



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 08:51 PM EST

PDB ID : 8SEO
EMDB ID : EMD-40423
Title : Cryo-EM Structure of RyR1 + ATP-gamma-S
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.92 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

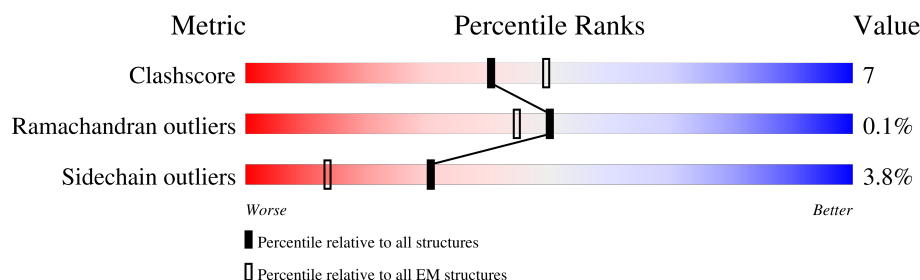
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.92 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	5037	<div> <div>13%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	B	5037	<div> <div>13%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	C	5037	<div> <div>13%</div> <div>68%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	D	5037	<div> <div>13%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
2	E	350	<div> <div>28%</div> <div>•</div> <div>69%</div> </div>
2	F	350	<div> <div>27%</div> <div>•</div> <div>69%</div> </div>
2	G	350	<div> <div>27%</div> <div>•</div> <div>69%</div> </div>
2	H	350	<div> <div>27%</div> <div>•</div> <div>69%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 143016 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		
1	B	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		
1	C	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		
1	D	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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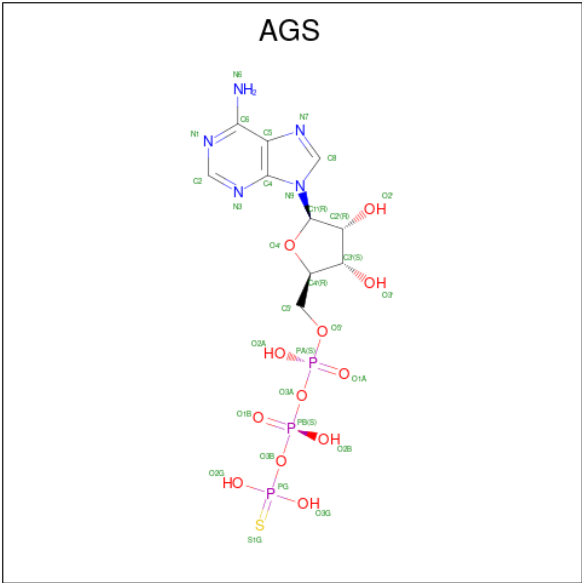
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

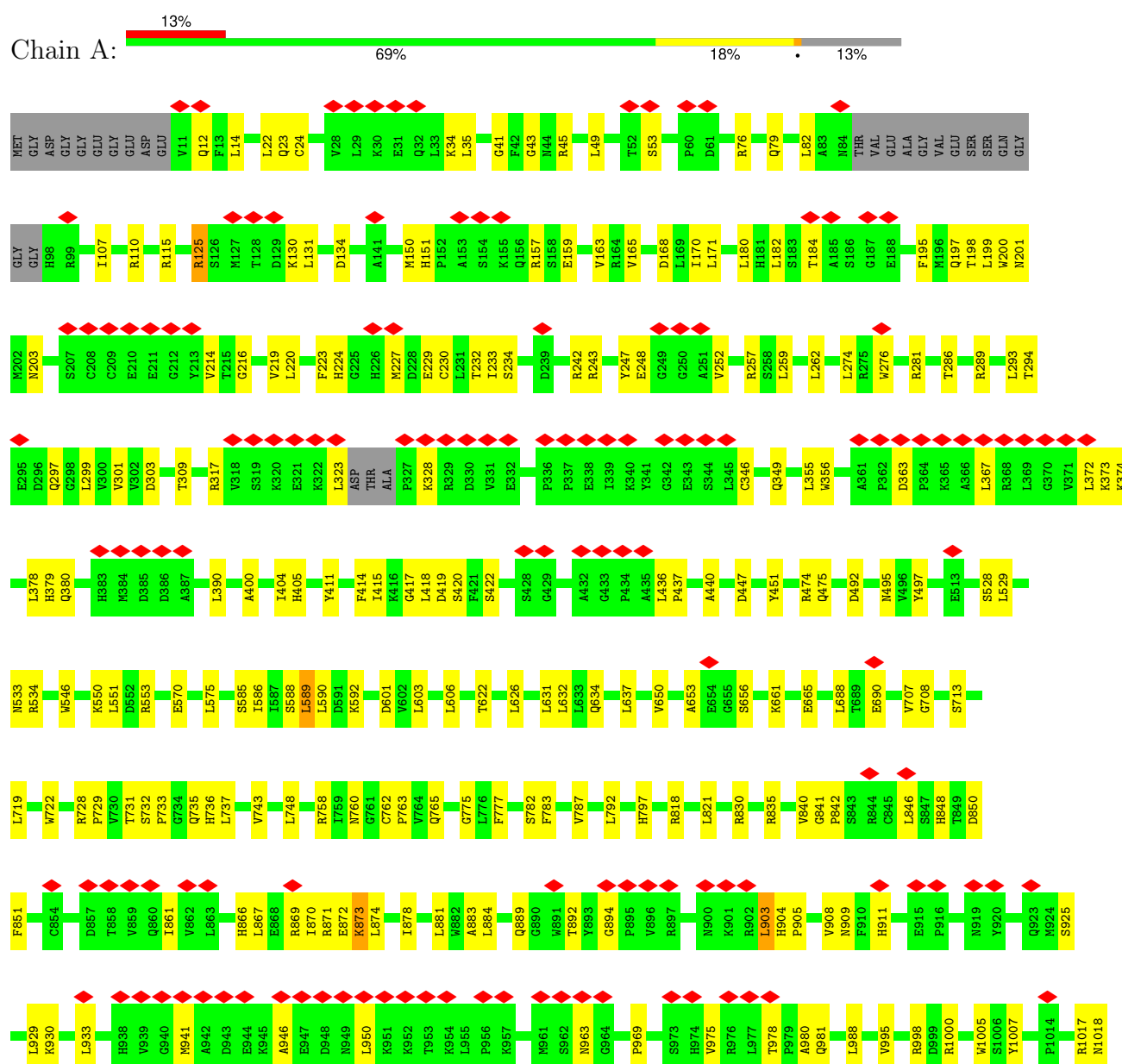
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ryanodine receptor 1



E2413	L2290	E2414	E2296	V2299	L2307	Q2308	L2313	L2314	A2315	D2320	I2321	R2336	V2339	V2353	R2359	G2365	P2366	A2367	G2468	I2469	I2470	S2471	L2472	P2473	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	K2499	A2500	S2501	N2502	R2508	V2509	Y2510	G2511	I2512	E2513	D2516	F2517	L2518	L2519
PRO	ALA	GLU	E2088	K2089	K2090	L2094	L2097	V2098	M2101	Q2107	Y2110	F2121	S2122	L2123	P2146	I2167	Q2173	V2190	Q2193	G2202	M2203	H2204	M2211	V2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	R2244	Q2245	L2254	L2258	L2263	N2283	L2286	A2287	P2410	P2411	E2412					
L1021	L1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	K1032	R1036	L1039	C1040	V1043	R1044	T1045	L1046	Y1051	N1052	P1055	P1056	D1057	Q1058	E1059	P1060	S1061	Q1062	V1063	E1064	N1065	R1068	W1069	I1074	F1075	A1076	R1087	W1088	Y1089	F1090	E1091	T1097	R1101	R1106	L1109	R1110			
P1111	L1115	G1116	L1120	A1121	R1128	R1131	W1132	W1143	M1152	I1153	D1154	L1155	T1156	I1160	D1172	S1173	S1175	T1177	A1178	E1181	I1182	E1183	G1197	Q1198	V1199	N1203	L1204	G1205	S1210	L1211	L1219	F1223	E1224	P1225	T1228	T1236	P1243	P1249	P1250								
E1251	H1252	P1253	L1254	Y1255	E1256	V1257	A1258	R1259	W1264	C1269	L1270	R1275	T1276	W1277	G1278	N1281	L1291	V1295	C1303	T1304	ALA	GLY	ALA	THR	PRO	VAL	GLY	GLN	ASP	PRO	ALA	THR	GLY	ASN	ARG	ALA	GLY	PHE	PHE	LYS	ALA	LYS	ALA				
ARG	SER	ALA	GLY	TRP	GLY	GLU	ALA	GLY	GLY	LYS	GLU	GLY	THR	ALA	LYS	GLY	THR	PRO	GLN	PRO	GLY	GLU	ALA	GLN	THR	PRO	VAL	ARG	ALA	ALA	PRO	GLY	LEU	LYS	GLN	ASP	PRO	ALA	GLY	GLU	PHE	PHE	LYS	ALA	LYS	ALA	
ALA	MET	THR	GLN	PRO	PRO	ALA	THR	PRO	ALA	LEU	PRO	ARG	LEU	HIS	ASP	VAL	VAL	PRO	D1419	N1420	R1421	D1422	T1427	L1428	T1432	Y1433	V1439	G1442	Q1443	V1448	G1451	P1455	H1458	D1461	K1468	V1474	M1475	G1477	D1478	E1479	S1485	S1486					
M1494	V1501	S1502	P1503	G1504	Q1505	Q1506	G1507	R1508	I1509	S1510	H1511	T1512	D1513	L1514	L1519	V1520	M1527	K1534	N1537	F1540	K1547	L1548	F1549	P1550	V1554	L1555	Q1559	M1560	V1561	I1562	Q1563	F1564	K1568	Q1569	K1570	P1574	M1579	P1589	Q1590	C1591	P1592	L1595	E1596	V1597			
P1602	E1616	A1620	A1627	Q1628	V1629	M1637	P1642	I1650	L1653	R1656	Q1660	H1665	L1676	V1681	L1685	L1694	L1715	E1721	R1725	S1726	R1727	L1731	L1738	E1741	T1742	R1743	A1744	I1745	F1748	R1752	K1753	G1754	G1755	N1756	A1757	R1758	L1759										
H1760	T1769	R1772	P1773	H1776	A1788	A1789	G1790	V1791	A1792	E1793	L1798	R1808	D1828	P1829	V1830	Q1837	L1842	S1846	M1851	G1852	I1853	F1854	D1858	V1870	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU			
LYS	GLU	ASP	GLU	GLU	GLU	LYS	ASP	ALA	GLU	LYS	GLU	GLU	ALA	PRO	GLY	GLU	LYS	GLU	ASP	L1922	E1944	E1956	K1968	Q1973	L1980	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	R1993	R1994	T1995	R1996	R1999	S2000	Q2003	E2004	Q2005	I2006				
N2007	K2013	D2014	E2015	E2018	E2019	D2020	C2021	R2028	Q2029	D2030	L2031	Q2032	L2039	I2044	Q2045	L2046	GLU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	
PRO	ALA	GLU	E2088	K2089	K2090	L2094	L2097	V2098	M2101	Q2107	Y2110	F2121	S2122	L2123	P2146	I2167	Q2173	V2190	Q2193	G2202	M2203	H2204	M2211	V2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	R2244	Q2245	L2254	L2258	L2263	N2283	L2286	A2287								
L2290	E2296	V2299	L2307	Q2308	L2313	L2314	A2315	D2320	I2321	R2336	V2339	V2353	R2359	G2365	P2366	A2367	G2468	I2469	I2470	S2471	L2472	P2473	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	K2499	A2500	S2501	N2502	R2508	V2509	Y2510	G2511	I2512	E2513	D2516	F2517	L2518	L2519		





Frequency	Percentage
Daily	69%
Weekly	18%
Monthly	13%
Other	13%

















Chain D:





E2893	L2894	A2895	A2896	K2897	G2898	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	P2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	K2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	Q2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	Q2971
I2874	L2877	E2878	A2879	V2880	V2881	S2882	S2883	L3075	D3076	A3077	R3078	T3079	V3080	K3081	K3082	V3088	D3102	I3103	E3104	V3107	L3110	L3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	T3130	Y3131	T3132	T3133	L3136	H3146	S3147	Q3151	P3152	G3153	D3154	P3155	V3156	I3157	L3158	V3163						
S3171	I3172	Y3173	S3174	L3175	N3180	T3181	Y3182	V3183	E3184	K3185	L3190	K3201	P3202	V3203	L3206	E3207	P3208	Q3209	L3210	N3214	A3215	C3216	S3217	V3218	V3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	P3244	V3245	L3246	D3247	R3248	I3253						
