLU:HG2	2:I:131:ILE:CD1	2.21	0.64
3:A:1766:PRO:HG3	3:A:1780:PRO:HB3	1.80	0.64
3:B:3477:GLY:HA2	3:B:3480:ILE:HD12	1.79	0.64
3:C:1766:PRO:HG3	3:C:1780:PRO:HB3	1.80	0.64
3:B:1766:PRO:HG3	3:B:1780:PRO:HB3	1.80	0.64
3:C:3427:ASN:CB	3:C:3463:THR:O	2.45	0.64
3:C:3478:LEU:HD21	3:D:1233:GLN:HB3	1.78	0.64
3:B:3695:MET:HB3	3:B:3731:LEU:HD11	1.80	0.64
3:B:4052:MET:HE2	3:B:4063:THR:HG23	1.78	0.64
3:A:2150:MET:HE1	3:A:2199:PHE:HA	1.80	0.63
3:A:3477:GLY:HA2	3:A:3480:ILE:HD12	1.79	0.63
3:B:2150:MET:HE1	3:B:2199:PHE:HA	1.80	0.63
3:D:3477:GLY:HA2	3:D:3480:ILE:HD12	1.79	0.63
3:A:3695:MET:HB3	3:A:3731:LEU:HD11	1.80	0.63
3:B:4664:ASP:OD1	3:B:4674:LYS:NZ	2.29	0.63
3:D:1729:MET:HE2	3:D:1930:ASP:HB2	1.78	0.63
2:L:6:THR:OG1	2:L:9:GLN:OE1	2.13	0.63
3:D:4751:LYS:HA	3:D:4754:ARG:HE	1.64	0.63
3:A:3412:PHE:O	3:A:3416:GLU:HB2	1.97	0.63
3:C:4751:LYS:HA	3:C:4754:ARG:HE	1.63	0.63
2:L:138:ASN:O	2:L:142:PHE:HB2	1.98	0.63
2:K:138:ASN:O	2:K:142:PHE:HB2	1.98	0.63
3:B:222:GLU:HB2	3:B:349:MET:HG3	1.80	0.63
1:G:83:TYR:OH	3:C:1768:PHE:O	2.15	0.63
3:B:3499:LYS:HE3	3:B:3564:LYS:NZ	2.14	0.63
3:A:3037:GLY:HA2	3:A:3040:LEU:HD13	1.81	0.63
3:B:4144:ARG:HB3	3:B:4961:GLN:HE22	1.64	0.63
3:B:4751:LYS:HA	3:B:4754:ARG:HE	1.64	0.63
3:A:2556:SER:HB2	3:A:2569:ILE:HG21	1.81	0.62
3:C:2150:MET:HE1	3:C:2199:PHE:HA	1.80	0.62
3:C:3499:LYS:HE3	3:C:3564:LYS:NZ	2.14	0.62
3:C:4664:ASP:OD1	3:C:4674:LYS:NZ	2.29	0.62
3:A:4751:LYS:HA	3:A:4754:ARG:HE	1.64	0.62
3:C:2830:ASN:HD22	3:D:1435:GLY:HA2	1.63	0.62
3:C:4169:LYS:NZ	5:C:5002:ATP:O1B	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3695:MET:HB3	3:D:3731:LEU:HD11	1.80	0.62
2:I:138:ASN:O	2:I:142:PHE:HB2	1.98	0.62
2:J:138:ASN:O	2:J:142:PHE:HB2	1.98	0.62
3:A:4664:ASP:OD1	3:A:4674:LYS:NZ	2.29	0.62
3:D:4169:LYS:NZ	5:D:5002:ATP:O1B	2.32	0.62
3:A:4144:ARG:HB3	3:A:4961:GLN:HE22	1.64	0.62
3:A:4169:LYS:NZ	5:A:5002:ATP:O1B	2.32	0.62
3:A:4622:SER:OG	3:A:4624:ASP:OD1	2.18	0.62
3:B:2556:SER:HB2	3:B:2569:ILE:HG21	1.81	0.62
3:B:4169:LYS:NZ	5:B:5002:ATP:O1B	2.32	0.62
3:A:222:GLU:HB2	3:A:349:MET:HG3	1.80	0.62
3:C:3477:GLY:HA2	3:C:3480:ILE:HD12	1.79	0.62
3:D:4622:SER:OG	3:D:4624:ASP:OD1	2.18	0.62
2:J:15:GLU:OE1	2:J:15:GLU:N	2.32	0.62
3:B:3653:GLU:HG2	3:B:3655:ASP:H	1.65	0.62
3:C:897:LYS:HB2	3:C:902:TRP:HB2	1.82	0.62
3:C:3695:MET:HB3	3:C:3731:LEU:HD11	1.80	0.62
3:C:4590:TYR:HA	3:C:4593:LEU:HB3	1.82	0.62
2:I:83:GLU:OE2	2:I:87:ARG:NH1	2.31	0.62
3:C:4144:ARG:HB3	3:C:4961:GLN:HE22	1.64	0.62
3:D:222:GLU:HB2	3:D:349:MET:HG3	1.80	0.62
3:D:3037:GLY:HA2	3:D:3040:LEU:HD13	1.81	0.62
3:D:3499:LYS:HE3	3:D:3564:LYS:NZ	2.14	0.62
2:K:128:GLU:HG2	2:K:131:ILE:CD1	2.21	0.62
3:D:897:LYS:HB2	3:D:902:TRP:HB2	1.82	0.62
3:D:4144:ARG:HB3	3:D:4961:GLN:HE22	1.64	0.62
3:A:3499:LYS:HE3	3:A:3564:LYS:NZ	2.14	0.62
3:B:3037:GLY:HA2	3:B:3040:LEU:HD13	1.81	0.62
3:C:3653:GLU:HG2	3:C:3655:ASP:H	1.65	0.62
3:D:2150:MET:HE1	3:D:2199:PHE:HA	1.80	0.62
3:D:3324:GLU:HG2	3:D:3327:LYS:HZ3	1.65	0.62
3:A:3653:GLU:HG2	3:A:3655:ASP:H	1.65	0.61
3:C:222:GLU:HB2	3:C:349:MET:HG3	1.80	0.61
3:D:3653:GLU:HG2	3:D:3655:ASP:H	1.65	0.61
3:B:3427:ASN:CB	3:B:3463:THR:O	2.45	0.61
3:C:3037:GLY:HA2	3:C:3040:LEU:HD13	1.81	0.61
2:L:83:GLU:OE2	2:L:87:ARG:NH1	2.31	0.61
3:B:163:HIS:HB2	3:B:182:ILE:HG13	1.83	0.61
3:D:3493:LYS:HZ2	3:D:3558:LEU:HB2	1.64	0.61
3:A:3274:ASN:HB2	3:A:3314:LEU:HD11	1.82	0.61
3:B:4590:TYR:HA	3:B:4593:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4590:TYR:HA	3:A:4593:LEU:HB3	1.82	0.61
3:B:15:ARG:HH11	3:B:15:ARG:HG3	1.66	0.61
3:B:3274:ASN:HB2	3:B:3314:LEU:HD11	1.82	0.61
3:B:3464:SER:HB3	3:B:3467:VAL:HG22	1.83	0.61
3:C:3493:LYS:HZ2	3:C:3558:LEU:HB2	1.65	0.61
3:C:15:ARG:HH11	3:C:15:ARG:HG3	1.66	0.61
3:C:3482:ALA:H	3:C:3485:ASP:HB3	1.65	0.61
3:A:163:HIS:HB2	3:A:182:ILE:HG13	1.83	0.61
3:A:3559:PHE:HD1	3:A:3563:GLN:HE21	1.48	0.61
3:D:4590:TYR:HA	3:D:4593:LEU:HB3	1.82	0.61
3:A:2920:ARG:NH1	3:A:2981:TYR:OH	2.34	0.61
3:B:3493:LYS:HZ2	3:B:3558:LEU:HB2	1.64	0.61
3:C:3464:SER:HB3	3:C:3467:VAL:HG22	1.83	0.61
3:D:314:LEU:HD11	3:D:372:LEU:HD11	1.83	0.61
2:I:15:GLU:OE1	2:I:15:GLU:N	2.32	0.60
3:A:3522:PRO:HA	3:A:3525:ARG:HG2	1.83	0.60
3:C:2556:SER:HB2	3:C:2569:ILE:HG21	1.81	0.60
3:D:2556:SER:HB2	3:D:2569:ILE:HG21	1.81	0.60
3:D:2920:ARG:NH1	3:D:2981:TYR:OH	2.34	0.60
3:D:3522:PRO:HA	3:D:3525:ARG:HG2	1.83	0.60
3:A:314:LEU:HD11	3:A:372:LEU:HD11	1.83	0.60
3:A:3427:ASN:CB	3:A:3463:THR:O	2.45	0.60
3:B:3482:ALA:H	3:B:3485:ASP:HB3	1.65	0.60
3:C:163:HIS:HB2	3:C:182:ILE:HG13	1.83	0.60
3:C:2920:ARG:NH1	3:C:2981:TYR:OH	2.34	0.60
3:C:3522:PRO:HA	3:C:3525:ARG:HG2	1.83	0.60
3:D:3274:ASN:HB2	3:D:3314:LEU:HD11	1.82	0.60
3:A:137:ARG:NE	3:A:139:SER:OG	2.35	0.60
3:B:3522:PRO:HA	3:B:3525:ARG:HG2	1.83	0.60
3:C:4622:SER:OG	3:C:4624:ASP:OD1	2.18	0.60
3:D:323:ASP:O	3:D:325:LYS:N	2.33	0.60
3:A:897:LYS:HB2	3:A:902:TRP:HB2	1.82	0.60
3:B:2920:ARG:NH1	3:B:2981:TYR:OH	2.34	0.60
3:B:3559:PHE:HD1	3:B:3563:GLN:HE21	1.48	0.60
3:D:799:LYS:HG2	3:D:1620:GLN:HG3	1.84	0.60
2:I:146:MET:O	3:A:3596:LYS:HD3	2.02	0.60
3:A:3482:ALA:H	3:A:3485:ASP:HB3	1.65	0.60
3:D:1839:LEU:HD12	3:D:1842:ILE:HD11	1.84	0.60
3:D:3559:PHE:HD1	3:D:3563:GLN:HE21	1.48	0.60
3:B:4622:SER:OG	3:B:4624:ASP:OD1	2.18	0.60
3:C:137:ARG:NE	3:C:139:SER:OG	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:163:HIS:HB2	3:D:182:ILE:HG13	1.83	0.60
2:J:83:GLU:OE2	2:J:87:ARG:NH1	2.31	0.60
2:K:15:GLU:OE1	2:K:15:GLU:N	2.32	0.60
3:C:799:LYS:HG2	3:C:1620:GLN:HG3	1.83	0.60
3:C:2830:ASN:ND2	3:D:1435:GLY:HA2	2.16	0.60
3:B:897:LYS:HB2	3:B:902:TRP:HB2	1.82	0.60
3:C:3559:PHE:HD1	3:C:3563:GLN:HE21	1.48	0.60
3:A:3464:SER:HB3	3:A:3467:VAL:HG22	1.83	0.60
3:A:4637:THR:HG21	3:A:4705:TYR:HB2	1.84	0.60
3:B:541:ILE:HD11	3:B:574:VAL:HG13	1.84	0.60
2:J:138:ASN:O	2:J:142:PHE:CB	2.50	0.60
3:D:15:ARG:HH11	3:D:15:ARG:HG3	1.66	0.60
2:I:138:ASN:O	2:I:142:PHE:CB	2.50	0.59
2:K:83:GLU:OE2	2:K:87:ARG:NH1	2.31	0.59
3:A:1839:LEU:HD12	3:A:1842:ILE:HD11	1.84	0.59
3:B:555:LEU:HD11	3:B:578:VAL:HG11	1.84	0.59
3:C:3274:ASN:HB2	3:C:3314:LEU:HD11	1.82	0.59
3:A:799:LYS:HG2	3:A:1620:GLN:HG3	1.84	0.59
3:B:137:ARG:NE	3:B:139:SER:OG	2.35	0.59
3:D:137:ARG:NE	3:D:139:SER:OG	2.35	0.59
3:D:2139:GLU:HG3	3:D:2192:MET:HB2	1.84	0.59
3:D:3464:SER:HB3	3:D:3467:VAL:HG22	1.83	0.59
3:D:3482:ALA:H	3:D:3485:ASP:HB3	1.65	0.59
3:B:1839:LEU:HD12	3:B:1842:ILE:HD11	1.84	0.59
3:C:3022:PHE:HD2	3:C:3029:ILE:HD13	1.67	0.59
3:D:925:PRO:HB2	3:D:928:GLU:HB2	1.84	0.59
3:C:314:LEU:HD11	3:C:372:LEU:HD11	1.83	0.59
3:C:541:ILE:HD11	3:C:574:VAL:HG13	1.84	0.59
3:D:4637:THR:HG21	3:D:4705:TYR:HB2	1.84	0.59
3:A:541:ILE:HD11	3:A:574:VAL:HG13	1.84	0.59
3:C:925:PRO:HB2	3:C:928:GLU:HB2	1.85	0.59
3:D:1129:GLY:HA3	3:D:1145:TRP:HB3	1.84	0.59
2:I:148:ALA:HB3	3:A:3597:ARG:NH2	2.18	0.59
2:K:138:ASN:O	2:K:142:PHE:CB	2.50	0.59
3:B:799:LYS:HG2	3:B:1620:GLN:HG3	1.83	0.59
3:B:4187:GLU:OE1	3:B:4949:TRP:NE1	2.31	0.59
3:C:323:ASP:O	3:C:325:LYS:N	2.33	0.59
3:A:925:PRO:HB2	3:A:928:GLU:HB2	1.85	0.59
3:A:1129:GLY:HA3	3:A:1145:TRP:HB3	1.84	0.59
3:A:2139:GLU:HG3	3:A:2192:MET:HB2	1.84	0.59
3:B:1936:LEU:HD11	3:B:1976:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1936:LEU:HD11	3:D:1976:LEU:HD22	1.84	0.59
3:D:4187:GLU:OE1	3:D:4949:TRP:NE1	2.31	0.59
2:L:138:ASN:O	2:L:142:PHE:CB	2.50	0.59
3:B:3022:PHE:HD2	3:B:3029:ILE:HD13	1.68	0.59
3:C:555:LEU:HD11	3:C:578:VAL:HG11	1.85	0.59
3:C:1839:LEU:HD12	3:C:1842:ILE:HD11	1.84	0.59
3:A:15:ARG:HG3	3:A:15:ARG:HH11	1.66	0.59
3:A:555:LEU:HD11	3:A:578:VAL:HG11	1.85	0.59
3:A:3022:PHE:HD2	3:A:3029:ILE:HD13	1.68	0.59
3:A:4028:SER:O	3:A:4033:LYS:NZ	2.36	0.59
3:A:4187:GLU:OE1	3:A:4949:TRP:NE1	2.31	0.59
3:B:314:LEU:HD11	3:B:372:LEU:HD11	1.83	0.59
3:B:4818:TYR:HE1	3:C:4847:ASP:HB2	1.66	0.59
3:D:3022:PHE:HD2	3:D:3029:ILE:HD13	1.68	0.59
3:A:1936:LEU:HD11	3:A:1976:LEU:HD22	1.84	0.58
3:D:841:LYS:O	3:D:848:ARG:NH2	2.34	0.58
3:D:1165:MET:HE1	3:D:1176:THR:HG23	1.84	0.58
3:B:4028:SER:O	3:B:4033:LYS:NZ	2.36	0.58
3:C:1129:GLY:HA3	3:C:1145:TRP:HB3	1.84	0.58
3:C:1936:LEU:HD11	3:C:1976:LEU:HD22	1.84	0.58
3:C:3348:MET:SD	3:C:3353:LEU:HB2	2.44	0.58
3:B:3348:MET:SD	3:B:3353:LEU:HB2	2.44	0.58
3:A:1165:MET:HE1	3:A:1176:THR:HG23	1.84	0.58
3:C:4637:THR:HG21	3:C:4705:TYR:HB2	1.84	0.58
3:D:541:ILE:HD11	3:D:574:VAL:HG13	1.84	0.58
1:H:50:ARG:HB3	1:H:50:ARG:HH11	1.69	0.58
2:L:15:GLU:OE1	2:L:15:GLU:N	2.32	0.58
3:C:1962:THR:HA	3:C:1965:PHE:HD2	1.69	0.58
3:A:3804:ASP:H	3:A:3829:VAL:HG13	1.68	0.58
3:C:2823:PRO:O	3:C:2824:ARG:NH1	2.37	0.58
3:D:3651:PRO:HB2	3:D:3652:PRO:HD3	1.85	0.58
2:J:109:VAL:HB	3:B:3603:PHE:HZ	1.69	0.58
2:L:128:GLU:CA	2:L:131:ILE:HD11	2.29	0.58
3:B:323:ASP:O	3:B:325:LYS:N	2.33	0.58
3:B:1129:GLY:HA3	3:B:1145:TRP:HB3	1.84	0.58
3:C:3246:MET:HG2	3:C:3268:LEU:HD11	1.85	0.58
3:D:555:LEU:HD11	3:D:578:VAL:HG11	1.85	0.58
3:D:3348:MET:SD	3:D:3353:LEU:HB2	2.44	0.58
2:J:6:THR:H	2:J:9:GLN:NE2	2.02	0.58
3:A:841:LYS:O	3:A:848:ARG:NH2	2.34	0.58
3:A:3269:ASN:HB3	3:A:3271:GLU:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3269:ASN:HB3	3:B:3271:GLU:HG3	1.86	0.58
3:C:3804:ASP:H	3:C:3829:VAL:HG13	1.68	0.58
2:I:111:THR:OG1	3:A:1960:ARG:NH2	2.32	0.58
3:A:2823:PRO:O	3:A:2824:ARG:NH1	2.37	0.58
3:A:3348:MET:SD	3:A:3353:LEU:HB2	2.44	0.58
3:B:925:PRO:HB2	3:B:928:GLU:HB2	1.85	0.58
3:B:2139:GLU:HG3	3:B:2192:MET:HB2	1.84	0.58
3:D:2823:PRO:O	3:D:2824:ARG:NH1	2.37	0.58
3:D:2895:PHE:HA	3:D:2898:ILE:HG12	1.86	0.58
3:A:1962:THR:HA	3:A:1965:PHE:HD2	1.69	0.58
3:B:2744:GLY:HA2	3:B:2753:VAL:HG13	1.86	0.58
3:C:2322:ARG:O	3:C:2326:ARG:HG2	2.04	0.58
3:C:2734:MET:HE2	3:C:2823:PRO:HB2	1.85	0.58
3:D:1097:LYS:NZ	3:D:1198:GLY:O	2.37	0.58
1:F:50:ARG:HB3	1:F:50:ARG:HH11	1.69	0.57
2:I:6:THR:H	2:I:9:GLN:NE2	2.02	0.57
3:B:1962:THR:HA	3:B:1965:PHE:HD2	1.69	0.57
3:B:4637:THR:HG21	3:B:4705:TYR:HB2	1.84	0.57
3:C:2139:GLU:HG3	3:C:2192:MET:HB2	1.84	0.57
3:C:2744:GLY:HA2	3:C:2753:VAL:HG13	1.86	0.57
3:C:3651:PRO:HB2	3:C:3652:PRO:HD3	1.85	0.57
3:C:3892:TYR:O	3:C:3957:LYS:NZ	2.37	0.57
3:D:1962:THR:HA	3:D:1965:PHE:HD2	1.69	0.57
3:D:2792:THR:HG23	3:D:2794:GLU:H	1.69	0.57
3:A:2792:THR:HG23	3:A:2794:GLU:H	1.69	0.57
3:A:2895:PHE:HA	3:A:2898:ILE:HG12	1.86	0.57
3:A:3320:LEU:HD23	3:A:3321:PRO:HD3	1.86	0.57
3:B:2545:ILE:HD12	3:B:2580:LEU:HD21	1.86	0.57
3:B:2734:MET:HE2	3:B:2823:PRO:HB2	1.85	0.57
3:B:2743:TYR:HA	3:B:2757:MET:HE1	1.86	0.57
3:B:3246:MET:HG2	3:B:3268:LEU:HD11	1.85	0.57
3:B:3534:LEU:HD13	3:B:3537:ARG:HG3	1.86	0.57
3:C:1165:MET:HE1	3:C:1176:THR:HG23	1.84	0.57
3:D:3892:TYR:O	3:D:3957:LYS:NZ	2.37	0.57
1:E:50:ARG:HB3	1:E:50:ARG:HH11	1.69	0.57
3:B:1165:MET:HE1	3:B:1176:THR:HG23	1.84	0.57
3:C:2826:ILE:HD12	3:D:1501:ASN:HD21	1.69	0.57
3:D:4913:HIS:O	5:D:5002:ATP:N6	2.37	0.57
2:K:6:THR:H	2:K:9:GLN:NE2	2.02	0.57
2:L:6:THR:H	2:L:9:GLN:NE2	2.02	0.57
3:A:2322:ARG:O	3:A:2326:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1097:LYS:NZ	3:B:1198:GLY:O	2.37	0.57
3:B:2322:ARG:O	3:B:2326:ARG:HG2	2.04	0.57
3:C:2758:LYS:HE3	3:C:2763:LEU:HA	1.87	0.57
3:A:2743:TYR:HA	3:A:2757:MET:HE1	1.86	0.57
3:A:4913:HIS:O	5:A:5002:ATP:N6	2.37	0.57
3:B:2895:PHE:HA	3:B:2898:ILE:HG12	1.86	0.57
3:B:4913:HIS:O	5:B:5002:ATP:N6	2.37	0.57
3:C:1097:LYS:NZ	3:C:1198:GLY:O	2.37	0.57
3:D:3246:MET:HG2	3:D:3268:LEU:HD11	1.85	0.57
2:I:82:SER:O	2:I:86:ILE:HG22	2.04	0.57
3:C:2895:PHE:HA	3:C:2898:ILE:HG12	1.86	0.57
3:C:4913:HIS:O	5:C:5002:ATP:N6	2.37	0.57
3:D:3269:ASN:HB3	3:D:3271:GLU:HG3	1.86	0.57
3:D:3320:LEU:HD23	3:D:3321:PRO:HD3	1.86	0.57
3:D:3804:ASP:H	3:D:3829:VAL:HG13	1.68	0.57
2:I:113:LEU:HD22	3:A:1963:LYS:HG3	1.87	0.57
3:A:394:HIS:CE1	3:A:396:GLU:HG3	2.40	0.57
3:A:1097:LYS:NZ	3:A:1198:GLY:O	2.37	0.57
3:A:1951:LEU:HD12	3:A:1958:THR:HG21	1.86	0.57
3:A:2545:ILE:HD12	3:A:2580:LEU:HD21	1.86	0.57
3:B:1268:ILE:HD11	3:B:1300:MET:HE2	1.86	0.57
3:B:1951:LEU:HD12	3:B:1958:THR:HG21	1.86	0.57
3:B:3651:PRO:HB2	3:B:3652:PRO:HD3	1.85	0.57
3:C:3269:ASN:HB3	3:C:3271:GLU:HG3	1.86	0.57
3:D:1951:LEU:HD12	3:D:1958:THR:HG21	1.86	0.57
3:D:3274:ASN:OD1	3:D:3275:THR:N	2.38	0.57
3:D:3406:TRP:HA	3:D:3412:PHE:CE2	2.40	0.57
3:D:3534:LEU:HD13	3:D:3537:ARG:HG3	1.86	0.57
1:G:50:ARG:HB3	1:G:50:ARG:HH11	1.69	0.57
2:J:82:SER:O	2:J:86:ILE:HG22	2.04	0.57
3:A:3184:TYR:HA	3:A:3192:ARG:NH1	2.20	0.57
3:C:3715:GLU:O	3:C:3719:MET:HG2	2.05	0.57
3:D:2545:ILE:HD12	3:D:2580:LEU:HD21	1.86	0.57
3:D:2734:MET:HE2	3:D:2823:PRO:HB2	1.85	0.57
3:D:2744:GLY:HA2	3:D:2753:VAL:HG13	1.86	0.57
3:A:3406:TRP:HA	3:A:3412:PHE:CE2	2.40	0.57
3:A:3651:PRO:HB2	3:A:3652:PRO:HD3	1.85	0.57
3:A:3715:GLU:O	3:A:3719:MET:HG2	2.05	0.57
3:B:2823:PRO:O	3:B:2824:ARG:NH1	2.37	0.57
3:B:3804:ASP:H	3:B:3829:VAL:HG13	1.68	0.57
3:C:394:HIS:CE1	3:C:396:GLU:HG3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:249:SER:HA	3:D:257:ARG:NH2	2.20	0.57
3:A:1682:GLU:HG2	3:A:1683:PRO:HD3	1.86	0.57
3:A:1911:GLN:OE1	3:A:2090:ARG:NH1	2.33	0.57
3:A:3246:MET:HG2	3:A:3268:LEU:HD11	1.85	0.57
3:B:4186:MET:HE2	3:B:4186:MET:HA	1.87	0.57
3:C:875:PRO:HD2	3:C:878:LEU:HD12	1.86	0.57
3:C:1682:GLU:HG2	3:C:1683:PRO:HD3	1.86	0.57
3:D:394:HIS:CE1	3:D:396:GLU:HG3	2.40	0.57
3:A:1243:THR:HG22	3:A:1808:ASP:HB2	1.87	0.56
3:B:1911:GLN:OE1	3:B:2090:ARG:NH1	2.32	0.56
3:C:4186:MET:HE2	3:C:4186:MET:HA	1.87	0.56
3:C:4640:PHE:HB3	3:C:4641:PRO:HD3	1.87	0.56
3:D:1682:GLU:HG2	3:D:1683:PRO:HD3	1.86	0.56
2:K:82:SER:O	2:K:86:ILE:HG22	2.04	0.56
2:K:128:GLU:CA	2:K:131:ILE:HD11	2.29	0.56
3:A:3324:GLU:HG2	3:A:3327:LYS:HZ3	1.69	0.56
3:B:249:SER:HA	3:B:257:ARG:NH2	2.20	0.56
3:C:2792:THR:HG23	3:C:2794:GLU:H	1.69	0.56
3:D:601:LEU:HG	3:D:610:VAL:HG11	1.87	0.56
3:D:2743:TYR:HA	3:D:2757:MET:HE1	1.86	0.56
3:A:249:SER:HA	3:A:257:ARG:NH2	2.20	0.56
3:A:558:LEU:HG	3:A:571:ILE:HG23	1.86	0.56
3:A:601:LEU:HG	3:A:610:VAL:HG11	1.87	0.56
3:A:875:PRO:HD2	3:A:878:LEU:HD12	1.86	0.56
3:A:1268:ILE:HD11	3:A:1300:MET:HE2	1.86	0.56
3:A:1272:ARG:NH2	3:A:1582:CYS:SG	2.79	0.56
3:A:3534:LEU:HD13	3:A:3537:ARG:HG3	1.86	0.56
3:B:394:HIS:CE1	3:B:396:GLU:HG3	2.40	0.56
3:B:2758:LYS:HE3	3:B:2763:LEU:HA	1.87	0.56
3:B:2792:THR:HG23	3:B:2794:GLU:H	1.69	0.56
3:B:3406:TRP:HA	3:B:3412:PHE:CE2	2.40	0.56
3:B:3715:GLU:O	3:B:3719:MET:HG2	2.05	0.56
3:B:3892:TYR:O	3:B:3957:LYS:NZ	2.37	0.56
3:C:3320:LEU:HD23	3:C:3321:PRO:HD3	1.86	0.56
3:C:3406:TRP:HA	3:C:3412:PHE:CE2	2.40	0.56
3:D:558:LEU:HG	3:D:571:ILE:HG23	1.86	0.56
3:D:1268:ILE:HD11	3:D:1300:MET:HE2	1.86	0.56
3:D:2758:LYS:HE3	3:D:2763:LEU:HA	1.87	0.56
3:D:3184:TYR:HA	3:D:3192:ARG:NH1	2.20	0.56
3:D:3715:GLU:O	3:D:3719:MET:HG2	2.05	0.56
3:D:4640:PHE:HB3	3:D:4641:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:VAL:HG22	1:H:48:LYS:HG2	1.88	0.56
2:L:82:SER:O	2:L:86:ILE:HG22	2.04	0.56
3:B:476:GLN:NE2	3:B:3678:GLU:OE1	2.39	0.56
3:B:3184:TYR:HA	3:B:3192:ARG:NH1	2.20	0.56
3:B:3493:LYS:HZ2	3:B:3558:LEU:CB	2.18	0.56
3:C:2426:LEU:HD21	3:D:143:LEU:HD22	1.86	0.56
3:C:3461:MET:HE3	3:C:3461:MET:C	2.31	0.56
3:C:3534:LEU:HD13	3:C:3537:ARG:HG3	1.86	0.56
3:D:1272:ARG:NH2	3:D:1582:CYS:SG	2.79	0.56
3:D:4186:MET:HE2	3:D:4186:MET:HA	1.87	0.56
3:B:3320:LEU:HD23	3:B:3321:PRO:HD3	1.86	0.56
3:B:4640:PHE:HB3	3:B:4641:PRO:HD3	1.88	0.56
3:D:1243:THR:HG22	3:D:1808:ASP:HB2	1.87	0.56
3:D:2322:ARG:O	3:D:2326:ARG:HG2	2.04	0.56
3:D:4028:SER:O	3:D:4033:LYS:NZ	2.36	0.56
3:A:1495:SER:OG	3:A:1496:PRO:HD2	2.06	0.56
3:A:4186:MET:HA	3:A:4186:MET:HE2	1.87	0.56
3:B:1682:GLU:HG2	3:B:1683:PRO:HD3	1.86	0.56
3:C:2743:TYR:HA	3:C:2757:MET:HE1	1.86	0.56
3:A:1176:THR:HG22	3:A:1181:ILE:HA	1.88	0.56
3:A:2171:VAL:HG21	3:A:2199:PHE:CD2	2.41	0.56
3:C:249:SER:HA	3:C:257:ARG:NH2	2.20	0.56
3:C:1272:ARG:NH2	3:C:1582:CYS:SG	2.79	0.56
3:D:476:GLN:NE2	3:D:3678:GLU:OE1	2.39	0.56
3:D:3461:MET:C	3:D:3461:MET:HE3	2.31	0.56
3:A:2734:MET:HE2	3:A:2823:PRO:HB2	1.85	0.56
3:A:2744:GLY:HA2	3:A:2753:VAL:HG13	1.86	0.56
3:A:3686:PHE:HA	3:A:3689:MET:HE2	1.88	0.56
3:B:1176:THR:HG22	3:B:1181:ILE:HA	1.88	0.56
3:B:1272:ARG:NH2	3:B:1582:CYS:SG	2.79	0.56
3:B:2171:VAL:HG21	3:B:2199:PHE:CD2	2.41	0.56
3:B:2830:ASN:ND2	3:C:1435:GLY:HA2	2.20	0.56
3:C:1951:LEU:HD12	3:C:1958:THR:HG21	1.86	0.56
3:C:2545:ILE:HD12	3:C:2580:LEU:HD21	1.86	0.56
3:C:3594:GLN:HA	3:C:3597:ARG:HD3	1.88	0.56
3:D:3594:GLN:HA	3:D:3597:ARG:HD3	1.88	0.56
1:G:24:VAL:HG22	1:G:48:LYS:HG2	1.88	0.56
3:A:323:ASP:O	3:A:325:LYS:N	2.33	0.56
3:A:3274:ASN:OD1	3:A:3275:THR:N	2.38	0.56
3:A:4640:PHE:HB3	3:A:4641:PRO:HD3	1.88	0.56
3:C:246:THR:HG21	3:C:267:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:476:GLN:NE2	3:C:3678:GLU:OE1	2.39	0.56
3:C:601:LEU:HG	3:C:610:VAL:HG11	1.87	0.56
3:C:1268:ILE:HD11	3:C:1300:MET:HE2	1.86	0.56
3:C:3184:TYR:HA	3:C:3192:ARG:NH1	2.20	0.56
3:C:4053:GLU:OE2	3:C:4060:GLN:NE2	2.39	0.56
2:J:92:VAL:HG12	2:J:93:PHE:HD1	1.71	0.56
3:A:2758:LYS:HE3	3:A:2763:LEU:HA	1.87	0.56
3:B:2488:LEU:HD21	3:B:2548:LEU:HD22	1.88	0.56
3:B:3594:GLN:HA	3:B:3597:ARG:HD3	1.88	0.56
3:B:3778:LEU:HB2	3:B:3854:PHE:CZ	2.41	0.56
3:D:875:PRO:HD2	3:D:878:LEU:HD12	1.86	0.56
3:D:1176:THR:HG22	3:D:1181:ILE:HA	1.88	0.56
3:D:2171:VAL:HG21	3:D:2199:PHE:CD2	2.41	0.56
3:D:3686:PHE:HA	3:D:3689:MET:HE2	1.88	0.56
3:D:4664:ASP:OD1	3:D:4674:LYS:NZ	2.29	0.56
1:F:50:ARG:HB3	1:F:50:ARG:NH1	2.22	0.55
3:A:419:ILE:HG21	3:A:492:GLU:HG3	1.88	0.55
3:A:476:GLN:NE2	3:A:3678:GLU:OE1	2.39	0.55
3:A:3461:MET:HE3	3:A:3461:MET:C	2.31	0.55
3:B:558:LEU:HG	3:B:571:ILE:HG23	1.86	0.55
3:B:3461:MET:C	3:B:3461:MET:HE3	2.31	0.55
3:C:558:LEU:HG	3:C:571:ILE:HG23	1.86	0.55
3:C:1243:THR:HG22	3:C:1808:ASP:HB2	1.87	0.55
1:E:24:VAL:HG22	1:E:48:LYS:HG2	1.88	0.55
2:K:92:VAL:HG12	2:K:93:PHE:HD1	1.71	0.55
3:A:3594:GLN:HA	3:A:3597:ARG:HD3	1.88	0.55
3:B:1243:THR:HG22	3:B:1808:ASP:HB2	1.87	0.55
3:B:2610:LEU:HD13	3:B:2644:LEU:HD21	1.89	0.55
3:C:1495:SER:OG	3:C:1496:PRO:HD2	2.06	0.55
3:C:2171:VAL:HG21	3:C:2199:PHE:CD2	2.41	0.55
3:C:2325:ILE:HD12	3:D:207:PHE:CZ	2.42	0.55
3:C:2610:LEU:HD13	3:C:2644:LEU:HD21	1.89	0.55
3:C:3274:ASN:OD1	3:C:3275:THR:N	2.38	0.55
3:A:246:THR:HG21	3:A:267:VAL:HG11	1.88	0.55
3:A:4053:GLU:OE2	3:A:4060:GLN:NE2	2.39	0.55
3:B:246:THR:HG21	3:B:267:VAL:HG11	1.88	0.55
3:B:875:PRO:HD2	3:B:878:LEU:HD12	1.86	0.55
3:B:4019:MET:HG2	3:B:4066:LEU:HD11	1.89	0.55
3:B:4053:GLU:OE2	3:B:4060:GLN:NE2	2.39	0.55
3:D:1495:SER:OG	3:D:1496:PRO:HD2	2.06	0.55
3:A:2488:LEU:HD21	3:A:2548:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3892:TYR:O	3:A:3957:LYS:NZ	2.37	0.55
3:B:3274:ASN:OD1	3:B:3275:THR:N	2.38	0.55
3:C:4155:SER:O	3:C:4159:GLN:HG2	2.07	0.55
3:D:4019:MET:HG2	3:D:4066:LEU:HD11	1.89	0.55
3:A:2947:SER:HA	3:A:2952:GLU:HA	1.88	0.55
3:A:4019:MET:HG2	3:A:4066:LEU:HD11	1.89	0.55
1:F:24:VAL:HG22	1:F:48:LYS:HG2	1.88	0.55
1:H:50:ARG:HB3	1:H:50:ARG:NH1	2.22	0.55
3:A:3778:LEU:HB2	3:A:3854:PHE:CZ	2.41	0.55
3:B:601:LEU:HG	3:B:610:VAL:HG11	1.87	0.55
3:C:3250:TRP:NE1	3:C:3309:LYS:HG2	2.22	0.55
3:C:3686:PHE:HA	3:C:3689:MET:HE2	1.88	0.55
3:C:4187:GLU:OE1	3:C:4949:TRP:NE1	2.31	0.55
3:D:419:ILE:HG21	3:D:492:GLU:HG3	1.88	0.55
1:G:50:ARG:HB3	1:G:50:ARG:NH1	2.22	0.55
2:L:14:LYS:HG2	3:D:2153:LYS:HD3	1.89	0.55
3:A:3493:LYS:HZ2	3:A:3558:LEU:HB2	1.72	0.55
3:B:2789:ILE:HD11	3:B:2901:TYR:HB3	1.88	0.55
3:C:2947:SER:HA	3:C:2952:GLU:HA	1.88	0.55
3:D:246:THR:HG21	3:D:267:VAL:HG11	1.88	0.55
3:A:3234:VAL:O	3:A:3238:ILE:HB	2.07	0.55
3:B:841:LYS:O	3:B:848:ARG:NH2	2.34	0.55
3:C:4019:MET:HG2	3:C:4066:LEU:HD11	1.89	0.55
3:D:11:ILE:HD12	3:D:176:ARG:HG2	1.89	0.55
3:D:3778:LEU:HB2	3:D:3854:PHE:CZ	2.41	0.55
3:D:4053:GLU:OE2	3:D:4060:GLN:NE2	2.39	0.55
1:E:50:ARG:HB3	1:E:50:ARG:NH1	2.22	0.55
2:L:61:ASN:CG	2:L:62:GLY:H	2.15	0.55
3:A:2405:GLU:OE1	3:A:2407:HIS:ND1	2.39	0.55
3:B:11:ILE:HD12	3:B:176:ARG:HG2	1.89	0.55
3:B:2947:SER:HA	3:B:2952:GLU:HA	1.88	0.55
3:C:1176:THR:HG22	3:C:1181:ILE:HA	1.88	0.55
3:D:2947:SER:HA	3:D:2952:GLU:HA	1.88	0.55
3:D:3250:TRP:NE1	3:D:3309:LYS:HG2	2.22	0.55
1:H:78:THR:OG1	1:H:80:ASP:OD1	2.23	0.55
2:K:61:ASN:CG	2:K:62:GLY:H	2.15	0.55
3:B:164:PRO:HB3	3:B:169:ARG:HB2	1.89	0.55
3:B:419:ILE:HG21	3:B:492:GLU:HG3	1.88	0.55
3:B:1495:SER:OG	3:B:1496:PRO:HD2	2.06	0.55
3:B:3188:SER:OG	3:B:3190:ARG:NH1	2.40	0.55
3:C:1937:GLN:NE2	3:C:3608:LEU:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4028:SER:O	3:C:4033:LYS:NZ	2.36	0.55
3:D:2610:LEU:HD13	3:D:2644:LEU:HD21	1.89	0.55
3:A:4155:SER:O	3:A:4159:GLN:HG2	2.07	0.54
3:B:1937:GLN:NE2	3:B:3608:LEU:O	2.40	0.54
3:B:2683:SER:OG	3:B:2685:TYR:O	2.25	0.54
3:C:3778:LEU:HB2	3:C:3854:PHE:CZ	2.41	0.54
3:D:2488:LEU:HD21	3:D:2548:LEU:HD22	1.89	0.54
2:K:4:GLN:HG2	2:K:5:LEU:HD12	1.90	0.54
3:C:2789:ILE:HD11	3:C:2901:TYR:HB3	1.88	0.54
3:C:3493:LYS:HZ2	3:C:3558:LEU:CB	2.18	0.54
2:I:92:VAL:HG12	2:I:93:PHE:HD1	1.71	0.54
2:J:4:GLN:HG2	2:J:5:LEU:HD12	1.90	0.54
3:A:1937:GLN:NE2	3:A:3608:LEU:O	2.40	0.54
3:A:2610:LEU:HD13	3:A:2644:LEU:HD21	1.89	0.54
3:C:3188:SER:OG	3:C:3190:ARG:NH1	2.40	0.54
3:D:629:GLN:OE1	3:D:1669:ASN:ND2	2.38	0.54
3:D:3072:MET:SD	3:D:3139:ALA:HB3	2.48	0.54
3:D:3234:VAL:O	3:D:3238:ILE:HB	2.07	0.54
2:I:107:ARG:HG2	2:I:121:GLU:HG3	1.89	0.54
2:I:128:GLU:CA	2:I:131:ILE:HD11	2.29	0.54
2:L:92:VAL:HG12	2:L:93:PHE:HD1	1.71	0.54
3:B:4155:SER:O	3:B:4159:GLN:HG2	2.07	0.54
3:C:2146:LEU:O	3:C:2150:MET:HG2	2.08	0.54
3:D:1273:ILE:HB	3:D:1282:CYS:HB2	1.90	0.54
3:D:1937:GLN:NE2	3:D:3608:LEU:O	2.40	0.54
3:D:2690:GLU:HB2	3:D:2692:GLN:HE22	1.72	0.54
2:I:4:GLN:HG2	2:I:5:LEU:HD12	1.90	0.54
2:L:33:LEU:O	2:L:37:MET:HG2	2.08	0.54
3:A:1273:ILE:HB	3:A:1282:CYS:HB2	1.90	0.54
3:A:3072:MET:SD	3:A:3139:ALA:HB3	2.48	0.54
3:B:3686:PHE:HA	3:B:3689:MET:HE2	1.88	0.54
3:C:2787:TRP:HE1	3:C:2905:ARG:HH21	1.56	0.54
3:D:896:ASN:O	3:D:900:LEU:HG	2.08	0.54
3:D:2146:LEU:O	3:D:2150:MET:HG2	2.08	0.54
3:D:3493:LYS:HZ2	3:D:3558:LEU:CB	2.18	0.54
2:I:61:ASN:CG	2:I:62:GLY:H	2.15	0.54
2:J:61:ASN:CG	2:J:62:GLY:H	2.15	0.54
3:A:1117:TRP:HB3	3:A:1201:PHE:HB3	1.90	0.54
3:A:1564:MET:SD	3:A:1565:PRO:HD2	2.48	0.54
3:A:2690:GLU:HB2	3:A:2692:GLN:HE22	1.72	0.54
3:B:2405:GLU:OE1	3:B:2407:HIS:ND1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3427:ASN:OD1	3:B:3463:THR:O	2.22	0.54
3:D:1117:TRP:HB3	3:D:1201:PHE:HB3	1.90	0.54
2:K:33:LEU:O	2:K:37:MET:HG2	2.08	0.54
3:A:896:ASN:O	3:A:900:LEU:HG	2.08	0.54
3:A:3188:SER:OG	3:A:3190:ARG:NH1	2.40	0.54
3:B:1048:ASP:OD1	3:B:1049:SER:N	2.41	0.54
3:B:1564:MET:SD	3:B:1565:PRO:HD2	2.48	0.54
3:B:3250:TRP:NE1	3:B:3309:LYS:HG2	2.22	0.54
3:C:141:ASP:HB3	3:C:144:ALA:HB3	1.90	0.54
3:C:164:PRO:HB3	3:C:169:ARG:HB2	1.89	0.54
3:D:2789:ILE:HD11	3:D:2901:TYR:HB3	1.89	0.54
2:I:128:GLU:HG3	2:I:131:ILE:HD11	1.89	0.54
2:J:107:ARG:HG2	2:J:121:GLU:HG3	1.89	0.54
2:K:140:GLU:O	2:K:143:VAL:HG22	2.08	0.54
3:B:2690:GLU:HB2	3:B:2692:GLN:HE22	1.72	0.54
3:C:3507:ASP:OD1	3:C:3510:ARG:NH2	2.41	0.54
3:D:4155:SER:O	3:D:4159:GLN:HG2	2.07	0.54
3:B:981:MET:HE1	3:B:1056:THR:HA	1.90	0.54
3:B:1722:ASN:O	3:B:1919:ARG:NH2	2.41	0.54
3:B:2146:LEU:O	3:B:2150:MET:HG2	2.08	0.54
3:B:3234:VAL:O	3:B:3238:ILE:HB	2.07	0.54
3:D:4107:GLU:OE1	3:D:4149:TYR:OH	2.23	0.54
3:A:2146:LEU:O	3:A:2150:MET:HG2	2.07	0.54
3:A:2683:SER:OG	3:A:2685:TYR:O	2.25	0.54
3:A:3493:LYS:HZ2	3:A:3558:LEU:CB	2.19	0.54
3:C:659:ILE:HD11	3:C:826:VAL:HG22	1.90	0.54
3:C:1273:ILE:HB	3:C:1282:CYS:HB2	1.90	0.54
3:D:1048:ASP:OD1	3:D:1049:SER:N	2.41	0.54
3:D:3427:ASN:CG	3:D:3463:THR:C	2.64	0.54
2:I:33:LEU:O	2:I:37:MET:HG2	2.08	0.53
2:J:140:GLU:O	2:J:143:VAL:HG22	2.08	0.53
3:A:11:ILE:HD12	3:A:176:ARG:HG2	1.89	0.53
3:B:659:ILE:HD11	3:B:826:VAL:HG22	1.90	0.53
3:B:2787:TRP:HE1	3:B:2905:ARG:HH21	1.56	0.53
3:C:2488:LEU:HD21	3:C:2548:LEU:HD22	1.89	0.53
3:C:2561:LEU:O	3:C:2566:ARG:NH1	2.42	0.53
3:C:3072:MET:SD	3:C:3139:ALA:HB3	2.48	0.53
3:D:141:ASP:HB3	3:D:144:ALA:HB3	1.90	0.53
2:J:138:ASN:HD21	2:J:141:GLU:HB2	1.74	0.53
2:K:11:ALA:O	2:K:15:GLU:OE1	2.26	0.53
2:L:107:ARG:HG2	2:L:121:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:896:ASN:O	3:B:900:LEU:HG	2.08	0.53
3:C:141:ASP:O	3:C:143:LEU:N	2.41	0.53
3:C:896:ASN:O	3:C:900:LEU:HG	2.08	0.53
3:C:3234:VAL:O	3:C:3238:ILE:HB	2.07	0.53
3:D:981:MET:HE1	3:D:1056:THR:HA	1.90	0.53
3:D:1564:MET:SD	3:D:1565:PRO:HD2	2.48	0.53
2:I:138:ASN:HD21	2:I:141:GLU:HB2	1.74	0.53
2:L:11:ALA:O	2:L:15:GLU:OE1	2.26	0.53
3:A:164:PRO:HB3	3:A:169:ARG:HB2	1.90	0.53
3:A:981:MET:HE1	3:A:1056:THR:HA	1.90	0.53
3:A:3145:SER:HB3	3:A:3148:VAL:HG22	1.91	0.53
3:B:3072:MET:SD	3:B:3139:ALA:HB3	2.48	0.53
3:C:981:MET:HE1	3:C:1056:THR:HA	1.90	0.53
3:C:1564:MET:SD	3:C:1565:PRO:HD2	2.48	0.53
3:C:2405:GLU:OE1	3:C:2407:HIS:ND1	2.39	0.53
1:G:78:THR:OG1	1:G:80:ASP:OD1	2.23	0.53
3:A:2789:ILE:HD11	3:A:2901:TYR:HB3	1.89	0.53
3:B:3507:ASP:OD1	3:B:3510:ARG:NH2	2.41	0.53
3:C:2690:GLU:HB2	3:C:2692:GLN:HE22	1.72	0.53
3:D:2202:TYR:O	3:D:2206:ILE:HG12	2.09	0.53
3:D:3507:ASP:OD1	3:D:3510:ARG:NH2	2.41	0.53
3:A:1722:ASN:O	3:A:1919:ARG:NH2	2.41	0.53
3:B:1273:ILE:HB	3:B:1282:CYS:HB2	1.90	0.53
3:B:3145:SER:HB3	3:B:3148:VAL:HG22	1.91	0.53
3:C:11:ILE:HD12	3:C:176:ARG:HG2	1.89	0.53
3:C:419:ILE:HG21	3:C:492:GLU:HG3	1.88	0.53
3:C:629:GLN:OE1	3:C:1669:ASN:ND2	2.37	0.53
3:C:2202:TYR:O	3:C:2206:ILE:HG12	2.09	0.53
3:C:2683:SER:OG	3:C:2685:TYR:O	2.25	0.53
3:D:2787:TRP:HE1	3:D:2905:ARG:HH21	1.56	0.53
3:D:3188:SER:OG	3:D:3190:ARG:NH1	2.40	0.53
2:J:33:LEU:O	2:J:37:MET:HG2	2.08	0.53
2:K:138:ASN:HD21	2:K:141:GLU:HB2	1.74	0.53
2:L:4:GLN:HG2	2:L:5:LEU:HD12	1.90	0.53
2:L:140:GLU:O	2:L:143:VAL:HG22	2.08	0.53
3:A:1973:ILE:HG21	3:A:3620:PHE:HA	1.91	0.53
3:A:2202:TYR:O	3:A:2206:ILE:HG12	2.08	0.53
3:C:3145:SER:HB3	3:C:3148:VAL:HG22	1.91	0.53
3:D:141:ASP:O	3:D:143:LEU:N	2.41	0.53
3:D:164:PRO:HB3	3:D:169:ARG:HB2	1.89	0.53
3:D:1722:ASN:O	3:D:1919:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4637:THR:HG22	3:D:4639:SER:H	1.74	0.53
1:F:50:ARG:NH1	1:F:53:LYS:HG3	2.24	0.53
3:A:141:ASP:O	3:A:143:LEU:N	2.41	0.53
3:A:1048:ASP:OD1	3:A:1049:SER:N	2.41	0.53
3:A:2561:LEU:O	3:A:2566:ARG:NH1	2.42	0.53
3:A:3250:TRP:NE1	3:A:3309:LYS:HG2	2.22	0.53
3:B:4107:GLU:OE1	3:B:4149:TYR:OH	2.23	0.53
3:B:4637:THR:HG22	3:B:4639:SER:H	1.74	0.53
3:C:841:LYS:O	3:C:848:ARG:NH2	2.34	0.53
3:C:1722:ASN:O	3:C:1919:ARG:NH2	2.41	0.53
3:D:1973:ILE:HG21	3:D:3620:PHE:HA	1.91	0.53
2:K:107:ARG:HG2	2:K:121:GLU:HG3	1.89	0.53
3:A:3507:ASP:OD1	3:A:3510:ARG:NH2	2.41	0.53
3:A:4107:GLU:OE1	3:A:4149:TYR:OH	2.23	0.53
3:B:1117:TRP:HB3	3:B:1201:PHE:HB3	1.90	0.53
3:B:1973:ILE:HG21	3:B:3620:PHE:HA	1.91	0.53
3:B:2202:TYR:O	3:B:2206:ILE:HG12	2.08	0.53
3:C:983:LEU:O	3:C:1055:ARG:NH2	2.41	0.53
3:C:1048:ASP:OD1	3:C:1049:SER:N	2.41	0.53
3:C:1117:TRP:HB3	3:C:1201:PHE:HB3	1.90	0.53
3:C:2730:ASP:OD1	3:C:2821:TYR:OH	2.27	0.53
3:C:3100:ALA:HB1	3:C:3104:MET:HE2	1.91	0.53
3:D:1911:GLN:OE1	3:D:2090:ARG:NH1	2.33	0.53
3:A:2285:TYR:OH	3:A:2380:ASP:O	2.27	0.53
3:A:4753:LEU:HG	3:B:4773:LEU:HD22	1.90	0.53
3:B:4775:ALA:HA	3:B:4817:MET:CE	2.39	0.53
3:C:4637:THR:HG22	3:C:4639:SER:H	1.74	0.53
3:C:4775:ALA:HA	3:C:4817:MET:CE	2.39	0.53
1:H:8:ILE:HA	3:D:730:LEU:HD11	1.90	0.53
2:I:140:GLU:O	2:I:143:VAL:HG22	2.08	0.53
2:L:49:LEU:O	2:L:53:ILE:HG12	2.09	0.53
3:A:1967:SER:O	3:A:3605:MET:HE2	2.09	0.53
3:A:2787:TRP:HE1	3:A:2905:ARG:HH21	1.56	0.53
3:A:3524:ILE:HG22	3:A:3528:MET:HE1	1.91	0.53
3:A:4637:THR:HG22	3:A:4639:SER:H	1.74	0.53
3:B:2730:ASP:OD1	3:B:2821:TYR:OH	2.27	0.53
3:B:3100:ALA:HB1	3:B:3104:MET:HE2	1.91	0.53
3:C:1973:ILE:HG21	3:C:3620:PHE:HA	1.91	0.53
2:I:111:THR:CB	3:A:1960:ARG:HH22	2.22	0.52
3:A:141:ASP:HB3	3:A:144:ALA:HB3	1.90	0.52
3:A:3280:ILE:O	3:A:3284:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1107:THR:HB	3:C:1113:MET:HE1	1.91	0.52
3:C:2826:ILE:HA	3:D:1501:ASN:HD21	1.73	0.52
3:C:3427:ASN:OD1	3:C:3463:THR:O	2.22	0.52
3:D:2730:ASP:OD1	3:D:2821:TYR:OH	2.27	0.52
1:G:50:ARG:NH1	1:G:53:LYS:HG3	2.24	0.52
2:J:128:GLU:CA	2:J:131:ILE:HD11	2.29	0.52
2:K:49:LEU:O	2:K:53:ILE:HG12	2.09	0.52
2:L:87:ARG:HA	2:L:90:PHE:CE1	2.45	0.52
2:L:138:ASN:HD21	2:L:141:GLU:HB2	1.74	0.52
3:A:1089:ARG:HB3	3:A:1204:VAL:HG23	1.91	0.52
3:A:2730:ASP:OD1	3:A:2821:TYR:OH	2.27	0.52
3:C:3524:ILE:HG22	3:C:3528:MET:HE1	1.91	0.52
3:D:1967:SER:O	3:D:3605:MET:HE2	2.09	0.52
1:H:50:ARG:NH1	1:H:53:LYS:HG3	2.24	0.52
2:J:11:ALA:O	2:J:15:GLU:OE1	2.27	0.52
2:K:110:MET:HE3	2:K:124:GLU:OE2	2.10	0.52
2:L:143:VAL:O	2:L:147:THR:HG22	2.10	0.52
3:B:515:ALA:HB2	3:B:523:GLY:HA3	1.91	0.52
3:B:983:LEU:O	3:B:1055:ARG:NH2	2.41	0.52
3:C:3280:ILE:O	3:C:3284:ILE:HG12	2.09	0.52
3:C:3627:SER:O	3:C:3631:THR:OG1	2.24	0.52
3:C:3997:LYS:HG2	3:C:4109:MET:HE1	1.92	0.52
3:D:515:ALA:HB2	3:D:523:GLY:HA3	1.91	0.52
3:D:3524:ILE:HG22	3:D:3528:MET:HE1	1.91	0.52
2:I:11:ALA:O	2:I:15:GLU:OE1	2.26	0.52
2:I:87:ARG:HA	2:I:90:PHE:CE1	2.45	0.52
2:J:87:ARG:HA	2:J:90:PHE:CE1	2.45	0.52
3:A:2722:ASN:O	3:A:2726:GLU:HG3	2.10	0.52
3:B:132:CYS:SG	3:B:187:SER:OG	2.68	0.52
3:B:1967:SER:O	3:B:3605:MET:HE2	2.09	0.52
3:C:132:CYS:SG	3:C:187:SER:OG	2.68	0.52
3:D:659:ILE:HD11	3:D:826:VAL:HG22	1.90	0.52
3:D:2285:TYR:OH	3:D:2380:ASP:O	2.27	0.52
3:D:2561:LEU:O	3:D:2566:ARG:NH1	2.42	0.52
1:E:50:ARG:NH1	1:E:53:LYS:HG3	2.24	0.52
2:K:87:ARG:HA	2:K:90:PHE:CE1	2.45	0.52
3:C:2285:TYR:OH	3:C:2380:ASP:O	2.27	0.52
3:D:2072:GLU:O	3:D:3660:ARG:NH1	2.43	0.52
3:D:3145:SER:HB3	3:D:3148:VAL:HG22	1.91	0.52
3:D:3280:ILE:O	3:D:3284:ILE:HG12	2.09	0.52
2:I:147:THR:HA	3:A:3596:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:544:ASN:HB3	3:A:547:ASN:HB2	1.91	0.52
3:A:659:ILE:HD11	3:A:826:VAL:HG22	1.90	0.52
3:A:849:ASP:OD1	3:A:1214:ARG:NE	2.43	0.52
3:A:2929:LEU:HD13	3:A:2971:ILE:HG12	1.91	0.52
3:B:544:ASN:HB3	3:B:547:ASN:HB2	1.91	0.52
3:B:3414:ARG:NH1	3:B:3417:GLN:OE1	2.43	0.52
3:B:3997:LYS:HG2	3:B:4109:MET:HE1	1.92	0.52
3:C:3427:ASN:CG	3:C:3463:THR:C	2.64	0.52
3:D:983:LEU:O	3:D:1055:ARG:NH2	2.41	0.52
3:D:3684:GLU:HG3	3:D:3689:MET:HE1	1.92	0.52
2:J:110:MET:HE3	2:J:124:GLU:OE2	2.10	0.52
3:A:983:LEU:O	3:A:1055:ARG:NH2	2.41	0.52
3:B:270:HIS:CD2	3:B:491:GLU:HG3	2.45	0.52
3:B:2561:LEU:O	3:B:2566:ARG:NH1	2.42	0.52
3:C:1089:ARG:HB3	3:C:1204:VAL:HG23	1.91	0.52
3:C:1911:GLN:OE1	3:C:2090:ARG:NH1	2.33	0.52
3:C:2436:ILE:HG22	3:C:2491:GLY:HA3	1.92	0.52
3:D:849:ASP:OD1	3:D:1214:ARG:NE	2.43	0.52
3:D:1107:THR:HB	3:D:1113:MET:HE1	1.91	0.52
3:D:2722:ASN:O	3:D:2726:GLU:HG3	2.10	0.52
3:A:629:GLN:OE1	3:A:1669:ASN:ND2	2.38	0.52
3:B:2285:TYR:OH	3:B:2380:ASP:O	2.27	0.52
3:C:3250:TRP:HB2	3:C:3273:MET:CE	2.40	0.52
1:E:80:ASP:OD1	1:E:81:VAL:N	2.43	0.52
2:I:49:LEU:O	2:I:53:ILE:HG12	2.09	0.52
2:K:143:VAL:O	2:K:147:THR:HG22	2.10	0.52
3:A:515:ALA:HB2	3:A:523:GLY:HA3	1.91	0.52
3:A:1107:THR:HB	3:A:1113:MET:HE1	1.91	0.52
3:B:3250:TRP:HB2	3:B:3273:MET:CE	2.40	0.52
3:B:4170:ARG:NH1	5:B:5002:ATP:O2G	2.40	0.52
3:C:544:ASN:HB3	3:C:547:ASN:HB2	1.91	0.52
3:C:814:LEU:HD12	3:C:815:PRO:HD2	1.92	0.52
3:C:3729:ALA:HA	3:C:3732:HIS:CD2	2.45	0.52
3:D:1009:ARG:O	3:D:1013:ARG:NE	2.42	0.52
3:D:2683:SER:OG	3:D:2685:TYR:O	2.25	0.52
3:D:3100:ALA:HB1	3:D:3104:MET:HE2	1.91	0.52
3:D:3414:ARG:NH1	3:D:3417:GLN:OE1	2.43	0.52
3:A:2541:HIS:O	3:A:2545:ILE:HG12	2.10	0.52
3:A:3729:ALA:HA	3:A:3732:HIS:CD2	2.45	0.52
3:B:629:GLN:OE1	3:B:1669:ASN:ND2	2.37	0.52
3:B:849:ASP:OD1	3:B:1214:ARG:NE	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:270:HIS:CD2	3:C:491:GLU:HG3	2.45	0.52
3:C:849:ASP:OD1	3:C:1214:ARG:NE	2.43	0.52
3:C:2722:ASN:O	3:C:2726:GLU:HG3	2.10	0.52
3:C:2929:LEU:HD13	3:C:2971:ILE:HG12	1.91	0.52
3:D:544:ASN:HB3	3:D:547:ASN:HB2	1.91	0.52
3:D:562:LEU:HD22	3:D:600:LEU:HD22	1.92	0.52
3:D:1089:ARG:HB3	3:D:1204:VAL:HG23	1.91	0.52
2:I:110:MET:HE3	2:I:124:GLU:OE2	2.10	0.51
2:I:143:VAL:O	2:I:147:THR:HG22	2.10	0.51
3:C:1967:SER:O	3:C:3605:MET:HE2	2.09	0.51
3:D:2405:GLU:OE1	3:D:2407:HIS:ND1	2.39	0.51
3:D:3250:TRP:HB2	3:D:3273:MET:CE	2.40	0.51
2:J:49:LEU:O	2:J:53:ILE:HG12	2.09	0.51
3:A:562:LEU:HD22	3:A:600:LEU:HD22	1.92	0.51
3:A:814:LEU:HD12	3:A:815:PRO:HD2	1.92	0.51
3:A:3414:ARG:NH1	3:A:3417:GLN:OE1	2.43	0.51
3:B:141:ASP:HB3	3:B:144:ALA:HB3	1.90	0.51
3:B:562:LEU:HD22	3:B:600:LEU:HD22	1.92	0.51
3:B:1107:THR:HB	3:B:1113:MET:HE1	1.91	0.51
3:B:2541:HIS:O	3:B:2545:ILE:HG12	2.10	0.51
3:B:3524:ILE:HG22	3:B:3528:MET:HE1	1.91	0.51
3:C:562:LEU:HD22	3:C:600:LEU:HD22	1.92	0.51
3:C:2072:GLU:O	3:C:3660:ARG:NH1	2.43	0.51
3:C:3684:GLU:HG3	3:C:3689:MET:HE1	1.92	0.51
3:D:1549:SER:OG	3:D:1551:ASN:O	2.28	0.51
3:D:3997:LYS:HG2	3:D:4109:MET:HE1	1.92	0.51
1:E:8:ILE:HA	3:A:730:LEU:HD11	1.93	0.51
2:L:110:MET:HE3	2:L:124:GLU:OE2	2.10	0.51
3:A:1549:SER:OG	3:A:1551:ASN:O	2.28	0.51
3:A:2478:ILE:HD13	3:A:2527:LEU:HD11	1.92	0.51
3:B:2072:GLU:O	3:B:3660:ARG:NH1	2.43	0.51
3:B:3560:HIS:O	3:B:3564:LYS:C	2.53	0.51
3:B:4091:ALA:C	3:B:4093:ASP:H	2.18	0.51
3:C:1009:ARG:O	3:C:1013:ARG:NE	2.42	0.51
3:C:3414:ARG:NH1	3:C:3417:GLN:OE1	2.43	0.51
3:C:4170:ARG:NH1	5:C:5002:ATP:O2G	2.40	0.51
3:D:132:CYS:SG	3:D:187:SER:OG	2.68	0.51
3:D:4775:ALA:HA	3:D:4817:MET:CE	2.39	0.51
1:E:78:THR:OG1	1:E:80:ASP:OD1	2.23	0.51
1:F:26:HIS:CD2	1:F:105:LEU:HD11	2.46	0.51
1:F:80:ASP:OD1	1:F:81:VAL:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:113:LEU:HD13	3:A:1966:ARG:HB2	1.92	0.51
2:L:128:GLU:HA	2:L:131:ILE:HD11	1.93	0.51
3:A:132:CYS:SG	3:A:187:SER:OG	2.68	0.51
3:A:3100:ALA:HB1	3:A:3104:MET:HE2	1.91	0.51
3:A:4775:ALA:HA	3:A:4817:MET:CE	2.39	0.51
3:B:1089:ARG:HB3	3:B:1204:VAL:HG23	1.91	0.51
3:B:1549:SER:OG	3:B:1551:ASN:O	2.28	0.51
3:B:3280:ILE:O	3:B:3284:ILE:HG12	2.09	0.51
3:C:1118:SER:HB3	3:C:1204:VAL:HG11	1.93	0.51
3:C:1549:SER:OG	3:C:1551:ASN:O	2.28	0.51
3:C:2541:HIS:O	3:C:2545:ILE:HG12	2.10	0.51
3:D:814:LEU:HD12	3:D:815:PRO:HD2	1.92	0.51
3:D:2929:LEU:HD13	3:D:2971:ILE:HG12	1.91	0.51
3:D:3427:ASN:OD1	3:D:3463:THR:O	2.22	0.51
1:G:80:ASP:OD1	1:G:81:VAL:N	2.43	0.51
3:A:270:HIS:CD2	3:A:491:GLU:HG3	2.45	0.51
3:A:1009:ARG:O	3:A:1013:ARG:NE	2.42	0.51
3:A:1772:SER:OG	3:A:1774:GLU:OE1	2.28	0.51
3:A:3684:GLU:HG3	3:A:3689:MET:HE1	1.92	0.51
3:B:2478:ILE:HD13	3:B:2527:LEU:HD11	1.91	0.51
3:C:3560:HIS:O	3:C:3564:LYS:C	2.54	0.51
3:C:4747:ALA:HA	3:C:4753:LEU:HB3	1.92	0.51
3:D:3560:HIS:O	3:D:3564:LYS:C	2.54	0.51
3:D:3729:ALA:HA	3:D:3732:HIS:CD2	2.45	0.51
3:D:4091:ALA:C	3:D:4093:ASP:H	2.18	0.51
3:D:4747:ALA:HA	3:D:4753:LEU:HB3	1.92	0.51
1:E:26:HIS:CD2	1:E:105:LEU:HD11	2.46	0.51
1:G:26:HIS:CD2	1:G:105:LEU:HD11	2.46	0.51
3:A:3427:ASN:HD21	3:A:3464:SER:HA	1.76	0.51
3:A:3560:HIS:O	3:A:3564:LYS:C	2.54	0.51
3:A:3997:LYS:HG2	3:A:4109:MET:HE1	1.92	0.51
3:B:141:ASP:O	3:B:143:LEU:N	2.41	0.51
3:B:2436:ILE:HG22	3:B:2491:GLY:HA3	1.92	0.51
3:B:4045:LYS:HD3	3:B:4078:LEU:HD23	1.93	0.51
3:C:2478:ILE:HD13	3:C:2527:LEU:HD11	1.92	0.51
3:C:3324:GLU:HG2	3:C:3327:LYS:NZ	2.26	0.51
3:D:1118:SER:HB3	3:D:1204:VAL:HG11	1.93	0.51
3:D:2478:ILE:HD13	3:D:2527:LEU:HD11	1.92	0.51
3:D:2779:LEU:HA	3:D:2782:MET:HG2	1.92	0.51
3:D:4045:LYS:HD3	3:D:4078:LEU:HD23	1.93	0.51
1:H:26:HIS:CD2	1:H:105:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:466:PRO:HG2	3:A:479:LEU:HG	1.93	0.51
3:A:2072:GLU:O	3:A:3660:ARG:NH1	2.43	0.51
3:A:4091:ALA:C	3:A:4093:ASP:H	2.18	0.51
3:B:1118:SER:HB3	3:B:1204:VAL:HG11	1.93	0.51
3:B:2929:LEU:HD13	3:B:2971:ILE:HG12	1.91	0.51
3:B:3015:VAL:HG23	3:B:3029:ILE:HD12	1.93	0.51
3:B:3427:ASN:HD21	3:B:3464:SER:HA	1.76	0.51
3:C:1932:PHE:CE1	3:C:1996:LEU:HB2	2.46	0.51
3:C:3047:LYS:HD2	3:C:3048:THR:HG23	1.93	0.51
3:C:4091:ALA:C	3:C:4093:ASP:H	2.18	0.51
3:D:1932:PHE:CE1	3:D:1996:LEU:HB2	2.46	0.51
3:D:3015:VAL:HG23	3:D:3029:ILE:HD12	1.93	0.51
3:A:1118:SER:HB3	3:A:1204:VAL:HG11	1.93	0.51
3:A:3493:LYS:NZ	3:A:3558:LEU:HB2	2.23	0.51
3:A:4045:LYS:HD3	3:A:4078:LEU:HD23	1.93	0.51
3:C:732:LEU:HB3	3:C:779:PHE:CZ	2.46	0.51
3:C:4045:LYS:HD3	3:C:4078:LEU:HD23	1.93	0.51
3:C:4107:GLU:OE1	3:C:4149:TYR:OH	2.23	0.51
3:D:270:HIS:CD2	3:D:491:GLU:HG3	2.45	0.51
3:D:2541:HIS:O	3:D:2545:ILE:HG12	2.10	0.51
2:J:143:VAL:O	2:J:147:THR:HG22	2.10	0.51
3:A:3015:VAL:HG23	3:A:3029:ILE:HD12	1.93	0.51
3:A:3250:TRP:HB2	3:A:3273:MET:CE	2.40	0.51
3:B:185:SER:OG	3:B:188:SER:OG	2.28	0.51
3:B:713:TRP:HZ2	3:B:1251:LEU:HD21	1.76	0.51
3:C:3015:VAL:HG23	3:C:3029:ILE:HD12	1.93	0.51
3:C:3803:LEU:HB2	3:C:3884:SER:HB2	1.93	0.51
3:D:3324:GLU:HG2	3:D:3327:LYS:NZ	2.26	0.51
1:H:80:ASP:OD1	1:H:81:VAL:N	2.43	0.51
2:K:128:GLU:HG3	2:K:131:ILE:HD11	1.89	0.51
3:A:3427:ASN:HB2	3:A:3463:THR:HG1	1.73	0.51
3:A:3455:LYS:O	3:A:3459:TYR:HB3	2.11	0.51
3:B:466:PRO:HG2	3:B:479:LEU:HG	1.93	0.51
3:B:3493:LYS:NZ	3:B:3558:LEU:HB2	2.23	0.51
3:B:3684:GLU:HG3	3:B:3689:MET:HE1	1.92	0.51
3:B:4620:GLN:OE1	3:B:4632:ARG:NH2	2.44	0.51
3:C:2508:SER:OG	3:C:2560:SER:OG	2.28	0.51
3:D:466:PRO:HG2	3:D:479:LEU:HG	1.93	0.51
3:D:2436:ILE:HG22	3:D:2491:GLY:HA3	1.92	0.51
2:I:12:GLU:HA	2:I:15:GLU:OE1	2.12	0.50
3:A:4620:GLN:OE1	3:A:4632:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:814:LEU:HD12	3:B:815:PRO:HD2	1.92	0.50
3:B:2722:ASN:O	3:B:2726:GLU:HG3	2.10	0.50
3:B:3455:LYS:O	3:B:3459:TYR:HB3	2.11	0.50
3:B:3729:ALA:HA	3:B:3732:HIS:CD2	2.45	0.50
3:D:3427:ASN:HD21	3:D:3464:SER:HA	1.76	0.50
2:I:88:GLU:OE1	2:I:91:ARG:NH2	2.45	0.50
3:A:4625:ASP:OD1	3:A:4625:ASP:N	2.43	0.50
3:B:4827:ILE:O	3:B:4831:ILE:HG12	2.11	0.50
3:C:515:ALA:HB2	3:C:523:GLY:HA3	1.91	0.50
3:C:4620:GLN:OE1	3:C:4632:ARG:NH2	2.44	0.50
3:D:732:LEU:HB3	3:D:779:PHE:CZ	2.46	0.50
3:A:307:SER:HB3	3:A:327:THR:HG22	1.94	0.50
3:A:1932:PHE:CE1	3:A:1996:LEU:HB2	2.46	0.50
3:A:2779:LEU:HA	3:A:2782:MET:HG2	1.92	0.50
3:A:3803:LEU:HB2	3:A:3884:SER:HB2	1.93	0.50
3:A:4827:ILE:O	3:A:4831:ILE:HG12	2.12	0.50
3:B:732:LEU:HB3	3:B:779:PHE:CZ	2.46	0.50
3:B:2779:LEU:HA	3:B:2782:MET:HG2	1.92	0.50
3:C:466:PRO:HG2	3:C:479:LEU:HG	1.93	0.50
3:C:1428:TYR:OH	3:C:1444:GLY:O	2.30	0.50
3:D:258:ARG:NE	3:D:316:LEU:O	2.33	0.50
3:D:3047:LYS:HD2	3:D:3048:THR:HG23	1.93	0.50
3:D:4827:ILE:O	3:D:4831:ILE:HG12	2.11	0.50
2:J:12:GLU:HA	2:J:15:GLU:OE1	2.12	0.50
2:K:128:GLU:HA	2:K:131:ILE:HD11	1.93	0.50
3:A:2436:ILE:HG22	3:A:2491:GLY:HA3	1.92	0.50
3:A:4747:ALA:HA	3:A:4753:LEU:HB3	1.92	0.50
3:B:1932:PHE:CE1	3:B:1996:LEU:HB2	2.46	0.50
3:C:1729:MET:CE	3:C:1930:ASP:HB2	2.41	0.50
3:D:737:ILE:HD12	3:D:1482:ARG:HD3	1.94	0.50
3:D:2322:ARG:HH22	3:D:2415:GLU:HG3	1.77	0.50
2:L:12:GLU:HA	2:L:15:GLU:OE1	2.12	0.50
2:L:88:GLU:OE1	2:L:91:ARG:NH2	2.45	0.50
3:A:317:MET:HB2	3:A:321:LYS:HD2	1.94	0.50
3:A:1729:MET:CE	3:A:1930:ASP:HB2	2.41	0.50
3:A:3047:LYS:HD2	3:A:3048:THR:HG23	1.93	0.50
3:B:1772:SER:OG	3:B:1774:GLU:OE1	2.28	0.50
3:B:2834:SER:O	3:B:2838[A]:HIS:HB2	2.11	0.50
3:C:4014:LEU:HD13	3:C:4122:ALA:HB2	1.94	0.50
3:D:4014:LEU:HD13	3:D:4122:ALA:HB2	1.94	0.50
3:D:4620:GLN:OE1	3:D:4632:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:115:TYR:HE2	3:A:169:ARG:HB3	1.77	0.50
3:A:1428:TYR:OH	3:A:1444:GLY:O	2.30	0.50
3:B:3076:LYS:O	3:B:3077:GLN:HG3	2.12	0.50
3:C:2779:LEU:HA	3:C:2782:MET:HG2	1.92	0.50
3:C:4896:ASP:HA	3:C:4899:ASP:HB2	1.94	0.50
3:D:317:MET:HB2	3:D:321:LYS:HD2	1.94	0.50
3:D:3467:VAL:HB	3:D:3471:LYS:NZ	2.27	0.50
2:K:88:GLU:OE1	2:K:91:ARG:NH2	2.45	0.50
3:A:737:ILE:HD12	3:A:1482:ARG:HD3	1.94	0.50
3:A:2834:SER:O	3:A:2838[A]:HIS:HB2	2.11	0.50
3:A:3427:ASN:OD1	3:A:3465:LEU:CD2	2.60	0.50
3:B:737:ILE:HD12	3:B:1482:ARG:HD3	1.94	0.50
3:B:1428:TYR:OH	3:B:1444:GLY:O	2.30	0.50
3:B:3336:GLU:HG3	3:B:3355:ILE:HG22	1.94	0.50
3:B:4014:LEU:HD13	3:B:4122:ALA:HB2	1.94	0.50
3:B:4747:ALA:HA	3:B:4753:LEU:HB3	1.92	0.50
3:C:559:ILE:HG23	3:C:562:LEU:HD12	1.93	0.50
3:C:713:TRP:HZ2	3:C:1251:LEU:HD21	1.76	0.50
3:C:3427:ASN:HD21	3:C:3464:SER:HA	1.75	0.50
3:C:3455:LYS:O	3:C:3459:TYR:HB3	2.11	0.50
3:D:3455:LYS:O	3:D:3459:TYR:HB3	2.11	0.50
2:J:128:GLU:HG3	2:J:131:ILE:HD11	1.89	0.50
3:A:242:ASP:OD1	3:A:242:ASP:N	2.45	0.50
3:A:3280:ILE:CG2	3:A:3299:LEU:HD21	2.42	0.50
3:B:1001:GLU:OE2	3:B:1005:ASN:ND2	2.45	0.50
3:C:3427:ASN:CB	3:C:3463:THR:OG1	2.42	0.50
3:D:1428:TYR:OH	3:D:1444:GLY:O	2.30	0.50
3:D:1844:GLN:NE2	3:D:1853:GLU:OE1	2.45	0.50
2:J:128:GLU:HA	2:J:131:ILE:HD11	1.93	0.50
3:A:3324:GLU:HG2	3:A:3327:LYS:NZ	2.26	0.50
3:B:2920:ARG:HG3	3:B:2923:TYR:HB2	1.93	0.50
3:B:3427:ASN:OD1	3:B:3465:LEU:CD2	2.60	0.50
3:C:2920:ARG:HG3	3:C:2923:TYR:HB2	1.93	0.50
3:C:3280:ILE:CG2	3:C:3299:LEU:HD21	2.42	0.50
3:C:4827:ILE:O	3:C:4831:ILE:HG12	2.12	0.50
3:D:115:TYR:HE2	3:D:169:ARG:HB3	1.77	0.50
3:D:2749:ASP:HA	3:D:2754:GLN:OE1	2.12	0.50
3:D:2857:LYS:HA	3:D:2860:LEU:HG	1.93	0.50
2:I:128:GLU:HA	2:I:131:ILE:HD11	1.93	0.49
2:J:67:PRO:HB2	3:B:2202:TYR:CZ	2.46	0.49
2:J:88:GLU:OE1	2:J:91:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:732:LEU:HB3	3:A:779:PHE:CZ	2.46	0.49
3:B:1009:ARG:O	3:B:1013:ARG:NE	2.42	0.49
3:B:4896:ASP:HA	3:B:4899:ASP:HB2	1.94	0.49
3:C:185:SER:OG	3:C:188:SER:OG	2.28	0.49
3:C:737:ILE:HD12	3:C:1482:ARG:HD3	1.94	0.49
3:C:3691:TYR:O	3:C:3695:MET:HG3	2.12	0.49
3:D:1729:MET:CE	3:D:1930:ASP:HB2	2.41	0.49
3:D:3280:ILE:CG2	3:D:3299:LEU:HD21	2.42	0.49
3:D:4116:GLN:HA	3:D:4119:LEU:HD12	1.94	0.49
3:D:4896:ASP:HA	3:D:4899:ASP:HB2	1.94	0.49
1:G:8:ILE:HA	3:C:730:LEU:HD11	1.93	0.49
3:A:1844:GLN:NE2	3:A:1853:GLU:OE1	2.45	0.49
3:A:2322:ARG:HH22	3:A:2415:GLU:HG3	1.77	0.49
3:A:3076:LYS:O	3:A:3077:GLN:HG3	2.12	0.49
3:B:2753:VAL:O	3:B:2753:VAL:HG12	2.12	0.49
3:B:3150:ARG:NH1	3:B:3151:GLN:HB3	2.28	0.49
3:B:3198:PRO:HG2	3:B:3204:VAL:HA	1.95	0.49
3:B:4116:GLN:HA	3:B:4119:LEU:HD12	1.94	0.49
3:C:1834:PHE:O	3:C:1835:HIS:ND1	2.45	0.49
3:C:1844:GLN:NE2	3:C:1853:GLU:OE1	2.45	0.49
3:C:2749:ASP:HA	3:C:2754:GLN:OE1	2.12	0.49
3:C:2834:SER:O	3:C:2838[A]:HIS:HB2	2.11	0.49
3:D:2508:SER:OG	3:D:2560:SER:OG	2.28	0.49
3:D:2837:LEU:HA	3:D:2840:MET:HE3	1.94	0.49
3:A:4014:LEU:HD13	3:A:4122:ALA:HB2	1.94	0.49
3:B:2171:VAL:HG21	3:B:2199:PHE:HD2	1.77	0.49
3:B:2749:ASP:HA	3:B:2754:GLN:OE1	2.12	0.49
3:B:2937:HIS:O	3:B:2940:ILE:HG22	2.12	0.49
3:B:3467:VAL:HB	3:B:3471:LYS:NZ	2.27	0.49
3:B:3691:TYR:O	3:B:3695:MET:HG3	2.12	0.49
3:C:2753:VAL:O	3:C:2753:VAL:HG12	2.13	0.49
3:C:4079:ASP:O	3:C:4082:GLU:HG3	2.12	0.49
3:D:59:PRO:HG3	3:D:296:ARG:CZ	2.43	0.49
3:D:242:ASP:OD1	3:D:242:ASP:N	2.45	0.49
3:D:1772:SER:OG	3:D:1774:GLU:OE1	2.28	0.49
2:I:146:MET:SD	3:A:3600:VAL:CG1	3.00	0.49
3:A:1440:ASN:HB3	3:A:1546:GLN:HB3	1.95	0.49
3:A:2857:LYS:HA	3:A:2860:LEU:HG	1.93	0.49
3:A:2920:ARG:HG3	3:A:2923:TYR:HB2	1.93	0.49
3:B:115:TYR:HE2	3:B:169:ARG:HB3	1.77	0.49
3:B:2834:SER:O	3:B:2838[B]:HIS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4079:ASP:O	3:B:4082:GLU:HG3	2.12	0.49
3:B:4796:SER:HB3	3:B:4803:ASP:H	1.77	0.49
3:C:3150:ARG:NH1	3:C:3151:GLN:HB3	2.28	0.49
3:C:3467:VAL:HB	3:C:3471:LYS:NZ	2.27	0.49
3:D:307:SER:HB3	3:D:327:THR:HG22	1.94	0.49
3:D:713:TRP:HZ2	3:D:1251:LEU:HD21	1.76	0.49
3:D:1001:GLU:OE2	3:D:1005:ASN:ND2	2.45	0.49
3:D:4637:THR:O	3:D:4650:LYS:NZ	2.41	0.49
2:J:51:ASP:OD1	2:J:52:MET:N	2.45	0.49
3:A:114:LEU:HB2	3:A:117:HIS:HD2	1.77	0.49
3:A:2937:HIS:O	3:A:2940:ILE:HG22	2.12	0.49
3:A:3198:PRO:HG2	3:A:3204:VAL:HA	1.94	0.49
3:A:3467:VAL:HB	3:A:3471:LYS:NZ	2.27	0.49
3:B:549:ALA:O	3:B:552:SER:OG	2.18	0.49
3:B:559:ILE:HG23	3:B:562:LEU:HD12	1.94	0.49
3:B:1844:GLN:NE2	3:B:1853:GLU:OE1	2.45	0.49
3:B:3280:ILE:CG2	3:B:3299:LEU:HD21	2.42	0.49
3:C:2937:HIS:O	3:C:2940:ILE:HG22	2.12	0.49
3:D:2834:SER:O	3:D:2838[A]:HIS:HB2	2.11	0.49
3:D:3242:LEU:HD12	3:D:3246:MET:HE3	1.95	0.49
3:D:3803:LEU:HB2	3:D:3884:SER:HB2	1.94	0.49
3:A:59:PRO:HG3	3:A:296:ARG:CZ	2.43	0.49
3:A:713:TRP:HZ2	3:A:1251:LEU:HD21	1.76	0.49
3:A:4896:ASP:HA	3:A:4899:ASP:HB2	1.94	0.49
3:B:2252:GLU:OE2	3:B:3819:MET:HG3	2.13	0.49
3:B:2322:ARG:HH22	3:B:2415:GLU:HG3	1.77	0.49
3:B:4172:PHE:O	3:B:4176:VAL:HG22	2.13	0.49
3:C:2154:VAL:HG13	3:C:2158:HIS:HD2	1.78	0.49
3:C:2322:ARG:HH22	3:C:2415:GLU:HG3	1.77	0.49
3:C:3076:LYS:O	3:C:3077:GLN:HG3	2.12	0.49
3:C:3198:PRO:HG2	3:C:3204:VAL:HA	1.94	0.49
3:C:3242:LEU:HD12	3:C:3246:MET:HE3	1.95	0.49
3:C:4886:THR:O	3:C:4895:ASN:N	2.46	0.49
3:D:643:LEU:O	3:D:645:GLN:NE2	2.46	0.49
3:D:3134:LEU:HB2	3:D:3162:PHE:CE1	2.48	0.49
3:D:4796:SER:HB3	3:D:4803:ASP:H	1.77	0.49
3:A:2252:GLU:OE2	3:A:3819:MET:HG3	2.13	0.49
3:A:3242:LEU:HD12	3:A:3246:MET:HE3	1.95	0.49
3:B:1440:ASN:HB3	3:B:1546:GLN:HB3	1.95	0.49
3:B:2338:GLU:HA	3:C:140:THR:HB	1.95	0.49
3:B:2857:LYS:HA	3:B:2860:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3803:LEU:HB2	3:B:3884:SER:HB2	1.93	0.49
3:C:307:SER:HB3	3:C:327:THR:HG22	1.94	0.49
3:C:3427:ASN:OD1	3:C:3465:LEU:CD2	2.60	0.49
3:C:4796:SER:HB3	3:C:4803:ASP:H	1.77	0.49
3:D:2154:VAL:HG13	3:D:2158:HIS:HD2	1.78	0.49
3:D:3076:LYS:O	3:D:3077:GLN:HG3	2.12	0.49
2:L:128:GLU:HG3	2:L:131:ILE:HD11	1.89	0.49
3:A:559:ILE:HG23	3:A:562:LEU:HD12	1.93	0.49
3:A:1001:GLU:OE2	3:A:1005:ASN:ND2	2.45	0.49
3:A:4079:ASP:O	3:A:4082:GLU:HG3	2.12	0.49
3:A:4796:SER:HB3	3:A:4803:ASP:H	1.77	0.49
3:B:2837:LEU:HA	3:B:2840:MET:HE3	1.94	0.49
3:B:3047:LYS:HD2	3:B:3048:THR:HG23	1.93	0.49
3:C:2837:LEU:HA	3:C:2840:MET:HE3	1.94	0.49
3:C:3426:ASN:C	3:C:3428:MET:H	2.21	0.49
3:C:3493:LYS:NZ	3:C:3558:LEU:HB2	2.23	0.49
3:C:4172:PHE:O	3:C:4176:VAL:HG22	2.13	0.49
3:D:2920:ARG:HG3	3:D:2923:TYR:HB2	1.93	0.49
3:D:3638:ASP:OD1	3:D:3730:ARG:NH2	2.37	0.49
3:D:3691:TYR:O	3:D:3695:MET:HG3	2.12	0.49
3:A:1834:PHE:O	3:A:1835:HIS:ND1	2.45	0.49
3:A:3426:ASN:C	3:A:3428:MET:H	2.21	0.49
3:A:4116:GLN:HA	3:A:4119:LEU:HD12	1.94	0.49
3:B:59:PRO:HG3	3:B:296:ARG:CZ	2.43	0.49
3:C:721:ASP:OD1	3:C:724:SER:OG	2.26	0.49
3:C:1001:GLU:OE2	3:C:1005:ASN:ND2	2.45	0.49
3:C:2857:LYS:HA	3:C:2860:LEU:HG	1.93	0.49
3:C:3134:LEU:HB2	3:C:3162:PHE:CE1	2.48	0.49
3:D:1644:LEU:HD23	3:D:1651:LEU:HA	1.95	0.49
3:D:2171:VAL:HG21	3:D:2199:PHE:HD2	1.77	0.49
3:D:2753:VAL:O	3:D:2753:VAL:HG12	2.13	0.49
3:D:3198:PRO:HG2	3:D:3204:VAL:HA	1.95	0.49
3:D:3427:ASN:OD1	3:D:3465:LEU:CD2	2.60	0.49
2:K:12:GLU:HA	2:K:15:GLU:OE1	2.12	0.49
3:A:2834:SER:O	3:A:2838[B]:HIS:HB2	2.12	0.49
3:A:3150:ARG:NH1	3:A:3151:GLN:HB3	2.28	0.49
3:A:3336:GLU:HG3	3:A:3355:ILE:HG22	1.94	0.49
3:A:3691:TYR:O	3:A:3695:MET:HG3	2.12	0.49
3:A:4172:PHE:O	3:A:4176:VAL:HG22	2.13	0.49
3:A:4196:THR:HB	3:A:4919:LEU:HD11	1.95	0.49
3:B:643:LEU:O	3:B:645:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2154:VAL:HG13	3:B:2158:HIS:HD2	1.78	0.49
3:B:3242:LEU:HD12	3:B:3246:MET:HE3	1.95	0.49
3:B:4196:THR:HB	3:B:4919:LEU:HD11	1.95	0.49
3:C:59:PRO:HG3	3:C:296:ARG:CZ	2.43	0.49
3:C:866:PRO:HG2	3:C:1009:ARG:HH11	1.78	0.49
3:C:3046:MET:HE2	3:C:3121:LEU:HD12	1.95	0.49
3:D:4079:ASP:O	3:D:4082:GLU:HG3	2.12	0.49
2:K:51:ASP:OD1	2:K:52:MET:N	2.45	0.48
3:A:3638:ASP:OD1	3:A:3730:ARG:NH2	2.37	0.48
3:A:3892:TYR:OH	3:A:3899:ASP:OD1	2.19	0.48
3:B:866:PRO:HG2	3:B:1009:ARG:HH11	1.78	0.48
3:B:3426:ASN:C	3:B:3428:MET:H	2.21	0.48
3:C:115:TYR:HE2	3:C:169:ARG:HB3	1.77	0.48
3:C:3467:VAL:HB	3:C:3471:LYS:HZ1	1.77	0.48
3:C:4196:THR:HB	3:C:4919:LEU:HD11	1.95	0.48
3:D:331:PHE:HE1	3:D:363:ILE:HG12	1.78	0.48
3:D:866:PRO:HG2	3:D:1009:ARG:HH11	1.78	0.48
3:D:2229:LEU:HB3	3:D:2297:ARG:HD3	1.95	0.48
3:D:4196:THR:HB	3:D:4919:LEU:HD11	1.95	0.48
1:G:88:HIS:HD2	1:G:89:PRO:HD2	1.78	0.48
2:J:15:GLU:O	2:J:19:LEU:HG	2.13	0.48
3:A:866:PRO:HG3	3:A:1005:ASN:HB3	1.95	0.48
3:B:307:SER:HB3	3:B:327:THR:HG22	1.94	0.48
3:B:2968:LEU:HB2	3:B:2969:PRO:HD3	1.96	0.48
3:B:3324:GLU:HG2	3:B:3327:LYS:NZ	2.26	0.48
3:B:3509:ILE:O	3:B:3513:ILE:HG12	2.14	0.48
3:C:2171:VAL:HG21	3:C:2199:PHE:HD2	1.77	0.48
3:C:2229:LEU:HB3	3:C:2297:ARG:HD3	1.95	0.48
3:C:4116:GLN:HA	3:C:4119:LEU:HD12	1.94	0.48
3:D:1834:PHE:O	3:D:1835:HIS:ND1	2.45	0.48
3:D:3426:ASN:C	3:D:3428:MET:H	2.21	0.48
3:A:2753:VAL:HG12	3:A:2753:VAL:O	2.13	0.48
3:A:2837:LEU:HA	3:A:2840:MET:HE3	1.94	0.48
3:A:2968:LEU:HB2	3:A:2969:PRO:HD3	1.95	0.48
3:B:1834:PHE:O	3:B:1835:HIS:ND1	2.45	0.48
3:C:2252:GLU:OE2	3:C:3819:MET:HG3	2.13	0.48
3:C:2834:SER:O	3:C:2838[B]:HIS:HB2	2.12	0.48
3:D:559:ILE:HG23	3:D:562:LEU:HD12	1.93	0.48
3:D:2252:GLU:OE2	3:D:3819:MET:HG3	2.13	0.48
3:D:2834:SER:O	3:D:2838[B]:HIS:HB2	2.12	0.48
3:D:3467:VAL:HA	3:D:3470:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3509:ILE:O	3:D:3513:ILE:HG12	2.14	0.48
3:A:331:PHE:HE1	3:A:363:ILE:HG12	1.78	0.48
3:A:2154:VAL:HG13	3:A:2158:HIS:HD2	1.78	0.48
3:A:2171:VAL:HG21	3:A:2199:PHE:HD2	1.77	0.48
3:A:4654:MET:HE1	3:A:4663:ARG:HB3	1.95	0.48
3:B:1729:MET:CE	3:B:1930:ASP:HB2	2.41	0.48
3:B:2736:LYS:HG3	3:B:2737:LEU:HD23	1.94	0.48
3:B:3134:LEU:HB2	3:B:3162:PHE:CE1	2.48	0.48
3:B:3496:PHE:CE2	3:B:3556:ASN:N	2.82	0.48
3:C:3404:ILE:O	3:C:3408:LYS:HG2	2.13	0.48
3:D:2582:PRO:HB3	3:D:2617:CYS:SG	2.54	0.48
3:D:2736:LYS:HG3	3:D:2737:LEU:HD23	1.94	0.48
3:D:2937:HIS:O	3:D:2940:ILE:HG22	2.12	0.48
3:D:3046:MET:HE2	3:D:3121:LEU:HD12	1.95	0.48
1:F:88:HIS:HD2	1:F:89:PRO:HD2	1.78	0.48
2:I:51:ASP:OD1	2:I:52:MET:N	2.45	0.48
3:A:866:PRO:HG2	3:A:1009:ARG:HH11	1.78	0.48
3:A:999:LEU:HD23	3:A:1050:LEU:HD21	1.96	0.48
3:A:1249:MET:HB3	3:A:1599:MET:HB3	1.96	0.48
3:A:2749:ASP:HA	3:A:2754:GLN:OE1	2.12	0.48
3:A:3397:ARG:NH2	3:A:3550:ARG:HD2	2.24	0.48
3:A:3467:VAL:HA	3:A:3470:LEU:HG	1.96	0.48
3:A:3740:VAL:HG13	3:A:3758:THR:HG22	1.95	0.48
3:A:4617:ILE:HG23	3:A:4665:ARG:HH22	1.78	0.48
3:B:2508:SER:OG	3:B:2560:SER:OG	2.28	0.48
3:B:3122:ILE:HG22	3:B:3127:GLN:HG2	1.96	0.48
3:B:3427:ASN:HD22	3:B:3463:THR:C	2.18	0.48
3:C:317:MET:HB2	3:C:321:LYS:HD2	1.94	0.48
3:D:2968:LEU:HB2	3:D:2969:PRO:HD3	1.95	0.48
3:D:3336:GLU:HG3	3:D:3355:ILE:HG22	1.94	0.48
3:D:3774:GLN:HB3	3:D:3854:PHE:HE2	1.79	0.48
1:E:88:HIS:HD2	1:E:89:PRO:HD2	1.78	0.48
2:L:15:GLU:O	2:L:19:LEU:HG	2.13	0.48
3:B:242:ASP:OD1	3:B:242:ASP:N	2.45	0.48
3:B:317:MET:HB2	3:B:321:LYS:HD2	1.94	0.48
3:C:1440:ASN:HB3	3:C:1546:GLN:HB3	1.95	0.48
3:C:2968:LEU:HB2	3:C:2969:PRO:HD3	1.96	0.48
3:C:3296:MET:HE2	3:C:3296:MET:HB2	1.68	0.48
3:D:999:LEU:HD23	3:D:1050:LEU:HD21	1.96	0.48
3:D:4170:ARG:NH1	5:D:5002:ATP:O2G	2.41	0.48
1:F:78:THR:OG1	1:F:80:ASP:OD1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:15:GLU:O	2:I:19:LEU:HG	2.13	0.48
2:K:15:GLU:O	2:K:19:LEU:HG	2.14	0.48
3:A:115:TYR:CE1	3:A:175:VAL:HG22	2.49	0.48
3:A:3134:LEU:HB2	3:A:3162:PHE:CE1	2.48	0.48
3:A:3427:ASN:OD1	3:A:3465:LEU:HD22	2.14	0.48
3:A:3509:ILE:O	3:A:3513:ILE:HG12	2.14	0.48
3:A:4933:HIS:HD2	3:A:4937:GLU:HB3	1.79	0.48
3:B:891:GLU:HA	3:B:894:VAL:HG22	1.96	0.48
3:B:891:GLU:O	3:B:895:MET:HG3	2.13	0.48
3:B:895:MET:HA	3:B:898:ILE:HD13	1.96	0.48
3:B:2283:LYS:HE3	3:B:2285:TYR:HE1	1.79	0.48
3:B:3467:VAL:HB	3:B:3471:LYS:HZ1	1.78	0.48
3:B:3476:ILE:O	3:B:3480:ILE:HG13	2.14	0.48
3:B:4654:MET:HE1	3:B:4663:ARG:HB3	1.95	0.48
3:C:891:GLU:O	3:C:895:MET:HG3	2.13	0.48
3:C:2283:LYS:HE3	3:C:2285:TYR:HE1	1.79	0.48
3:C:3476:ILE:O	3:C:3480:ILE:HG13	2.14	0.48
3:C:4617:ILE:HG23	3:C:4665:ARG:HH22	1.78	0.48
3:D:3122:ILE:HG22	3:D:3127:GLN:HG2	1.96	0.48
3:D:3476:ILE:O	3:D:3480:ILE:HG13	2.14	0.48
1:H:88:HIS:HD2	1:H:89:PRO:HD2	1.78	0.48
2:K:108:HIS:HE1	3:C:1956:ALA:HA	1.79	0.48
3:A:185:SER:OG	3:A:188:SER:OG	2.28	0.48
3:A:891:GLU:HA	3:A:894:VAL:HG22	1.96	0.48
3:A:4170:ARG:NH1	5:A:5002:ATP:O2G	2.40	0.48
3:B:3046:MET:HE2	3:B:3121:LEU:HD12	1.95	0.48
3:B:4617:ILE:HG23	3:B:4665:ARG:HH22	1.78	0.48
3:C:2736:LYS:HG3	3:C:2737:LEU:HD23	1.94	0.48
3:C:4933:HIS:HD2	3:C:4937:GLU:HB3	1.79	0.48
3:D:891:GLU:O	3:D:895:MET:HG3	2.13	0.48
3:D:891:GLU:HA	3:D:894:VAL:HG22	1.96	0.48
3:D:3150:ARG:NH1	3:D:3151:GLN:HB3	2.27	0.48
3:D:3404:ILE:O	3:D:3408:LYS:HG2	2.13	0.48
3:D:4172:PHE:O	3:D:4176:VAL:HG22	2.13	0.48
3:D:4933:HIS:HD2	3:D:4937:GLU:HB3	1.79	0.48
3:A:882:ARG:CZ	3:A:937:LEU:HD12	2.44	0.48
3:A:2283:LYS:HE3	3:A:2285:TYR:HE1	1.79	0.48
3:A:2582:PRO:HB3	3:A:2617:CYS:SG	2.54	0.48
3:A:3345:ARG:NH1	3:A:3347:ASP:OD1	2.44	0.48
3:A:3496:PHE:CE2	3:A:3556:ASN:N	2.82	0.48
3:B:2229:LEU:HB3	3:B:2297:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2565:GLN:O	3:B:2569:ILE:HG13	2.14	0.48
3:C:986:ILE:O	3:C:1055:ARG:NH2	2.47	0.48
3:C:2582:PRO:HB3	3:C:2617:CYS:SG	2.54	0.48
3:C:3033:LEU:HD13	3:C:3104:MET:SD	2.54	0.48
3:D:986:ILE:O	3:D:1055:ARG:NH2	2.47	0.48
3:D:4617:ILE:HG23	3:D:4665:ARG:HH22	1.78	0.48
3:A:643:LEU:O	3:A:645:GLN:NE2	2.46	0.48
3:A:2229:LEU:HB3	3:A:2297:ARG:HD3	1.95	0.48
3:A:3122:ILE:HG22	3:A:3127:GLN:HG2	1.96	0.48
3:A:3404:ILE:O	3:A:3408:LYS:HG2	2.13	0.48
3:A:4615:LEU:HA	3:A:4619:GLU:HB2	1.96	0.48
3:A:4886:THR:O	3:A:4895:ASN:N	2.46	0.48
3:B:331:PHE:HE1	3:B:363:ILE:HG12	1.78	0.48
3:B:2582:PRO:HB3	3:B:2617:CYS:SG	2.54	0.48
3:B:4933:HIS:HD2	3:B:4937:GLU:HB3	1.79	0.48
3:C:514:PHE:CE2	3:C:522:ALA:HB1	2.49	0.48
3:C:1249:MET:HB3	3:C:1599:MET:HB3	1.96	0.48
3:C:1644:LEU:HD23	3:C:1651:LEU:HA	1.95	0.48
3:C:3122:ILE:HG22	3:C:3127:GLN:HG2	1.96	0.48
3:C:3427:ASN:OD1	3:C:3465:LEU:HD22	2.14	0.48
3:C:3496:PHE:CE2	3:C:3556:ASN:N	2.82	0.48
3:C:3740:VAL:HG13	3:C:3758:THR:HG22	1.95	0.48
3:C:3774:GLN:HB3	3:C:3854:PHE:HE2	1.79	0.48
3:D:882:ARG:CZ	3:D:937:LEU:HD12	2.44	0.48
3:D:4654:MET:HE1	3:D:4663:ARG:HB3	1.95	0.48
3:A:1644:LEU:HD23	3:A:1651:LEU:HA	1.95	0.47
3:A:3476:ILE:O	3:A:3480:ILE:HG13	2.14	0.47
3:B:115:TYR:CE1	3:B:175:VAL:HG22	2.49	0.47
3:B:3033:LEU:HD13	3:B:3104:MET:SD	2.54	0.47
3:C:189:GLU:HG2	3:C:207:PHE:HE1	1.79	0.47
3:C:271:ALA:HB2	3:C:488:LEU:HD22	1.96	0.47
3:C:331:PHE:HE1	3:C:363:ILE:HG12	1.78	0.47
3:C:891:GLU:HA	3:C:894:VAL:HG22	1.96	0.47
3:D:115:TYR:CE1	3:D:175:VAL:HG22	2.49	0.47
3:D:555:LEU:HD23	3:D:589:ILE:HD11	1.96	0.47
3:D:3221:LEU:C	3:D:3223:GLU:H	2.22	0.47
3:D:3496:PHE:CE2	3:D:3556:ASN:N	2.82	0.47
3:D:4660:PHE:C	3:D:4660:PHE:CD2	2.92	0.47
3:A:891:GLU:O	3:A:895:MET:HG3	2.13	0.47
3:A:3427:ASN:CG	3:A:3463:THR:C	2.64	0.47
3:B:986:ILE:O	3:B:1055:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3297:LYS:HE3	3:B:3297:LYS:HB3	1.34	0.47
3:B:3404:ILE:O	3:B:3408:LYS:HG2	2.14	0.47
3:B:3697:LYS:HA	3:B:3700:HIS:CD2	2.49	0.47
3:C:643:LEU:O	3:C:645:GLN:NE2	2.46	0.47
3:C:2565:GLN:O	3:C:2569:ILE:HG13	2.14	0.47
3:C:2788:ARG:HB2	3:C:2904:SER:OG	2.14	0.47
3:C:3336:GLU:HG3	3:C:3355:ILE:HG22	1.94	0.47
3:C:3467:VAL:HA	3:C:3470:LEU:HG	1.96	0.47
3:D:189:GLU:HG2	3:D:207:PHE:HE1	1.79	0.47
3:D:514:PHE:CE2	3:D:522:ALA:HB1	2.49	0.47
3:D:928:GLU:HA	3:D:931:TYR:CE2	2.49	0.47
3:D:2283:LYS:HE3	3:D:2285:TYR:HE1	1.79	0.47
3:D:2758:LYS:HB2	3:D:2762:LEU:HD23	1.96	0.47
3:D:3454:ARG:N	3:D:3457:ASP:OD2	2.47	0.47
3:D:3697:LYS:HA	3:D:3700:HIS:CD2	2.49	0.47
2:I:145:MET:C	2:I:145:MET:HE3	2.39	0.47
2:L:145:MET:C	2:L:145:MET:HE3	2.39	0.47
3:A:4660:PHE:C	3:A:4660:PHE:CD2	2.92	0.47
3:B:882:ARG:CZ	3:B:937:LEU:HD12	2.44	0.47
3:B:1644:LEU:HD23	3:B:1651:LEU:HA	1.95	0.47
3:B:2758:LYS:HB2	3:B:2762:LEU:HD23	1.96	0.47
3:C:2849:HIS:CE1	3:C:2877:LEU:HD11	2.50	0.47
3:C:3183:ILE:HG13	3:C:3187:LYS:HB2	1.96	0.47
3:C:3523:ALA:HA	3:C:3526:TRP:CD1	2.50	0.47
3:C:3638:ASP:OD1	3:C:3730:ARG:NH2	2.37	0.47
3:D:2788:ARG:HB2	3:D:2904:SER:OG	2.14	0.47
3:D:3145:SER:O	3:D:3149:GLU:HG2	2.14	0.47
2:K:145:MET:HE3	2:K:145:MET:C	2.39	0.47
3:A:514:PHE:CE2	3:A:522:ALA:HB1	2.49	0.47
3:A:895:MET:HA	3:A:898:ILE:HD13	1.96	0.47
3:A:1114:ARG:NH1	3:A:1128:LEU:O	2.45	0.47
3:A:1220:ASP:O	3:A:1223:THR:OG1	2.28	0.47
3:A:2736:LYS:HG3	3:A:2737:LEU:HD23	1.94	0.47
3:A:2767:GLU:O	3:A:2770:ILE:HG12	2.14	0.47
3:A:2849:HIS:CE1	3:A:2877:LEU:HD11	2.50	0.47
3:A:3454:ARG:N	3:A:3457:ASP:OD2	2.47	0.47
3:B:111:ARG:HD3	3:B:111:ARG:HA	1.69	0.47
3:B:514:PHE:CE2	3:B:522:ALA:HB1	2.49	0.47
3:B:2767:GLU:O	3:B:2770:ILE:HG12	2.14	0.47
3:C:555:LEU:HD23	3:C:589:ILE:HD11	1.97	0.47
3:C:882:ARG:CZ	3:C:937:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:895:MET:HA	3:C:898:ILE:HD13	1.96	0.47
3:D:2290:TRP:CZ2	3:D:2388:ILE:HG12	2.50	0.47
3:D:2849:HIS:CE1	3:D:2877:LEU:HD11	2.50	0.47
3:D:3740:VAL:HG13	3:D:3758:THR:HG22	1.95	0.47
2:J:146:MET:HE2	2:J:146:MET:O	2.15	0.47
3:A:928:GLU:HA	3:A:931:TYR:CE2	2.49	0.47
3:A:2508:SER:OG	3:A:2560:SER:OG	2.28	0.47
3:B:1249:MET:HB3	3:B:1599:MET:HB3	1.96	0.47
3:C:866:PRO:HG3	3:C:1005:ASN:HB3	1.95	0.47
3:C:3509:ILE:O	3:C:3513:ILE:HG12	2.13	0.47
3:D:271:ALA:HB2	3:D:488:LEU:HD22	1.96	0.47
3:D:866:PRO:HG3	3:D:1005:ASN:HB3	1.95	0.47
3:D:2767:GLU:O	3:D:2770:ILE:HG12	2.14	0.47
3:D:4886:THR:O	3:D:4895:ASN:N	2.46	0.47
3:A:674:TYR:CE1	3:A:756:SER:HB3	2.49	0.47
3:A:877:HIS:HA	3:A:880:ARG:CD	2.45	0.47
3:A:986:ILE:O	3:A:1055:ARG:NH2	2.47	0.47
3:A:2565:GLN:O	3:A:2569:ILE:HG13	2.14	0.47
3:A:3697:LYS:HA	3:A:3700:HIS:CD2	2.50	0.47
3:A:3774:GLN:HB3	3:A:3854:PHE:HE2	1.79	0.47
3:B:866:PRO:HG3	3:B:1005:ASN:HB3	1.95	0.47
3:B:2788:ARG:HB2	3:B:2904:SER:OG	2.14	0.47
3:B:3072:MET:HG3	3:B:3140:LEU:HG	1.96	0.47
3:B:3462:GLN:OE1	3:C:1187:GLY:HA3	2.15	0.47
3:C:756:SER:HB2	3:C:769:ARG:HB2	1.97	0.47
3:C:877:HIS:HA	3:C:880:ARG:CD	2.45	0.47
3:C:928:GLU:HA	3:C:931:TYR:CE2	2.49	0.47
3:C:3145:SER:O	3:C:3149:GLU:HG2	2.15	0.47
3:C:3454:ARG:N	3:C:3457:ASP:OD2	2.47	0.47
3:D:877:HIS:HA	3:D:880:ARG:CD	2.45	0.47
3:D:3033:LEU:HD13	3:D:3104:MET:SD	2.54	0.47
3:D:3219:VAL:HA	3:D:3279:ASN:OD1	2.15	0.47
2:I:33:LEU:HD22	2:I:49:LEU:HD12	1.97	0.47
2:J:33:LEU:HD22	2:J:49:LEU:HD12	1.97	0.47
2:J:145:MET:HE3	2:J:145:MET:C	2.39	0.47
3:A:189:GLU:HG2	3:A:207:PHE:HE1	1.79	0.47
3:A:434:ASP:O	3:A:438:LYS:NZ	2.48	0.47
3:A:555:LEU:HD23	3:A:589:ILE:HD11	1.97	0.47
3:A:2758:LYS:HB2	3:A:2762:LEU:HD23	1.96	0.47
3:A:3033:LEU:HD13	3:A:3104:MET:SD	2.54	0.47
3:A:3046:MET:HE2	3:A:3121:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:363:ILE:HD12	3:B:372:LEU:HD22	1.97	0.47
3:B:555:LEU:HD23	3:B:589:ILE:HD11	1.96	0.47
3:B:877:HIS:HA	3:B:880:ARG:CD	2.45	0.47
3:B:896:ASN:HA	3:B:899:GLU:CD	2.40	0.47
3:B:928:GLU:HA	3:B:931:TYR:CE2	2.49	0.47
3:B:3345:ARG:NH1	3:B:3347:ASP:OD1	2.44	0.47
3:B:3774:GLN:HB3	3:B:3854:PHE:HE2	1.79	0.47
3:B:4615:LEU:HA	3:B:4619:GLU:HB2	1.96	0.47
3:B:4660:PHE:C	3:B:4660:PHE:CD2	2.92	0.47
3:C:114:LEU:HB2	3:C:117:HIS:HD2	1.78	0.47
3:C:749:LEU:HD22	3:C:755:ILE:HD11	1.97	0.47
3:C:3184:TYR:CE2	3:C:3201:VAL:HA	2.50	0.47
3:C:3219:VAL:HA	3:C:3279:ASN:OD1	2.15	0.47
3:C:3461:MET:HE3	3:C:3462:GLN:N	2.30	0.47
3:C:4654:MET:HE1	3:C:4663:ARG:HB3	1.95	0.47
3:D:114:LEU:HB2	3:D:117:HIS:HD2	1.77	0.47
3:D:227:TYR:HB3	3:D:352:SER:HB2	1.97	0.47
3:D:434:ASP:O	3:D:438:LYS:NZ	2.48	0.47
3:D:674:TYR:CE1	3:D:756:SER:HB3	2.50	0.47
3:D:2565:GLN:O	3:D:2569:ILE:HG13	2.14	0.47
3:D:3427:ASN:OD1	3:D:3465:LEU:HD22	2.14	0.47
3:D:4928:LYS:HE2	3:D:4932:GLU:HG3	1.97	0.47
3:A:3427:ASN:OD1	3:A:3463:THR:O	2.22	0.47
3:A:3920:LEU:O	3:A:3924:ILE:HG12	2.15	0.47
3:B:3184:TYR:CE2	3:B:3201:VAL:HA	2.50	0.47
3:B:3523:ALA:HA	3:B:3526:TRP:CD1	2.50	0.47
3:B:3740:VAL:HG13	3:B:3758:THR:HG22	1.95	0.47
3:B:3939:ARG:NH2	3:C:172:GLY:O	2.47	0.47
3:C:115:TYR:CE1	3:C:175:VAL:HG22	2.48	0.47
3:D:3393:GLU:CD	3:D:3537:ARG:HH22	2.23	0.47
3:D:3493:LYS:NZ	3:D:3558:LEU:HB2	2.23	0.47
2:L:146:MET:HE2	2:L:146:MET:O	2.15	0.47
3:A:2290:TRP:CZ2	3:A:2388:ILE:HG12	2.50	0.47
3:A:4637:THR:O	3:A:4650:LYS:NZ	2.41	0.47
3:B:189:GLU:HG2	3:B:207:PHE:HE1	1.79	0.47
3:B:3219:VAL:HA	3:B:3279:ASN:OD1	2.15	0.47
3:B:3427:ASN:OD1	3:B:3465:LEU:HD22	2.14	0.47
3:B:3454:ARG:N	3:B:3457:ASP:OD2	2.47	0.47
3:B:3467:VAL:HA	3:B:3470:LEU:HG	1.96	0.47
3:B:3920:LEU:O	3:B:3924:ILE:HG12	2.15	0.47
3:C:674:TYR:CE1	3:C:756:SER:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3221:LEU:C	3:C:3223:GLU:H	2.22	0.47
3:C:3548:VAL:O	3:C:3552:LEU:HG	2.15	0.47
3:D:895:MET:HA	3:D:898:ILE:HD13	1.96	0.47
3:D:3523:ALA:HA	3:D:3526:TRP:CD1	2.50	0.47
3:A:3072:MET:HG3	3:A:3140:LEU:HG	1.96	0.47
3:B:2290:TRP:CZ2	3:B:2388:ILE:HG12	2.50	0.47
3:B:2787:TRP:CH2	3:B:2840:MET:HB3	2.50	0.47
3:B:3638:ASP:OD1	3:B:3730:ARG:NH2	2.37	0.47
3:B:3892:TYR:OH	3:B:3899:ASP:OD1	2.19	0.47
3:B:4590:TYR:OH	3:B:4718:SER:HB2	2.15	0.47
3:C:227:TYR:HB3	3:C:352:SER:HB2	1.97	0.47
3:C:964:MET:HE3	3:C:964:MET:HB2	1.74	0.47
3:C:2290:TRP:CZ2	3:C:2388:ILE:HG12	2.50	0.47
3:C:3427:ASN:HD22	3:C:3463:THR:C	2.18	0.47
3:C:4590:TYR:OH	3:C:4718:SER:HB2	2.15	0.47
3:D:896:ASN:HA	3:D:899:GLU:CD	2.40	0.47
3:D:1440:ASN:HB3	3:D:1546:GLN:HB3	1.95	0.47
3:D:3427:ASN:CB	3:D:3463:THR:OG1	2.43	0.47
3:D:4615:LEU:HA	3:D:4619:GLU:HB2	1.96	0.47
1:F:63:GLY:O	1:F:67:MET:HG3	2.16	0.46
2:K:96:ASP:OD1	2:K:96:ASP:N	2.48	0.46
2:L:38:ARG:HD2	2:L:44:PRO:HD2	1.97	0.46
3:A:3461:MET:HE3	3:A:3462:GLN:N	2.30	0.46
3:A:3774:GLN:HB3	3:A:3854:PHE:CE2	2.51	0.46
3:B:310:GLU:H	3:B:310:GLU:CD	2.21	0.46
3:B:756:SER:HB2	3:B:769:ARG:HB2	1.97	0.46
3:B:1429:SER:OG	3:B:1556:GLU:HB2	2.15	0.46
3:C:1429:SER:OG	3:C:1556:GLU:HB2	2.15	0.46
3:C:3072:MET:HG3	3:C:3140:LEU:HG	1.97	0.46
3:C:3697:LYS:HA	3:C:3700:HIS:CD2	2.49	0.46
3:D:1249:MET:HB3	3:D:1599:MET:HB3	1.96	0.46
3:D:2765:GLU:HA	3:D:2768:LYS:HD2	1.97	0.46
3:D:3184:TYR:CE2	3:D:3201:VAL:HA	2.50	0.46
3:D:3774:GLN:HB3	3:D:3854:PHE:CE2	2.50	0.46
3:A:1114:ARG:HG2	3:A:1138:ASP:HB2	1.97	0.46
3:A:2788:ARG:HB2	3:A:2904:SER:OG	2.14	0.46
3:A:3183:ILE:HG13	3:A:3187:LYS:HB2	1.96	0.46
3:A:3184:TYR:CE2	3:A:3201:VAL:HA	2.50	0.46
3:B:749:LEU:HD22	3:B:755:ILE:HD11	1.97	0.46
3:B:999:LEU:HD23	3:B:1050:LEU:HD21	1.96	0.46
3:B:4661:TYR:HB3	3:B:4665:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:896:ASN:HA	3:C:899:GLU:CD	2.40	0.46
3:C:3774:GLN:O	3:C:3854:PHE:HZ	1.99	0.46
3:C:3920:LEU:O	3:C:3924:ILE:HG12	2.15	0.46
3:D:756:SER:HB2	3:D:769:ARG:HB2	1.97	0.46
3:D:3166:PHE:CE2	3:D:3168:VAL:HB	2.51	0.46
2:I:14:LYS:HG2	3:A:2153:LYS:HD3	1.97	0.46
3:A:271:ALA:HB2	3:A:488:LEU:HD22	1.96	0.46
3:A:363:ILE:HD12	3:A:372:LEU:HD22	1.97	0.46
3:A:1010:ASP:OD1	3:A:1013:ARG:NH2	2.48	0.46
3:A:3145:SER:O	3:A:3149:GLU:HG2	2.14	0.46
3:A:3308:ASN:OD1	3:A:3437:SER:CB	2.61	0.46
3:A:4928:LYS:HE2	3:A:4932:GLU:HG3	1.97	0.46
3:B:271:ALA:HB2	3:B:488:LEU:HD22	1.96	0.46
3:B:2765:GLU:HA	3:B:2768:LYS:HD2	1.97	0.46
3:C:1010:ASP:OD1	3:C:1013:ARG:NH2	2.48	0.46
3:C:2767:GLU:O	3:C:2770:ILE:HG12	2.14	0.46
3:C:3505:VAL:HG23	3:C:3552:LEU:HD13	1.97	0.46
3:C:3774:GLN:HB3	3:C:3854:PHE:CE2	2.50	0.46
3:D:1269:GLU:HB2	3:D:1288:LYS:HE2	1.97	0.46
3:D:3183:ILE:HG13	3:D:3187:LYS:HB2	1.96	0.46
3:D:3505:VAL:HG23	3:D:3552:LEU:HD13	1.97	0.46
2:K:38:ARG:HD2	2:K:44:PRO:HD2	1.97	0.46
3:A:33:GLN:OE1	3:A:53:SER:OG	2.34	0.46
3:A:227:TYR:HB3	3:A:352:SER:HB2	1.97	0.46
3:A:310:GLU:H	3:A:310:GLU:CD	2.21	0.46
3:A:1799:VAL:HG13	3:A:1896:MET:HE1	1.98	0.46
3:A:2787:TRP:CH2	3:A:2840:MET:HB3	2.50	0.46
3:A:3250:TRP:CE2	3:A:3309:LYS:HG2	2.51	0.46
3:A:3548:VAL:O	3:A:3552:LEU:HG	2.15	0.46
3:A:3774:GLN:O	3:A:3854:PHE:HZ	1.99	0.46
3:A:4661:TYR:HB3	3:A:4665:ARG:HH21	1.80	0.46
3:B:1010:ASP:OD1	3:B:1013:ARG:NH2	2.48	0.46
3:B:3774:GLN:HB3	3:B:3854:PHE:CE2	2.50	0.46
3:B:3774:GLN:O	3:B:3854:PHE:HZ	1.99	0.46
3:B:4891:CYS:HB3	3:B:4913:HIS:CE1	2.50	0.46
3:C:999:LEU:HD23	3:C:1050:LEU:HD21	1.96	0.46
3:C:4637:THR:O	3:C:4650:LYS:NZ	2.41	0.46
3:D:1494:MET:HE3	3:D:1494:MET:HB3	1.77	0.46
3:D:3774:GLN:O	3:D:3854:PHE:HZ	1.99	0.46
1:H:63:GLY:O	1:H:67:MET:HG3	2.16	0.46
2:J:38:ARG:HD2	2:J:44:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:111:ARG:HD3	3:A:111:ARG:HA	1.69	0.46
3:A:1429:SER:OG	3:A:1556:GLU:HB2	2.15	0.46
3:B:674:TYR:CE1	3:B:756:SER:HB3	2.50	0.46
3:B:1269:GLU:HB2	3:B:1288:LYS:HE2	1.98	0.46
3:B:1799:VAL:HG13	3:B:1896:MET:HE1	1.98	0.46
3:B:3221:LEU:C	3:B:3223:GLU:H	2.22	0.46
3:B:3559:PHE:HA	3:B:3563:GLN:NE2	2.31	0.46
3:C:1718:ARG:HD3	3:C:1831:MET:HA	1.98	0.46
3:C:3335:SER:O	3:C:3339:HIS:ND1	2.49	0.46
3:C:4928:LYS:HE2	3:C:4932:GLU:HG3	1.97	0.46
3:D:1010:ASP:OD1	3:D:1013:ARG:NH2	2.48	0.46
3:D:1114:ARG:HG2	3:D:1138:ASP:HB2	1.97	0.46
3:D:3250:TRP:CE2	3:D:3309:LYS:HG2	2.51	0.46
3:D:3307:ILE:HD11	3:D:3372:LEU:HD13	1.98	0.46
3:D:4590:TYR:OH	3:D:4718:SER:HB2	2.15	0.46
3:D:4863:GLN:O	3:D:4867:ILE:HG12	2.16	0.46
1:G:85:ALA:O	1:G:94:PRO:HB3	2.16	0.46
3:A:156:GLU:HG3	3:A:187:SER:HB3	1.98	0.46
3:A:1269:GLU:HB2	3:A:1288:LYS:HE2	1.98	0.46
3:A:3166:PHE:CE2	3:A:3168:VAL:HB	2.51	0.46
3:A:3307:ILE:HD11	3:A:3372:LEU:HD13	1.98	0.46
3:A:3523:ALA:HA	3:A:3526:TRP:CD1	2.50	0.46
3:A:3559:PHE:HA	3:A:3563:GLN:NE2	2.31	0.46
3:A:4634:VAL:HG13	3:A:4640:PHE:HE1	1.81	0.46
3:B:1718:ARG:HD3	3:B:1831:MET:HA	1.98	0.46
3:B:2849:HIS:CE1	3:B:2877:LEU:HD11	2.50	0.46
3:C:363:ILE:HD12	3:C:372:LEU:HD22	1.97	0.46
3:C:1114:ARG:NH1	3:C:1128:LEU:O	2.45	0.46
3:C:1494:MET:HE3	3:C:1494:MET:HB3	1.77	0.46
3:C:2758:LYS:HB2	3:C:2762:LEU:HD23	1.96	0.46
3:C:2787:TRP:CH2	3:C:2840:MET:HB3	2.51	0.46
3:D:878:LEU:HA	3:D:881:ILE:HG22	1.98	0.46
3:D:3920:LEU:O	3:D:3924:ILE:HG12	2.15	0.46
2:I:38:ARG:HD2	2:I:44:PRO:HD2	1.97	0.46
2:I:146:MET:HE2	2:I:146:MET:O	2.15	0.46
3:A:896:ASN:HA	3:A:899:GLU:CD	2.40	0.46
3:A:2765:GLU:HA	3:A:2768:LYS:HD2	1.97	0.46
3:B:227:TYR:HB3	3:B:352:SER:HB2	1.97	0.46
3:B:1114:ARG:HG2	3:B:1138:ASP:HB2	1.97	0.46
3:B:3145:SER:O	3:B:3149:GLU:HG2	2.14	0.46
3:B:3335:SER:O	3:B:3339:HIS:ND1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3401:GLU:HA	3:B:3404:ILE:HG12	1.98	0.46
3:C:878:LEU:HA	3:C:881:ILE:HG22	1.98	0.46
3:C:1825:PHE:CE1	3:C:1842:ILE:HD12	2.51	0.46
3:C:3374:ILE:HA	3:C:3377:VAL:HG22	1.97	0.46
3:C:3892:TYR:OH	3:C:3899:ASP:OD1	2.19	0.46
3:C:4615:LEU:HA	3:C:4619:GLU:HB2	1.96	0.46
3:D:252:HIS:C	3:D:257:ARG:HH12	2.24	0.46
3:D:1114:ARG:NH1	3:D:1128:LEU:O	2.45	0.46
3:D:2697:SER:O	3:D:2699:GLY:N	2.48	0.46
3:D:4891:CYS:HB3	3:D:4913:HIS:CE1	2.50	0.46
2:K:10:ILE:HD11	2:K:70:LEU:HD11	1.98	0.46
3:A:878:LEU:HA	3:A:881:ILE:HG22	1.98	0.46
3:A:1979:PHE:CZ	3:A:1996:LEU:HD23	2.51	0.46
3:A:4590:TYR:OH	3:A:4718:SER:HB2	2.15	0.46
3:B:3183:ILE:HG13	3:B:3187:LYS:HB2	1.96	0.46
3:C:181:LEU:HD21	3:C:214:VAL:HG23	1.98	0.46
3:C:1014:GLN:HG2	3:C:1027:ARG:NH2	2.31	0.46
3:C:1772:SER:OG	3:C:1774:GLU:OE1	2.28	0.46
3:C:3166:PHE:CE2	3:C:3168:VAL:HB	2.51	0.46
3:C:3393:GLU:CD	3:C:3537:ARG:HH22	2.23	0.46
3:C:3401:GLU:HA	3:C:3404:ILE:HG12	1.98	0.46
3:C:4891:CYS:HB3	3:C:4913:HIS:CE1	2.50	0.46
3:D:1979:PHE:CZ	3:D:1996:LEU:HD23	2.51	0.46
3:D:2187:ILE:HD13	3:D:2227:VAL:HG13	1.98	0.46
3:D:3072:MET:HG3	3:D:3140:LEU:HG	1.96	0.46
3:D:3461:MET:HE3	3:D:3462:GLN:N	2.30	0.46
1:H:85:ALA:O	1:H:94:PRO:HB3	2.16	0.46
2:K:67:PRO:HB2	3:C:2202:TYR:CZ	2.51	0.46
3:A:252:HIS:C	3:A:257:ARG:HH12	2.24	0.46
3:A:756:SER:HB2	3:A:769:ARG:HB2	1.97	0.46
3:A:3219:VAL:HA	3:A:3279:ASN:OD1	2.15	0.46
3:B:114:LEU:HB2	3:B:117:HIS:HD2	1.77	0.46
3:B:3427:ASN:CG	3:B:3463:THR:C	2.64	0.46
3:B:4137:GLU:O	3:B:4918:TYR:OH	2.32	0.46
3:C:1269:GLU:HB2	3:C:1288:LYS:HE2	1.98	0.46
3:C:1799:VAL:HG13	3:C:1896:MET:HE1	1.98	0.46
3:C:4863:GLN:O	3:C:4867:ILE:HG12	2.16	0.46
3:D:181:LEU:HD21	3:D:214:VAL:HG23	1.98	0.46
3:D:749:LEU:HD22	3:D:755:ILE:HD11	1.97	0.46
3:D:1429:SER:OG	3:D:1556:GLU:HB2	2.15	0.46
3:D:2658:GLU:HB3	3:D:2661:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2787:TRP:CH2	3:D:2840:MET:HB3	2.50	0.46
3:D:3335:SER:O	3:D:3339:HIS:ND1	2.49	0.46
3:D:3467:VAL:HB	3:D:3471:LYS:HZ1	1.81	0.46
3:D:4137:GLU:O	3:D:4918:TYR:OH	2.32	0.46
2:L:10:ILE:HD11	2:L:70:LEU:HD11	1.98	0.46
3:A:2296:GLU:HG3	3:A:2390:THR:HG22	1.98	0.46
3:A:4863:GLN:O	3:A:4867:ILE:HG12	2.16	0.46
3:B:721:ASP:OD1	3:B:724:SER:OG	2.26	0.46
3:B:1825:PHE:CE1	3:B:1842:ILE:HD12	2.51	0.46
3:B:1979:PHE:CZ	3:B:1996:LEU:HD23	2.51	0.46
3:B:2142:MET:SD	3:B:2174:VAL:HG11	2.56	0.46
3:B:3393:GLU:CD	3:B:3537:ARG:HH22	2.23	0.46
3:B:3505:VAL:HG23	3:B:3552:LEU:HD13	1.97	0.46
3:C:349:MET:HE3	3:C:349:MET:HA	1.97	0.46
3:C:1708:ASP:HA	3:C:1712:SER:HB2	1.98	0.46
3:C:2658:GLU:HB3	3:C:2661:LEU:HB3	1.98	0.46
3:C:4661:TYR:HB3	3:C:4665:ARG:HH21	1.80	0.46
3:D:1718:ARG:HD3	3:D:1831:MET:HA	1.98	0.46
2:L:33:LEU:HD22	2:L:49:LEU:HD12	1.97	0.45
2:L:51:ASP:OD1	2:L:52:MET:N	2.45	0.45
3:A:3393:GLU:CD	3:A:3537:ARG:HH22	2.23	0.45
3:A:3427:ASN:HD22	3:A:3463:THR:C	2.18	0.45
3:A:4190:VAL:HG11	3:A:4949:TRP:CH2	2.52	0.45
3:B:1014:GLN:HG2	3:B:1027:ARG:NH2	2.31	0.45
3:B:1986:CYS:O	3:B:1993:ARG:NH2	2.50	0.45
3:B:2607:LEU:HD23	3:B:2665:ALA:HA	1.98	0.45
3:B:3250:TRP:CE2	3:B:3309:LYS:HG2	2.51	0.45
3:B:3374:ILE:HA	3:B:3377:VAL:HG22	1.97	0.45
3:B:3548:VAL:O	3:B:3552:LEU:HG	2.15	0.45
3:B:4832:GLU:O	3:B:4843:ARG:NH2	2.49	0.45
3:B:4928:LYS:HE2	3:B:4932:GLU:HG3	1.97	0.45
3:C:3454:ARG:O	3:C:3458:ARG:HG2	2.16	0.45
3:C:4660:PHE:C	3:C:4660:PHE:CD2	2.92	0.45
3:D:801:ARG:HG2	3:D:1618:LEU:HA	1.98	0.45
3:D:1799:VAL:HG13	3:D:1896:MET:HE1	1.98	0.45
3:D:2607:LEU:HD23	3:D:2665:ALA:HA	1.98	0.45
3:D:3454:ARG:O	3:D:3458:ARG:HG2	2.17	0.45
1:E:45:LYS:HB2	1:E:45:LYS:HE2	1.68	0.45
1:F:45:LYS:HE2	1:F:45:LYS:HB2	1.68	0.45
2:K:33:LEU:HD22	2:K:49:LEU:HD12	1.97	0.45
2:K:146:MET:HE2	2:K:146:MET:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2697:SER:O	3:A:2699:GLY:N	2.48	0.45
3:B:935:MET:O	3:B:939:THR:OG1	2.30	0.45
3:B:948:CYS:HB3	3:B:1064:LEU:HD12	1.99	0.45
3:B:3323:MET:HE1	3:B:3326:LEU:HD22	1.99	0.45
3:C:1979:PHE:CZ	3:C:1996:LEU:HD23	2.51	0.45
3:C:2689:MET:HE1	3:C:2785:TRP:CD1	2.52	0.45
3:C:2771:TYR:O	3:C:2774:PRO:HD2	2.16	0.45
3:C:3250:TRP:CE2	3:C:3309:LYS:HG2	2.51	0.45
3:C:3277:LEU:O	3:C:3281:LEU:HD23	2.16	0.45
3:C:3333:VAL:HA	3:C:3336:GLU:CD	2.42	0.45
3:C:4190:VAL:HG11	3:C:4949:TRP:CH2	2.52	0.45
3:C:4832:GLU:O	3:C:4843:ARG:NH2	2.50	0.45
3:D:363:ILE:HD12	3:D:372:LEU:HD22	1.97	0.45
3:D:1014:GLN:HG2	3:D:1027:ARG:NH2	2.31	0.45
3:D:1986:CYS:O	3:D:1993:ARG:NH2	2.49	0.45
1:E:63:GLY:O	1:E:67:MET:HG3	2.16	0.45
2:J:10:ILE:HD11	2:J:70:LEU:HD11	1.98	0.45
2:L:61:ASN:OD1	2:L:62:GLY:N	2.49	0.45
3:A:749:LEU:HD22	3:A:755:ILE:HD11	1.97	0.45
3:A:1718:ARG:HD3	3:A:1831:MET:HA	1.98	0.45
3:A:2658:GLU:HB3	3:A:2661:LEU:HB3	1.98	0.45
3:A:2689:MET:HE1	3:A:2785:TRP:CD1	2.52	0.45
3:A:3221:LEU:C	3:A:3223:GLU:H	2.22	0.45
3:A:3335:SER:O	3:A:3339:HIS:ND1	2.49	0.45
3:B:181:LEU:HD21	3:B:214:VAL:HG23	1.98	0.45
3:B:349:MET:HA	3:B:349:MET:HE3	1.97	0.45
3:B:587:ASN:OD1	3:B:2133:ARG:NH1	2.49	0.45
3:B:2296:GLU:HG3	3:B:2390:THR:HG22	1.98	0.45
3:B:2771:TYR:O	3:B:2774:PRO:HD2	2.16	0.45
3:B:3277:LEU:O	3:B:3281:LEU:HD23	2.16	0.45
3:B:3454:ARG:O	3:B:3458:ARG:HG2	2.16	0.45
3:B:4822:ARG:HG2	3:C:4851:PHE:CD2	2.51	0.45
3:C:513:HIS:O	3:C:517:VAL:HG23	2.17	0.45
3:C:1114:ARG:HG2	3:C:1138:ASP:HB2	1.97	0.45
3:C:2590:ARG:O	3:C:2593:VAL:HG12	2.17	0.45
3:C:2765:GLU:HA	3:C:2768:LYS:HD2	1.97	0.45
3:C:3323:MET:HE1	3:C:3326:LEU:HD22	1.99	0.45
2:L:11:ALA:O	2:L:14:LYS:HB3	2.17	0.45
3:A:1986:CYS:O	3:A:1993:ARG:NH2	2.50	0.45
3:A:2142:MET:SD	3:A:2174:VAL:HG11	2.56	0.45
3:A:2187:ILE:HD13	3:A:2227:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2863:LYS:HE2	3:A:2865:GLY:O	2.17	0.45
3:A:4898:PHE:O	3:A:4904:GLY:HA3	2.17	0.45
3:B:3327:LYS:HB3	3:B:3398:MET:HE1	1.99	0.45
3:B:3333:VAL:HA	3:B:3336:GLU:CD	2.41	0.45
3:C:252:HIS:C	3:C:257:ARG:HH12	2.24	0.45
3:C:948:CYS:HB3	3:C:1064:LEU:HD12	1.98	0.45
3:C:3154:ALA:O	3:C:3157:GLU:HG3	2.17	0.45
3:C:3345:ARG:NH1	3:C:3347:ASP:OD1	2.44	0.45
3:D:1825:PHE:CE1	3:D:1842:ILE:HD12	2.51	0.45
3:D:2296:GLU:HG3	3:D:2390:THR:HG22	1.99	0.45
3:D:3345:ARG:NH1	3:D:3347:ASP:OD1	2.44	0.45
3:D:3401:GLU:HA	3:D:3404:ILE:HG12	1.98	0.45
3:D:3559:PHE:HA	3:D:3563:GLN:NE2	2.31	0.45
3:D:3892:TYR:OH	3:D:3899:ASP:OD1	2.19	0.45
3:D:4832:GLU:O	3:D:4843:ARG:NH2	2.50	0.45
3:A:2771:TYR:O	3:A:2774:PRO:HD2	2.16	0.45
3:A:3233:HIS:O	3:A:3237:VAL:HG22	2.17	0.45
3:A:3454:ARG:O	3:A:3458:ARG:HG2	2.16	0.45
3:A:4832:GLU:O	3:A:4843:ARG:NH2	2.50	0.45
3:A:4891:CYS:HB3	3:A:4913:HIS:CE1	2.50	0.45
3:B:434:ASP:O	3:B:438:LYS:NZ	2.48	0.45
3:B:866:PRO:HG2	3:B:1009:ARG:NH1	2.32	0.45
3:B:3233:HIS:O	3:B:3237:VAL:HG22	2.17	0.45
3:B:3461:MET:HE3	3:B:3462:GLN:N	2.30	0.45
3:B:4898:PHE:O	3:B:4904:GLY:HA3	2.17	0.45
3:C:549:ALA:O	3:C:552:SER:OG	2.18	0.45
3:C:801:ARG:HA	3:C:1617:TRP:O	2.17	0.45
3:C:1986:CYS:O	3:C:1993:ARG:NH2	2.50	0.45
3:C:2187:ILE:HD13	3:C:2227:VAL:HG13	1.98	0.45
3:C:2911:GLU:HG2	3:C:2912:LEU:HD23	1.99	0.45
3:D:624:ALA:HB2	3:D:1667:LEU:HD12	1.99	0.45
3:D:644:LEU:HD13	3:D:1630:LEU:HD21	1.99	0.45
3:D:2142:MET:SD	3:D:2174:VAL:HG11	2.56	0.45
3:D:3323:MET:HE1	3:D:3326:LEU:HD22	1.99	0.45
3:D:4634:VAL:HG13	3:D:4640:PHE:HE1	1.81	0.45
1:E:85:ALA:O	1:E:94:PRO:HB3	2.16	0.45
1:G:63:GLY:O	1:G:67:MET:HG3	2.16	0.45
2:L:6:THR:HG1	2:L:9:GLN:CD	2.17	0.45
3:A:1494:MET:HE3	3:A:1494:MET:HB3	1.77	0.45
3:A:1708:ASP:HA	3:A:1712:SER:HB2	1.98	0.45
3:A:1960:ARG:HA	3:A:1960:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3426:ASN:HD22	3:A:3426:ASN:HA	1.63	0.45
3:A:3505:VAL:HG23	3:A:3552:LEU:HD13	1.97	0.45
3:B:801:ARG:HG2	3:B:1618:LEU:HA	1.98	0.45
3:B:2187:ILE:HD13	3:B:2227:VAL:HG13	1.98	0.45
3:B:2689:MET:HE1	3:B:2785:TRP:CD1	2.52	0.45
3:B:3166:PHE:CE2	3:B:3168:VAL:HB	2.51	0.45
3:B:3861:GLN:H	3:B:3867:THR:HG23	1.82	0.45
3:B:4634:VAL:HG13	3:B:4640:PHE:HE1	1.81	0.45
3:B:4863:GLN:O	3:B:4867:ILE:HG12	2.16	0.45
3:B:4886:THR:O	3:B:4895:ASN:N	2.46	0.45
3:C:434:ASP:O	3:C:438:LYS:NZ	2.48	0.45
3:C:866:PRO:HG2	3:C:1009:ARG:NH1	2.32	0.45
3:D:33:GLN:OE1	3:D:53:SER:OG	2.34	0.45
3:D:587:ASN:OD1	3:D:2133:ARG:NH1	2.49	0.45
3:D:1708:ASP:HA	3:D:1712:SER:HB2	1.98	0.45
3:D:2590:ARG:O	3:D:2593:VAL:HG12	2.17	0.45
3:D:2689:MET:HE1	3:D:2785:TRP:CD1	2.52	0.45
3:D:3374:ILE:HA	3:D:3377:VAL:HG22	1.97	0.45
3:D:3548:VAL:O	3:D:3552:LEU:HG	2.15	0.45
1:F:85:ALA:O	1:F:94:PRO:HB3	2.16	0.45
2:I:11:ALA:O	2:I:14:LYS:HB3	2.17	0.45
2:I:61:ASN:OD1	2:I:62:GLY:N	2.49	0.45
3:A:181:LEU:HD21	3:A:214:VAL:HG23	1.98	0.45
3:A:349:MET:HA	3:A:349:MET:HE3	1.97	0.45
3:A:1825:PHE:CE1	3:A:1842:ILE:HD12	2.51	0.45
3:A:3374:ILE:HA	3:A:3377:VAL:HG22	1.97	0.45
3:A:3401:GLU:HA	3:A:3404:ILE:HG12	1.98	0.45
3:B:801:ARG:HA	3:B:1617:TRP:O	2.17	0.45
3:B:878:LEU:HA	3:B:881:ILE:HG22	1.98	0.45
3:B:1114:ARG:NH1	3:B:1128:LEU:O	2.45	0.45
3:B:1960:ARG:HA	3:B:1960:ARG:HE	1.82	0.45
3:B:3167:PRO:HA	3:B:3248:ARG:NH2	2.32	0.45
3:B:3553:ASP:O	3:B:3557:VAL:HG23	2.17	0.45
3:C:188:SER:HB2	3:C:190:ARG:HH11	1.82	0.45
3:C:644:LEU:HD13	3:C:1630:LEU:HD21	1.99	0.45
3:C:3307:ILE:HD11	3:C:3372:LEU:HD13	1.98	0.45
3:C:4509:VAL:HG11	3:C:4579:HIS:HB2	1.99	0.45
3:C:4634:VAL:HG13	3:C:4640:PHE:HE1	1.81	0.45
3:D:801:ARG:HA	3:D:1617:TRP:O	2.17	0.45
3:D:2771:TYR:O	3:D:2774:PRO:HD2	2.16	0.45
3:D:2863:LYS:HE2	3:D:2865:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3154:ALA:O	3:D:3157:GLU:HG3	2.17	0.45
3:D:4580:THR:OG1	3:D:4733:HIS:NE2	2.44	0.45
3:D:4661:TYR:HB3	3:D:4665:ARG:HH21	1.80	0.45
2:I:132:ASP:C	2:I:137:VAL:HG23	2.40	0.45
2:J:11:ALA:O	2:J:14:LYS:HB3	2.17	0.45
3:A:587:ASN:OD1	3:A:2133:ARG:NH1	2.49	0.45
3:A:624:ALA:HB2	3:A:1667:LEU:HD12	1.98	0.45
3:A:1014:GLN:HG2	3:A:1027:ARG:NH2	2.31	0.45
3:A:2607:LEU:HD23	3:A:2665:ALA:HA	1.98	0.45
3:B:1113:MET:HB2	3:B:1156:TRP:HZ2	1.82	0.45
3:B:2255:LEU:O	3:B:3810:ARG:NH1	2.47	0.45
3:B:2863:LYS:HE2	3:B:2865:GLY:O	2.17	0.45
3:B:4509:VAL:HG11	3:B:4579:HIS:HB2	1.99	0.45
3:C:1960:ARG:HA	3:C:1960:ARG:HE	1.82	0.45
3:C:2787:TRP:HA	3:C:2906:GLY:HA3	1.99	0.45
3:C:3861:GLN:H	3:C:3867:THR:HG23	1.82	0.45
3:D:188:SER:HB2	3:D:190:ARG:HH11	1.82	0.45
3:D:3233:HIS:O	3:D:3237:VAL:HG22	2.17	0.45
3:D:3370:TYR:HB3	3:D:3465:LEU:HD12	1.99	0.45
3:D:3427:ASN:HD22	3:D:3463:THR:C	2.18	0.45
1:G:45:LYS:HB2	1:G:45:LYS:HE2	1.68	0.45
2:I:10:ILE:HD11	2:I:70:LEU:HD11	1.98	0.45
2:K:11:ALA:O	2:K:14:LYS:HB3	2.17	0.45
3:A:513:HIS:O	3:A:517:VAL:HG23	2.17	0.45
3:A:801:ARG:HG2	3:A:1618:LEU:HA	1.98	0.45
3:B:2658:GLU:HB3	3:B:2661:LEU:HB3	1.98	0.45
3:B:2911:GLU:HG2	3:B:2912:LEU:HD23	1.99	0.45
3:C:976:TYR:O	3:C:978:PRO:HD3	2.17	0.45
3:C:2863:LYS:HE2	3:C:2865:GLY:O	2.17	0.45
3:C:3559:PHE:HA	3:C:3563:GLN:NE2	2.31	0.45
3:C:3651:PRO:CB	3:C:3652:PRO:HD3	2.47	0.45
3:C:3872:ILE:HA	3:C:3875:VAL:HG12	1.99	0.45
3:D:349:MET:HA	3:D:349:MET:HE3	1.97	0.45
3:D:2075:ILE:HG22	3:D:2077:ASP:H	1.82	0.45
3:D:2605:MET:HB3	3:D:2606:PRO:HD3	1.99	0.45
3:D:3651:PRO:CB	3:D:3652:PRO:HD3	2.47	0.45
3:D:4190:VAL:HG11	3:D:4949:TRP:CH2	2.52	0.45
2:K:61:ASN:OD1	2:K:62:GLY:N	2.49	0.45
3:A:1113:MET:HB2	3:A:1156:TRP:HZ2	1.82	0.45
3:A:1910:LEU:HB2	3:A:2087:LEU:HD21	1.99	0.45
3:A:2075:ILE:HG22	3:A:2077:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3312:PRO:HA	3:A:3376:PHE:HZ	1.82	0.45
3:A:3313:GLN:HA	3:A:3316:LYS:HD3	1.99	0.45
3:A:3323:MET:HE1	3:A:3326:LEU:HD22	1.99	0.45
3:A:4480:PHE:O	3:A:4484:ILE:HG23	2.17	0.45
3:B:188:SER:HB2	3:B:190:ARG:HH11	1.82	0.45
3:B:2590:ARG:O	3:B:2593:VAL:HG12	2.17	0.45
3:B:2596:VAL:HG21	3:B:2610:LEU:HD11	1.99	0.45
3:B:3307:ILE:HD11	3:B:3372:LEU:HD13	1.98	0.45
3:C:801:ARG:HG2	3:C:1618:LEU:HA	1.98	0.45
3:C:1113:MET:HB2	3:C:1156:TRP:HZ2	1.82	0.45
3:C:1910:LEU:HB2	3:C:2087:LEU:HD21	1.99	0.45
3:C:2607:LEU:HD23	3:C:2665:ALA:HA	1.98	0.45
3:C:3397:ARG:NH2	3:C:3550:ARG:HD2	2.24	0.45
3:D:976:TYR:O	3:D:978:PRO:HD3	2.17	0.45
3:D:1960:ARG:HA	3:D:1960:ARG:HE	1.82	0.45
3:D:3312:PRO:HA	3:D:3376:PHE:HZ	1.82	0.45
3:D:3333:VAL:HA	3:D:3336:GLU:CD	2.41	0.45
3:D:4898:PHE:O	3:D:4904:GLY:HA3	2.17	0.45
1:H:25:VAL:HG12	1:H:104:LEU:HA	1.99	0.44
3:A:188:SER:HB2	3:A:190:ARG:HH11	1.82	0.44
3:A:3333:VAL:HA	3:A:3336:GLU:CD	2.41	0.44
3:B:513:HIS:O	3:B:517:VAL:HG23	2.17	0.44
3:B:2605:MET:HB3	3:B:2606:PRO:HD3	1.99	0.44
3:C:156:GLU:HG3	3:C:187:SER:HB3	1.98	0.44
3:C:258:ARG:NE	3:C:316:LEU:O	2.33	0.44
3:C:881:ILE:O	3:C:885:LEU:HD23	2.18	0.44
3:C:2075:ILE:HG22	3:C:2077:ASP:H	1.82	0.44
3:C:3399:VAL:HG21	3:C:3473:LEU:HD22	2.00	0.44
3:C:3840:PHE:HE1	3:C:3874:THR:HG23	1.82	0.44
3:D:156:GLU:HG3	3:D:187:SER:HB3	1.98	0.44
3:D:866:PRO:HG2	3:D:1009:ARG:NH1	2.32	0.44
3:D:1910:LEU:HB2	3:D:2087:LEU:HD21	1.99	0.44
3:D:2482:ASP:OD1	3:D:2483:PHE:N	2.50	0.44
1:E:25:VAL:HG12	1:E:104:LEU:HA	1.99	0.44
2:J:96:ASP:N	2:J:96:ASP:OD1	2.48	0.44
3:A:644:LEU:HD13	3:A:1630:LEU:HD21	1.99	0.44
3:A:2590:ARG:O	3:A:2593:VAL:HG12	2.17	0.44
3:A:2688:MET:HE2	3:A:2905:ARG:CD	2.48	0.44
3:A:3167:PRO:HA	3:A:3248:ARG:NH2	2.32	0.44
3:A:3327:LYS:HB3	3:A:3398:MET:HE1	1.99	0.44
3:A:3496:PHE:HE2	3:A:3552:LEU:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:33:GLN:OE1	3:B:53:SER:OG	2.34	0.44
3:B:4190:VAL:HG11	3:B:4949:TRP:CH2	2.52	0.44
3:C:587:ASN:OD1	3:C:2133:ARG:NH1	2.49	0.44
3:C:2142:MET:SD	3:C:2174:VAL:HG11	2.56	0.44
3:C:2296:GLU:HG3	3:C:2390:THR:HG22	1.99	0.44
3:C:2697:SER:O	3:C:2699:GLY:N	2.48	0.44
3:C:3070:LYS:O	3:C:3073:GLU:HG3	2.17	0.44
3:C:3327:LYS:HB3	3:C:3398:MET:HE1	1.99	0.44
3:C:3553:ASP:O	3:C:3557:VAL:HG23	2.17	0.44
3:C:3840:PHE:CE1	3:C:3874:THR:HG23	2.53	0.44
3:C:4589:GLY:O	3:C:4590:TYR:HB3	2.17	0.44
3:D:513:HIS:O	3:D:517:VAL:HG23	2.17	0.44
3:D:3277:LEU:O	3:D:3281:LEU:HD23	2.16	0.44
3:A:557:TRP:NE1	3:A:561:ARG:HH12	2.16	0.44
3:A:976:TYR:O	3:A:978:PRO:HD3	2.17	0.44
3:A:2605:MET:HB3	3:A:2606:PRO:HD3	1.99	0.44
3:A:3277:LEU:O	3:A:3281:LEU:HD23	2.16	0.44
3:A:3840:PHE:CE1	3:A:3874:THR:HG23	2.53	0.44
3:B:76:ARG:HH11	3:B:80:GLU:HG3	1.82	0.44
3:B:1708:ASP:HA	3:B:1712:SER:HB2	1.98	0.44
3:B:1910:LEU:HB2	3:B:2087:LEU:HD21	1.99	0.44
3:B:2075:ILE:HG22	3:B:2077:ASP:H	1.82	0.44
3:B:2688:MET:HE2	3:B:2905:ARG:CD	2.48	0.44
3:B:3313:GLN:HA	3:B:3316:LYS:HD3	1.99	0.44
3:B:3423:ASN:O	3:B:3425:ILE:CD1	2.46	0.44
3:C:2596:VAL:HG21	3:C:2610:LEU:HD11	1.99	0.44
3:C:4898:PHE:O	3:C:4904:GLY:HA3	2.17	0.44
3:D:1914:CYS:SG	3:D:2091:GLN:NE2	2.78	0.44
3:D:3174:HIS:ND1	3:D:3175:LEU:HG	2.33	0.44
3:D:3313:GLN:HA	3:D:3316:LYS:HD3	1.99	0.44
3:D:3553:ASP:O	3:D:3557:VAL:HG23	2.17	0.44
3:D:3861:GLN:H	3:D:3867:THR:HG23	1.82	0.44
3:A:948:CYS:HB3	3:A:1064:LEU:HD12	1.98	0.44
3:A:995:MET:HE3	3:A:995:MET:HB3	1.56	0.44
3:B:3427:ASN:CB	3:B:3463:THR:OG1	2.42	0.44
3:B:3840:PHE:CE1	3:B:3874:THR:HG23	2.53	0.44
3:B:4480:PHE:O	3:B:4484:ILE:HG23	2.17	0.44
3:C:1091:GLU:HB3	3:C:1094:TYR:CD2	2.53	0.44
3:C:2688:MET:HE2	3:C:2905:ARG:CD	2.48	0.44
3:C:3545:GLU:HG2	3:C:3546:LYS:N	2.32	0.44
3:D:2580:LEU:HD23	3:D:2580:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4509:VAL:HG11	3:D:4579:HIS:HB2	1.99	0.44
1:G:90:GLY:HA2	3:C:638:PRO:HD3	2.00	0.44
3:A:1091:GLU:HB3	3:A:1094:TYR:CD2	2.53	0.44
3:A:1694:MET:HE2	3:A:1694:MET:HB2	1.77	0.44
3:A:3190:ARG:HG2	3:A:3191:GLU:OE1	2.17	0.44
3:A:3861:GLN:H	3:A:3867:THR:HG23	1.82	0.44
3:B:1494:MET:HE3	3:B:1494:MET:HB3	1.77	0.44
3:B:2482:ASP:OD1	3:B:2483:PHE:N	2.50	0.44
3:B:4610:LEU:HD11	3:B:4635:ILE:HG12	2.00	0.44
3:C:33:GLN:OE1	3:C:53:SER:OG	2.34	0.44
3:C:2605:MET:HB3	3:C:2606:PRO:HD3	1.99	0.44
3:C:3190:ARG:HG2	3:C:3191:GLU:OE1	2.17	0.44
3:C:3233:HIS:O	3:C:3237:VAL:HG22	2.17	0.44
3:C:3499:LYS:CE	3:C:3564:LYS:NZ	2.81	0.44
3:C:4888:CYS:HB3	3:C:4891:CYS:SG	2.58	0.44
3:D:3327:LYS:HB3	3:D:3398:MET:HE1	1.99	0.44
3:D:3399:VAL:HG21	3:D:3473:LEU:HD22	2.00	0.44
3:D:3840:PHE:HE1	3:D:3874:THR:HG23	1.82	0.44
2:L:21:ASP:OD1	2:L:22:LYS:N	2.51	0.44
2:L:96:ASP:OD1	2:L:96:ASP:N	2.48	0.44
3:A:2884:LYS:O	3:A:2887:GLU:HG3	2.18	0.44
3:A:3493:LYS:HZ3	3:A:3558:LEU:HB3	1.81	0.44
3:A:3661:VAL:HG23	3:A:3666:GLN:HG2	2.00	0.44
3:A:4610:LEU:HD11	3:A:4635:ILE:HG12	2.00	0.44
3:B:252:HIS:C	3:B:257:ARG:HH12	2.24	0.44
3:B:258:ARG:NE	3:B:316:LEU:O	2.33	0.44
3:B:976:TYR:O	3:B:978:PRO:HD3	2.17	0.44
3:B:3190:ARG:HG2	3:B:3191:GLU:OE1	2.17	0.44
3:B:4589:GLY:O	3:B:4590:TYR:HB3	2.17	0.44