T3264	E3265	T3273	W3284	G3288	P3289	P3292	P3293	P3294	A3295	L3296	P3297	A3298	Q3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	V3324	I3329	D3330	E3331	A3332	V3340	F3341	A3342	I3345	V3346	S3347	L3354	F3358	T3361	R3364	E3377	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387													
E3388	E3389	G3390	E3391	L3392	R3403	Y3409	R3414	Y3415	V3416	W3423	L3424	P3427	I3443	Y3444	V3445	F3451	E3454	N3457	F3458	V3459	V3460	Q3461	N3465	N3466	K3467	S3468	L3470	T3471	A3472	D3473	S3474	K3475	S3476	K3477	N3478	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN										
GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	S3503	V3505	Q3506	S3508	L3509	V3511	K3515	N3523	D3531	L3532	I3533	M3534	K3537	T3538	A3541	L3542	K3543	D3544	N3555	N3556	L3557	H3558	L3559	Q3560	K3561	K3562	V3563	E3564	F3565	S3566	L3569	R3570	L3575	Y3576	R3577	P3580	G3581											
R3582	E3583	E3584	D3585	A3586	D3587	P3589	I3592	R3595	V3596	A3601	Y3604	E3607	E3610	H3611	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	P3640	A3659	A3660	V3661	I3662	L3663	E3670	D3675											
D3676	L3677	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	L3698	H3699	Q3700	F3705	T3708	A3730	K3731	I3732	E3736	GLU	GLY	GLY	ASN	GLY	ALA	ALA	GLU	GLU	GLU	GLU	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3760	R3769	L3770	H3771	T3772	R3773	L3780	G3788										
L3798	S3803	K3815	L3820	K3821	K3824	L3835	L3842	D3843	L3844	K3858	V3859	N3860	E3861	D3862	T3864	I3865	I3866	N3867	R3868	Q3869	N3870	G3871	K3872	V3874	M3875	D3878	L3884	L3888	Q3889	L3890	L3891	F3899	L3903	T3915	T3919	S3929	D3932	V3935	Y3936	Y3937																	
S3938	G3939	K3940	E3945	Q3946	R3949	K3953	A3954	M3955	L3965	T3966	E3967	L3980	L3985	V3995	M3999	K4002	L4019	V4036	M4039	Q4043	V4049	L4068	I4071	S4074	E4075	A4076	D4079	T4082	L4088	S4089	K4090	K4091	L4092	F4093	Q4094	K4095	N4097	D4098																			
S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	A4117	E4118	M4119	E4120	E4121	M4122	I4123	N4124	F4125	D4138	N4142	E4152	P4155	R4159	L4160	R4161	L4164	E4165	E4172	R4175	L4178	Q4179	R4180	I4183	M4184	S4187	R4188	R4189	I4190	I4193	Y4194	F4195	E4196	I4197	S4198	E4199	T4200	N4201	R4202											
K4203	Q4204	E4205	N4207	K4211	E4212	S4213	E4224	E4227	M4245	Q4246	I4247	S4252	E4253	P4254	GLU	GLY	PRO	GLU	ALA	ASP	GLU	ASP	GLU	GLY	GLY	GLY	GLU	ALA	ALA	ALA	ALA	GLY	ALA	ALA	GLY	THR	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR												



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55892	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.268	Depositor
Minimum map value	-0.637	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.287	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	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, AGS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	1/35721 (0.0%)	0.65	11/48375 (0.0%)
1	B	0.32	1/35721 (0.0%)	0.65	10/48375 (0.0%)
1	C	0.32	1/35721 (0.0%)	0.65	10/48375 (0.0%)
1	D	0.32	1/35721 (0.0%)	0.65	10/48375 (0.0%)
2	E	0.32	0/834	0.64	0/1123
2	F	0.32	0/834	0.64	0/1123
2	G	0.32	0/834	0.64	0/1123
2	H	0.32	0/834	0.64	0/1123
All	All	0.32	4/146220 (0.0%)	0.65	41/197992 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	904	HIS	C-N	5.54	1.44	1.34
1	B	904	HIS	C-N	5.54	1.44	1.34
1	C	904	HIS	C-N	5.54	1.44	1.34
1	D	904	HIS	C-N	5.54	1.44	1.34

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	903	LEU	CA-CB-CG	6.24	129.64	115.30
1	C	903	LEU	CA-CB-CG	6.24	129.64	115.30
1	D	903	LEU	CA-CB-CG	6.24	129.64	115.30
1	A	903	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	4945	ASP	CB-CG-OD1	6.03	123.73	118.30
1	C	4945	ASP	CB-CG-OD1	6.03	123.73	118.30
1	D	4945	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	4945	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	3296	LEU	CA-CB-CG	5.90	128.87	115.30
1	C	3296	LEU	CA-CB-CG	5.90	128.87	115.30
1	D	3296	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	3296	LEU	CA-CB-CG	5.90	128.86	115.30
1	A	227	MET	CA-CB-CG	5.72	123.03	113.30
1	B	227	MET	CA-CB-CG	5.71	123.00	113.30
1	C	227	MET	CA-CB-CG	5.71	123.00	113.30
1	D	227	MET	CA-CB-CG	5.71	123.00	113.30
1	D	589	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	589	LEU	CA-CB-CG	5.62	128.24	115.30
1	C	589	LEU	CA-CB-CG	5.62	128.24	115.30
1	A	589	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	4164	LEU	CA-CB-CG	5.61	128.21	115.30
1	C	4164	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	4164	LEU	CA-CB-CG	5.60	128.17	115.30
1	D	4164	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	1152	MET	CA-CB-CG	5.24	122.21	113.30
1	C	1152	MET	CA-CB-CG	5.24	122.21	113.30
1	D	1152	MET	CA-CB-CG	5.23	122.18	113.30
1	A	1152	MET	CA-CB-CG	5.22	122.17	113.30
1	B	2751	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	2751	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	2751	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	2751	LEU	CA-CB-CG	5.12	127.06	115.30
1	A	1152	MET	CB-CG-SD	5.10	127.70	112.40
1	D	1152	MET	CB-CG-SD	5.10	127.69	112.40
1	B	1152	MET	CB-CG-SD	5.07	127.61	112.40
1	C	1152	MET	CB-CG-SD	5.07	127.61	112.40
1	A	1478	ASP	CB-CG-OD1	5.05	122.85	118.30
1	D	1478	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	1478	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	1478	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	2101	MET	CA-CB-CG	5.01	121.81	113.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	841	GLY	Mainchain
1	B	841	GLY	Mainchain
1	C	841	GLY	Mainchain
1	D	841	GLY	Mainchain

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	A	34904	0	34524	484	0
1	B	34904	0	34524	480	0
1	C	34904	0	34524	489	0
1	D	34904	0	34524	483	0
2	E	818	0	824	5	0
2	F	818	0	824	7	0
2	G	818	0	824	10	0
2	H	818	0	824	7	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	143016	0	141440	1931	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 7.