3:B:4660:PHE:C	3:B:4660:PHE:HD2	2.26	0.44
3:B:4752:THR:HG23	3:B:4753:LEU:HD12	2.00	0.44
3:C:76:ARG:HH11	3:C:80:GLU:HG3	1.82	0.44
3:C:624:ALA:HB2	3:C:1667:LEU:HD12	1.99	0.44
3:C:2062:ILE:O	3:C:2066:MET:HG2	2.18	0.44
3:C:3496:PHE:HE2	3:C:3552:LEU:O	2.00	0.44
3:C:4480:PHE:O	3:C:4484:ILE:HG23	2.17	0.44
3:C:4610:LEU:HD11	3:C:4635:ILE:HG12	2.00	0.44
3:C:4753:LEU:HG	3:D:4773:LEU:HD22	1.99	0.44
3:D:557:TRP:NE1	3:D:561:ARG:HH12	2.15	0.44
3:D:2193:VAL:HG11	3:D:2227:VAL:HG11	2.00	0.44
3:D:3123:LEU:HB3	3:D:3124:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3872:ILE:HA	3:D:3875:VAL:HG12	1.99	0.44
3:D:4480:PHE:O	3:D:4484:ILE:HG23	2.18	0.44
3:D:4589:GLY:O	3:D:4590:TYR:HB3	2.16	0.44
3:D:4770:THR:HG23	3:D:4862:ILE:HG12	2.00	0.44
3:A:881:ILE:O	3:A:885:LEU:HD23	2.17	0.44
3:A:1896:MET:HG2	3:A:1896:MET:O	2.18	0.44
3:A:2773:TRP:NE1	3:A:2777:GLU:OE2	2.51	0.44
3:A:3123:LEU:HB3	3:A:3124:GLU:OE1	2.17	0.44
3:A:3553:ASP:O	3:A:3557:VAL:HG23	2.17	0.44
3:A:4660:PHE:C	3:A:4660:PHE:HD2	2.26	0.44
3:A:4770:THR:HG23	3:A:4862:ILE:HG12	2.00	0.44
3:B:2787:TRP:HA	3:B:2906:GLY:HA3	1.99	0.44
3:B:3070:LYS:O	3:B:3073:GLU:HG3	2.17	0.44
3:B:3154:ALA:O	3:B:3157:GLU:HG3	2.17	0.44
3:B:3296:MET:HE2	3:B:3296:MET:HB2	1.68	0.44
3:B:3399:VAL:HG21	3:B:3473:LEU:HD22	2.00	0.44
3:B:4584:PHE:O	3:B:4587:ILE:HG22	2.18	0.44
3:C:3313:GLN:HA	3:C:3316:LYS:HD3	1.99	0.44
3:C:3370:TYR:HB3	3:C:3465:LEU:HD12	1.99	0.44
3:C:3506:ARG:NH2	3:C:3549:GLU:OE1	2.42	0.44
3:D:3190:ARG:HG2	3:D:3191:GLU:OE1	2.17	0.44
3:D:3297:LYS:HE3	3:D:3297:LYS:HB3	1.34	0.44
3:A:514:PHE:HD2	3:A:526:TRP:HB2	1.83	0.44
3:A:758:CYS:HB3	3:A:819:TYR:CE2	2.53	0.44
3:A:1914:CYS:SG	3:A:2091:GLN:NE2	2.78	0.44
3:A:2176:VAL:HG22	3:A:2220:TYR:CZ	2.53	0.44
3:A:3070:LYS:O	3:A:3073:GLU:HG3	2.17	0.44
3:A:3154:ALA:O	3:A:3157:GLU:HG3	2.17	0.44
3:A:3215:MET:O	3:A:3219:VAL:HG23	2.18	0.44
3:A:3545:GLU:HG2	3:A:3546:LYS:N	2.32	0.44
3:A:4509:VAL:HG11	3:A:4579:HIS:HB2	1.99	0.44
3:B:156:GLU:HG3	3:B:187:SER:HB3	1.98	0.44
3:B:644:LEU:HD13	3:B:1630:LEU:HD21	1.99	0.44
3:B:3840:PHE:HE1	3:B:3874:THR:HG23	1.82	0.44
3:C:2884:LYS:O	3:C:2887:GLU:HG3	2.18	0.44
3:C:3167:PRO:HA	3:C:3248:ARG:NH2	2.32	0.44
3:D:115:TYR:CD1	3:D:175:VAL:HG22	2.53	0.44
3:D:1694:MET:HE2	3:D:1694:MET:HB2	1.77	0.44
3:D:2062:ILE:O	3:D:2066:MET:HG2	2.18	0.44
3:D:2787:TRP:HA	3:D:2906:GLY:HA3	1.99	0.44
1:F:83:TYR:OH	3:B:1768:PHE:O	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:100:TYR:HD1	2:K:137:VAL:C	2.26	0.44
3:A:115:TYR:CD1	3:A:175:VAL:HG22	2.53	0.44
3:A:866:PRO:HG2	3:A:1009:ARG:NH1	2.32	0.44
3:A:964:MET:HE3	3:A:964:MET:HB2	1.74	0.44
3:A:2193:VAL:HG11	3:A:2227:VAL:HG11	2.00	0.44
3:A:2482:ASP:OD1	3:A:2483:PHE:N	2.50	0.44
3:A:2787:TRP:HA	3:A:2906:GLY:HA3	1.99	0.44
3:A:3174:HIS:ND1	3:A:3175:LEU:HG	2.33	0.44
3:A:3399:VAL:HG21	3:A:3473:LEU:HD22	2.00	0.44
3:A:3653:GLU:OE1	3:A:3653:GLU:N	2.46	0.44
3:A:3872:ILE:HA	3:A:3875:VAL:HG12	1.99	0.44
3:A:4569:GLU:HB3	3:A:4570:PRO:HD3	2.00	0.44
3:A:4589:GLY:O	3:A:4590:TYR:HB3	2.17	0.44
3:B:557:TRP:NE1	3:B:561:ARG:HH12	2.15	0.44
3:B:758:CYS:HB3	3:B:819:TYR:CE2	2.53	0.44
3:B:2258:ARG:HB3	3:B:2260:PRO:HD2	2.00	0.44
3:B:3215:MET:O	3:B:3219:VAL:HG23	2.18	0.44
3:B:3307:ILE:HD12	3:B:3375:ARG:HD3	2.00	0.44
3:B:3308:ASN:OD1	3:B:3437:SER:CB	2.61	0.44
3:B:3496:PHE:HE2	3:B:3552:LEU:O	2.00	0.44
3:B:3651:PRO:CB	3:B:3652:PRO:HD3	2.47	0.44
3:B:4637:THR:O	3:B:4650:LYS:NZ	2.41	0.44
3:C:758:CYS:HB3	3:C:819:TYR:CE2	2.53	0.44
3:C:2482:ASP:OD1	3:C:2483:PHE:N	2.50	0.44
3:C:2773:TRP:NE1	3:C:2777:GLU:OE2	2.51	0.44
3:C:4584:PHE:O	3:C:4587:ILE:HG22	2.18	0.44
3:D:948:CYS:HB3	3:D:1064:LEU:HD12	1.98	0.44
3:D:2773:TRP:NE1	3:D:2777:GLU:OE2	2.51	0.44
3:D:3215:MET:O	3:D:3219:VAL:HG23	2.18	0.44
3:D:4584:PHE:O	3:D:4587:ILE:HG22	2.18	0.44
3:A:801:ARG:HA	3:A:1617:TRP:O	2.17	0.43
3:A:981:MET:HE3	3:A:981:MET:HB2	1.76	0.43
3:A:1097:LYS:HA	3:A:1168:MET:HE2	2.00	0.43
3:A:2087:LEU:O	3:A:2091:GLN:HG2	2.18	0.43
3:A:2757:MET:HE2	3:A:2757:MET:HB2	1.65	0.43
3:A:3366:LEU:HG	3:A:3370:TYR:CD1	2.53	0.43
3:A:3370:TYR:HB3	3:A:3465:LEU:HD12	1.99	0.43
3:A:3651:PRO:CB	3:A:3652:PRO:HD3	2.47	0.43
3:A:3840:PHE:HE1	3:A:3874:THR:HG23	1.82	0.43
3:A:4137:GLU:O	3:A:4918:TYR:OH	2.32	0.43
3:B:514:PHE:HD2	3:B:526:TRP:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2759:PRO:O	3:B:2762:LEU:N	2.51	0.43
3:B:3872:ILE:HA	3:B:3875:VAL:HG12	1.99	0.43
3:B:4753:LEU:HD11	3:C:4769:LEU:HB3	2.00	0.43
3:C:115:TYR:CD1	3:C:175:VAL:HG22	2.53	0.43
3:C:3215:MET:O	3:C:3219:VAL:HG23	2.18	0.43
3:C:3366:LEU:HG	3:C:3370:TYR:CD1	2.53	0.43
3:C:3496:PHE:CE2	3:C:3555:ALA:HB3	2.53	0.43
3:C:3794:ALA:HB2	3:C:3868:VAL:HG11	2.00	0.43
3:C:4792:PHE:HB3	3:C:4843:ARG:NH2	2.33	0.43
3:D:514:PHE:HD2	3:D:526:TRP:HB2	1.83	0.43
3:D:881:ILE:O	3:D:885:LEU:HD23	2.18	0.43
3:D:3167:PRO:HA	3:D:3248:ARG:NH2	2.32	0.43
3:D:3366:LEU:HG	3:D:3370:TYR:CD1	2.53	0.43
3:A:1829:LEU:HG	3:A:1912:TYR:CE2	2.53	0.43
3:A:2596:VAL:HG21	3:A:2610:LEU:HD11	1.99	0.43
3:A:2911:GLU:HG2	3:A:2912:LEU:HD23	1.99	0.43
3:A:3235:MET:HE1	3:A:3295:TRP:CZ3	2.53	0.43
3:A:3324:GLU:HA	3:A:3327:LYS:HZ3	1.83	0.43
3:A:3627:SER:O	3:A:3631:THR:OG1	2.24	0.43
3:B:624:ALA:HB2	3:B:1667:LEU:HD12	1.99	0.43
3:B:881:ILE:O	3:B:885:LEU:HD23	2.17	0.43
3:B:1829:LEU:HG	3:B:1912:TYR:CE2	2.53	0.43
3:B:1896:MET:O	3:B:1896:MET:HG2	2.18	0.43
3:B:2087:LEU:O	3:B:2091:GLN:HG2	2.18	0.43
3:B:2176:VAL:HG22	3:B:2220:TYR:CZ	2.53	0.43
3:B:3123:LEU:HB3	3:B:3124:GLU:OE1	2.17	0.43
3:B:3174:HIS:ND1	3:B:3175:LEU:HG	2.33	0.43
3:C:557:TRP:NE1	3:C:561:ARG:HH12	2.16	0.43
3:C:2082:ARG:HG3	3:C:3687:LEU:HD22	2.01	0.43
3:C:2176:VAL:HG22	3:C:2220:TYR:CZ	2.53	0.43
3:C:3307:ILE:HD12	3:C:3375:ARG:HD3	2.00	0.43
3:C:3496:PHE:HE2	3:C:3555:ALA:HB3	1.83	0.43
3:D:2688:MET:HE2	3:D:2905:ARG:CD	2.48	0.43
3:D:3070:LYS:O	3:D:3073:GLU:HG3	2.17	0.43
3:D:3235:MET:HE1	3:D:3295:TRP:CZ3	2.53	0.43
3:D:4606:VAL:HA	3:D:4609:LYS:HE2	2.01	0.43
3:D:4610:LEU:HD11	3:D:4635:ILE:HG12	2.00	0.43
1:F:25:VAL:HG12	1:F:104:LEU:HA	1.99	0.43
2:J:21:ASP:OD1	2:J:22:LYS:N	2.51	0.43
2:K:21:ASP:OD1	2:K:22:LYS:N	2.51	0.43
2:K:108:HIS:CE1	3:C:1956:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3499:LYS:CE	3:A:3564:LYS:NZ	2.81	0.43
3:B:2062:ILE:O	3:B:2066:MET:HG2	2.18	0.43
3:B:2082:ARG:HG3	3:B:3687:LEU:HD22	2.01	0.43
3:B:2884:LYS:O	3:B:2887:GLU:HG3	2.18	0.43
3:B:3483:PRO:O	3:B:3486:GLN:HB2	2.18	0.43
3:B:3763:ILE:HD11	3:B:3838:ASP:O	2.18	0.43
3:B:4162:LYS:HD2	3:B:4203:ALA:HB1	2.00	0.43
3:C:739:ARG:HD2	3:C:739:ARG:HA	1.81	0.43
3:C:2193:VAL:HG11	3:C:2227:VAL:HG11	2.00	0.43
3:C:3035:ILE:O	3:C:3039:THR:HG23	2.19	0.43
3:C:3123:LEU:HB3	3:C:3124:GLU:OE1	2.17	0.43
3:C:3312:PRO:HA	3:C:3376:PHE:HZ	1.82	0.43
3:C:3653:GLU:OE1	3:C:3653:GLU:N	2.47	0.43
3:C:4752:THR:HG23	3:C:4753:LEU:HD12	2.00	0.43
3:D:964:MET:HE3	3:D:964:MET:HB2	1.74	0.43
3:D:1113:MET:HB2	3:D:1156:TRP:HZ2	1.82	0.43
3:D:4203:ALA:HA	3:D:4206:ILE:HG12	2.00	0.43
2:I:17:PHE:CZ	2:I:28:ILE:HG13	2.54	0.43
3:A:2062:ILE:O	3:A:2066:MET:HG2	2.18	0.43
3:A:3109:PHE:O	3:A:3165:ALA:HB2	2.19	0.43
3:B:1694:MET:HE2	3:B:1694:MET:HB2	1.77	0.43
3:B:2773:TRP:NE1	3:B:2777:GLU:OE2	2.51	0.43
3:B:3235:MET:HE1	3:B:3295:TRP:CZ3	2.53	0.43
3:B:3496:PHE:CE2	3:B:3555:ALA:HB3	2.53	0.43
3:B:3496:PHE:HE2	3:B:3555:ALA:HB3	1.83	0.43
3:B:4888:CYS:HB3	3:B:4891:CYS:SG	2.58	0.43
3:C:1829:LEU:HG	3:C:1912:TYR:CE2	2.53	0.43
3:C:1896:MET:HG2	3:C:1896:MET:O	2.18	0.43
3:C:2087:LEU:O	3:C:2091:GLN:HG2	2.18	0.43
3:C:2988:ARG:HD2	3:C:2990:LEU:O	2.19	0.43
3:C:4902:PRO:HA	3:D:4183:LYS:HZ2	1.83	0.43
3:D:931:TYR:HA	3:D:934:GLN:HB2	2.01	0.43
3:D:981:MET:HE3	3:D:981:MET:HB2	1.76	0.43
3:D:995:MET:HE3	3:D:995:MET:HB3	1.56	0.43
3:D:1097:LYS:HA	3:D:1168:MET:HE2	2.01	0.43
3:D:3840:PHE:CE1	3:D:3874:THR:HG23	2.53	0.43
1:G:25:VAL:HG12	1:G:104:LEU:HA	1.99	0.43
2:I:83:GLU:O	2:I:87:ARG:HG2	2.18	0.43
2:I:100:TYR:HD1	2:I:137:VAL:C	2.26	0.43
2:J:17:PHE:CZ	2:J:28:ILE:HG13	2.54	0.43
2:J:100:TYR:HD1	2:J:137:VAL:C	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2224:ASN:O	3:A:2227:VAL:HG23	2.19	0.43
3:A:4888:CYS:HB3	3:A:4891:CYS:SG	2.58	0.43
3:B:3427:ASN:HB2	3:B:3463:THR:HG1	1.76	0.43
3:B:3499:LYS:CE	3:B:3564:LYS:NZ	2.81	0.43
3:B:3661:VAL:HG23	3:B:3666:GLN:HG2	2.00	0.43
3:C:3109:PHE:O	3:C:3165:ALA:HB2	2.18	0.43
3:C:3235:MET:HE1	3:C:3295:TRP:CZ3	2.53	0.43
3:D:721:ASP:OD1	3:D:724:SER:OG	2.26	0.43
3:D:1896:MET:O	3:D:1896:MET:HG2	2.18	0.43
3:D:3483:PRO:O	3:D:3486:GLN:HB2	2.18	0.43
3:D:3794:ALA:HB2	3:D:3868:VAL:HG11	2.00	0.43
2:K:83:GLU:O	2:K:87:ARG:HG2	2.18	0.43
3:A:76:ARG:HH11	3:A:80:GLU:HG3	1.82	0.43
3:A:721:ASP:OD1	3:A:724:SER:OG	2.26	0.43
3:A:2082:ARG:HG3	3:A:3687:LEU:HD22	2.01	0.43
3:A:2759:PRO:O	3:A:2762:LEU:N	2.51	0.43
3:A:3763:ILE:HD11	3:A:3838:ASP:O	2.18	0.43
3:A:4584:PHE:O	3:A:4587:ILE:HG22	2.18	0.43
3:B:1097:LYS:HA	3:B:1168:MET:HE2	2.00	0.43
3:B:3370:TYR:HB3	3:B:3465:LEU:HD12	1.99	0.43
3:B:3545:GLU:HG2	3:B:3546:LYS:N	2.32	0.43
3:C:931:TYR:HA	3:C:934:GLN:HB2	2.01	0.43
3:C:2255:LEU:O	3:C:3810:ARG:NH1	2.47	0.43
3:C:2716:LYS:HG3	3:C:2717:LEU:HD22	2.00	0.43
3:C:2759:PRO:O	3:C:2762:LEU:N	2.51	0.43
3:C:4660:PHE:C	3:C:4660:PHE:HD2	2.26	0.43
3:D:1051:ARG:HA	3:D:1054:VAL:HG12	2.00	0.43
3:D:2759:PRO:HD3	3:D:2821:TYR:HB2	2.01	0.43
3:D:3109:PHE:O	3:D:3165:ALA:HB2	2.18	0.43
3:D:3250:TRP:HB2	3:D:3273:MET:HE1	2.01	0.43
3:D:3296:MET:HE2	3:D:3296:MET:HB2	1.68	0.43
3:D:3496:PHE:HE2	3:D:3555:ALA:HB3	1.83	0.43
3:D:4660:PHE:C	3:D:4660:PHE:HD2	2.25	0.43
2:I:21:ASP:OD1	2:I:22:LYS:N	2.51	0.43
2:J:83:GLU:O	2:J:87:ARG:HG2	2.18	0.43
3:A:935:MET:O	3:A:939:THR:OG1	2.31	0.43
3:A:2258:ARG:HB3	3:A:2260:PRO:HD2	2.00	0.43
3:A:3483:PRO:O	3:A:3486:GLN:HB2	2.18	0.43
3:B:964:MET:HE3	3:B:964:MET:HB2	1.74	0.43
3:B:1091:GLU:HB3	3:B:1094:TYR:CD2	2.53	0.43
3:B:2716:LYS:HG3	3:B:2717:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3035:ILE:O	3:B:3039:THR:HG23	2.19	0.43
3:C:2736:LYS:HD2	3:C:2757:MET:SD	2.59	0.43
3:C:4162:LYS:HD2	3:C:4203:ALA:HB1	2.01	0.43
3:C:4606:VAL:HA	3:C:4609:LYS:HE2	2.01	0.43
3:D:758:CYS:HB3	3:D:819:TYR:CE2	2.53	0.43
3:D:1091:GLU:HB3	3:D:1094:TYR:CD2	2.53	0.43
3:D:1829:LEU:HG	3:D:1912:TYR:CE2	2.53	0.43
3:D:2176:VAL:HG22	3:D:2220:TYR:CZ	2.53	0.43
3:D:2596:VAL:HG21	3:D:2610:LEU:HD11	1.99	0.43
3:D:2884:LYS:O	3:D:2887:GLU:HG3	2.18	0.43
3:D:3470:LEU:HD12	3:D:3471:LYS:HD3	2.01	0.43
2:I:96:ASP:OD1	2:I:96:ASP:N	2.48	0.43
2:J:61:ASN:OD1	2:J:62:GLY:N	2.49	0.43
2:L:17:PHE:CZ	2:L:28:ILE:HG13	2.54	0.43
3:A:514:PHE:CD2	3:A:526:TRP:HB2	2.54	0.43
3:A:3331:ALA:HA	3:A:3334:VAL:HG22	2.01	0.43
3:A:3496:PHE:CE2	3:A:3555:ALA:HB3	2.53	0.43
3:A:3496:PHE:HE2	3:A:3555:ALA:HB3	1.83	0.43
3:B:115:TYR:CD1	3:B:175:VAL:HG22	2.53	0.43
3:B:330:THR:HG23	3:B:366:VAL:HG22	2.01	0.43
3:B:514:PHE:CD2	3:B:526:TRP:HB2	2.54	0.43
3:B:3312:PRO:HA	3:B:3376:PHE:HZ	1.82	0.43
3:B:4569:GLU:HB3	3:B:4570:PRO:HD3	2.00	0.43
3:C:514:PHE:CD2	3:C:526:TRP:HB2	2.54	0.43
3:C:1097:LYS:HA	3:C:1168:MET:HE2	2.00	0.43
3:C:1298:ASP:OD1	3:C:1299:ILE:N	2.52	0.43
3:C:2224:ASN:O	3:C:2227:VAL:HG23	2.19	0.43
3:C:3308:ASN:OD1	3:C:3437:SER:CB	2.61	0.43
3:C:4921:PHE:HE2	3:C:4940:VAL:HG11	1.84	0.43
3:D:150:GLN:NE2	3:D:158:CYS:SG	2.72	0.43
3:D:1966:ARG:NH2	3:D:3605:MET:O	2.52	0.43
3:D:2082:ARG:HG3	3:D:3687:LEU:HD22	2.00	0.43
3:D:2911:GLU:HG2	3:D:2912:LEU:HD23	1.99	0.43
3:D:2988:ARG:HD2	3:D:2990:LEU:O	2.19	0.43
3:D:3606:ALA:HA	3:D:3607:PRO:HD3	1.86	0.43
3:D:3661:VAL:HG23	3:D:3666:GLN:HG2	2.00	0.43
3:D:4752:THR:HG23	3:D:4753:LEU:HD12	2.00	0.43
3:D:4792:PHE:HB3	3:D:4843:ARG:NH2	2.33	0.43
3:A:3488:LEU:HA	3:A:3491:LEU:HD23	2.01	0.43
3:A:4113:THR:HA	3:A:4116:GLN:HB2	2.01	0.43
3:A:4753:LEU:HD23	3:B:4773:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:766:ILE:HB	3:B:779:PHE:HB2	2.01	0.43
3:B:3109:PHE:O	3:B:3165:ALA:HB2	2.18	0.43
3:B:4113:THR:HA	3:B:4116:GLN:HB2	2.01	0.43
3:C:1091:GLU:HB3	3:C:1094:TYR:HD2	1.84	0.43
3:C:1966:ARG:NH2	3:C:3605:MET:O	2.52	0.43
3:C:2422:ILE:HD11	3:D:189:GLU:OE2	2.19	0.43
3:C:3174:HIS:ND1	3:C:3175:LEU:HG	2.33	0.43
3:C:3250:TRP:HB2	3:C:3273:MET:HE1	2.01	0.43
3:C:3522:PRO:O	3:C:3525:ARG:HG2	2.19	0.43
3:C:3661:VAL:HG23	3:C:3666:GLN:HG2	2.00	0.43
3:C:4903:HIS:H	3:D:4183:LYS:CD	2.27	0.43
3:D:674:TYR:CD2	3:D:815:PRO:HB3	2.54	0.43
3:D:3426:ASN:HD22	3:D:3426:ASN:HA	1.63	0.43
3:D:3545:GLU:HG2	3:D:3546:LYS:N	2.32	0.43
2:L:83:GLU:O	2:L:87:ARG:HG2	2.18	0.43
3:A:766:ILE:HB	3:A:779:PHE:HB2	2.01	0.43
3:A:2603:ALA:C	3:A:2606:PRO:HD2	2.44	0.43
3:A:3794:ALA:HB2	3:A:3868:VAL:HG11	2.00	0.43
3:A:4023:LEU:HD12	3:A:4026:LEU:HD23	2.01	0.43
3:A:4752:THR:HG23	3:A:4753:LEU:HD12	2.00	0.43
3:B:1966:ARG:NH2	3:B:3605:MET:O	2.52	0.43
3:B:2224:ASN:O	3:B:2227:VAL:HG23	2.19	0.43
3:B:2603:ALA:C	3:B:2606:PRO:HD2	2.44	0.43
3:B:3794:ALA:HB2	3:B:3868:VAL:HG11	2.00	0.43
3:B:4555:ILE:HD12	3:B:4555:ILE:HA	1.79	0.43
3:B:4770:THR:HG23	3:B:4862:ILE:HG12	2.00	0.43
3:B:4792:PHE:HB3	3:B:4843:ARG:NH2	2.33	0.43
3:B:4921:PHE:HE2	3:B:4940:VAL:HG11	1.84	0.43
3:C:1559:ARG:HD2	3:C:1565:PRO:HD3	2.00	0.43
3:C:4061:SER:O	3:C:4064:GLU:HG3	2.19	0.43
3:D:2087:LEU:O	3:D:2091:GLN:HG2	2.18	0.43
3:D:3763:ILE:HD11	3:D:3838:ASP:O	2.18	0.43
3:A:330:THR:HG23	3:A:366:VAL:HG22	2.01	0.42
3:A:3250:TRP:HB2	3:A:3273:MET:HE1	2.01	0.42
3:A:3307:ILE:HD12	3:A:3375:ARG:HD3	2.00	0.42
3:A:4606:VAL:HA	3:A:4609:LYS:HE2	2.01	0.42
3:B:3071:THR:HG23	3:B:3094:ILE:HD12	2.01	0.42
3:B:3482:ALA:O	3:B:3486:GLN:HG2	2.19	0.42
3:B:3522:PRO:O	3:B:3525:ARG:HG2	2.19	0.42
3:B:4023:LEU:HD12	3:B:4026:LEU:HD23	2.01	0.42
3:B:4606:VAL:HA	3:B:4609:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4625:ASP:OD1	3:B:4625:ASP:N	2.43	0.42
3:B:4863:GLN:NE2	3:C:4860:ALA:HB2	2.34	0.42
3:B:4903:HIS:H	3:C:4183:LYS:HD2	1.84	0.42
3:C:3483:PRO:O	3:C:3486:GLN:HB2	2.18	0.42
3:C:4569:GLU:HB3	3:C:4570:PRO:HD3	2.00	0.42
3:C:4770:THR:HG23	3:C:4862:ILE:HG12	2.00	0.42
3:D:76:ARG:HH11	3:D:80:GLU:HG3	1.82	0.42
3:D:766:ILE:HB	3:D:779:PHE:HB2	2.01	0.42
3:D:1559:ARG:HD2	3:D:1565:PRO:HD3	2.01	0.42
3:D:3035:ILE:O	3:D:3039:THR:HG23	2.18	0.42
2:J:77:MET:O	2:J:79:ASP:N	2.47	0.42
2:K:17:PHE:CZ	2:K:28:ILE:HG13	2.54	0.42
2:L:100:TYR:HD1	2:L:137:VAL:C	2.26	0.42
3:A:1943:ARG:O	3:A:1946:GLU:HG2	2.19	0.42
3:A:2988:ARG:HD2	3:A:2990:LEU:O	2.19	0.42
3:A:3035:ILE:O	3:A:3039:THR:HG23	2.19	0.42
3:A:3296:MET:HB2	3:A:3296:MET:HE2	1.68	0.42
3:A:4792:PHE:HB3	3:A:4843:ARG:NH2	2.33	0.42
3:B:674:TYR:CD2	3:B:815:PRO:HB3	2.54	0.42
3:B:718:VAL:HG23	3:B:793:SER:HB3	2.01	0.42
3:B:739:ARG:HD2	3:B:739:ARG:HA	1.81	0.42
3:B:1051:ARG:HA	3:B:1054:VAL:HG12	2.00	0.42
3:B:2193:VAL:HG11	3:B:2227:VAL:HG11	2.00	0.42
3:B:3250:TRP:HB2	3:B:3273:MET:HE1	2.01	0.42
3:B:3366:LEU:HG	3:B:3370:TYR:CD1	2.53	0.42
3:C:514:PHE:HD2	3:C:526:TRP:HB2	1.83	0.42
3:C:718:VAL:HG23	3:C:793:SER:HB3	2.01	0.42
3:C:1898:LEU:HD13	3:C:1902:VAL:HG12	2.01	0.42
3:C:2759:PRO:HD3	3:C:2821:TYR:HB2	2.01	0.42
3:C:4555:ILE:HD12	3:C:4555:ILE:HA	1.79	0.42
3:D:2547:SER:OG	3:D:2876:THR:O	2.30	0.42
3:D:2736:LYS:HD2	3:D:2757:MET:SD	2.59	0.42
3:D:3071:THR:HG23	3:D:3094:ILE:HD12	2.02	0.42
3:D:3187:LYS:O	3:D:3188:SER:OG	2.35	0.42
3:D:3307:ILE:HD12	3:D:3375:ARG:HD3	2.00	0.42
3:A:938:GLU:O	3:A:942:THR:HG23	2.20	0.42
3:A:1298:ASP:OD1	3:A:1299:ILE:N	2.52	0.42
3:A:1427:TYR:HB2	3:A:1563:VAL:HG11	2.02	0.42
3:A:2641:SER:HB3	3:A:2676:LEU:HD21	2.01	0.42
3:A:4203:ALA:HA	3:A:4206:ILE:HG12	2.00	0.42
3:B:1559:ARG:HD2	3:B:1565:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:674:TYR:CD2	3:C:815:PRO:HB3	2.54	0.42
3:C:3470:LEU:HD12	3:C:3471:LYS:HD3	2.00	0.42
3:C:4113:THR:HA	3:C:4116:GLN:HB2	2.01	0.42
3:D:2224:ASN:O	3:D:2227:VAL:HG23	2.19	0.42
3:D:2258:ARG:HB3	3:D:2260:PRO:HD2	2.00	0.42
3:D:2872:VAL:HG22	3:D:2873:PRO:HD2	2.02	0.42
3:D:3496:PHE:CE2	3:D:3555:ALA:HB3	2.53	0.42
3:D:3496:PHE:HE2	3:D:3552:LEU:O	2.00	0.42
3:D:4569:GLU:HB3	3:D:4570:PRO:HD3	2.00	0.42
3:D:4888:CYS:HB3	3:D:4891:CYS:SG	2.58	0.42
2:K:101:ILE:HD12	2:K:137:VAL:O	2.19	0.42
3:A:931:TYR:HA	3:A:934:GLN:HB2	2.01	0.42
3:A:931:TYR:O	3:A:935:MET:HG2	2.19	0.42
3:B:3214:LEU:CD2	3:B:3242:LEU:HD21	2.49	0.42
3:B:3338:ASP:HA	3:B:3341:LYS:HD2	2.01	0.42
3:D:931:TYR:O	3:D:935:MET:HG2	2.19	0.42
3:D:1220:ASP:O	3:D:1223:THR:OG1	2.28	0.42
3:D:3331:ALA:HA	3:D:3334:VAL:HG22	2.01	0.42
3:D:3522:PRO:O	3:D:3525:ARG:HG2	2.19	0.42
3:D:4023:LEU:HD12	3:D:4026:LEU:HD23	2.01	0.42
2:I:101:ILE:HD12	2:I:137:VAL:O	2.19	0.42
2:J:104:ALA:O	2:J:108:HIS:CD2	2.73	0.42
3:A:1966:ARG:NH2	3:A:3605:MET:O	2.52	0.42
3:A:3071:THR:HG23	3:A:3094:ILE:HD12	2.01	0.42
3:A:3089:GLY:O	3:A:3093:ILE:HG12	2.20	0.42
3:A:3427:ASN:CB	3:A:3463:THR:OG1	2.42	0.42
3:A:4921:PHE:HE2	3:A:4940:VAL:HG11	1.84	0.42
3:B:674:TYR:HE1	3:B:756:SER:HB3	1.84	0.42
3:B:675:TYR:CE1	3:B:790:PRO:HB3	2.55	0.42
3:B:931:TYR:HA	3:B:934:GLN:HB2	2.01	0.42
3:B:1427:TYR:HB2	3:B:1563:VAL:HG11	2.02	0.42
3:B:2486:HIS:O	3:B:2490:VAL:HG22	2.20	0.42
3:B:2736:LYS:HD2	3:B:2757:MET:SD	2.59	0.42
3:B:3280:ILE:HG23	3:B:3299:LEU:HD21	2.02	0.42
3:B:3488:LEU:HA	3:B:3491:LEU:HD23	2.01	0.42
3:C:1051:ARG:HA	3:C:1054:VAL:HG12	2.01	0.42
3:C:2486:HIS:O	3:C:2490:VAL:HG22	2.20	0.42
3:C:2603:ALA:C	3:C:2606:PRO:HD2	2.44	0.42
3:C:2641:SER:HB3	3:C:2676:LEU:HD21	2.01	0.42
3:C:3496:PHE:CE2	3:C:3552:LEU:O	2.73	0.42
3:C:3763:ILE:HD11	3:C:3838:ASP:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4756:ILE:O	3:C:4759:SER:OG	2.32	0.42
3:D:1298:ASP:OD1	3:D:1299:ILE:N	2.52	0.42
3:D:1898:LEU:HD13	3:D:1902:VAL:HG12	2.01	0.42
3:D:3214:LEU:CD2	3:D:3242:LEU:HD21	2.49	0.42
3:D:3488:LEU:HA	3:D:3491:LEU:HD23	2.01	0.42
1:H:45:LYS:HE2	1:H:45:LYS:HB2	1.68	0.42
1:H:83:TYR:OH	3:D:1768:PHE:O	2.21	0.42
2:J:20:PHE:O	2:J:22:LYS:HB2	2.20	0.42
2:K:132:ASP:C	2:K:137:VAL:HG23	2.40	0.42
3:A:2716:LYS:HG3	3:A:2717:LEU:HD22	2.00	0.42
3:A:3338:ASP:HA	3:A:3341:LYS:HD2	2.01	0.42
3:A:3496:PHE:CE2	3:A:3552:LEU:O	2.73	0.42
3:B:1100:ARG:HB3	3:B:1236:TYR:CD1	2.55	0.42
3:B:3478:LEU:HD21	3:C:1233:GLN:HB3	2.01	0.42
3:C:330:THR:HG23	3:C:366:VAL:HG22	2.01	0.42
3:C:1100:ARG:HB3	3:C:1236:TYR:CD1	2.55	0.42
3:C:2828:MET:O	3:C:2894:LYS:HD3	2.19	0.42
3:C:3482:ALA:O	3:C:3486:GLN:HG2	2.19	0.42
3:C:4203:ALA:HA	3:C:4206:ILE:HG12	2.00	0.42
3:D:514:PHE:CD2	3:D:526:TRP:HB2	2.54	0.42
3:D:675:TYR:CE1	3:D:790:PRO:HB3	2.55	0.42
3:D:2545:ILE:HD11	3:D:2584:MET:HE1	2.02	0.42
3:D:3089:GLY:O	3:D:3093:ILE:HG12	2.20	0.42
3:D:3308:ASN:OD1	3:D:3437:SER:CB	2.61	0.42
3:D:3496:PHE:CE2	3:D:3552:LEU:O	2.73	0.42
3:D:4162:LYS:HD2	3:D:4203:ALA:HB1	2.00	0.42
3:D:4166:LYS:O	3:D:4170:ARG:HG3	2.20	0.42
3:A:1051:ARG:HA	3:A:1054:VAL:HG12	2.01	0.42
3:A:1897:LYS:HB2	3:A:1897:LYS:HE2	1.81	0.42
3:A:2545:ILE:HD11	3:A:2584:MET:HE1	2.02	0.42
3:A:2789:ILE:HD13	3:A:2903:VAL:HB	2.02	0.42
3:A:3214:LEU:CD2	3:A:3242:LEU:HD21	2.49	0.42
3:A:3470:LEU:HD12	3:A:3471:LYS:HD3	2.01	0.42
3:A:3522:PRO:O	3:A:3525:ARG:HG2	2.19	0.42
3:A:4162:LYS:HD2	3:A:4203:ALA:HB1	2.01	0.42
3:B:931:TYR:O	3:B:935:MET:HG2	2.19	0.42
3:C:1446:ILE:HG12	3:C:1542:ALA:HB2	2.01	0.42
3:C:2580:LEU:HD23	3:C:2580:LEU:HA	1.81	0.42
3:C:2872:VAL:HG22	3:C:2873:PRO:HD2	2.02	0.42
3:C:4137:GLU:O	3:C:4918:TYR:OH	2.32	0.42
3:D:1446:ILE:HG12	3:D:1542:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4113:THR:HA	3:D:4116:GLN:HB2	2.01	0.42
3:D:4641:PRO:HG2	3:D:4647:LYS:HA	2.01	0.42
2:I:77:MET:O	2:I:79:ASP:N	2.47	0.42
2:J:101:ILE:HD12	2:J:137:VAL:O	2.19	0.42
2:K:131:ILE:H	2:K:131:ILE:HG13	1.55	0.42
2:L:20:PHE:O	2:L:22:LYS:HB2	2.20	0.42
3:A:2736:LYS:HD2	3:A:2757:MET:SD	2.59	0.42
3:A:2828:MET:O	3:A:2894:LYS:HD3	2.20	0.42
3:B:3089:GLY:O	3:B:3093:ILE:HG12	2.20	0.42
3:B:3467:VAL:O	3:B:3470:LEU:HG	2.20	0.42
3:B:3496:PHE:CE2	3:B:3552:LEU:O	2.73	0.42
3:B:3855:GLN:NE2	3:B:3925:GLN:O	2.53	0.42
3:B:4061:SER:O	3:B:4064:GLU:HG3	2.19	0.42
3:B:4203:ALA:HA	3:B:4206:ILE:HG12	2.00	0.42
3:C:938:GLU:O	3:C:942:THR:HG23	2.20	0.42
3:C:3331:ALA:HA	3:C:3334:VAL:HG22	2.01	0.42
3:C:3467:VAL:O	3:C:3470:LEU:HG	2.20	0.42
3:C:4166:LYS:O	3:C:4170:ARG:HG3	2.20	0.42
3:D:1785:ASP:OD1	3:D:1785:ASP:N	2.53	0.42
3:D:3467:VAL:O	3:D:3470:LEU:HG	2.20	0.42
3:D:4091:ALA:O	3:D:4092:LYS:HB3	2.20	0.42
2:I:141:GLU:HA	2:I:144:GLN:CD	2.45	0.42
3:A:674:TYR:CD2	3:A:815:PRO:HB3	2.54	0.42
3:A:674:TYR:HE1	3:A:756:SER:HB3	1.83	0.42
3:A:718:VAL:HG23	3:A:793:SER:HB3	2.01	0.42
3:A:1091:GLU:HB3	3:A:1094:TYR:HD2	1.84	0.42
3:A:1444:GLY:HA3	3:A:1487:MET:HA	2.02	0.42
3:A:1559:ARG:HD2	3:A:1565:PRO:HD3	2.00	0.42
3:A:3482:ALA:O	3:A:3486:GLN:HG2	2.19	0.42
3:B:1091:GLU:HB3	3:B:1094:TYR:HD2	1.84	0.42
3:B:1298:ASP:OD1	3:B:1299:ILE:N	2.52	0.42
3:B:2222:LEU:HD23	3:B:2222:LEU:HA	1.92	0.42
3:B:2708:THR:HB	3:B:2780:LYS:HB3	2.02	0.42
3:B:2828:MET:O	3:B:2894:LYS:HD3	2.20	0.42
3:B:2988:ARG:HD2	3:B:2990:LEU:O	2.19	0.42
3:B:4641:PRO:HG2	3:B:4647:LYS:HA	2.02	0.42
3:C:931:TYR:O	3:C:935:MET:HG2	2.20	0.42
3:C:3071:THR:HG23	3:C:3094:ILE:HD12	2.01	0.42
3:C:3596:LYS:HD2	3:C:3597:ARG:NH1	2.35	0.42
3:D:330:THR:HG23	3:D:366:VAL:HG22	2.01	0.42
3:D:938:GLU:O	3:D:942:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1943:ARG:O	3:D:1946:GLU:HG2	2.19	0.42
3:D:1959:ALA:HA	3:D:1962:THR:HG22	2.01	0.42
3:D:2716:LYS:HG3	3:D:2717:LEU:HD22	2.00	0.42
3:D:2759:PRO:O	3:D:2762:LEU:N	2.51	0.42
1:F:90:GLY:HA2	3:B:638:PRO:HD3	2.01	0.42
2:L:93:PHE:HE2	2:L:101:ILE:HG23	1.85	0.42
3:A:1100:ARG:HB3	3:A:1236:TYR:CD1	2.55	0.42
3:A:1966:ARG:NE	3:A:3602:CYS:O	2.50	0.42
3:A:4091:ALA:O	3:A:4092:LYS:HB3	2.20	0.42
3:A:4092:LYS:HA	3:A:4129:PHE:CE1	2.55	0.42
3:B:2545:ILE:HD11	3:B:2584:MET:HE1	2.02	0.42
3:B:2759:PRO:HD3	3:B:2821:TYR:HB2	2.01	0.42
3:B:3331:ALA:HA	3:B:3334:VAL:HG22	2.01	0.42
3:B:3466:ILE:H	3:B:3466:ILE:HD12	1.85	0.42
3:B:4092:LYS:HA	3:B:4129:PHE:CE1	2.55	0.42
3:B:4859:LEU:HD12	3:B:4859:LEU:HA	1.94	0.42
3:C:674:TYR:HE1	3:C:756:SER:HB3	1.83	0.42
3:C:897:LYS:HE3	5:C:5005:ATP:HN62	1.84	0.42
3:C:1419:PHE:O	3:C:1423:THR:HB	2.20	0.42
3:C:2344:LEU:HD22	3:C:2434:GLY:HA3	2.02	0.42
3:C:3495:ARG:NH1	3:C:3500:ASP:OD2	2.53	0.42
3:C:4023:LEU:HD12	3:C:4026:LEU:HD23	2.01	0.42
3:C:4091:ALA:O	3:C:4092:LYS:HB3	2.20	0.42
3:D:1091:GLU:HB3	3:D:1094:TYR:HD2	1.84	0.42
3:D:1419:PHE:O	3:D:1423:THR:HB	2.20	0.42
3:D:1444:GLY:HA3	3:D:1487:MET:HA	2.02	0.42
3:D:2690:GLU:HB2	3:D:2692:GLN:NE2	2.35	0.42
3:D:3022:PHE:CD2	3:D:3029:ILE:HD13	2.53	0.42
3:D:3596:LYS:HD2	3:D:3597:ARG:NH1	2.35	0.42
2:I:104:ALA:O	2:I:108:HIS:CD2	2.73	0.41
2:L:101:ILE:HD12	2:L:137:VAL:O	2.19	0.41
2:L:104:ALA:O	2:L:108:HIS:CD2	2.73	0.41
3:A:489:PHE:CD2	3:A:494:MET:HG3	2.55	0.41
3:A:675:TYR:CE1	3:A:790:PRO:HB3	2.55	0.41
3:B:489:PHE:CD2	3:B:494:MET:HG3	2.55	0.41
3:B:680:ASP:OD2	3:B:801:ARG:NE	2.53	0.41
3:B:1419:PHE:O	3:B:1423:THR:HB	2.20	0.41
3:B:2641:SER:HB3	3:B:2676:LEU:HD21	2.01	0.41
3:B:3396:PHE:HE1	3:B:3474:LEU:HD23	1.85	0.41
3:C:489:PHE:CD2	3:C:494:MET:HG3	2.55	0.41
3:C:766:ILE:HB	3:C:779:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2258:ARG:HB3	3:C:2260:PRO:HD2	2.00	0.41
3:C:3466:ILE:H	3:C:3466:ILE:HD12	1.85	0.41
3:C:4650:LYS:HB3	3:C:4672:MET:HE2	2.02	0.41
3:D:169:ARG:NE	3:D:179:ASP:OD2	2.39	0.41
3:D:1100:ARG:HB3	3:D:1236:TYR:CD1	2.55	0.41
3:D:2486:HIS:O	3:D:2490:VAL:HG22	2.20	0.41
3:D:2603:ALA:C	3:D:2606:PRO:HD2	2.44	0.41
3:D:2828:MET:O	3:D:2894:LYS:HD3	2.19	0.41
3:D:3482:ALA:O	3:D:3486:GLN:HG2	2.19	0.41
3:D:3495:ARG:NH1	3:D:3500:ASP:OD2	2.53	0.41
1:G:3:VAL:HG11	1:G:62:GLU:HG3	2.02	0.41
2:I:101:ILE:HD11	2:I:139:TYR:CD1	2.55	0.41
2:I:123:ASP:O	2:I:127:ARG:HD3	2.21	0.41
2:K:20:PHE:O	2:K:22:LYS:HB2	2.20	0.41
2:K:101:ILE:HD11	2:K:139:TYR:CD1	2.55	0.41
2:L:38:ARG:HD2	2:L:43:ASN:HA	2.03	0.41
3:A:1196:ASP:OD1	3:A:1196:ASP:N	2.53	0.41
3:A:2690:GLU:HB2	3:A:2692:GLN:NE2	2.35	0.41
3:A:3297:LYS:HB3	3:A:3297:LYS:HE3	1.34	0.41
3:B:1943:ARG:O	3:B:1946:GLU:HG2	2.19	0.41
3:B:2720:PHE:CE1	3:B:2896:LEU:HD23	2.55	0.41
3:B:3606:ALA:HA	3:B:3607:PRO:HD3	1.86	0.41
3:B:3890:TRP:CD2	3:C:76:ARG:HD3	2.55	0.41
3:B:4091:ALA:O	3:B:4092:LYS:HB3	2.20	0.41
3:C:614:LEU:HD22	3:C:632:ILE:HG12	2.02	0.41
3:C:935:MET:O	3:C:939:THR:OG1	2.30	0.41
3:C:1785:ASP:OD1	3:C:1785:ASP:N	2.53	0.41
3:C:3214:LEU:CD2	3:C:3242:LEU:HD21	2.49	0.41
3:C:3378:ASP:OD1	3:C:3379:TYR:N	2.53	0.41
3:C:4191:ASN:OD1	3:C:4608:ARG:NH1	2.52	0.41
3:C:4641:PRO:HG2	3:C:4647:LYS:HA	2.01	0.41
3:D:1972:GLN:O	3:D:1975:MET:HG3	2.21	0.41
3:D:2247:VAL:HG11	3:D:2257:LEU:HD21	2.03	0.41
3:D:3338:ASP:HA	3:D:3341:LYS:HD2	2.01	0.41
1:E:83:TYR:OH	3:A:1768:PHE:O	2.24	0.41
2:J:101:ILE:HD11	2:J:139:TYR:CD1	2.55	0.41
2:L:4:GLN:OE1	2:L:4:GLN:N	2.53	0.41
2:L:141:GLU:HA	2:L:144:GLN:CD	2.45	0.41
3:A:614:LEU:HD22	3:A:632:ILE:HG12	2.02	0.41
3:A:2759:PRO:HD3	3:A:2821:TYR:HB2	2.01	0.41
3:A:3505:VAL:CG2	3:A:3552:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4061:SER:O	3:A:4064:GLU:HG3	2.19	0.41
3:A:4191:ASN:OD1	3:A:4608:ARG:NH1	2.52	0.41
3:A:4660:PHE:HD2	3:A:4660:PHE:O	2.04	0.41
3:B:614:LEU:HD22	3:B:632:ILE:HG12	2.02	0.41
3:B:897:LYS:HE3	5:B:5005:ATP:HN62	1.85	0.41
3:B:938:GLU:O	3:B:942:THR:HG23	2.20	0.41
3:B:2847:ASN:HD22	3:B:2847:ASN:C	2.26	0.41
3:B:3378:ASP:OD1	3:B:3379:TYR:N	2.53	0.41
3:B:3495:ARG:NH1	3:B:3500:ASP:OD2	2.53	0.41
3:B:3505:VAL:CG2	3:B:3552:LEU:HD13	2.50	0.41
3:B:4650:LYS:HB3	3:B:4672:MET:HE2	2.02	0.41
3:C:675:TYR:CE1	3:C:790:PRO:HB3	2.55	0.41
3:C:3022:PHE:CD2	3:C:3029:ILE:HD13	2.53	0.41
3:D:698:ALA:HB3	3:D:789:PHE:CE1	2.56	0.41
3:D:2332:GLY:O	3:D:2336:ARG:HG3	2.21	0.41
3:D:2344:LEU:HD22	3:D:2434:GLY:HA3	2.02	0.41
3:D:2641:SER:HB3	3:D:2676:LEU:HD21	2.01	0.41
3:D:3378:ASP:OD1	3:D:3379:TYR:N	2.53	0.41
3:D:4921:PHE:HE2	3:D:4940:VAL:HG11	1.84	0.41
1:G:43:ARG:HA	3:C:1682:GLU:OE2	2.20	0.41
2:I:93:PHE:HE2	2:I:101:ILE:HG23	1.85	0.41
2:K:123:ASP:O	2:K:127:ARG:HD3	2.21	0.41
2:K:141:GLU:HA	2:K:144:GLN:CD	2.45	0.41
3:A:612:ASP:OD1	3:A:1656:HIS:ND1	2.54	0.41
3:A:1898:LEU:HD13	3:A:1902:VAL:HG12	2.01	0.41
3:A:2235:ARG:HG2	3:A:2297:ARG:NH1	2.31	0.41
3:A:2332:GLY:O	3:A:2336:ARG:HG3	2.20	0.41
3:A:2872:VAL:HG22	3:A:2873:PRO:HD2	2.02	0.41
3:A:2917:ILE:HD11	3:A:2999:LYS:HB3	2.03	0.41
3:A:3378:ASP:OD1	3:A:3379:TYR:N	2.53	0.41
3:A:3596:LYS:HD2	3:A:3597:ARG:NH1	2.35	0.41
3:A:3975:GLN:O	3:A:3979:VAL:HG23	2.20	0.41
3:B:505:LEU:HD23	3:B:505:LEU:HA	1.92	0.41
3:B:1898:LEU:HD13	3:B:1902:VAL:HG12	2.01	0.41
3:B:2872:VAL:HG22	3:B:2873:PRO:HD2	2.02	0.41
3:B:3470:LEU:HD12	3:B:3471:LYS:HD3	2.01	0.41
3:C:1444:GLY:HA3	3:C:1487:MET:HA	2.02	0.41
3:C:1959:ALA:HA	3:C:1962:THR:HG22	2.01	0.41
3:C:1972:GLN:O	3:C:1975:MET:HG3	2.21	0.41
3:C:2545:ILE:HD11	3:C:2584:MET:HE1	2.02	0.41
3:C:2708:THR:HB	3:C:2780:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3280:ILE:HG23	3:C:3299:LEU:HD21	2.02	0.41
3:C:3338:ASP:HA	3:C:3341:LYS:HD2	2.01	0.41
3:C:3396:PHE:HE1	3:C:3474:LEU:HD23	1.86	0.41
3:C:3649:ALA:C	3:C:3652:PRO:HD2	2.46	0.41
3:C:3855:GLN:NE2	3:C:3925:GLN:O	2.53	0.41
3:D:552:SER:HA	3:D:555:LEU:HD13	2.02	0.41
3:D:2724:TYR:HB3	3:D:2775:ILE:HD13	2.02	0.41
1:H:3:VAL:HG11	1:H:62:GLU:HG3	2.02	0.41
2:I:38:ARG:HD2	2:I:43:ASN:HA	2.02	0.41
3:A:713:TRP:CZ2	3:A:1251:LEU:HD21	2.55	0.41
3:A:1959:ALA:HA	3:A:1962:THR:HG22	2.01	0.41
3:A:2486:HIS:O	3:A:2490:VAL:HG22	2.20	0.41
3:A:2720:PHE:CE1	3:A:2896:LEU:HD23	2.56	0.41
3:B:2789:ILE:HD13	3:B:2903:VAL:HB	2.02	0.41
3:B:2856:LYS:HD3	3:B:2859:GLU:OE2	2.21	0.41
3:B:4166:LYS:O	3:B:4170:ARG:HG3	2.20	0.41
3:C:680:ASP:OD2	3:C:801:ARG:NE	2.53	0.41
3:C:995:MET:HB3	3:C:995:MET:HE3	1.56	0.41
3:C:1943:ARG:O	3:C:1946:GLU:HG2	2.19	0.41
3:C:2332:GLY:O	3:C:2336:ARG:HG3	2.20	0.41
3:C:3488:LEU:HA	3:C:3491:LEU:HD23	2.01	0.41
3:D:612:ASP:OD1	3:D:1656:HIS:ND1	2.54	0.41
3:D:1427:TYR:HB2	3:D:1563:VAL:HG11	2.02	0.41
3:D:4660:PHE:HD2	3:D:4660:PHE:O	2.03	0.41
1:F:3:VAL:HG11	1:F:62:GLU:HG3	2.03	0.41
2:J:141:GLU:HA	2:J:144:GLN:CD	2.45	0.41
2:K:4:GLN:OE1	2:K:4:GLN:N	2.53	0.41
3:A:162:ILE:O	3:A:163:HIS:ND1	2.54	0.41
3:A:2261:ASP:O	3:A:2265:VAL:HG23	2.21	0.41
3:A:2934:ASP:O	3:A:2938:GLN:HG2	2.21	0.41
3:B:1972:GLN:O	3:B:1975:MET:HG3	2.21	0.41
3:B:2697:SER:O	3:B:2699:GLY:N	2.48	0.41
3:B:2893:LEU:HD13	3:B:2896:LEU:HD12	2.03	0.41
3:B:3596:LYS:HD2	3:B:3597:ARG:NH1	2.35	0.41
3:C:612:ASP:OD1	3:C:1656:HIS:ND1	2.54	0.41
3:C:1711:LEU:HB3	3:C:1831:MET:SD	2.61	0.41
3:C:2247:VAL:HG11	3:C:2257:LEU:HD21	2.03	0.41
3:C:2856:LYS:HD3	3:C:2859:GLU:OE2	2.21	0.41
3:D:614:LEU:HD22	3:D:632:ILE:HG12	2.02	0.41
3:D:674:TYR:HE1	3:D:756:SER:HB3	1.83	0.41
3:D:1196:ASP:OD1	3:D:1196:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2154:VAL:HG13	3:D:2158:HIS:CD2	2.56	0.41
3:D:2847:ASN:C	3:D:2847:ASN:HD22	2.26	0.41
3:D:4509:VAL:CG1	3:D:4579:HIS:HB2	2.51	0.41
3:D:4721:TYR:OH	3:D:4745:ASP:OD1	2.31	0.41
1:E:3:VAL:HG11	1:E:62:GLU:HG3	2.03	0.41
2:J:1:MET:O	2:J:1:MET:SD	2.79	0.41
2:J:4:GLN:OE1	2:J:4:GLN:N	2.53	0.41
2:K:93:PHE:HE2	2:K:101:ILE:HG23	1.85	0.41
3:A:967:PRO:HB2	3:A:969:ASN:OD1	2.21	0.41
3:A:1785:ASP:OD1	3:A:1785:ASP:N	2.53	0.41
3:A:2708:THR:HB	3:A:2780:LYS:HB3	2.03	0.41
3:A:3280:ILE:HG23	3:A:3299:LEU:HD21	2.02	0.41
3:A:3488:LEU:HA	3:A:3491:LEU:CD2	2.51	0.41
3:A:4166:LYS:O	3:A:4170:ARG:HG3	2.20	0.41
3:A:4509:VAL:CG1	3:A:4579:HIS:HB2	2.51	0.41
3:B:612:ASP:OD1	3:B:1656:HIS:ND1	2.54	0.41
3:B:2247:VAL:HG11	3:B:2257:LEU:HD21	2.03	0.41
3:B:3649:ALA:C	3:B:3652:PRO:HD2	2.46	0.41
3:C:2760:TYR:CE1	3:C:2768:LYS:HG2	2.56	0.41
3:C:3975:GLN:O	3:C:3979:VAL:HG23	2.21	0.41
3:C:4092:LYS:HA	3:C:4129:PHE:CE1	2.55	0.41
3:C:4172:PHE:CZ	3:C:4189:PHE:HA	2.56	0.41
3:D:3397:ARG:NH2	3:D:3550:ARG:HD2	2.24	0.41
2:L:1:MET:SD	2:L:1:MET:O	2.79	0.41
3:A:897:LYS:HE3	5:A:5005:ATP:HN62	1.85	0.41
3:A:2241:ASP:OD2	3:A:2297:ARG:NH2	2.54	0.41
3:A:2247:VAL:HG11	3:A:2257:LEU:HD21	2.03	0.41
3:A:2255:LEU:O	3:A:3810:ARG:NH1	2.47	0.41
3:A:3152:ARG:HA	3:A:3155:LEU:HD12	2.03	0.41
3:A:3396:PHE:HE1	3:A:3474:LEU:HD23	1.86	0.41
3:A:3466:ILE:H	3:A:3466:ILE:HD12	1.85	0.41
3:A:3495:ARG:NH1	3:A:3500:ASP:OD2	2.53	0.41
3:B:1446:ILE:HG12	3:B:1542:ALA:HB2	2.01	0.41
3:B:1711:LEU:HB3	3:B:1831:MET:SD	2.61	0.41
3:B:2241:ASP:OD2	3:B:2297:ARG:NH2	2.54	0.41
3:B:3312:PRO:HA	3:B:3376:PHE:CZ	2.56	0.41
3:B:3890:TRP:CE3	3:C:76:ARG:HD3	2.55	0.41
3:B:4753:LEU:CD1	3:C:4769:LEU:HB3	2.50	0.41
3:C:1914:CYS:SG	3:C:2091:GLN:NE2	2.78	0.41
3:C:2488:LEU:HD11	3:C:2548:LEU:HD13	2.03	0.41
3:C:2893:LEU:HD13	3:C:2896:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:ILE:O	3:D:163:HIS:ND1	2.54	0.41
3:D:661:LEU:HD13	3:D:673:TRP:CD1	2.56	0.41
3:D:1711:LEU:HB3	3:D:1831:MET:SD	2.61	0.41
3:D:2488:LEU:HD11	3:D:2548:LEU:HD13	2.03	0.41
3:D:2917:ILE:HD11	3:D:2999:LYS:HB3	2.03	0.41
3:D:2984:SER:O	3:D:3001:LYS:NZ	2.32	0.41
3:D:3102:LEU:HB2	3:D:3103:PRO:HD3	2.03	0.41
3:D:3499:LYS:CE	3:D:3564:LYS:NZ	2.81	0.41
3:D:3505:VAL:CG2	3:D:3552:LEU:HD13	2.50	0.41
2:J:132:ASP:C	2:J:137:VAL:HG23	2.40	0.41
2:K:104:ALA:O	2:K:108:HIS:CD2	2.73	0.41
2:L:101:ILE:HD11	2:L:139:TYR:CD1	2.55	0.41
2:L:123:ASP:O	2:L:127:ARG:HD3	2.21	0.41
3:A:229:ILE:HG22	3:A:288:HIS:CD2	2.56	0.41
3:A:552:SER:HA	3:A:555:LEU:HD13	2.02	0.41
3:A:661:LEU:HD13	3:A:673:TRP:CD1	2.56	0.41
3:A:680:ASP:OD2	3:A:801:ARG:NE	2.53	0.41
3:A:698:ALA:HB3	3:A:789:PHE:CE1	2.56	0.41
3:A:739:ARG:HD2	3:A:739:ARG:HA	1.81	0.41
3:A:1972:GLN:O	3:A:1975:MET:HG3	2.21	0.41
3:A:2154:VAL:HG13	3:A:2158:HIS:CD2	2.56	0.41
3:A:2724:TYR:HB3	3:A:2775:ILE:HD13	2.02	0.41
3:A:2760:TYR:CE1	3:A:2768:LYS:HG2	2.56	0.41
3:A:3467:VAL:O	3:A:3470:LEU:HG	2.20	0.41
3:A:3855:GLN:NE2	3:A:3925:GLN:O	2.53	0.41
3:B:698:ALA:HB3	3:B:789:PHE:CE1	2.56	0.41
3:B:713:TRP:CZ2	3:B:1251:LEU:HD21	2.55	0.41
3:B:1267:HIS:HB3	3:B:1287:GLN:NE2	2.36	0.41
3:B:1444:GLY:HA3	3:B:1487:MET:HA	2.02	0.41
3:B:1914:CYS:SG	3:B:2091:GLN:NE2	2.78	0.41
3:B:2645:PHE:HB2	3:B:2672:VAL:HG11	2.03	0.41
3:B:2934:ASP:O	3:B:2938:GLN:HG2	2.21	0.41
3:B:3152:ARG:HA	3:B:3155:LEU:HD12	2.03	0.41
3:B:3488:LEU:HA	3:B:3491:LEU:CD2	2.51	0.41
3:B:3493:LYS:HZ3	3:B:3558:LEU:HB3	1.84	0.41
3:B:3534:LEU:HA	3:B:3535:PRO:HD3	1.97	0.41
3:C:147:VAL:HG21	3:C:192:LEU:HD23	2.03	0.41
3:C:229:ILE:HG22	3:C:288:HIS:CD2	2.56	0.41
3:C:698:ALA:HB3	3:C:789:PHE:CE1	2.56	0.41
3:C:1267:HIS:HB3	3:C:1287:GLN:NE2	2.36	0.41
3:C:1427:TYR:HB2	3:C:1563:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2261:ASP:O	3:C:2265:VAL:HG23	2.21	0.41
3:C:2720:PHE:CE1	3:C:2896:LEU:HD23	2.55	0.41
3:C:2789:ILE:HD13	3:C:2903:VAL:HB	2.02	0.41
3:C:3089:GLY:O	3:C:3093:ILE:HG12	2.20	0.41
3:D:21:VAL:HG23	3:D:215:ALA:HB3	2.03	0.41
3:D:111:ARG:HA	3:D:111:ARG:HD3	1.69	0.41
3:D:147:VAL:HG21	3:D:192:LEU:HD23	2.03	0.41
3:D:192:LEU:O	3:D:210:THR:HG22	2.21	0.41
3:D:489:PHE:CD2	3:D:494:MET:HG3	2.55	0.41
3:D:648:LEU:HD23	3:D:648:LEU:HA	1.94	0.41
3:D:718:VAL:HG23	3:D:793:SER:HB3	2.01	0.41
3:D:1267:HIS:HB3	3:D:1287:GLN:NE2	2.36	0.41
3:D:1843:LEU:HD23	3:D:1843:LEU:HA	1.95	0.41
3:D:2261:ASP:O	3:D:2265:VAL:HG23	2.21	0.41
3:D:2708:THR:HB	3:D:2780:LYS:HB3	2.02	0.41
3:D:2720:PHE:CE1	3:D:2896:LEU:HD23	2.56	0.41
3:D:2856:LYS:HD3	3:D:2859:GLU:OE2	2.21	0.41
3:D:3159:LEU:HD12	3:D:3159:LEU:HA	1.95	0.41
3:D:3396:PHE:HE1	3:D:3474:LEU:HD23	1.85	0.41
3:D:3488:LEU:HA	3:D:3491:LEU:CD2	2.51	0.41
3:D:3649:ALA:C	3:D:3652:PRO:HD2	2.46	0.41
3:D:4061:SER:O	3:D:4064:GLU:HG3	2.19	0.41
2:I:45:THR:N	2:I:48:GLU:HB2	2.36	0.41
2:J:45:THR:N	2:J:48:GLU:HB2	2.36	0.41
2:K:45:THR:N	2:K:48:GLU:HB2	2.36	0.41
3:A:1419:PHE:O	3:A:1423:THR:HB	2.20	0.41
3:A:1728:PRO:HD3	3:A:1757:LEU:HG	2.03	0.41
3:A:3102:LEU:HB2	3:A:3103:PRO:HD3	2.03	0.41
3:A:3398:MET:O	3:A:3402:VAL:HG23	2.21	0.41
3:A:3493:LYS:HZ2	3:A:3558:LEU:CD1	2.34	0.41
3:A:4649:VAL:HA	3:A:4652:LYS:HG2	2.03	0.41
3:B:150:GLN:NE2	3:B:158:CYS:SG	2.72	0.41
3:B:808:HIS:CG	3:B:832:LEU:HD23	2.56	0.41
3:B:877:HIS:O	3:B:880:ARG:HD3	2.21	0.41
3:B:2261:ASP:O	3:B:2265:VAL:HG23	2.21	0.41
3:B:2655:LYS:O	3:B:2958:GLN:NE2	2.54	0.41
3:B:2724:TYR:HB3	3:B:2775:ILE:HD13	2.02	0.41
3:B:4883:ASP:C	3:B:4885:GLU:H	2.29	0.41
3:C:3423:ASN:O	3:C:3425:ILE:CD1	2.46	0.41
3:D:310:GLU:OE1	3:D:310:GLU:N	2.31	0.41
3:D:877:HIS:O	3:D:880:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1728:PRO:HD3	3:D:1757:LEU:HG	2.03	0.41
3:D:2255:LEU:O	3:D:3810:ARG:NH1	2.47	0.41
3:D:2760:TYR:CE1	3:D:2768:LYS:HG2	2.56	0.41
3:D:4092:LYS:HA	3:D:4129:PHE:CE1	2.55	0.41
3:D:4832:GLU:HG2	3:D:4833:ASP:H	1.86	0.41
1:G:88:HIS:CD2	1:G:89:PRO:HD2	2.56	0.40
2:I:20:PHE:O	2:I:22:LYS:HB2	2.20	0.40
2:I:141:GLU:HA	2:I:144:GLN:NE2	2.36	0.40
2:L:22:LYS:HA	2:L:22:LYS:HD2	1.81	0.40
3:A:192:LEU:O	3:A:210:THR:HG22	2.21	0.40
3:A:808:HIS:CG	3:A:832:LEU:HD23	2.56	0.40
3:A:2419:ILE:HA	3:A:2422:ILE:HD12	2.03	0.40
3:A:2837:LEU:HD22	3:A:2897:GLN:NE2	2.37	0.40
3:A:4641:PRO:HG2	3:A:4647:LYS:HA	2.01	0.40
3:B:349:MET:HA	3:B:349:MET:CE	2.51	0.40
3:B:552:SER:HA	3:B:555:LEU:HD13	2.02	0.40
3:B:1959:ALA:HA	3:B:1962:THR:HG22	2.01	0.40
3:B:2332:GLY:O	3:B:2336:ARG:HG3	2.21	0.40
3:B:3102:LEU:HB2	3:B:3103:PRO:HD3	2.03	0.40
3:B:4191:ASN:OD1	3:B:4608:ARG:NH1	2.52	0.40
3:B:4660:PHE:HD2	3:B:4660:PHE:O	2.04	0.40
3:C:21:VAL:HG23	3:C:215:ALA:HB3	2.03	0.40
3:C:192:LEU:O	3:C:210:THR:HG22	2.21	0.40
3:C:967:PRO:HB2	3:C:969:ASN:OD1	2.21	0.40
3:C:2826:ILE:HD12	3:D:1501:ASN:ND2	2.35	0.40
3:C:3152:ARG:HA	3:C:3155:LEU:HD12	2.03	0.40
3:C:3315:LEU:HA	3:C:3319:PHE:HB2	2.04	0.40
3:C:3478:LEU:HD21	3:D:1233:GLN:CB	2.46	0.40
3:C:4509:VAL:CG1	3:C:4579:HIS:HB2	2.51	0.40
3:C:4678:ASP:OD1	3:C:4678:ASP:N	2.55	0.40
3:D:2241:ASP:OD2	3:D:2297:ARG:NH2	2.54	0.40
3:D:3505:VAL:HG23	3:D:3552:LEU:CD1	2.52	0.40
3:D:4650:LYS:HG2	3:D:4670:LEU:HD22	2.03	0.40
1:E:88:HIS:CD2	1:E:89:PRO:HD2	2.56	0.40
2:I:1:MET:O	2:I:1:MET:SD	2.79	0.40
2:J:123:ASP:O	2:J:127:ARG:HD3	2.21	0.40
2:L:45:THR:N	2:L:48:GLU:HB2	2.36	0.40
3:A:23:GLN:HG2	3:A:36:CYS:SG	2.61	0.40
3:A:147:VAL:HG21	3:A:192:LEU:HD23	2.03	0.40
3:A:2763:LEU:O	3:A:2768:LYS:HE2	2.22	0.40
3:A:4176:VAL:HA	3:A:4180:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:23:GLN:HG2	3:B:36:CYS:SG	2.61	0.40
3:B:3975:GLN:O	3:B:3979:VAL:HG23	2.21	0.40
3:B:4172:PHE:CZ	3:B:4189:PHE:HA	2.56	0.40
3:C:552:SER:HA	3:C:555:LEU:HD13	2.02	0.40
3:C:2426:LEU:HG	3:D:143:LEU:HD13	2.03	0.40
3:C:2724:TYR:HB3	3:C:2775:ILE:HD13	2.02	0.40
3:C:2917:ILE:HD11	3:C:2999:LYS:HB3	2.03	0.40
3:C:2934:ASP:O	3:C:2938:GLN:HG2	2.21	0.40
3:C:4883:ASP:C	3:C:4885:GLU:H	2.29	0.40
3:D:897:LYS:HE3	5:D:5005:ATP:HN62	1.84	0.40
3:D:967:PRO:HB2	3:D:969:ASN:OD1	2.21	0.40
3:D:3152:ARG:HA	3:D:3155:LEU:HD12	2.03	0.40
3:D:4172:PHE:CZ	3:D:4189:PHE:HA	2.56	0.40
3:A:911:ASN:OD1	3:A:912:LYS:N	2.55	0.40
3:A:992:GLN:O	3:A:996:VAL:HG23	2.22	0.40
3:A:2645:PHE:HB2	3:A:2672:VAL:HG11	2.03	0.40
3:A:2893:LEU:HD13	3:A:2896:LEU:HD12	2.03	0.40
3:A:3122:ILE:O	3:A:3123:LEU:HD22	2.22	0.40
3:A:4650:LYS:HB3	3:A:4672:MET:HE2	2.02	0.40
3:A:4832:GLU:HG2	3:A:4833:ASP:H	1.86	0.40
3:B:229:ILE:HG22	3:B:288:HIS:CD2	2.56	0.40
3:B:967:PRO:HB2	3:B:969:ASN:OD1	2.21	0.40
3:B:3315:LEU:HA	3:B:3319:PHE:HB2	2.04	0.40
3:B:3505:VAL:HG23	3:B:3552:LEU:CD1	2.51	0.40
3:B:4509:VAL:CG1	3:B:4579:HIS:HB2	2.51	0.40
3:B:4832:GLU:HG2	3:B:4833:ASP:H	1.86	0.40
3:C:111:ARG:HD3	3:C:111:ARG:HA	1.69	0.40
3:C:2407:HIS:CE1	3:C:2408:LEU:HG	2.56	0.40
3:C:2763:LEU:O	3:C:2768:LYS:HE2	2.22	0.40
3:C:2837:LEU:HD22	3:C:2897:GLN:NE2	2.36	0.40
3:C:3312:PRO:HA	3:C:3376:PHE:CZ	2.56	0.40
3:C:3505:VAL:CG2	3:C:3552:LEU:HD13	2.50	0.40
3:C:4650:LYS:HG2	3:C:4670:LEU:HD22	2.04	0.40
3:D:2655:LYS:O	3:D:2958:GLN:NE2	2.54	0.40
3:D:2893:LEU:HD13	3:D:2896:LEU:HD12	2.03	0.40
3:D:3329:LYS:O	3:D:3333:VAL:HG23	2.21	0.40
3:D:4649:VAL:HA	3:D:4652:LYS:HG2	2.03	0.40
2:J:38:ARG:HD2	2:J:43:ASN:HA	2.02	0.40
2:J:93:PHE:HE2	2:J:101:ILE:HG23	1.85	0.40
2:L:67:PRO:HB2	3:D:2202:TYR:CZ	2.57	0.40
2:L:121:GLU:HG2	2:L:122:VAL:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1446:ILE:HG12	3:A:1542:ALA:HB2	2.01	0.40
3:A:3505:VAL:HG23	3:A:3552:LEU:CD1	2.52	0.40
3:A:4172:PHE:CZ	3:A:4189:PHE:HA	2.56	0.40
3:A:4678:ASP:OD1	3:A:4678:ASP:N	2.55	0.40
3:B:1792:ILE:HD11	3:B:1838:ASP:HB3	2.04	0.40
3:B:1897:LYS:HB2	3:B:1897:LYS:HE2	1.80	0.40
3:B:2760:TYR:CE1	3:B:2768:LYS:HG2	2.56	0.40
3:B:4600:PHE:HB2	3:B:4643:ASN:HB3	2.04	0.40
3:B:4650:LYS:HG2	3:B:4670:LEU:HD22	2.03	0.40
3:C:495:ILE:H	3:C:495:ILE:HD12	1.87	0.40
3:C:969:ASN:OD1	3:C:970:TYR:N	2.55	0.40
3:C:1220:ASP:O	3:C:1223:THR:OG1	2.28	0.40
3:C:1415:ASP:OD1	3:C:1415:ASP:N	2.55	0.40
3:C:3102:LEU:HB2	3:C:3103:PRO:HD3	2.03	0.40
3:C:3122:ILE:O	3:C:3123:LEU:HD22	2.22	0.40
3:C:3505:VAL:HG23	3:C:3552:LEU:CD1	2.52	0.40
3:D:349:MET:HA	3:D:349:MET:CE	2.51	0.40
3:D:765:SER:HA	3:D:779:PHE:O	2.21	0.40
3:D:1139:GLY:HA3	3:D:1156:TRP:CE3	2.56	0.40
3:D:1792:ILE:HD11	3:D:1838:ASP:HB3	2.04	0.40
3:D:2407:HIS:CE1	3:D:2408:LEU:HG	2.56	0.40
3:D:2487:LEU:HA	3:D:2490:VAL:HG22	2.04	0.40
3:D:2837:LEU:HD22	3:D:2897:GLN:NE2	2.36	0.40
3:D:3280:ILE:HG23	3:D:3299:LEU:HD21	2.02	0.40
3:D:3509:ILE:CD1	3:D:3552:LEU:CD2	2.95	0.40
1:E:90:GLY:HA2	3:A:638:PRO:HD3	2.04	0.40
2:K:1:MET:O	2:K:1:MET:SD	2.79	0.40
2:L:141:GLU:HA	2:L:144:GLN:NE2	2.36	0.40
3:A:648:LEU:HD23	3:A:648:LEU:HA	1.94	0.40
3:A:1711:LEU:HB3	3:A:1831:MET:SD	2.61	0.40
3:A:2635:GLU:OE2	3:A:2680:TYR:OH	2.35	0.40
3:A:2856:LYS:HD3	3:A:2859:GLU:OE2	2.21	0.40
3:A:3649:ALA:C	3:A:3652:PRO:HD2	2.46	0.40
3:A:4847:ASP:OD2	3:D:4818:TYR:OH	2.29	0.40
3:B:992:GLN:O	3:B:996:VAL:HG23	2.22	0.40
3:B:1988:CYS:HA	3:B:1989:PRO:HD3	1.97	0.40
3:B:2419:ILE:HA	3:B:2422:ILE:HD12	2.03	0.40
3:B:3320:LEU:CD2	3:B:3321:PRO:HD3	2.51	0.40
3:B:3366:LEU:HG	3:B:3370:TYR:CE1	2.57	0.40
3:B:4176:VAL:HA	3:B:4180:GLY:HA3	2.03	0.40
3:C:877:HIS:O	3:C:880:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1139:GLY:HA3	3:C:1156:TRP:CE3	2.56	0.40
3:C:1792:ILE:HD11	3:C:1838:ASP:HB3	2.04	0.40
3:C:2241:ASP:OD2	3:C:2297:ARG:NH2	2.54	0.40
3:C:2496:LEU:HD23	3:C:2520:LEU:HD13	2.03	0.40
3:C:2655:LYS:O	3:C:2958:GLN:NE2	2.55	0.40
3:D:739:ARG:HA	3:D:739:ARG:HD2	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	I	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
2	J	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
2	K	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
2	L	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
3	A	4343/4967 (87%)	4192 (96%)	147 (3%)	4 (0%)	48	71
3	B	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	48	71
3	C	4343/4967 (87%)	4192 (96%)	147 (3%)	4 (0%)	48	71
3	D	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	48	71
All	All	18336/20896 (88%)	17666 (96%)	654 (4%)	16 (0%)	49	71