All (1931) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2283:ASN:HD22	1:C:2286:LEU:HG	1.56	0.71
1:B:2283:ASN:HD22	1:B:2286:LEU:HG	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2283:ASN:HD22	1:D:2286:LEU:HG	1.56	0.70
1:B:1561:VAL:HG12	1:B:1562:ILE:HG13	1.74	0.69
1:C:317:ARG:NH2	1:C:349:GLN:OE1	2.25	0.69
1:A:2283:ASN:HD22	1:A:2286:LEU:HG	1.56	0.69
1:D:1561:VAL:HG12	1:D:1562:ILE:HG13	1.74	0.69
1:A:3577:ARG:HH21	1:A:3582:ARG:HB3	1.58	0.69
1:D:3577:ARG:HH21	1:D:3582:ARG:HB3	1.58	0.69
1:C:3577:ARG:HH21	1:C:3582:ARG:HB3	1.58	0.68
1:A:1561:VAL:HG12	1:A:1562:ILE:HG13	1.74	0.68
1:B:3577:ARG:HH21	1:B:3582:ARG:HB3	1.58	0.68
1:C:1561:VAL:HG12	1:C:1562:ILE:HG13	1.74	0.68
1:A:317:ARG:NH2	1:A:349:GLN:OE1	2.25	0.68
1:D:317:ARG:NH2	1:D:349:GLN:OE1	2.25	0.68
1:A:2530:MET:SD	1:A:2531:ARG:NH1	2.68	0.67
1:B:2530:MET:SD	1:B:2531:ARG:NH1	2.68	0.67
1:D:2530:MET:SD	1:D:2531:ARG:NH1	2.68	0.67
1:C:2530:MET:SD	1:C:2531:ARG:NH1	2.68	0.67
1:D:946:ALA:O	1:D:950:LEU:HB2	1.95	0.67
1:A:946:ALA:O	1:A:950:LEU:HB2	1.95	0.66
1:C:946:ALA:O	1:C:950:LEU:HB2	1.95	0.66
1:B:317:ARG:NH2	1:B:349:GLN:OE1	2.25	0.66
1:A:3980:LEU:HD12	1:A:3985:LEU:HD22	1.77	0.66
1:C:3980:LEU:HD12	1:C:3985:LEU:HD22	1.77	0.66
1:B:475:GLN:NE2	1:B:528:SER:O	2.29	0.65
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.29	0.65
1:B:946:ALA:O	1:B:950:LEU:HB2	1.95	0.65
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.30	0.65
1:A:475:GLN:NE2	1:A:528:SER:O	2.29	0.65
1:A:2430:ILE:HD13	1:A:2502:MET:HG3	1.79	0.65
1:D:2430:ILE:HD13	1:D:2502:MET:HG3	1.79	0.65
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.29	0.65
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.29	0.65
1:B:3980:LEU:HD12	1:B:3985:LEU:HD22	1.77	0.65
1:D:3980:LEU:HD12	1:D:3985:LEU:HD22	1.77	0.65
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.79	0.65
1:D:3932:ASP:HA	1:D:3935:TRP:HB2	1.78	0.65
1:C:3932:ASP:HA	1:C:3935:TRP:HB2	1.78	0.64
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.79	0.64
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.79	0.64
1:C:2430:ILE:HD13	1:C:2502:MET:HG3	1.79	0.64
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.30	0.64
1:D:1476:MET:HB3	1:D:1485:SER:HB3	1.80	0.64
1:B:247:TYR:HB2	1:B:374:LYS:HB3	1.80	0.64
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.30	0.64
1:B:2430:ILE:HD13	1:B:2502:MET:HG3	1.79	0.64
1:D:475:GLN:NE2	1:D:528:SER:O	2.29	0.64
1:A:3031:ALA:HB3	1:A:3036:LYS:HZ3	1.63	0.64
1:C:1476:MET:HB3	1:C:1485:SER:HB3	1.80	0.64
1:A:1476:MET:HB3	1:A:1485:SER:HB3	1.80	0.63
1:C:475:GLN:NE2	1:C:528:SER:O	2.29	0.63
1:A:1023:PRO:HD2	1:A:1026:LEU:HD12	1.80	0.63
1:A:3932:ASP:HA	1:A:3935:TRP:HB2	1.78	0.63
1:B:3031:ALA:HB3	1:B:3036:LYS:HZ3	1.64	0.63
1:C:842:PRO:O	1:C:1197:GLY:N	2.26	0.63
1:B:3932:ASP:HA	1:B:3935:TRP:HB2	1.78	0.63
1:B:1023:PRO:HD2	1:B:1026:LEU:HD12	1.81	0.63
1:B:1476:MET:HB3	1:B:1485:SER:HB3	1.80	0.63
1:C:247:TYR:HB2	1:C:374:LYS:HB3	1.80	0.63
1:C:1023:PRO:HD2	1:C:1026:LEU:HD12	1.81	0.63
1:D:247:TYR:HB2	1:D:374:LYS:HB3	1.80	0.63
1:D:1029:GLU:HA	1:D:1032:LYS:HB2	1.81	0.62
1:A:247:TYR:HB2	1:A:374:LYS:HB3	1.80	0.62
1:B:842:PRO:O	1:B:1197:GLY:N	2.26	0.62
1:C:1029:GLU:HA	1:C:1032:LYS:HB2	1.81	0.62
1:A:2431:ASP:HB2	1:A:2501:SER:HB3	1.82	0.62
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.82	0.62
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	1.82	0.62
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.82	0.62
1:D:1023:PRO:HD2	1:D:1026:LEU:HD12	1.81	0.62
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.65	0.61
1:D:4152:GLU:OE2	1:D:4180:ARG:NH2	2.33	0.61
1:B:286:THR:HA	1:B:405:HIS:HB2	1.81	0.61
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.65	0.61
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.29	0.61
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.33	0.61
1:C:4152:GLU:OE2	1:C:4180:ARG:NH2	2.33	0.61
1:D:3688:GLU:HG3	1:D:3690:VAL:HG12	1.82	0.61
1:A:286:THR:HA	1:A:405:HIS:HB2	1.81	0.61
1:B:2431:ASP:HB2	1:B:2501:SER:HB3	1.82	0.61
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	1.82	0.61
1:C:286:THR:HA	1:C:405:HIS:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	1.82	0.61
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.82	0.61
1:A:3688:GLU:HG3	1:A:3690:VAL:HG12	1.82	0.61
1:B:1029:GLU:HA	1:B:1032:LYS:HB2	1.81	0.61
1:A:4152:GLU:OE2	1:A:4180:ARG:NH2	2.33	0.61
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.33	0.61
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.34	0.61
1:C:2431:ASP:HB2	1:C:2501:SER:HB3	1.82	0.61
1:D:286:THR:HA	1:D:405:HIS:HB2	1.81	0.61
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.34	0.61
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.74	0.61
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.74	0.61
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.74	0.61
1:B:866:HIS:HA	1:B:869:ARG:HE	1.66	0.61
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.82	0.61
1:B:4152:GLU:OE2	1:B:4180:ARG:NH2	2.33	0.61
1:A:842:PRO:O	1:A:1197:GLY:N	2.26	0.61
1:A:866:HIS:HA	1:A:869:ARG:HE	1.66	0.61
1:A:1029:GLU:HA	1:A:1032:LYS:HB2	1.81	0.61
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.29	0.61
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.34	0.61
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.34	0.60
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.83	0.60
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.83	0.60
1:C:3688:GLU:HG3	1:C:3690:VAL:HG12	1.82	0.60
1:D:1520:VAL:HG12	1:D:1527:MET:HG3	1.83	0.60
1:D:3031:ALA:HB3	1:D:3036:LYS:HZ3	1.65	0.60
1:B:3688:GLU:HG3	1:B:3690:VAL:HG12	1.82	0.60
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.83	0.60