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1495	SER
3	A	2358	SER
3	B	1495	SER
3	B	2358	SER
3	C	1495	SER
3	C	2358	SER
3	D	1495	SER
3	D	2358	SER
3	A	1955	ALA
3	B	1955	ALA
3	C	1955	ALA
3	D	1955	ALA
3	A	313	ASN
3	B	313	ASN
3	C	313	ASN
3	D	313	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	88/89 (99%)	85 (97%)	3 (3%)	32	58
1	F	88/89 (99%)	85 (97%)	3 (3%)	32	58
1	G	88/89 (99%)	85 (97%)	3 (3%)	32	58
1	H	88/89 (99%)	85 (97%)	3 (3%)	32	58
2	I	119/127 (94%)	105 (88%)	14 (12%)	5	14
2	J	119/127 (94%)	105 (88%)	14 (12%)	5	14
2	K	119/127 (94%)	105 (88%)	14 (12%)	5	14
2	L	119/127 (94%)	105 (88%)	14 (12%)	5	14
3	A	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81
3	B	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81
3	C	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81
3	D	3836/4358 (88%)	3799 (99%)	37 (1%)	68	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	16172/18296 (88%)	15956 (99%)	216 (1%)	59	77

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	GLU
1	E	50	ARG
1	E	86	THR
1	F	4	GLU
1	F	50	ARG
1	F	86	THR
1	G	4	GLU
1	G	50	ARG
1	G	86	THR
1	H	4	GLU
1	H	50	ARG
1	H	86	THR
2	I	15	GLU
2	I	22	LYS
2	I	75	ARG
2	I	76	LYS
2	I	77	MET
2	I	86	ILE
2	I	92	VAL
2	I	110	MET
2	I	118	THR
2	I	128	GLU
2	I	131	ILE
2	I	137	VAL
2	I	145	MET
2	I	146	MET
2	J	15	GLU
2	J	22	LYS
2	J	75	ARG
2	J	76	LYS
2	J	77	MET
2	J	86	ILE
2	J	92	VAL
2	J	110	MET
2	J	118	THR
2	J	128	GLU
2	J	131	ILE

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Mol	Chain	Res	Type
2	J	137	VAL
2	J	145	MET
2	J	146	MET
2	K	15	GLU
2	K	22	LYS
2	K	75	ARG
2	K	76	LYS
2	K	77	MET
2	K	86	ILE
2	K	92	VAL
2	K	110	MET
2	K	118	THR
2	K	128	GLU
2	K	131	ILE
2	K	137	VAL
2	K	145	MET
2	K	146	MET
2	L	15	GLU
2	L	22	LYS
2	L	75	ARG
2	L	76	LYS
2	L	77	MET
2	L	86	ILE
2	L	92	VAL
2	L	110	MET
2	L	118	THR
2	L	128	GLU
2	L	131	ILE
2	L	137	VAL
2	L	145	MET
2	L	146	MET
3	A	111	ARG
3	A	309	MET
3	A	349	MET
3	A	778	MET
3	A	995	MET
3	A	1249	MET
3	A	1494	MET
3	A	1721	MET
3	A	2512	MET
3	A	2681	MET
3	A	2737	LEU

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Mol	Chain	Res	Type
3	A	2757	MET
3	A	2760	TYR
3	A	2761	LYS
3	A	2838[A]	HIS
3	A	2838[B]	HIS
3	A	2884	LYS
3	A	3190	ARG
3	A	3215	MET
3	A	3221	LEU
3	A	3231	MET
3	A	3281	LEU
3	A	3296	MET
3	A	3297	LYS
3	A	3381	ARG
3	A	3398	MET
3	A	3420	VAL
3	A	3422	GLN
3	A	3426	ASN
3	A	3461	MET
3	A	3719	MET
3	A	4186	MET
3	A	4555	ILE
3	A	4672	MET
3	A	4925	LEU
3	A	4942	LYS
3	A	4951	PHE
3	B	111	ARG
3	B	309	MET
3	B	349	MET
3	B	778	MET
3	B	995	MET
3	B	1249	MET
3	B	1494	MET
3	B	1721	MET
3	B	2512	MET
3	B	2681	MET
3	B	2737	LEU
3	B	2757	MET
3	B	2760	TYR
3	B	2761	LYS
3	B	2838[A]	HIS
3	B	2838[B]	HIS