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.83	0.60
1:A:975:VAL:O	1:A:1044:ARG:NH1	2.35	0.60
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.33	0.60
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.83	0.60
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.34	0.60
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	1.82	0.60
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.74	0.60
1:C:866:HIS:HA	1:C:869:ARG:HE	1.66	0.60
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.83	0.60
1:A:1520:VAL:HG12	1:A:1527:MET:HG3	1.83	0.60
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.83	0.60
1:D:866:HIS:HA	1:D:869:ARG:HE	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.83	0.60
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.65	0.60
1:D:363:ASP:OD1	1:D:374:LYS:NZ	2.35	0.60
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.33	0.60
1:D:2431:ASP:HB2	1:D:2501:SER:HB3	1.82	0.60
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.65	0.60
1:B:2003:GLN:OE1	1:B:2007:ASN:ND2	2.35	0.60
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.34	0.60
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.83	0.60
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.34	0.60
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.83	0.60
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.20	0.60
1:B:975:VAL:O	1:B:1044:ARG:NH1	2.35	0.60
1:B:1520:VAL:HG12	1:B:1527:MET:HG3	1.83	0.60
1:D:975:VAL:O	1:D:1044:ARG:NH1	2.35	0.60
1:D:2003:GLN:OE1	1:D:2007:ASN:ND2	2.35	0.60
1:A:107:ILE:HD13	1:A:150:MET:HG2	1.84	0.60
1:C:622:THR:HA	1:C:626:LEU:HD23	1.84	0.59
1:D:622:THR:HA	1:D:626:LEU:HD23	1.84	0.59
1:A:363:ASP:OD1	1:A:374:LYS:NZ	2.35	0.59
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.34	0.59
1:B:363:ASP:OD1	1:B:374:LYS:NZ	2.35	0.59
1:C:1520:VAL:HG12	1:C:1527:MET:HG3	1.83	0.59
1:D:107:ILE:HD13	1:D:150:MET:HG2	1.84	0.59
1:C:363:ASP:OD1	1:C:374:LYS:NZ	2.35	0.59
1:D:248:GLU:OE1	1:D:257:ARG:NH2	2.36	0.59
1:C:248:GLU:OE1	1:C:257:ARG:NH2	2.36	0.59
1:C:975:VAL:O	1:C:1044:ARG:NH1	2.35	0.59
1:C:2003:GLN:OE1	1:C:2007:ASN:ND2	2.35	0.59
1:A:4179:GLY:O	1:A:4194:TYR:HA	2.03	0.59
1:B:24:CYS:HB2	1:B:35:LEU:HB2	1.84	0.59
1:B:4179:GLY:O	1:B:4194:TYR:HA	2.03	0.59
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.36	0.59
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.20	0.59
1:A:2003:GLN:OE1	1:A:2007:ASN:ND2	2.35	0.59
1:C:107:ILE:HD13	1:C:150:MET:HG2	1.84	0.59
1:D:276:TRP:O	1:D:328:LYS:NZ	2.34	0.59
1:D:2499:LYS:NZ	1:D:2529:ASP:OD2	2.33	0.59
1:A:3946:GLN:OE1	1:A:3949:ARG:NH2	2.36	0.59
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.36	0.59
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.83	0.59
1:B:248:GLU:OE1	1:B:257:ARG:NH2	2.36	0.59
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.20	0.59
1:B:3946:GLN:OE1	1:B:3949:ARG:NH2	2.36	0.59
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.36	0.59
1:A:248:GLU:OE1	1:A:257:ARG:NH2	2.36	0.58
1:A:622:THR:HA	1:A:626:LEU:HD23	1.84	0.58
1:B:622:THR:HA	1:B:626:LEU:HD23	1.84	0.58
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.83	0.58
1:C:276:TRP:HE1	1:C:346:CYS:HG	1.43	0.58
1:C:3946:GLN:OE1	1:C:3949:ARG:NH2	2.36	0.58
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.36	0.58
1:A:157:ARG:HH12	1:A:163:VAL:HA	1.68	0.58
1:B:157:ARG:HH12	1:B:163:VAL:HA	1.68	0.58
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.36	0.58
1:A:2499:LYS:NZ	1:A:2529:ASP:OD2	2.33	0.58
1:B:3459:VAL:HG11	1:B:3503:TYR:HB2	1.85	0.58
1:C:157:ARG:HH12	1:C:163:VAL:HA	1.68	0.58
1:C:3459:VAL:HG11	1:C:3503:TYR:HB2	1.85	0.58
1:C:4179:GLY:O	1:C:4194:TYR:HA	2.03	0.58
1:D:157:ARG:HH12	1:D:163:VAL:HA	1.68	0.58
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.36	0.58
1:B:22:LEU:HD11	1:B:200:TRP:HB3	1.85	0.58
1:B:1259:ARG:NH1	1:B:1595:LEU:O	2.37	0.58
1:C:24:CYS:HB2	1:C:35:LEU:HB2	1.84	0.58
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.36	0.58
1:A:276:TRP:O	1:A:328:LYS:NZ	2.35	0.58
1:D:3459:VAL:HG11	1:D:3503:TYR:HB2	1.85	0.58
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.36	0.58
1:C:34:LYS:H	1:C:53:SER:HB3	1.69	0.58
1:C:197:GLN:NE2	1:C:198:THR:O	2.37	0.58
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.20	0.58
1:D:4179:GLY:O	1:D:4194:TYR:HA	2.03	0.58
1:A:24:CYS:HB2	1:A:35:LEU:HB2	1.84	0.58
1:A:1259:ARG:NH1	1:A:1595:LEU:O	2.37	0.58
1:A:2443:ILE:HD12	1:A:2454:ARG:HH21	1.69	0.58
1:A:3459:VAL:HG11	1:A:3503:TYR:HB2	1.85	0.58
1:B:107:ILE:HD13	1:B:150:MET:HG2	1.84	0.58
1:C:276:TRP:O	1:C:328:LYS:NZ	2.34	0.58
1:C:3244:PRO:HA	1:C:3248:ARG:HH21	1.69	0.58
1:D:3946:GLN:OE1	1:D:3949:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.86	0.58
1:C:534:ARG:HH11	1:C:570:GLU:HG3	1.69	0.58
1:D:2470:ILE:HA	1:D:2499:LYS:HE3	1.86	0.58
1:B:3675:ASP:OD1	1:B:3769:ARG:NH1	2.37	0.58
1:C:22:LEU:HD11	1:C:200:TRP:HB3	1.85	0.58
1:C:3675:ASP:OD1	1:C:3769:ARG:NH1	2.37	0.58
1:A:197:GLN:NE2	1:A:198:THR:O	2.37	0.57
1:A:2107:GLN:O	1:A:3683:GLN:NE2	2.37	0.57
1:C:1259:ARG:NH1	1:C:1595:LEU:O	2.37	0.57
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.36	0.57
1:D:34:LYS:H	1:D:53:SER:HB3	1.69	0.57
1:D:878:ILE:HD11	1:D:925:SER:HB2	1.86	0.57
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.86	0.57
1:D:3244:PRO:HA	1:D:3248:ARG:HH21	1.69	0.57
1:A:2470:ILE:HA	1:A:2499:LYS:HE3	1.86	0.57
1:B:197:GLN:NE2	1:B:198:THR:O	2.37	0.57
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.36	0.57
1:C:2365:GLY:O	1:C:2369[B]:ARG:NH2	2.38	0.57
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.86	0.57
1:A:878:ILE:HD11	1:A:925:SER:HB2	1.86	0.57