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Mol	Chain	Res	Type
3	B	2884	LYS
3	B	3190	ARG
3	B	3215	MET
3	B	3221	LEU
3	B	3231	MET
3	B	3281	LEU
3	B	3296	MET
3	B	3297	LYS
3	B	3381	ARG
3	B	3398	MET
3	B	3420	VAL
3	B	3422	GLN
3	B	3426	ASN
3	B	3461	MET
3	B	3719	MET
3	B	4186	MET
3	B	4555	ILE
3	B	4672	MET
3	B	4925	LEU
3	B	4942	LYS
3	B	4951	PHE
3	C	111	ARG
3	C	309	MET
3	C	349	MET
3	C	778	MET
3	C	995	MET
3	C	1249	MET
3	C	1494	MET
3	C	1721	MET
3	C	2512	MET
3	C	2681	MET
3	C	2737	LEU
3	C	2757	MET
3	C	2760	TYR
3	C	2761	LYS
3	C	2838[A]	HIS
3	C	2838[B]	HIS
3	C	2884	LYS
3	C	3190	ARG
3	C	3215	MET
3	C	3221	LEU
3	C	3231	MET

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Mol	Chain	Res	Type
3	C	3281	LEU
3	C	3296	MET
3	C	3297	LYS
3	C	3381	ARG
3	C	3398	MET
3	C	3420	VAL
3	C	3422	GLN
3	C	3426	ASN
3	C	3461	MET
3	C	3719	MET
3	C	4186	MET
3	C	4555	ILE
3	C	4672	MET
3	C	4925	LEU
3	C	4942	LYS
3	C	4951	PHE
3	D	111	ARG
3	D	309	MET
3	D	349	MET
3	D	778	MET
3	D	995	MET
3	D	1249	MET
3	D	1494	MET
3	D	1721	MET
3	D	2512	MET
3	D	2681	MET
3	D	2737	LEU
3	D	2757	MET
3	D	2760	TYR
3	D	2761	LYS
3	D	2838[A]	HIS
3	D	2838[B]	HIS
3	D	2884	LYS
3	D	3190	ARG
3	D	3215	MET
3	D	3221	LEU
3	D	3231	MET
3	D	3281	LEU
3	D	3296	MET
3	D	3297	LYS
3	D	3381	ARG
3	D	3398	MET

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Mol	Chain	Res	Type
3	D	3420	VAL
3	D	3422	GLN
3	D	3426	ASN
3	D	3461	MET
3	D	3719	MET
3	D	4186	MET
3	D	4555	ILE
3	D	4672	MET
3	D	4925	LEU
3	D	4942	LYS
3	D	4951	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	108	HIS
2	J	108	HIS
2	K	108	HIS
2	L	108	HIS
3	A	209	GLN
3	A	746	GLN
3	A	836	HIS
3	A	1071	HIS
3	A	1498	GLN
3	A	1577	ASN
3	A	1691	ASN
3	A	1805	HIS
3	A	2386	ASN
3	A	2540	HIS
3	A	2550	HIS
3	A	2754	GLN
3	A	2897	GLN
3	A	2998	ASN
3	A	3063	ASN
3	A	3151	GLN
3	A	3230	GLN
3	A	3252	HIS
3	A	3256	ASN
3	A	3426	ASN
3	A	3563	GLN
3	A	3770	ASN
3	A	3775	GLN