1:A:3244:PRO:HA	1:A:3248:ARG:HH21	1.69	0.57
1:B:34:LYS:H	1:B:53:SER:HB3	1.69	0.57
1:B:1748:PHE:HB2	1:B:1758:ARG:HH21	1.69	0.57
1:C:2107:GLN:O	1:C:3683:GLN:NE2	2.37	0.57
1:D:534:ARG:HH11	1:D:570:GLU:HG3	1.69	0.57
1:D:2107:GLN:O	1:D:3683:GLN:NE2	2.37	0.57
1:A:22:LEU:HD11	1:A:200:TRP:HB3	1.85	0.57
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.36	0.57
1:D:1259:ARG:NH1	1:D:1595:LEU:O	2.37	0.57
1:D:3107:VAL:HG21	1:D:3171:SER:HB2	1.86	0.57
1:D:22:LEU:HD11	1:D:200:TRP:HB3	1.85	0.57
1:D:197:GLN:NE2	1:D:198:THR:O	2.37	0.57
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.87	0.57
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.38	0.57
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.38	0.57
1:B:534:ARG:HH11	1:B:570:GLU:HG3	1.69	0.57
1:B:941:MET:SD	1:B:1052:ASN:ND2	2.78	0.57
1:B:2107:GLN:O	1:B:3683:GLN:NE2	2.37	0.57
1:C:878:ILE:HD11	1:C:925:SER:HB2	1.86	0.57
1:D:24:CYS:HB2	1:D:35:LEU:HB2	1.84	0.57
1:D:2365:GLY:O	1:D:2369[B]:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:H	1:A:53:SER:HB3	1.69	0.57
1:A:2365:GLY:O	1:A:2369[B]:ARG:NH2	2.38	0.57
1:B:276:TRP:O	1:B:328:LYS:NZ	2.34	0.57
1:B:2443:ILE:HD12	1:B:2454:ARG:HH21	1.69	0.57
1:B:3244:PRO:HA	1:B:3248:ARG:HH21	1.69	0.57
1:A:1748:PHE:HB2	1:A:1758:ARG:HH21	1.70	0.57
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.38	0.57
1:A:3675:ASP:OD1	1:A:3769:ARG:NH1	2.37	0.57
1:B:632:LEU:O	1:B:634:GLN:NE2	2.38	0.57
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.38	0.57
1:C:941:MET:SD	1:C:1052:ASN:ND2	2.78	0.57
1:D:2013:LYS:NZ	1:D:3661:TRP:O	2.38	0.57
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.38	0.57
1:A:941:MET:SD	1:A:1052:ASN:ND2	2.78	0.57
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.87	0.57
1:D:941:MET:SD	1:D:1052:ASN:ND2	2.78	0.57
1:D:3675:ASP:OD1	1:D:3769:ARG:NH1	2.37	0.57
1:A:534:ARG:HH11	1:A:570:GLU:HG3	1.69	0.57
1:A:632:LEU:O	1:A:634:GLN:NE2	2.38	0.57
1:A:1504:GLY:O	1:A:1508:ARG:NH2	2.38	0.57
1:B:2365:GLY:O	1:B:2369[B]:ARG:NH2	2.38	0.57
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.86	0.57
1:B:3107:VAL:HG21	1:B:3171:SER:HB2	1.86	0.57
1:C:1748:PHE:HB2	1:C:1758:ARG:HH21	1.69	0.57
1:C:2499:LYS:NZ	1:C:2529:ASP:OD2	2.33	0.57
1:C:3107:VAL:HG21	1:C:3171:SER:HB2	1.86	0.57
1:D:2443:ILE:HD12	1:D:2454:ARG:HH21	1.69	0.57
1:A:3107:VAL:HG21	1:A:3171:SER:HB2	1.86	0.56
1:B:878:ILE:HD11	1:B:925:SER:HB2	1.86	0.56
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.38	0.56
1:B:4738:ALA:HA	1:B:4743:MET:HG3	1.87	0.56
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.38	0.56
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.87	0.56
1:D:1243:PRO:O	1:D:1458:HIS:ND1	2.38	0.56
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.38	0.56
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.38	0.56
1:B:2470:ILE:HA	1:B:2499:LYS:HE3	1.86	0.56
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.38	0.56
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.87	0.56
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.87	0.56
1:A:4738:ALA:HA	1:A:4743:MET:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:884:LEU:HD13	1:B:969:PRO:HD2	1.87	0.56
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.87	0.56
1:C:632:LEU:O	1:C:634:GLN:NE2	2.38	0.56
1:C:1504:GLY:O	1:C:1508:ARG:NH2	2.38	0.56
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.38	0.56
1:D:1504:GLY:O	1:D:1508:ARG:NH2	2.38	0.56
1:C:2443:ILE:HD12	1:C:2454:ARG:HH21	1.69	0.56
1:D:3236:VAL:HA	1:D:3239:MET:HG2	1.88	0.56
1:B:1504:GLY:O	1:B:1508:ARG:NH2	2.38	0.56
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	1.88	0.56
1:C:2470:ILE:HA	1:C:2499:LYS:HE3	1.86	0.56
1:C:3236:VAL:HA	1:C:3239:MET:HG2	1.88	0.56
1:D:884:LEU:HD13	1:D:969:PRO:HD2	1.87	0.56
1:A:1243:PRO:O	1:A:1458:HIS:ND1	2.38	0.56
1:B:869:ARG:NH1	1:B:1051:TYR:OH	2.39	0.56
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.38	0.56
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.38	0.56
1:D:688:LEU:HD23	1:D:690:GLU:H	1.71	0.56
1:D:1748:PHE:HB2	1:D:1758:ARG:HH21	1.69	0.56
1:A:688:LEU:HD23	1:A:690:GLU:H	1.71	0.56
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.38	0.56
1:C:884:LEU:HD13	1:C:969:PRO:HD2	1.87	0.56
1:D:632:LEU:O	1:D:634:GLN:NE2	2.38	0.56
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.38	0.56
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.38	0.56
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	1.88	0.56
1:A:3788:GLY:HA2	1:A:3835:LEU:HG	1.88	0.56
1:B:3788:GLY:HA2	1:B:3835:LEU:HG	1.88	0.56
1:D:451:TYR:O	1:D:474:ARG:NH1	2.39	0.56
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.38	0.56
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.87	0.56
1:C:2620:GLN:HE22	1:C:2674:LEU:HD22	1.71	0.56
1:A:869:ARG:NH1	1:A:1051:TYR:OH	2.39	0.56
1:A:1731:LEU:HD13	1:A:1772:ARG:HH21	1.72	0.56
1:B:234:SER:HB2	1:B:242:ARG:HA	1.88	0.56
1:B:2620:GLN:HE22	1:B:2674:LEU:HD22	1.71	0.56
1:B:3236:VAL:HA	1:B:3239:MET:HG2	1.88	0.56
1:C:451:TYR:O	1:C:474:ARG:NH1	2.39	0.56
1:D:869:ARG:NH1	1:D:1051:TYR:OH	2.39	0.56
1:A:229:GLU:HB3	1:A:247:TYR:HB3	1.88	0.55
1:B:229:GLU:HB3	1:B:247:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2215:LEU:O	1:B:2219:GLU:HA	2.05	0.55
1:C:1005:TRP:HB3	1:C:1021:LEU:HD11	1.88	0.55
1:C:1243:PRO:O	1:C:1458:HIS:ND1	2.38	0.55
1:C:2215:LEU:O	1:C:2219:GLU:HA	2.05	0.55
1:D:229:GLU:HB3	1:D:247:TYR:HB3	1.88	0.55
1:D:861:ILE:O	1:D:930:LYS:NZ	2.39	0.55
1:B:1731:LEU:HD13	1:B:1772:ARG:HH21	1.72	0.55
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	1.88	0.55
1:A:1005:TRP:HB3	1:A:1021:LEU:HD11	1.88	0.55
1:A:2215:LEU:O	1:A:2219:GLU:HA	2.06	0.55
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.87	0.55
1:C:229:GLU:HB3	1:C:247:TYR:HB3	1.88	0.55
1:C:869:ARG:NH1	1:C:1051:TYR:OH	2.39	0.55
1:C:2013:LYS:NZ	1:C:3661:TRP:O	2.38	0.55
1:C:2715:VAL:HG21	1:C:2950:SER:HB2	1.88	0.55
1:C:4738:ALA:HA	1:C:4743:MET:HG3	1.87	0.55
1:D:2715:VAL:HG21	1:D:2950:SER:HB2	1.88	0.55
1:A:861:ILE:O	1:A:930:LYS:NZ	2.39	0.55
1:A:884:LEU:HD13	1:A:969:PRO:HD2	1.87	0.55
1:A:451:TYR:O	1:A:474:ARG:NH1	2.39	0.55
1:C:861:ILE:O	1:C:930:LYS:NZ	2.39	0.55
1:D:2215:LEU:O	1:D:2219:GLU:HA	2.05	0.55
1:A:234:SER:HB2	1:A:242:ARG:HA	1.88	0.55
1:C:234:SER:HB2	1:C:242:ARG:HA	1.88	0.55
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.40	0.55
1:D:842:PRO:O	1:D:1197:GLY:N	2.26	0.55
1:D:4738:ALA:HA	1:D:4743:MET:HG3	1.87	0.55
2:E:24:VAL:HG12	2:E:103:LEU:HA	1.88	0.55
1:A:2827:ARG:HE	1:A:2933:ASN:HB3	1.71	0.55
1:A:3206:LEU:HB3	1:A:3246:LEU:HB2	1.88	0.55
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.40	0.55
1:C:2827:ARG:HE	1:C:2933:ASN:HB3	1.71	0.55
1:D:2827:ARG:HE	1:D:2933:ASN:HB3	1.71	0.55
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.07	0.55
1:A:3236:VAL:HA	1:A:3239:MET:HG2	1.88	0.55
1:C:688:LEU:HD23	1:C:690:GLU:H	1.71	0.55
1:D:883:ALA:HB1	1:D:905:PRO:HA	1.89	0.55
1:A:2715:VAL:HG21	1:A:2950:SER:HB2	1.88	0.55
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.07	0.55
1:B:1243:PRO:O	1:B:1458:HIS:ND1	2.38	0.55
1:B:1527:MET:HB2	1:B:1540:PHE:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3324:VAL:HG11	1:B:3361:THR:HB	1.89	0.55
1:C:3031:ALA:HB3	1:C:3036:LYS:HZ3	1.71	0.55
1:C:3206:LEU:HB3	1:C:3246:LEU:HB2	1.89	0.55
1:C:3324:VAL:HG11	1:C:3361:THR:HB	1.89	0.55
1:D:1527:MET:HB2	1:D:1540:PHE:HB2	1.89	0.55
1:D:1731:LEU:HD13	1:D:1772:ARG:HH21	1.72	0.55
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	1.88	0.55
1:B:451:TYR:O	1:B:474:ARG:NH1	2.39	0.55
1:B:688:LEU:HD23	1:B:690:GLU:H	1.71	0.55
1:B:883:ALA:HB1	1:B:905:PRO:HA	1.89	0.55
1:B:988:LEU:HG	1:B:1039:LEU:HD13	1.89	0.55
1:C:988:LEU:HG	1:C:1039:LEU:HD13	1.89	0.55
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.07	0.55
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.40	0.55
1:A:883:ALA:HB1	1:A:905:PRO:HA	1.89	0.54
1:B:861:ILE:O	1:B:930:LYS:NZ	2.39	0.54
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.38	0.54
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.90	0.54
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.40	0.54
1:C:3788:GLY:HA2	1:C:3835:LEU:HG	1.88	0.54
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.38	0.54
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	1.88	0.54
1:D:1005:TRP:HB3	1:D:1021:LEU:HD11	1.88	0.54
1:D:2620:GLN:HE22	1:D:2674:LEU:HD22	1.71	0.54
2:F:24:VAL:HG12	2:F:103:LEU:HA	1.88	0.54
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.89	0.54
1:B:1005:TRP:HB3	1:B:1021:LEU:HD11	1.88	0.54
1:B:2827:ARG:HE	1:B:2933:ASN:HB3	1.71	0.54
1:B:3151:GLN:NE2	1:B:3154:ASP:OD2	2.41	0.54
1:C:883:ALA:HB1	1:C:905:PRO:HA	1.89	0.54
1:A:1527:MET:HB2	1:A:1540:PHE:HB2	1.89	0.54
1:A:3151:GLN:NE2	1:A:3154:ASP:OD2	2.41	0.54
1:A:3207:GLU:OE1	1:A:3305:THR:OG1	2.26	0.54
1:B:846:LEU:HD22	1:B:851:PHE:HE1	1.73	0.54
1:B:1097:THR:HA	1:B:1143:TRP:HE1	1.73	0.54
1:B:2715:VAL:HG21	1:B:2950:SER:HB2	1.88	0.54
1:C:1097:THR:HA	1:C:1143:TRP:HE1	1.73	0.54
1:C:3151:GLN:NE2	1:C:3154:ASP:OD2	2.41	0.54
2:G:24:VAL:HG12	2:G:103:LEU:HA	1.88	0.54
1:A:988:LEU:HG	1:A:1039:LEU:HD13	1.89	0.54
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:846:LEU:HD22	1:D:851:PHE:HE1	1.73	0.54
1:D:3172:ILE:HD11	1:D:3190:LEU:HB3	1.90	0.54
1:A:1074:ILE:HD11	1:A:1111:PRO:HA	1.89	0.54
1:A:2620:GLN:HE22	1:A:2674:LEU:HD22	1.71	0.54
1:C:1074:ILE:HD11	1:C:1111:PRO:HA	1.89	0.54
1:C:1527:MET:HB2	1:C:1540:PHE:HB2	1.89	0.54
1:C:3172:ILE:HD11	1:C:3190:LEU:HB3	1.90	0.54
1:D:234:SER:HB2	1:D:242:ARG:HA	1.88	0.54
1:D:3771:HIS:O	1:D:3815:LYS:NZ	2.40	0.54
1:A:731:THR:O	1:A:765:GLN:NE2	2.41	0.54
1:A:846:LEU:HD22	1:A:851:PHE:HE1	1.73	0.54
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.90	0.54
1:D:988:LEU:HG	1:D:1039:LEU:HD13	1.89	0.54
1:D:2287:ALA:HA	1:D:2290:LEU:HB2	1.90	0.54
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.90	0.54
1:D:3324:VAL:HG11	1:D:3361:THR:HB	1.89	0.54
1:A:2792:ARG:NH2	1:A:2798:SER:OG	2.41	0.54
1:B:219:VAL:HG12	1:B:259:LEU:HD12	1.90	0.54
1:B:2499:LYS:NZ	1:B:2529:ASP:OD2	2.33	0.54
2:H:24:VAL:HG12	2:H:103:LEU:HA	1.88	0.54
1:A:2287:ALA:HA	1:A:2290:LEU:HB2	1.90	0.54
1:B:3206:LEU:HB3	1:B:3246:LEU:HB2	1.89	0.54
1:D:650:VAL:O	1:D:777:PHE:N	2.41	0.54
1:D:2792:ARG:NH2	1:D:2798:SER:OG	2.41	0.54
1:D:3151:GLN:NE2	1:D:3154:ASP:OD2	2.41	0.54
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.38	0.53
1:C:1731:LEU:HD13	1:C:1772:ARG:HH21	1.72	0.53
1:D:1074:ILE:HD11	1:D:1111:PRO:HA	1.89	0.53
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	1.90	0.53
1:D:3206:LEU:HB3	1:D:3246:LEU:HB2	1.89	0.53
1:A:4721:LYS:NZ	1:A:4741:LEU:O	2.41	0.53
1:B:2792:ARG:NH2	1:B:2798:SER:OG	2.41	0.53
1:A:3324:VAL:HG11	1:A:3361:THR:HB	1.89	0.53
1:B:41:GLY:O	1:B:45:ARG:NH1	2.41	0.53
1:B:731:THR:O	1:B:765:GLN:NE2	2.41	0.53
1:C:2287:ALA:HA	1:C:2290:LEU:HB2	1.90	0.53
1:A:4088:ILE:O	1:A:4123:ILE:N	2.42	0.53
1:B:1295:VAL:HG12	1:B:1579:MET:HB3	1.90	0.53
1:B:4088:ILE:O	1:B:4123:ILE:N	2.42	0.53
1:C:650:VAL:O	1:C:777:PHE:N	2.41	0.53
1:D:1097:THR:HA	1:D:1143:TRP:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1295:VAL:HG12	1:D:1579:MET:HB3	1.90	0.53
1:A:1097:THR:HA	1:A:1143:TRP:HE1	1.73	0.53
1:C:731:THR:O	1:C:765:GLN:NE2	2.41	0.53
1:D:3207:GLU:OE1	1:D:3305:THR:OG1	2.26	0.53
1:D:4117:ALA:HB1	1:D:4121:GLU:HA	1.91	0.53
1:A:3172:ILE:HD11	1:A:3190:LEU:HB3	1.90	0.53
1:C:219:VAL:HG12	1:C:259:LEU:HD12	1.90	0.53