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Mol	Chain	Res	Type
3	A	3869	ASN
3	A	3901	GLN
3	A	4009	ASN
3	A	4159	GLN
3	A	4178	ASN
3	A	4642	ASN
3	A	4699	ASN
3	A	4762	HIS
3	A	4766	GLN
3	A	4945	GLN
3	B	209	GLN
3	B	746	GLN
3	B	836	HIS
3	B	1071	HIS
3	B	1498	GLN
3	B	1501	ASN
3	B	1691	ASN
3	B	1805	HIS
3	B	2386	ASN
3	B	2540	HIS
3	B	2550	HIS
3	B	2754	GLN
3	B	2897	GLN
3	B	2998	ASN
3	B	3038	GLN
3	B	3063	ASN
3	B	3151	GLN
3	B	3179	ASN
3	B	3230	GLN
3	B	3252	HIS
3	B	3256	ASN
3	B	3426	ASN
3	B	3563	GLN
3	B	3770	ASN
3	B	3775	GLN
3	B	3869	ASN
3	B	4009	ASN
3	B	4159	GLN
3	B	4178	ASN
3	B	4642	ASN
3	B	4699	ASN
3	B	4762	HIS

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Mol	Chain	Res	Type
3	B	4766	GLN
3	B	4945	GLN
3	C	209	GLN
3	C	836	HIS
3	C	1071	HIS
3	C	1498	GLN
3	C	1501	ASN
3	C	1577	ASN
3	C	1691	ASN
3	C	1805	HIS
3	C	2386	ASN
3	C	2540	HIS
3	C	2550	HIS
3	C	2754	GLN
3	C	2847	ASN
3	C	2897	GLN
3	C	2998	ASN
3	C	3038	GLN
3	C	3063	ASN
3	C	3151	GLN
3	C	3179	ASN
3	C	3252	HIS
3	C	3256	ASN
3	C	3426	ASN
3	C	3563	GLN
3	C	3634	HIS
3	C	3770	ASN
3	C	3775	GLN
3	C	3869	ASN
3	C	3901	GLN
3	C	4009	ASN
3	C	4159	GLN
3	C	4178	ASN
3	C	4699	ASN
3	C	4762	HIS
3	C	4766	GLN
3	C	4945	GLN
3	D	208	GLN
3	D	209	GLN
3	D	651	HIS
3	D	746	GLN
3	D	836	HIS

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Mol	Chain	Res	Type
3	D	1498	GLN
3	D	1501	ASN
3	D	1577	ASN
3	D	1691	ASN
3	D	1805	HIS
3	D	2550	HIS
3	D	2754	GLN
3	D	2897	GLN
3	D	2998	ASN
3	D	3038	GLN
3	D	3063	ASN
3	D	3151	GLN
3	D	3179	ASN
3	D	3252	HIS
3	D	3256	ASN
3	D	3426	ASN
3	D	3462	GLN
3	D	3563	GLN
3	D	3770	ASN
3	D	3775	GLN
3	D	3869	ASN
3	D	3901	GLN
3	D	4009	ASN
3	D	4159	GLN
3	D	4178	ASN
3	D	4699	ASN
3	D	4762	HIS
3	D	4945	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	XAN	A	5004	-	12,12,12	0.92	1 (8%)	14,17,17	0.93	0
5	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	C	5005	-	32,33,33	0.54	0	48,52,52	0.57	0
7	XAN	D	5004	-	12,12,12	0.91	1 (8%)	14,17,17	0.92	0
7	XAN	C	5004	-	12,12,12	0.92	1 (8%)	14,17,17	0.92	0
5	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	D	5005	-	32,33,33	0.53	0	48,52,52	0.57	0
5	ATP	A	5005	-	32,33,33	0.53	0	48,52,52	0.57	0
5	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
5	ATP	B	5005	-	32,33,33	0.54	0	48,52,52	0.57	0
7	XAN	B	5004	-	12,12,12	0.92	1 (8%)	14,17,17	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	XAN	A	5004	-	-	-	0/2/2/2
5	ATP	B	5002	-	-	4/22/38/38	0/3/3/3
5	ATP	C	5005	-	-	4/22/38/38	0/3/3/3
7	XAN	D	5004	-	-	-	0/2/2/2
7	XAN	C	5004	-	-	-	0/2/2/2
5	ATP	D	5002	-	-	4/22/38/38	0/3/3/3
5	ATP	A	5002	-	-	4/22/38/38	0/3/3/3
5	ATP	D	5005	-	-	4/22/38/38	0/3/3/3
5	ATP	A	5005	-	-	4/22/38/38	0/3/3/3
5	ATP	C	5002	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	5005	-	-	4/22/38/38	0/3/3/3
7	XAN	B	5004	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5004	XAN	C4-N3	-2.59	1.33	1.37
7	B	5004	XAN	C4-N3	-2.58	1.33	1.37
7	C	5004	XAN	C4-N3	-2.56	1.33	1.37
7	D	5004	XAN	C4-N3	-2.55	1.33	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	C5'-O5'-PA-O1A
5	A	5002	ATP	C5'-O5'-PA-O3A
5	A	5005	ATP	C5'-O5'-PA-O3A
5	A	5005	ATP	O4'-C4'-C5'-O5'
5	B	5002	ATP	C5'-O5'-PA-O1A
5	B	5002	ATP	C5'-O5'-PA-O3A
5	B	5005	ATP	C5'-O5'-PA-O3A
5	B	5005	ATP	O4'-C4'-C5'-O5'
5	C	5002	ATP	C5'-O5'-PA-O1A
5	C	5002	ATP	C5'-O5'-PA-O3A
5	C	5005	ATP	C5'-O5'-PA-O3A
5	C	5005	ATP	O4'-C4'-C5'-O5'
5	D	5002	ATP	C5'-O5'-PA-O1A
5	D	5002	ATP	C5'-O5'-PA-O3A
5	D	5005	ATP	C5'-O5'-PA-O3A
5	D	5005	ATP	O4'-C4'-C5'-O5'
5	A	5005	ATP	C3'-C4'-C5'-O5'
5	B	5005	ATP	C3'-C4'-C5'-O5'
5	C	5005	ATP	C3'-C4'-C5'-O5'
5	D	5005	ATP	C3'-C4'-C5'-O5'
5	A	5002	ATP	C5'-O5'-PA-O2A
5	A	5005	ATP	C5'-O5'-PA-O1A
5	B	5002	ATP	C5'-O5'-PA-O2A
5	B	5005	ATP	C5'-O5'-PA-O1A
5	C	5002	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	C	5005	ATP	C5'-O5'-PA-O1A
5	D	5002	ATP	C5'-O5'-PA-O2A
5	D	5005	ATP	C5'-O5'-PA-O1A
5	A	5002	ATP	C4'-C5'-O5'-PA
5	B	5002	ATP	C4'-C5'-O5'-PA
5	C	5002	ATP	C4'-C5'-O5'-PA
5	D	5002	ATP	C4'-C5'-O5'-PA

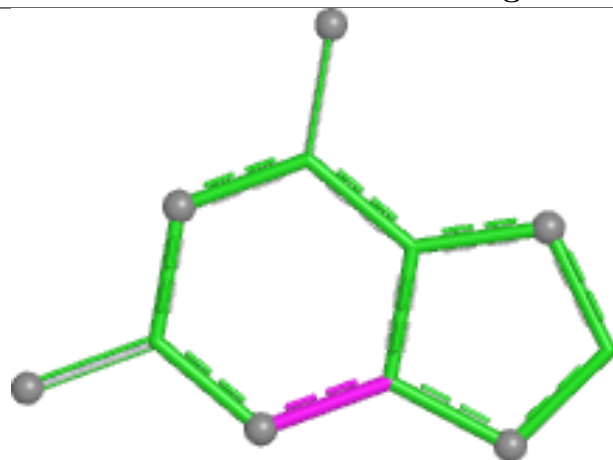
There are no ring outliers.

8 monomers are involved in 16 short contacts:

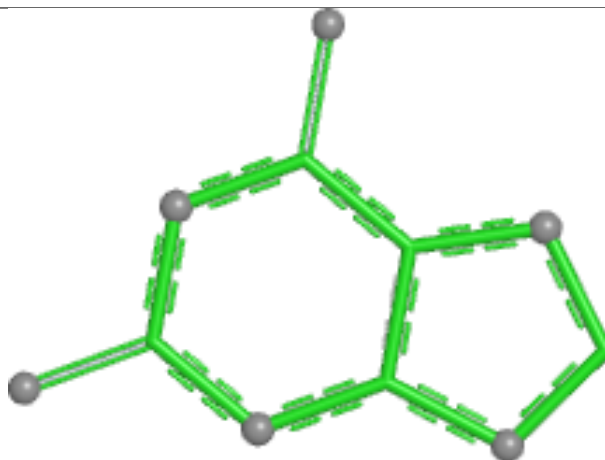
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5002	ATP	3	0
5	C	5005	ATP	1	0
5	D	5002	ATP	3	0
5	A	5002	ATP	3	0
5	D	5005	ATP	1	0
5	A	5005	ATP	1	0
5	C	5002	ATP	3	0
5	B	5005	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