1:B:1830:VAL:HB	1:B:1837:GLN:HG3	1.91	0.53
1:C:1574:PRO:HG3	1:C:1589:PRO:HG3	1.91	0.53
1:A:1295:VAL:HG12	1:A:1579:MET:HB3	1.90	0.53
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.74	0.53
1:B:1074:ILE:HD11	1:B:1111:PRO:HA	1.89	0.53
1:B:3771:HIS:O	1:B:3815:LYS:NZ	2.40	0.53
1:C:846:LEU:HD22	1:C:851:PHE:HE1	1.73	0.53
1:D:731:THR:O	1:D:765:GLN:NE2	2.41	0.53
1:A:219:VAL:HG12	1:A:259:LEU:HD12	1.90	0.53
1:A:650:VAL:O	1:A:777:PHE:N	2.41	0.53
1:A:1776:HIS:HB3	1:A:1798:LEU:HD13	1.91	0.53
1:B:2287:ALA:HA	1:B:2290:LEU:HB2	1.90	0.53
1:B:3172:ILE:HD11	1:B:3190:LEU:HB3	1.90	0.53
1:C:3955:MET:HB2	1:C:4019:LEU:HD22	1.91	0.53
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.91	0.53
1:A:3955:MET:HB2	1:A:4019:LEU:HD22	1.91	0.53
1:B:743:VAL:HB	1:B:760:ASN:HA	1.91	0.53
1:B:3955:MET:HB2	1:B:4019:LEU:HD22	1.91	0.53
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.91	0.53
1:D:1432:THR:HA	1:D:1520:VAL:O	2.09	0.53
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.74	0.53
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.43	0.52
1:B:650:VAL:O	1:B:777:PHE:N	2.41	0.52
1:B:1432:THR:HA	1:B:1520:VAL:O	2.09	0.52
1:C:732:SER:HB2	1:C:735:GLN:HB3	1.91	0.52
1:C:3207:GLU:OE1	1:C:3305:THR:OG1	2.26	0.52
1:C:3575:LEU:HD23	1:D:1219:LEU:HD22	1.91	0.52
1:D:603:LEU:HD23	1:D:606:LEU:HD12	1.91	0.52
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.74	0.52
1:C:603:LEU:HD23	1:C:606:LEU:HD12	1.91	0.52
1:C:1295:VAL:HG12	1:C:1579:MET:HB3	1.90	0.52
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.43	0.52
1:C:4117:ALA:HB1	1:C:4121:GLU:HA	1.91	0.52
1:B:214:VAL:HG12	1:B:274:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:LEU:HD23	1:B:606:LEU:HD12	1.91	0.52
1:B:995:VAL:HG22	1:B:998:ARG:HH21	1.74	0.52
1:B:1574:PRO:HG3	1:B:1589:PRO:HG3	1.91	0.52
1:B:2107:GLN:NE2	1:B:3682:GLU:OE1	2.43	0.52
1:C:214:VAL:HG12	1:C:274:LEU:HD12	1.92	0.52
1:C:2792:ARG:NH2	1:C:2798:SER:OG	2.41	0.52
1:C:4088:ILE:O	1:C:4123:ILE:N	2.42	0.52
1:D:3955:MET:HB2	1:D:4019:LEU:HD22	1.91	0.52
1:D:4088:ILE:O	1:D:4123:ILE:N	2.42	0.52
1:A:1830:VAL:HB	1:A:1837:GLN:HG3	1.91	0.52
1:A:2107:GLN:NE2	1:A:3682:GLU:OE1	2.43	0.52
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.43	0.52
1:C:1432:THR:HA	1:C:1520:VAL:O	2.09	0.52
1:C:3051:ARG:NH2	1:C:3102:ASP:OD1	2.43	0.52
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.92	0.52
1:A:276:TRP:NE1	1:A:346:CYS:SG	2.75	0.52
1:A:4117:ALA:HB1	1:A:4121:GLU:HA	1.91	0.52
1:B:3677:LEU:HB3	1:B:3698:LEU:HB2	1.92	0.52
1:C:3677:LEU:HB3	1:C:3698:LEU:HB2	1.92	0.52
1:D:1830:VAL:HB	1:D:1837:GLN:HG3	1.91	0.52
1:D:3677:LEU:HB3	1:D:3698:LEU:HB2	1.92	0.52
1:B:3330:ASP:O	1:B:3403:ARG:NH2	2.43	0.52
1:D:732:SER:HB2	1:D:735:GLN:HB3	1.91	0.52
1:D:1243:PRO:HA	1:D:1602:PRO:HA	1.92	0.52
1:A:1243:PRO:HA	1:A:1602:PRO:HA	1.92	0.52
1:A:3677:LEU:HB3	1:A:3698:LEU:HB2	1.92	0.52
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.92	0.52
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	1.90	0.52
1:B:2519:LEU:HD13	1:B:2522:LEU:HD12	1.92	0.52
1:B:3670:GLU:HB3	1:B:3732:SER:HB3	1.92	0.52
1:C:743:VAL:HB	1:C:760:ASN:HA	1.91	0.52
1:C:1106:ARG:NH2	1:C:1183:GLU:O	2.39	0.52
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.74	0.52
1:D:219:VAL:HG12	1:D:259:LEU:HD12	1.90	0.52
1:D:2519:LEU:HD13	1:D:2522:LEU:HD12	1.92	0.52
1:A:214:VAL:HG12	1:A:274:LEU:HD12	1.92	0.52
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.91	0.52
1:A:878:ILE:HG22	1:A:881:LEU:HD13	1.92	0.52
1:A:1432:THR:HA	1:A:1520:VAL:O	2.09	0.52
1:A:1574:PRO:HG3	1:A:1589:PRO:HG3	1.91	0.52
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1243:PRO:HA	1:C:1602:PRO:HA	1.92	0.52
1:D:214:VAL:HG12	1:D:274:LEU:HD12	1.92	0.52
1:D:3051:ARG:NH2	1:D:3102:ASP:OD1	2.43	0.52
1:A:41:GLY:O	1:A:45:ARG:NH1	2.41	0.52
1:A:743:VAL:HB	1:A:760:ASN:HA	1.91	0.52
1:A:2013:LYS:NZ	1:A:3661:TRP:O	2.38	0.52
1:A:2519:LEU:HD13	1:A:2522:LEU:HD12	1.92	0.52
1:A:3051:ARG:NH2	1:A:3102:ASP:OD1	2.43	0.52
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.92	0.52
1:C:1043:VAL:HA	1:C:1046:LEU:HD12	1.92	0.52
1:C:1474:VAL:O	1:C:1486:SER:HA	2.10	0.52
1:C:3330:ASP:O	1:C:3403:ARG:NH2	2.43	0.52
1:C:3670:GLU:HB3	1:C:3732:SER:HB3	1.92	0.52
1:D:3330:ASP:O	1:D:3403:ARG:NH2	2.43	0.52
1:A:3330:ASP:O	1:A:3403:ARG:NH2	2.43	0.52
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	1.92	0.52
1:C:2107:GLN:NE2	1:C:3682:GLU:OE1	2.43	0.52
1:C:2519:LEU:HD13	1:C:2522:LEU:HD12	1.92	0.52
1:B:1106:ARG:NH2	1:B:1183:GLU:O	2.39	0.51
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.10	0.51
1:D:1474:VAL:O	1:D:1486:SER:HA	2.10	0.51
1:D:2107:GLN:NE2	1:D:3682:GLU:OE1	2.43	0.51
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.10	0.51
1:B:3051:ARG:NH2	1:B:3102:ASP:OD1	2.43	0.51
1:C:76:ARG:HA	1:C:79:GLN:HG2	1.92	0.51
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.92	0.51
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.92	0.51
1:D:1043:VAL:HA	1:D:1046:LEU:HD12	1.92	0.51
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.92	0.51
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.43	0.51
1:A:995:VAL:HG22	1:A:998:ARG:HH21	1.74	0.51
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.43	0.51
1:A:3443:ILE:HD11	1:A:3601:ALA:HB1	1.93	0.51
1:B:732:SER:HB2	1:B:735:GLN:HB3	1.91	0.51
1:B:4117:ALA:HB1	1:B:4121:GLU:HA	1.91	0.51
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	1.90	0.51
1:C:3771:HIS:O	1:C:3815:LYS:NZ	2.40	0.51
1:C:4721:LYS:NZ	1:C:4741:LEU:O	2.41	0.51
1:D:1574:PRO:HG3	1:D:1589:PRO:HG3	1.91	0.51
1:D:2997:PHE:O	1:D:3001:ILE:HB	2.10	0.51
1:D:3443:ILE:HD11	1:D:3601:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4721:LYS:NZ	1:D:4741:LEU:O	2.41	0.51