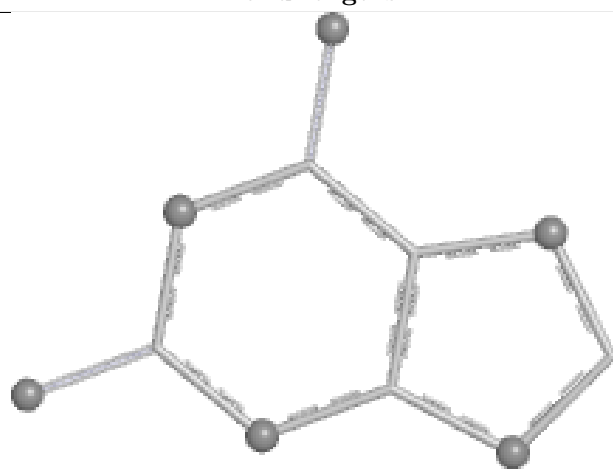
Ligand XAN A 5004



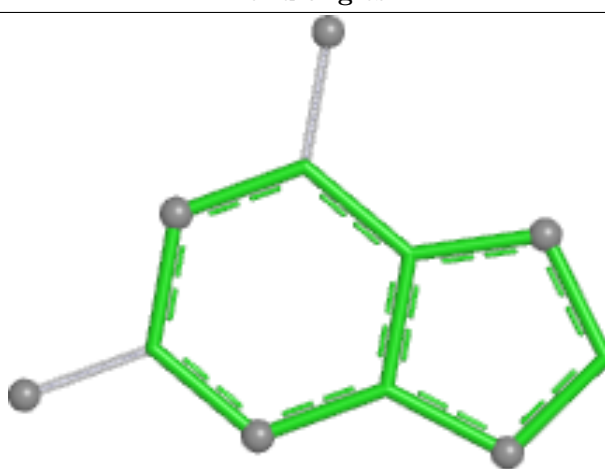
Bond lengths



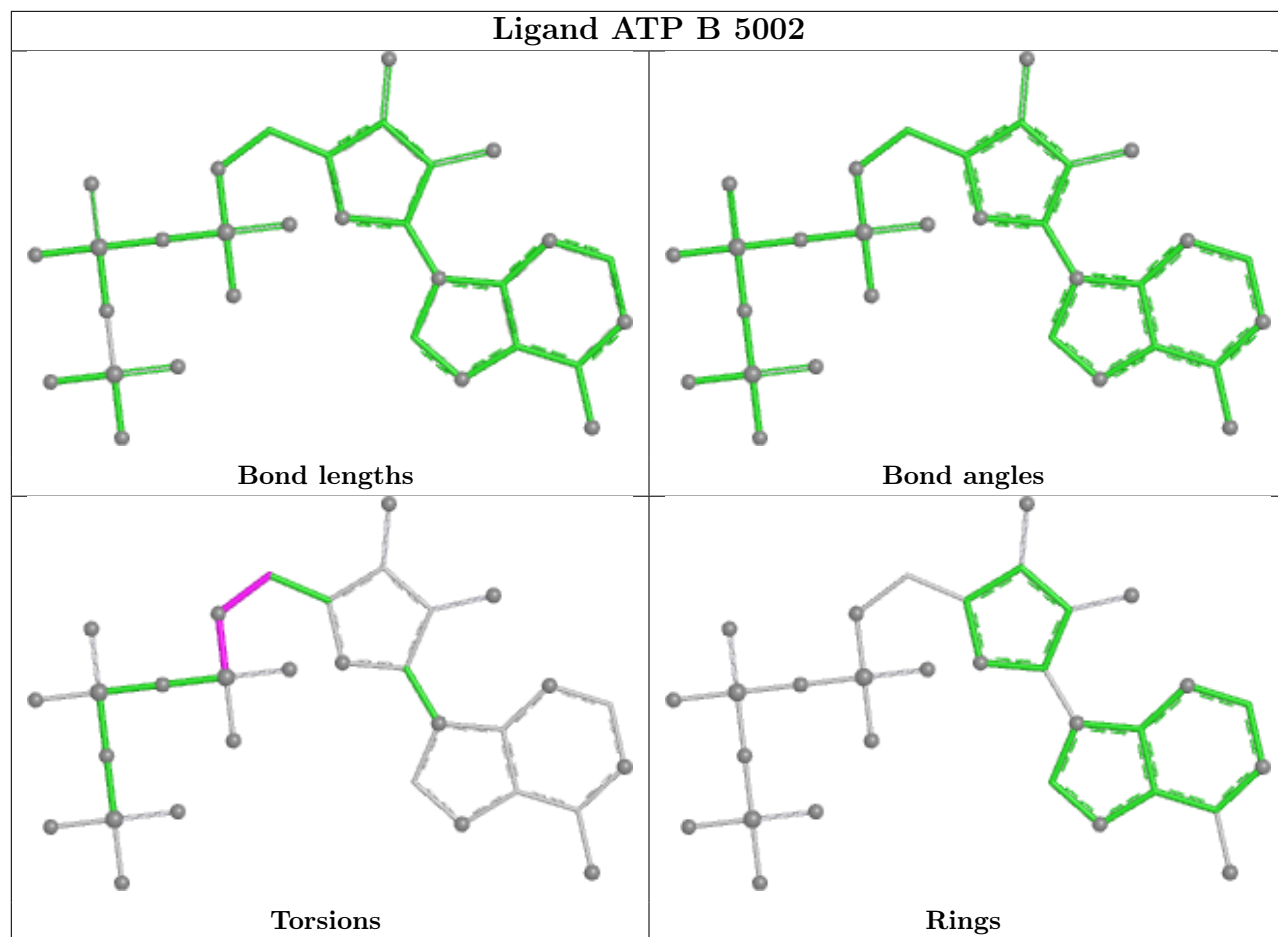
Bond angles

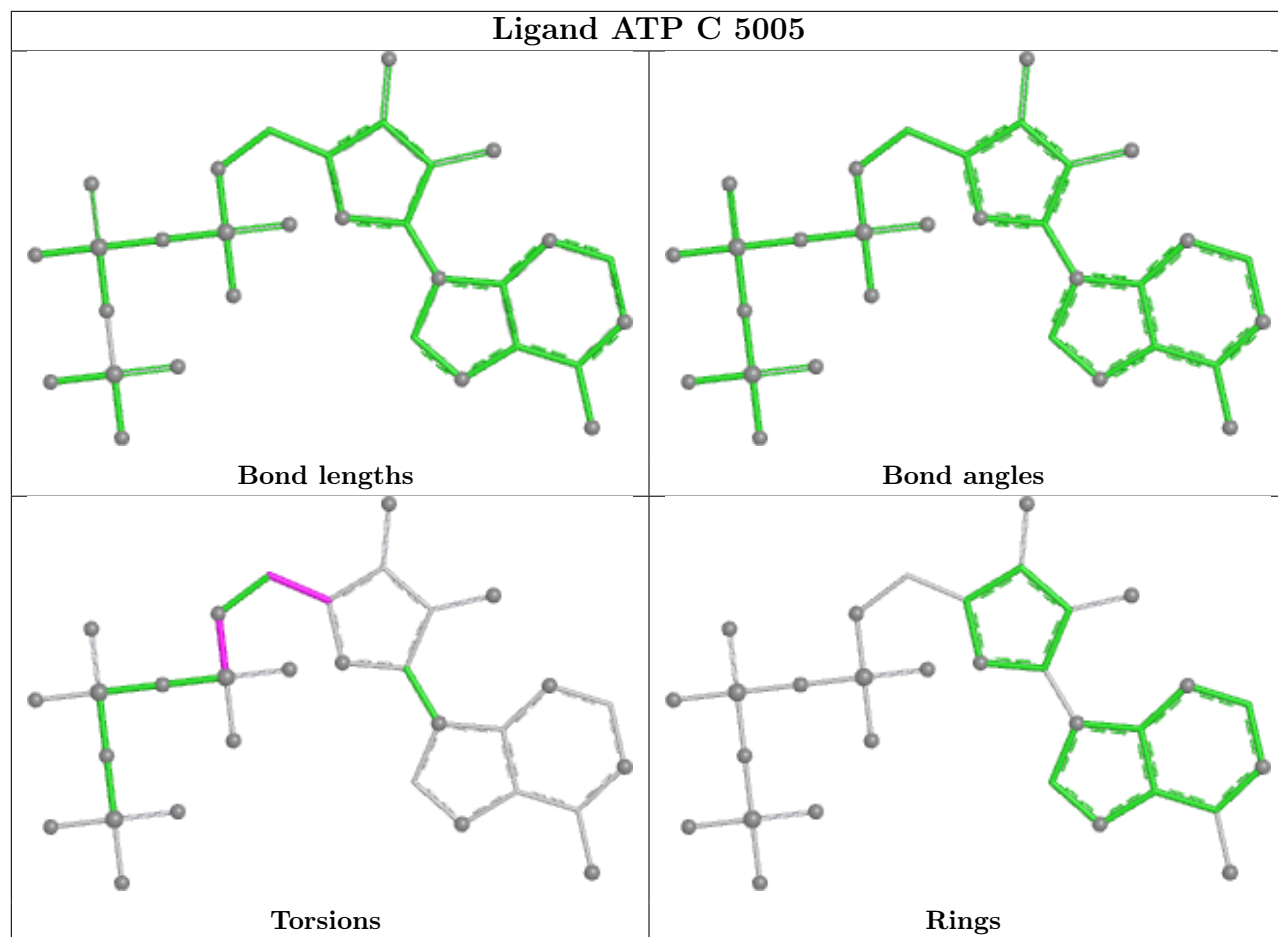


Torsions

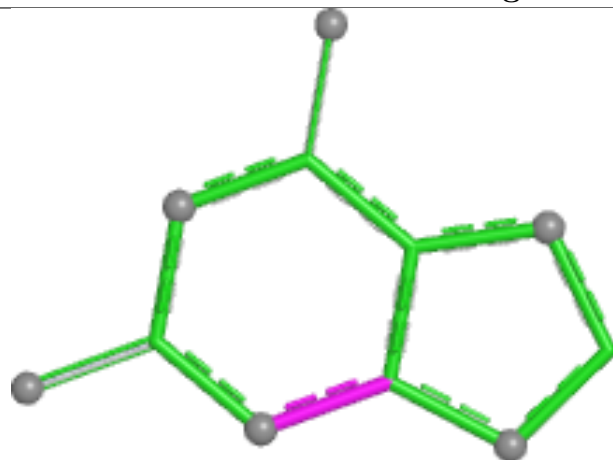


Rings

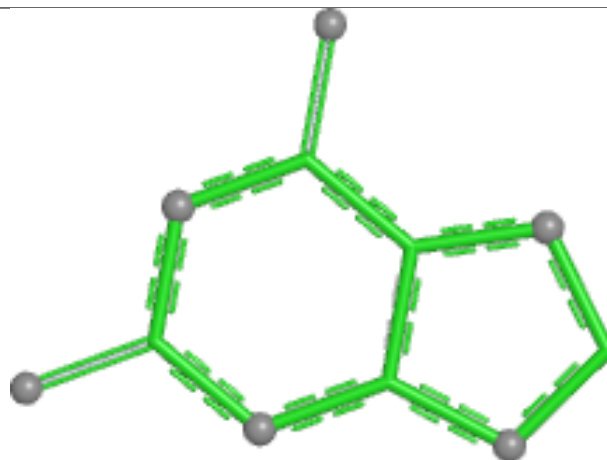




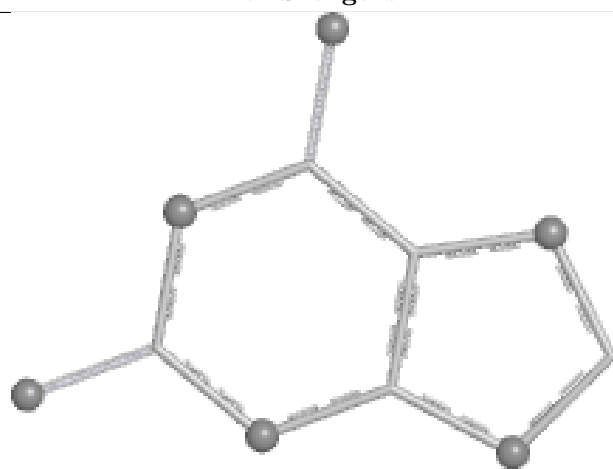
Ligand XAN D 5004



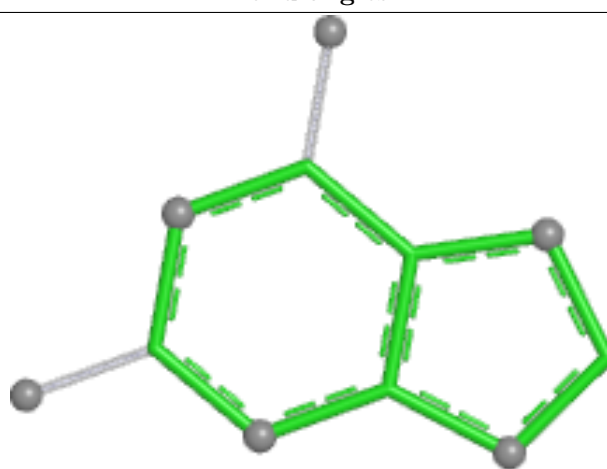
Bond lengths



Bond angles

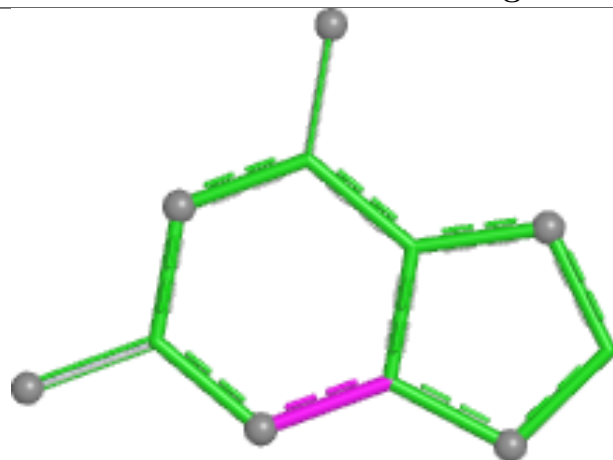


Torsions

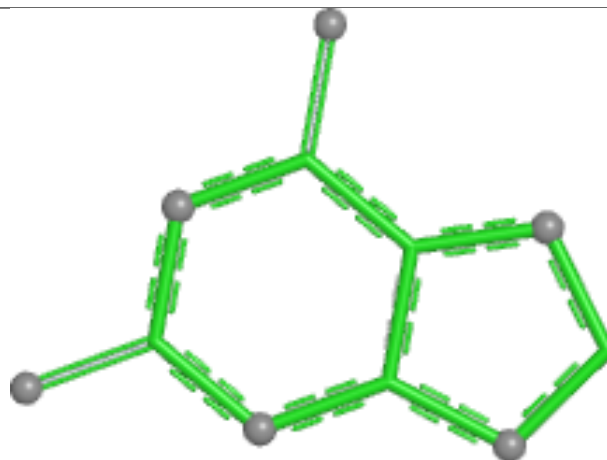


Rings

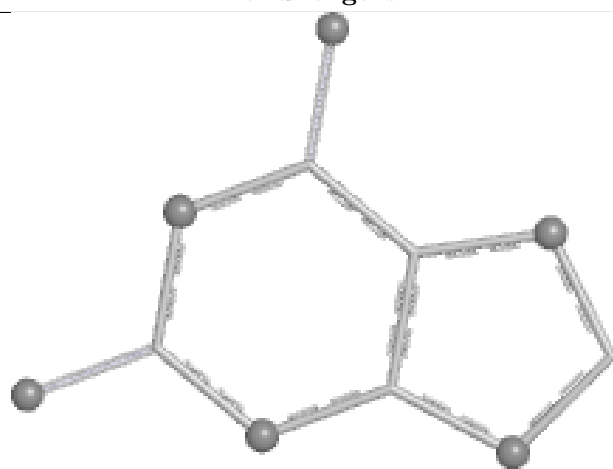
Ligand XAN C 5004



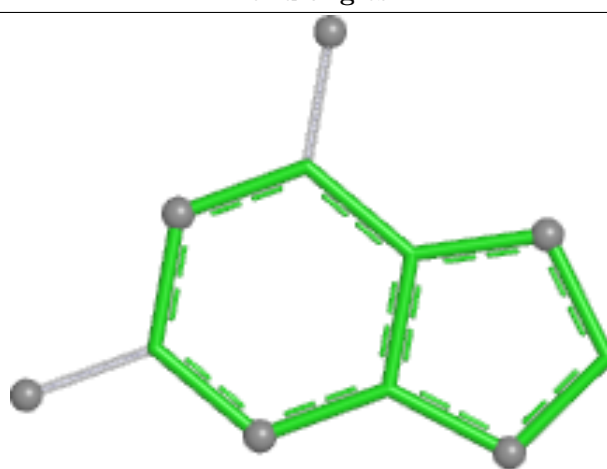
Bond lengths



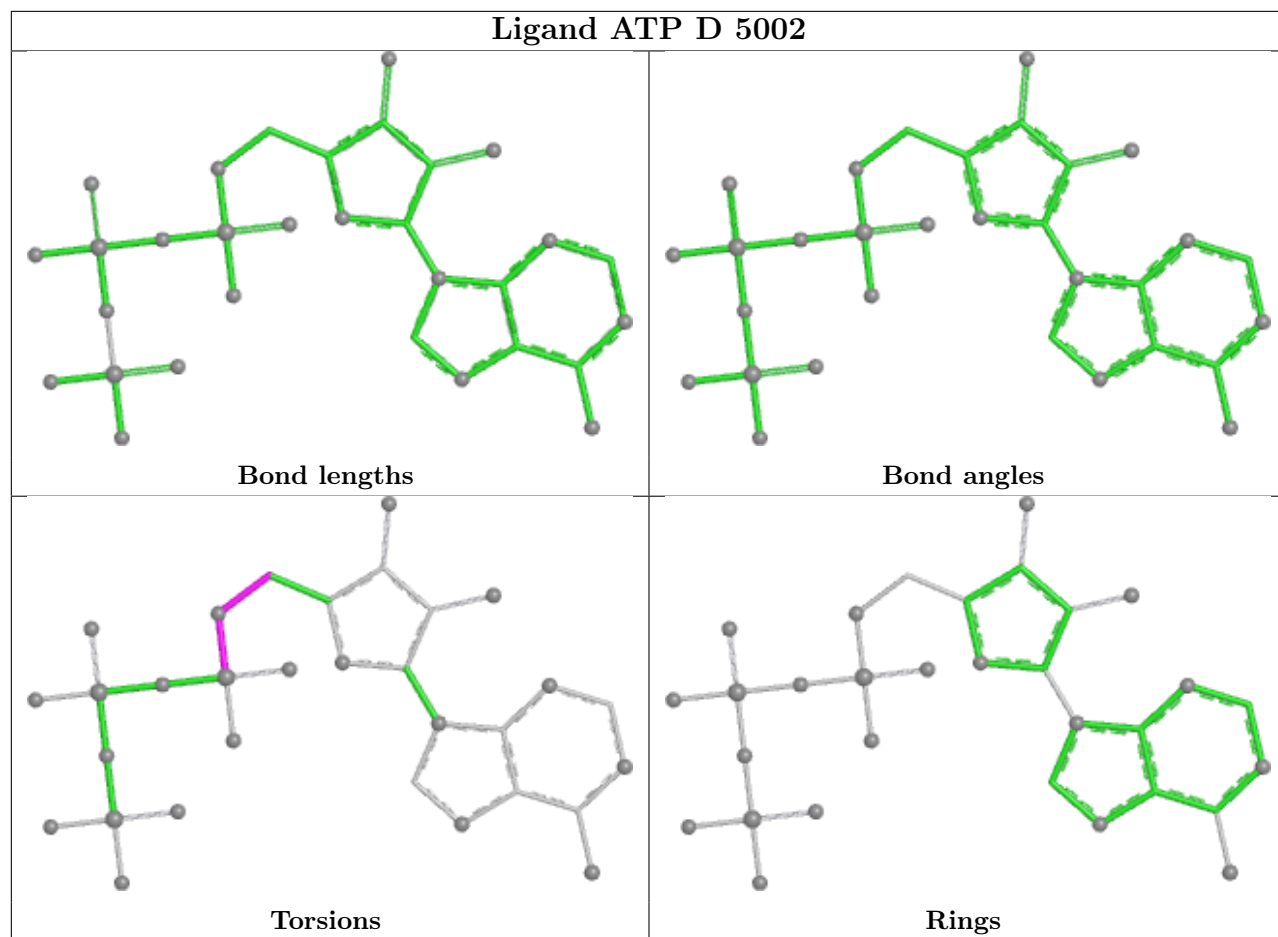
Bond angles

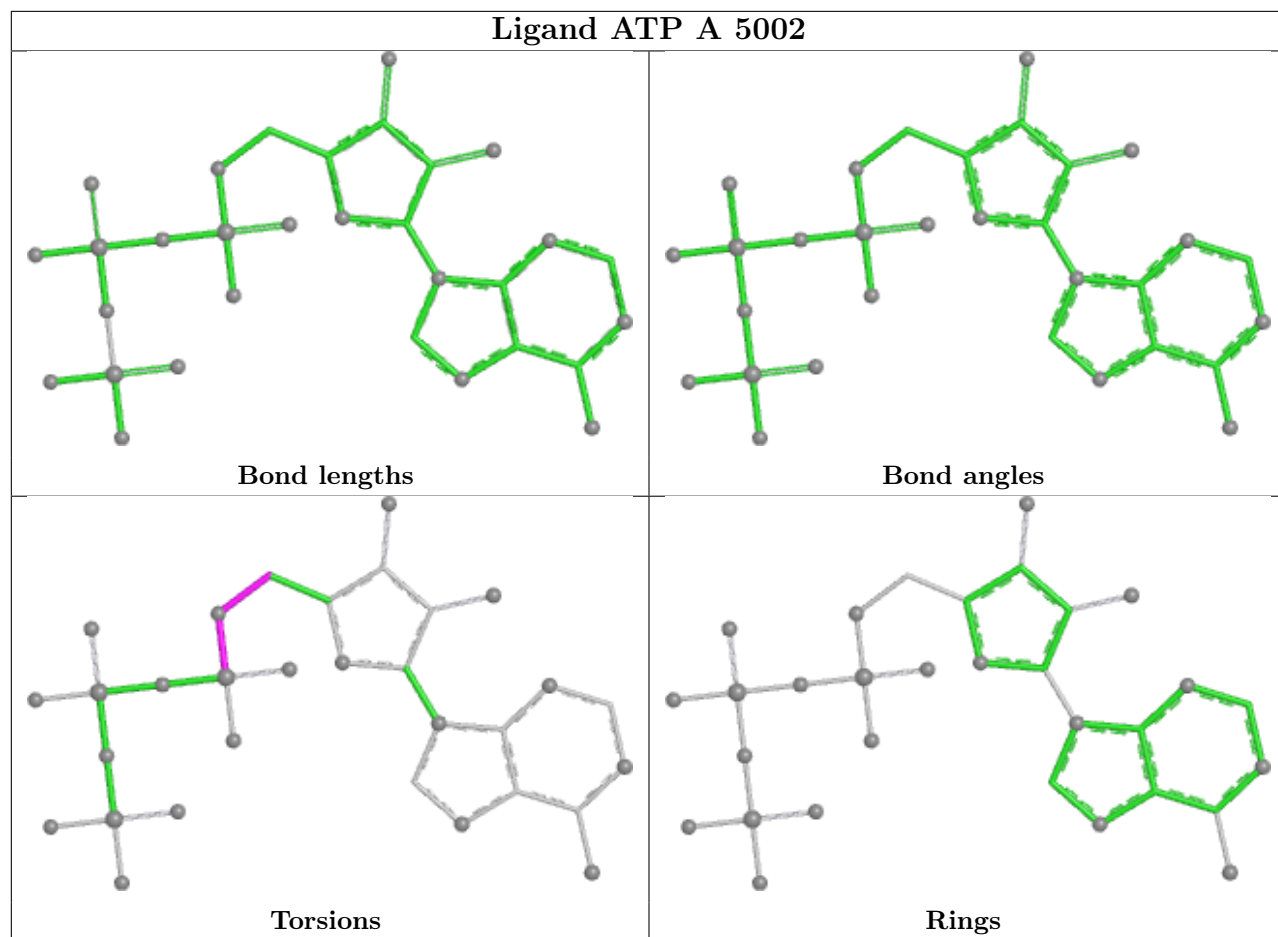


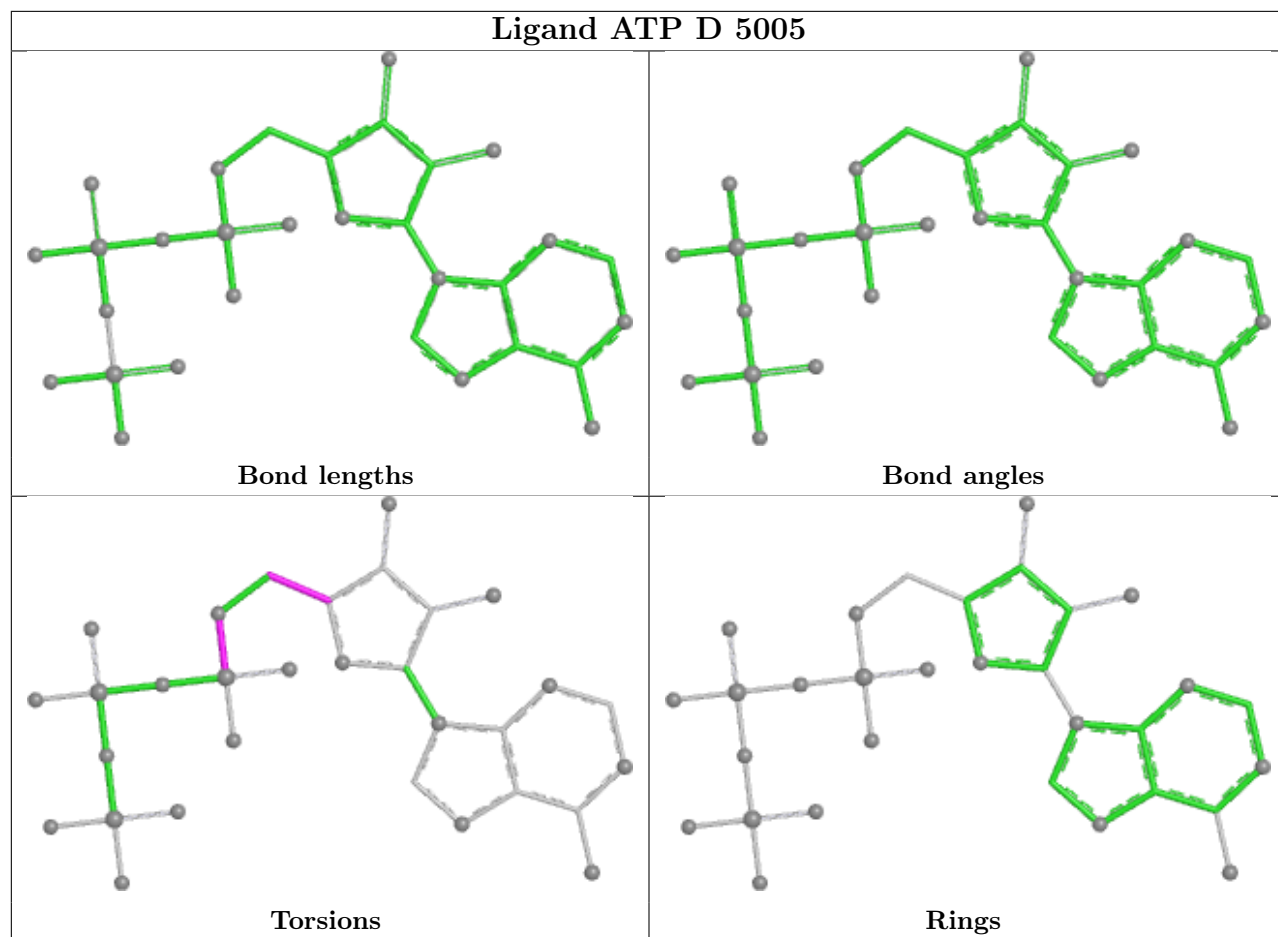
Torsions

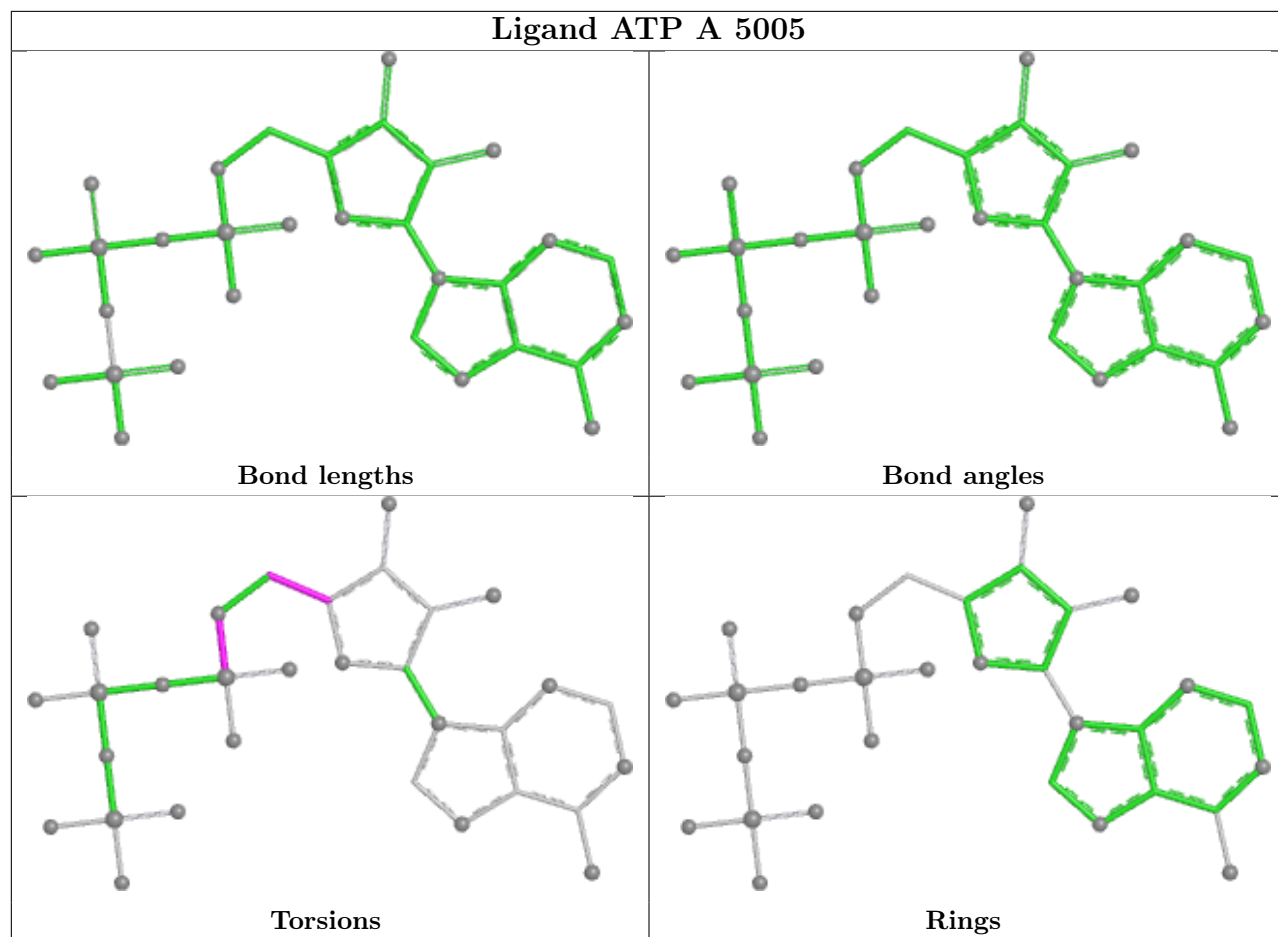


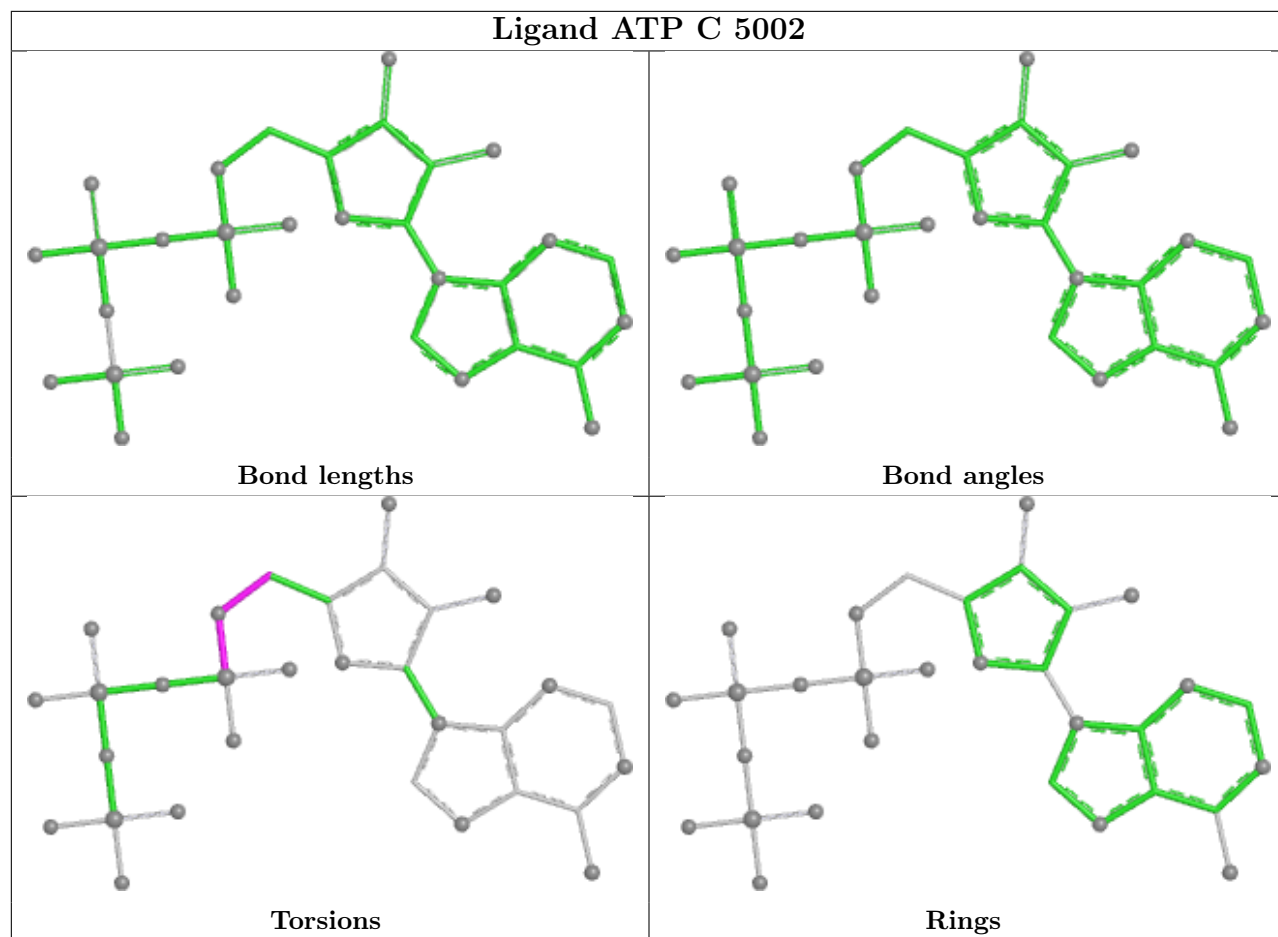
Rings

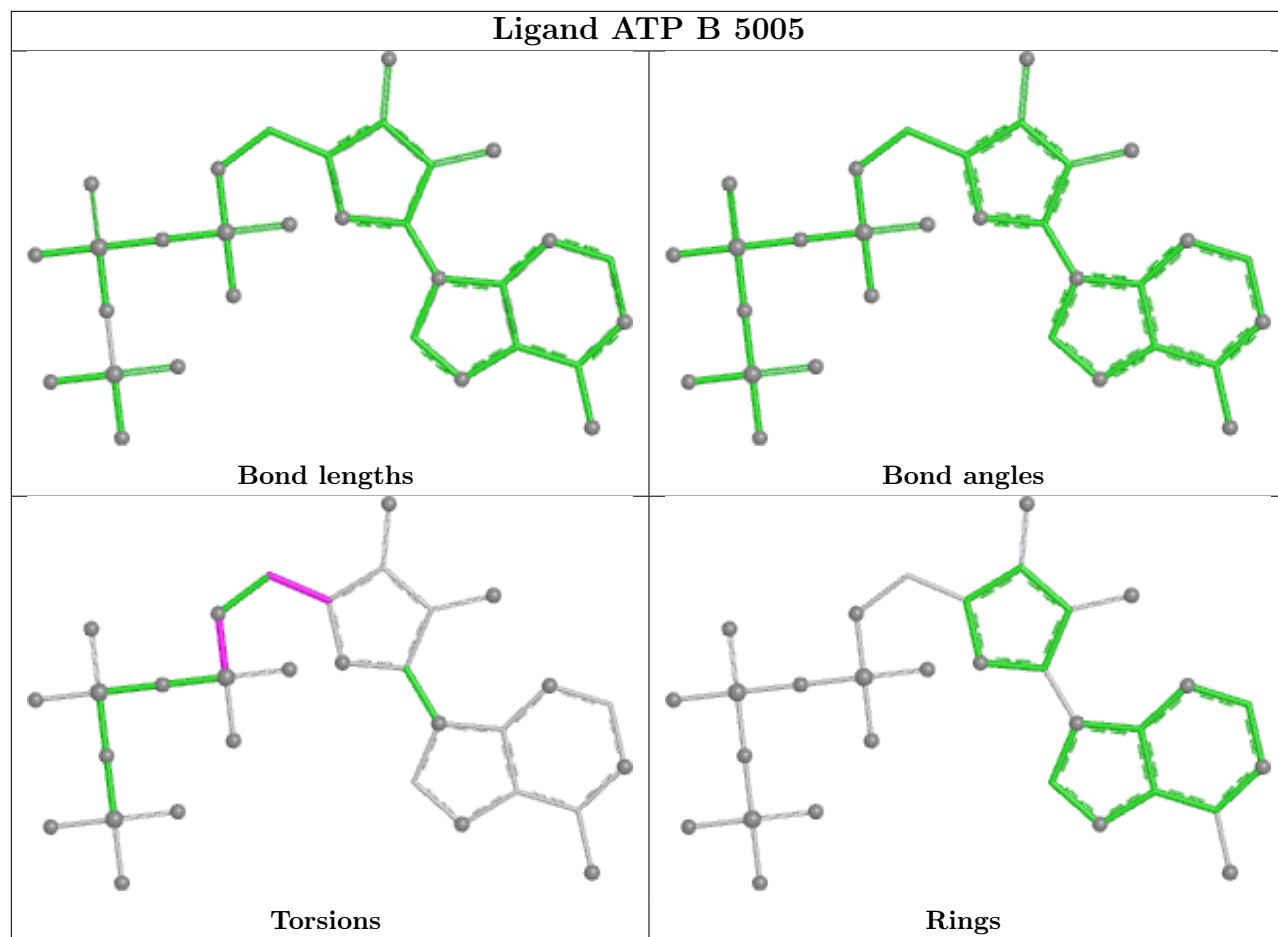


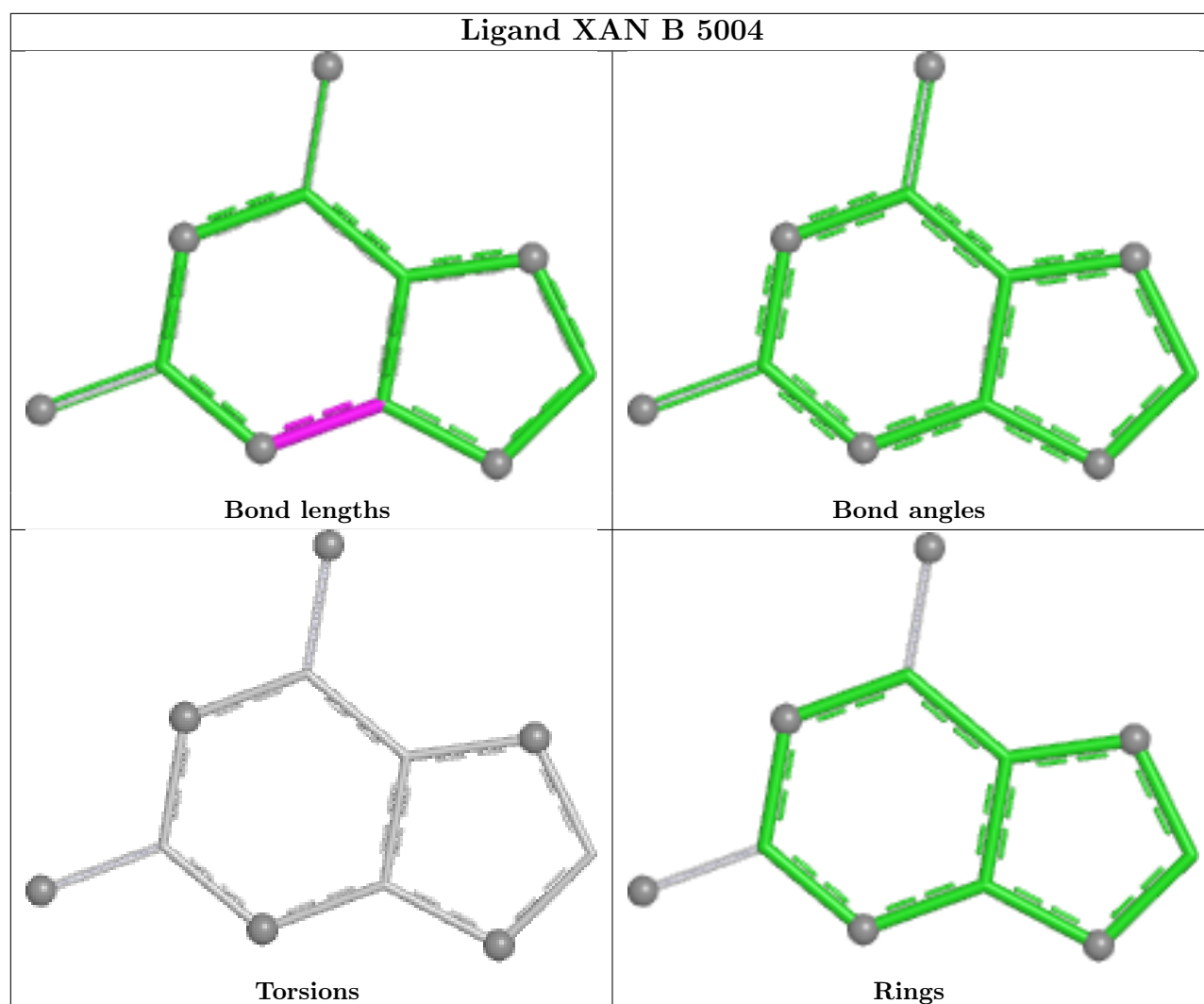












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

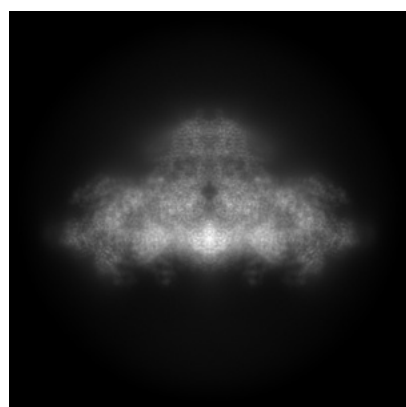
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26414. These allow visual inspection of the internal detail of the map and identification of artifacts.

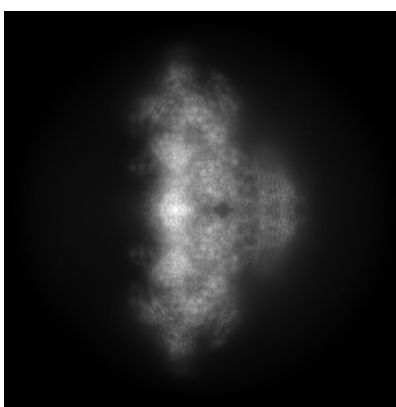
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

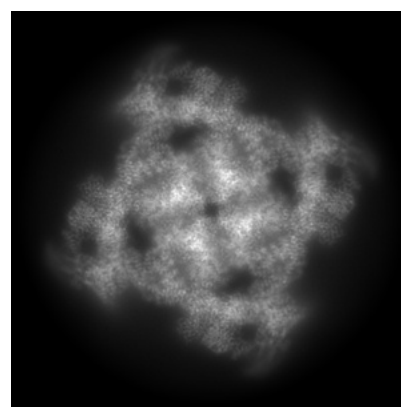
6.1.1 Primary map



X



Y

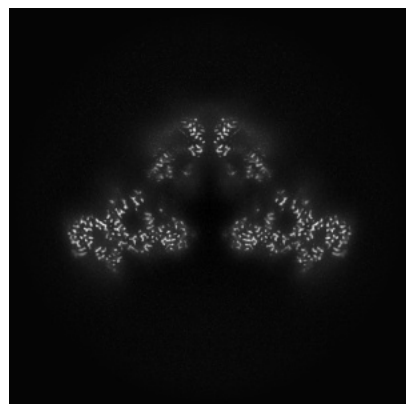


Z

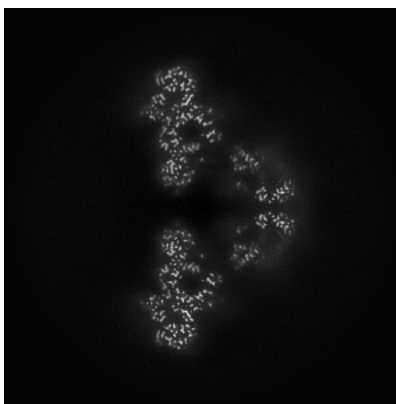
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

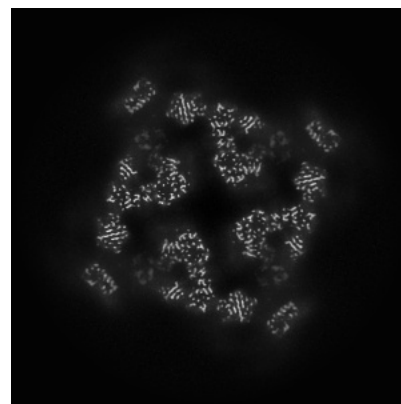
6.2.1 Primary map



X Index: 256



Y Index: 256

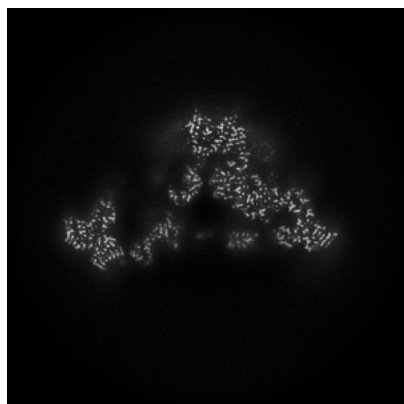


Z Index: 256

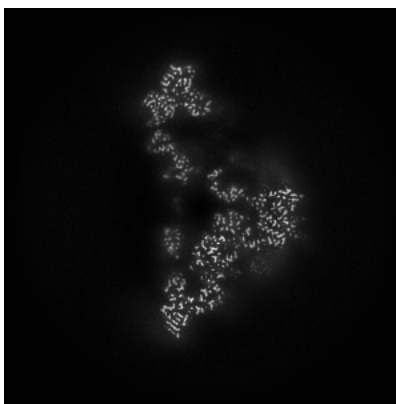
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

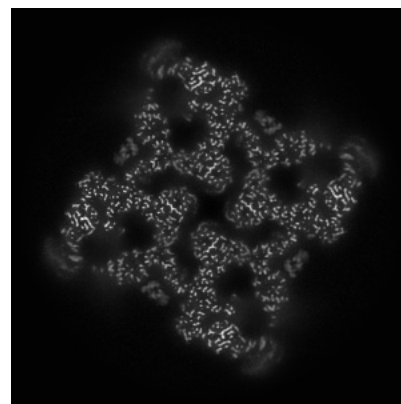
6.3.1 Primary map



X Index: 275



Y Index: 274

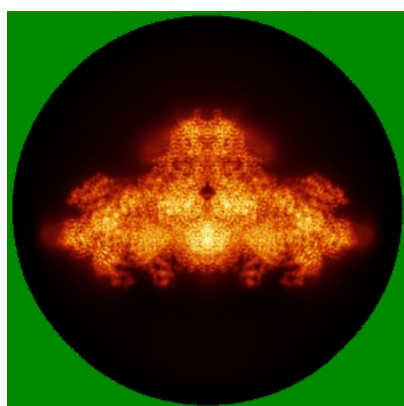


Z Index: 220

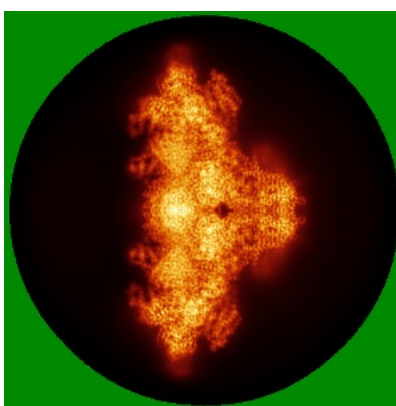
The images above show the largest variance slices of the map in three orthogonal directions.

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

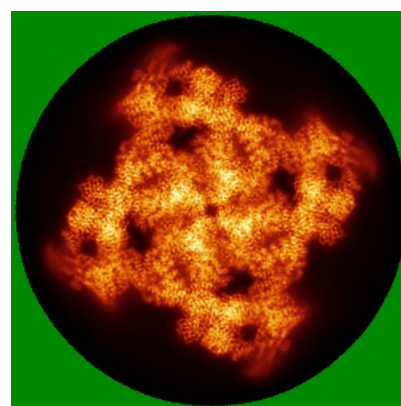
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

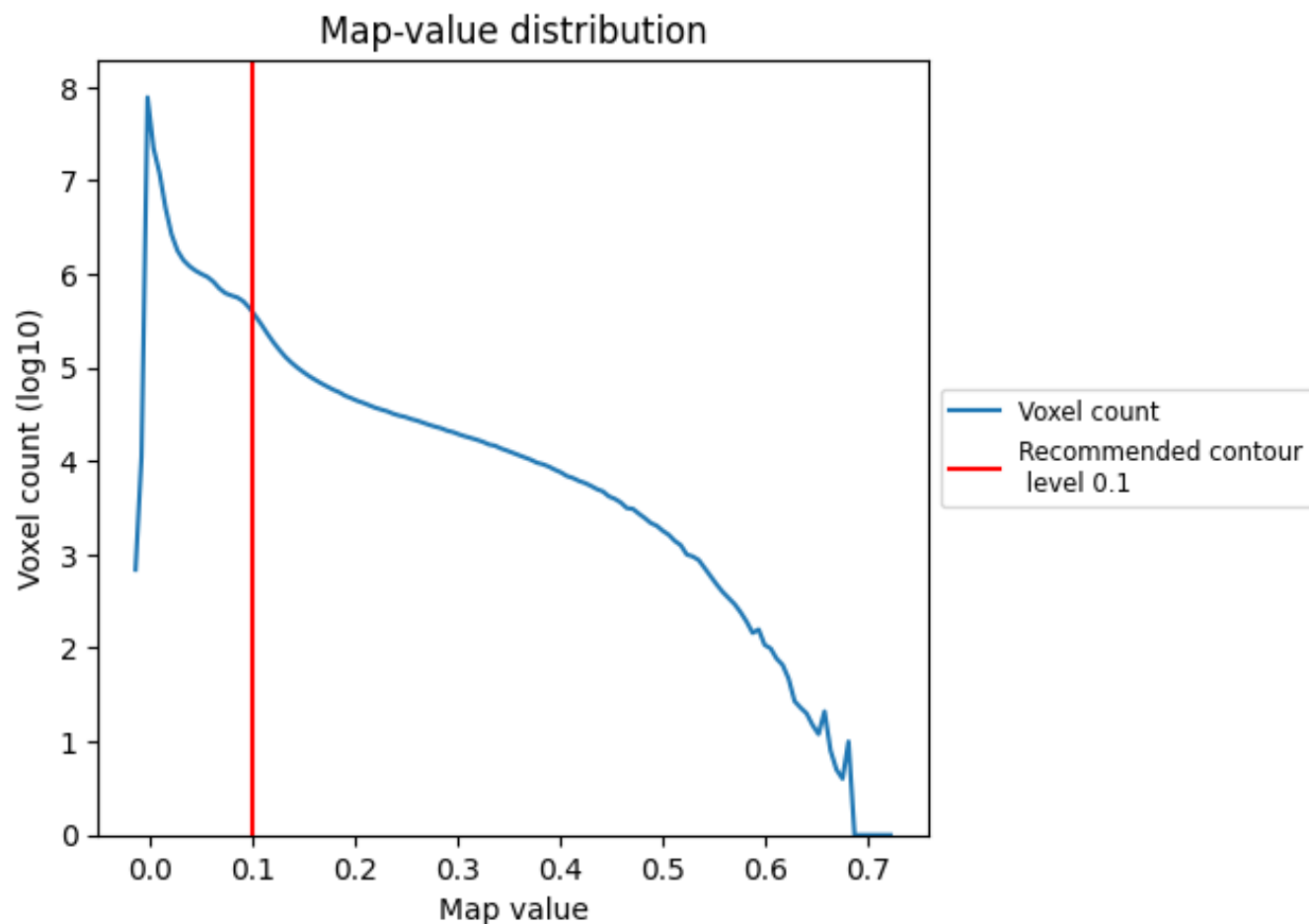
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

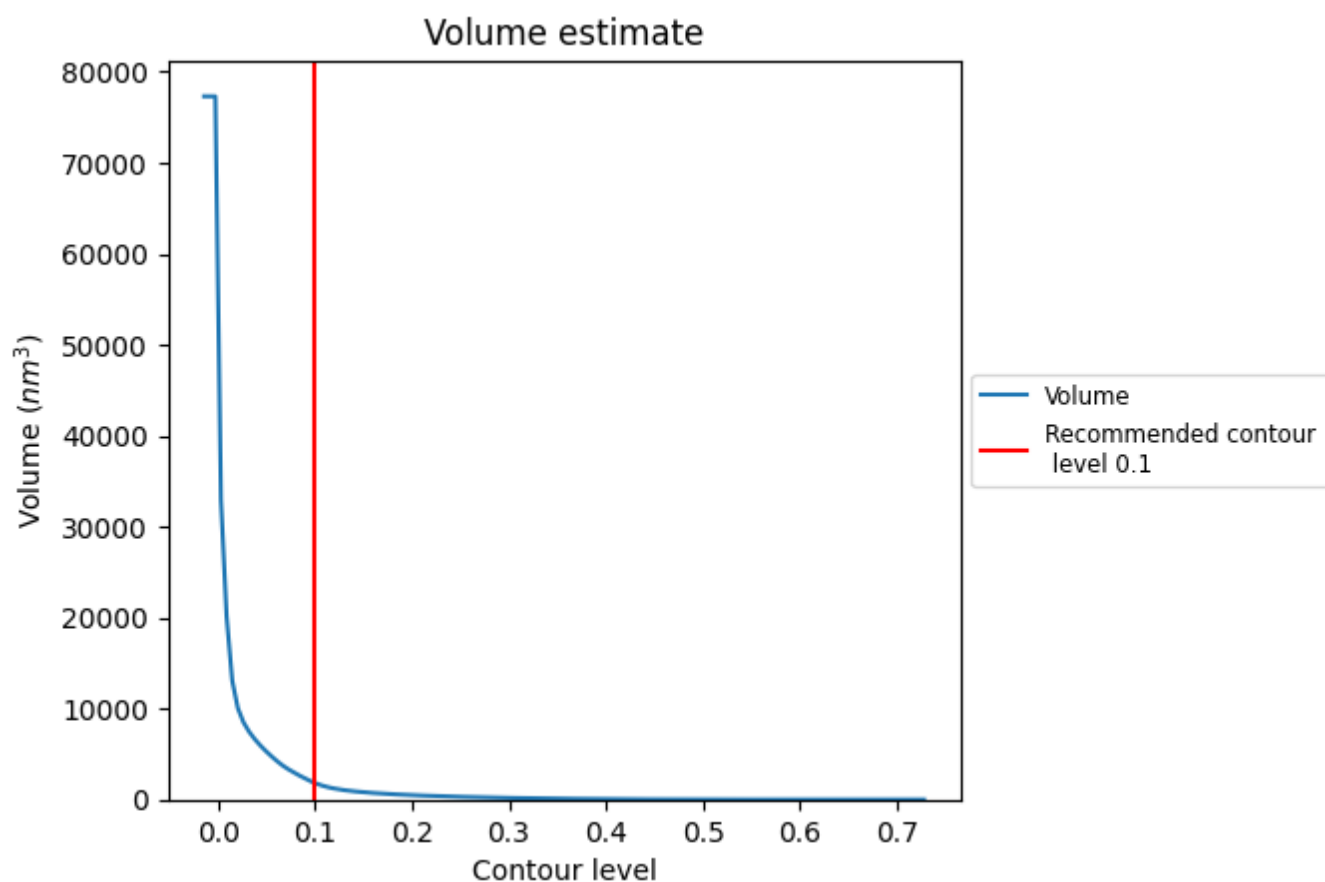
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

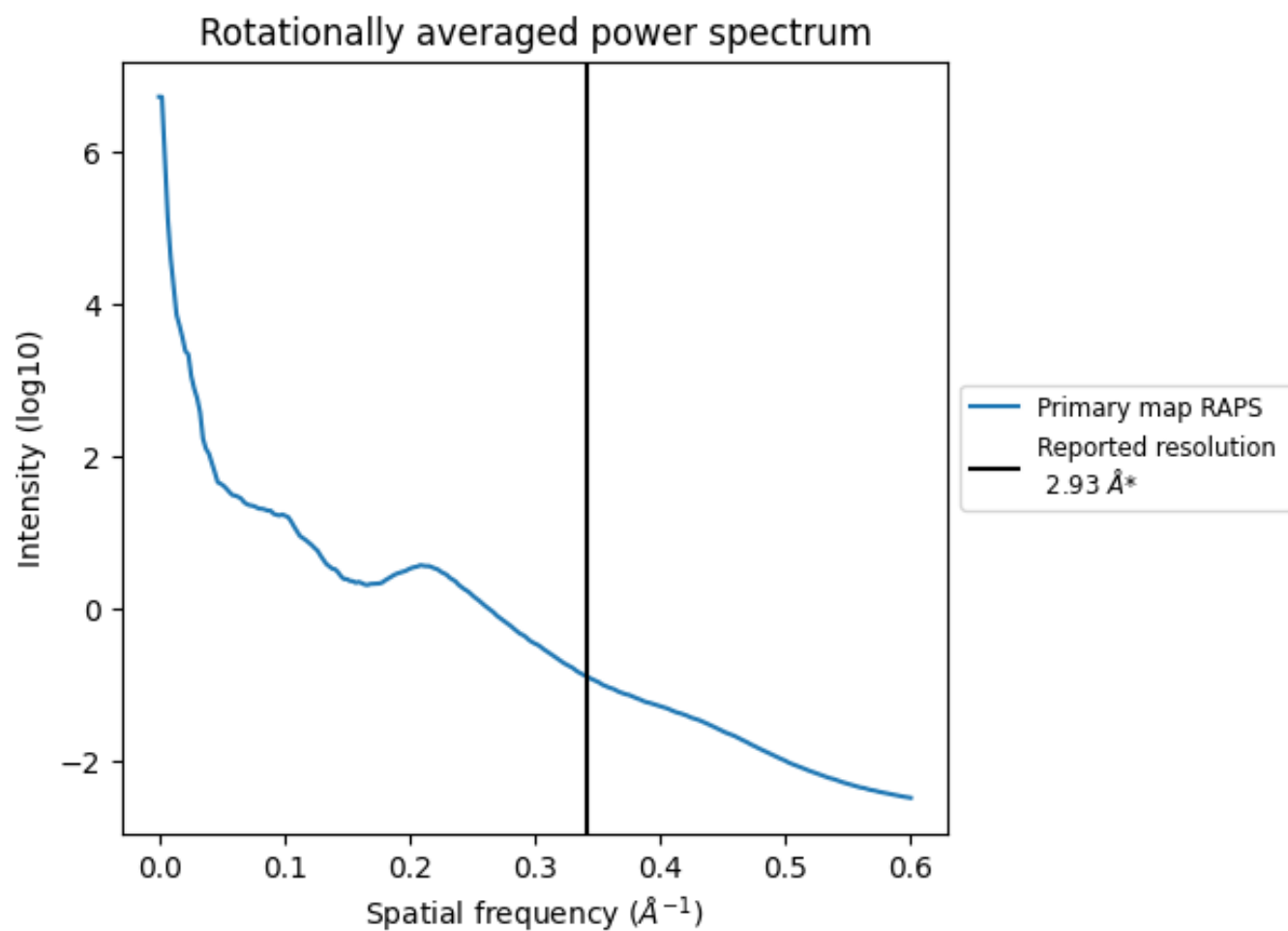
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1824 nm^3 ; this corresponds to an approximate mass of 1648 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 0.341 Å⁻¹

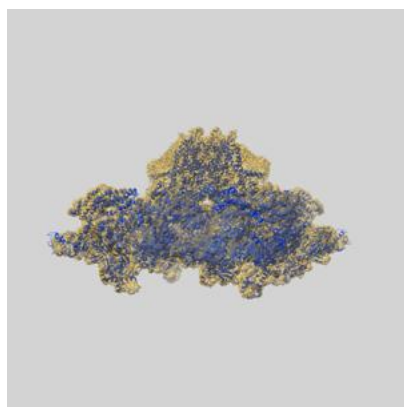
8 Fourier-Shell correlation

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

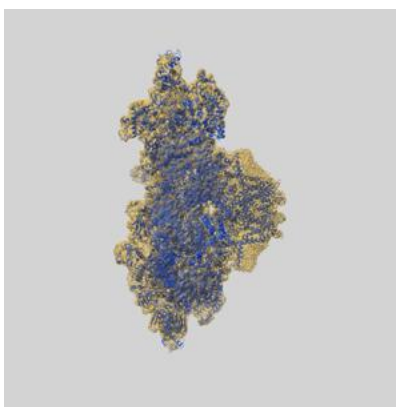
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26414 and PDB model 7UA4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

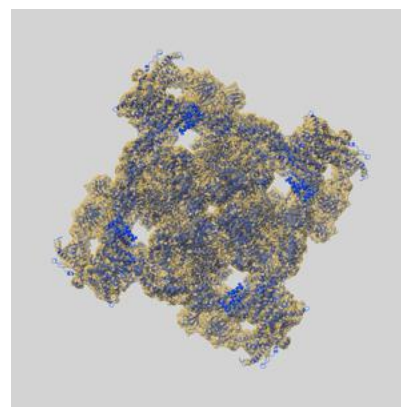
9.1 Map-model overlay [i](#)



X



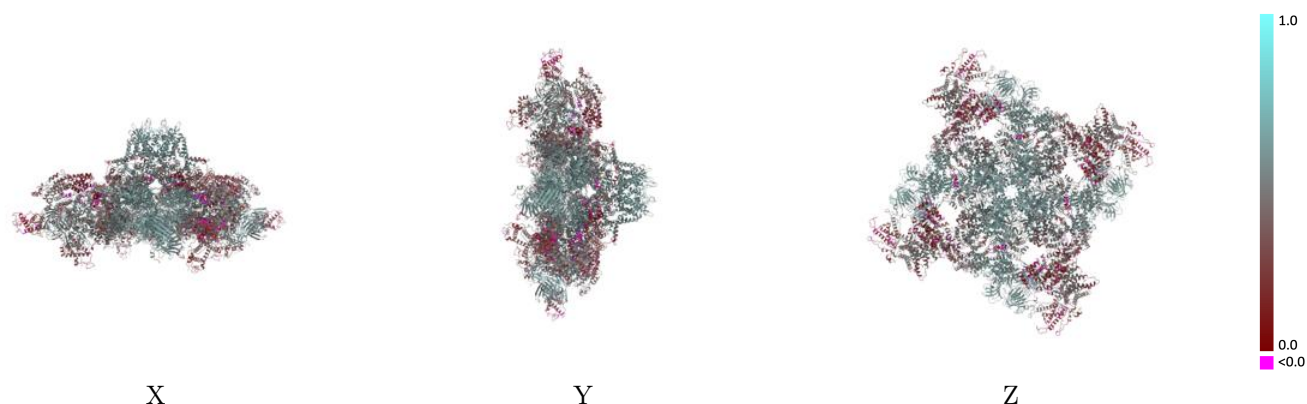
Y



Z

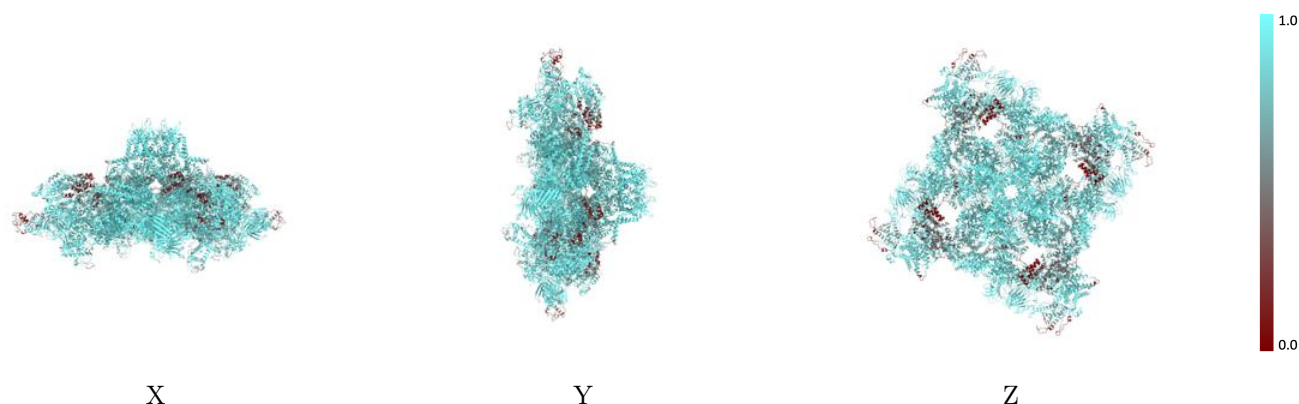
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



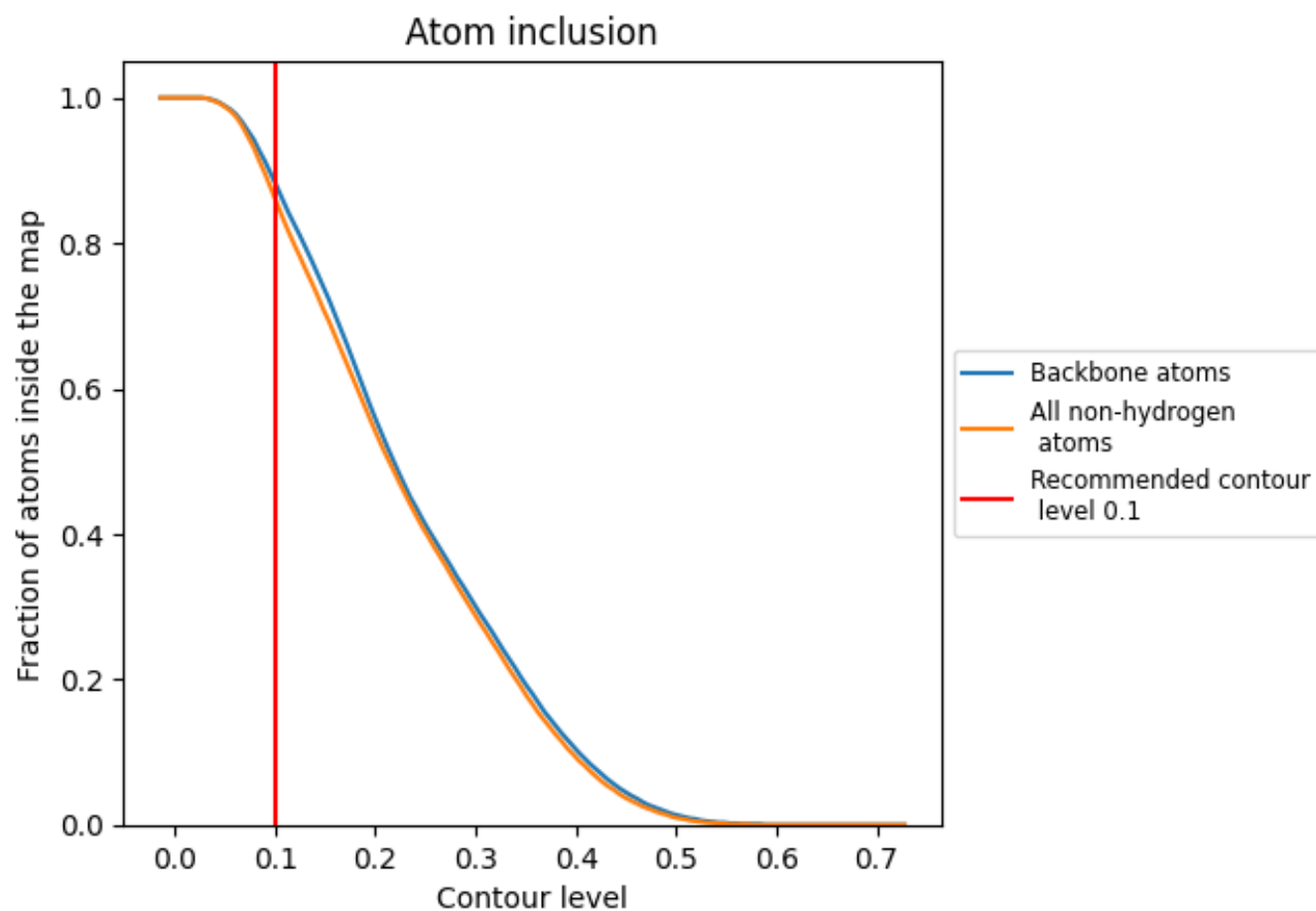
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.4560
A	0.8680	0.4670
B	0.8670	0.4580
C	0.8660	0.4570
D	0.8660	0.4610
E	0.9670	0.5880
F	0.9720	0.5700
G	0.9720	0.5710
H	0.9690	0.5730
I	0.6900	0.2200
J	0.6640	0.2040
K	0.6880	0.2240
L	0.6650	0.2110