1:A:2477:PRO:HG3	1:A:2546:MET:HE2	1.93	0.51
1:A:2997:PHE:O	1:A:3001:ILE:HB	2.10	0.51
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.92	0.51
1:B:76:ARG:HA	1:B:79:GLN:HG2	1.92	0.51
1:B:130:LYS:HD3	1:B:131:LEU:HG	1.93	0.51
1:B:3888:LEU:HD23	1:B:3891:LEU:HD21	1.92	0.51
1:C:2997:PHE:O	1:C:3001:ILE:HB	2.10	0.51
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.93	0.51
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	1.92	0.51
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	1.93	0.51
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	1.92	0.51
1:A:3888:LEU:HD23	1:A:3891:LEU:HD21	1.92	0.51
1:B:1243:PRO:HA	1:B:1602:PRO:HA	1.92	0.51
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.43	0.51
1:C:130:LYS:HD3	1:C:131:LEU:HG	1.93	0.51
1:D:3670:GLU:HB3	1:D:3732:SER:HB3	1.92	0.51
1:A:529:LEU:O	1:A:533:ASN:ND2	2.44	0.51
1:A:603:LEU:HD23	1:A:606:LEU:HD12	1.91	0.51
1:A:732:SER:HB2	1:A:735:GLN:HB3	1.91	0.51
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.91	0.51
1:B:878:ILE:HG22	1:B:881:LEU:HD13	1.92	0.51
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.92	0.51
1:D:995:VAL:HG22	1:D:998:ARG:HH21	1.74	0.51
1:A:3670:GLU:HB3	1:A:3732:SER:HB3	1.92	0.51
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.93	0.51
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	1.93	0.51
1:B:1443:GLN:NE2	1:B:1555:LEU:O	2.35	0.51
1:B:3575:LEU:HD23	1:C:1219:LEU:HD22	1.91	0.51
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.93	0.51
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.91	0.51
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.39	0.51
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.10	0.51
1:C:1830:VAL:HB	1:C:1837:GLN:HG3	1.91	0.51
1:D:878:ILE:HG22	1:D:881:LEU:HD13	1.92	0.51
1:B:1043:VAL:HA	1:B:1046:LEU:HD12	1.92	0.51
1:B:1474:VAL:O	1:B:1486:SER:HA	2.10	0.51
1:C:529:LEU:O	1:C:533:ASN:ND2	2.44	0.51
1:D:743:VAL:HB	1:D:760:ASN:HA	1.91	0.51
1:A:2517:PHE:HA	1:A:2520:HIS:HB3	1.93	0.51
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3443:ILE:HD11	1:B:3601:ALA:HB1	1.93	0.51
1:D:76:ARG:HA	1:D:79:GLN:HG2	1.92	0.51
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.92	0.51
1:A:1256:GLU:HB3	1:A:1275:ARG:HD2	1.93	0.51
1:C:995:VAL:HG22	1:C:998:ARG:HH21	1.74	0.51
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	1.93	0.51
1:D:835:ARG:NH2	1:D:1210:SER:O	2.44	0.51
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.43	0.51
1:D:1968:LYS:NZ	1:D:2030:ASP:OD2	2.44	0.51
1:D:2517:PHE:HA	1:D:2520:HIS:HB3	1.93	0.51
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.92	0.51
1:A:417:GLY:HA3	1:A:436:LEU:HD21	1.93	0.50
1:A:835:ARG:NH2	1:A:1210:SER:O	2.44	0.50
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.39	0.50
1:A:3203:VAL:HG12	1:A:3214:ASN:HD22	1.76	0.50
1:A:4686:LEU:HA	1:A:4690:GLU:HG3	1.92	0.50
1:C:4686:LEU:HA	1:C:4690:GLU:HG3	1.92	0.50
1:D:2477:PRO:HG3	1:D:2546:MET:HE2	1.91	0.50
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.93	0.50
1:A:76:ARG:NH1	1:D:3938:SER:OG	2.44	0.50
1:A:3690:VAL:HG13	1:A:3692:GLU:H	1.75	0.50
1:A:4544:LEU:O	1:A:4548:ARG:HB2	2.12	0.50
1:B:529:LEU:O	1:B:533:ASN:ND2	2.44	0.50
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.45	0.50
1:C:835:ARG:NH2	1:C:1210:SER:O	2.44	0.50
1:C:1256:GLU:HB3	1:C:1275:ARG:HD2	1.93	0.50
1:C:1443:GLN:NE2	1:C:1555:LEU:O	2.35	0.50
1:C:2477:PRO:HG3	1:C:2546:MET:HE2	1.93	0.50
1:D:41:GLY:O	1:D:45:ARG:NH1	2.41	0.50
1:D:4544:LEU:O	1:D:4548:ARG:HB2	2.12	0.50
1:A:1474:VAL:O	1:A:1486:SER:HA	2.10	0.50
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.10	0.50
1:B:1870:VAL:HG11	1:B:2097:LEU:HD22	1.93	0.50
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.34	0.50
1:C:878:ILE:HG22	1:C:881:LEU:HD13	1.92	0.50
1:C:2611:CYS:HA	1:C:2614:ILE:HG22	1.94	0.50
1:C:2755:ILE:HD12	1:C:2813:LEU:HG	1.93	0.50
1:D:1851:MET:HB2	1:D:1853:ILE:HG12	1.93	0.50
1:D:3592:ILE:HG13	1:D:3595:ARG:HE	1.76	0.50
1:D:4686:LEU:HA	1:D:4690:GLU:HG3	1.92	0.50
1:A:1968:LYS:NZ	1:A:2030:ASP:OD2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3592:ILE:HG13	1:A:3595:ARG:HE	1.76	0.50
1:D:529:LEU:O	1:D:533:ASN:ND2	2.44	0.50
1:B:1944:GLU:HB3	1:B:2123:LEU:HD21	1.94	0.50
1:B:2997:PHE:O	1:B:3001:ILE:HB	2.10	0.50
1:C:417:GLY:HA3	1:C:436:LEU:HD21	1.94	0.50
1:C:1870:VAL:HG11	1:C:2097:LEU:HD22	1.93	0.50
1:D:417:GLY:HA3	1:D:436:LEU:HD21	1.94	0.50
1:D:1721:GLU:OE1	1:D:1725:ARG:NH2	2.45	0.50
1:D:3218:VAL:HB	1:D:3227:ARG:HD3	1.93	0.50
1:A:1043:VAL:HA	1:A:1046:LEU:HD12	1.92	0.50
1:A:1851:MET:HB2	1:A:1853:ILE:HG12	1.94	0.50
1:B:417:GLY:HA3	1:B:436:LEU:HD21	1.94	0.50
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.92	0.50
1:B:835:ARG:NH2	1:B:1210:SER:O	2.44	0.50
1:B:2517:PHE:HA	1:B:2520:HIS:HB3	1.93	0.50
1:B:3207:GLU:OE1	1:B:3305:THR:OG1	2.26	0.50
1:B:3690:VAL:HG13	1:B:3692:GLU:H	1.75	0.50
1:B:4721:LYS:NZ	1:B:4741:LEU:O	2.41	0.50
1:C:1721:GLU:OE1	1:C:1725:ARG:NH2	2.45	0.50
1:C:3443:ILE:HD11	1:C:3601:ALA:HB1	1.93	0.50
1:C:3888:LEU:HD23	1:C:3891:LEU:HD21	1.92	0.50
1:D:3690:VAL:HG13	1:D:3692:GLU:H	1.75	0.50
1:D:4155:PRO:O	1:D:4161:ARG:NH1	2.45	0.50
1:A:76:ARG:HA	1:A:79:GLN:HG2	1.92	0.50
1:A:1870:VAL:HG11	1:A:2097:LEU:HD22	1.93	0.50
1:A:3607:GLU:HA	1:A:3610:GLU:HG2	1.94	0.50
1:B:1851:MET:HB2	1:B:1853:ILE:HG12	1.94	0.50
1:B:2755:ILE:HD12	1:B:2813:LEU:HG	1.93	0.50
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.45	0.50
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.45	0.50
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	1.93	0.50
1:D:2695:LEU:O	1:D:2699:ALA:HB2	2.12	0.50
1:A:653:ALA:HB3	1:A:656:SER:HB2	1.94	0.50
1:A:2755:ILE:HD12	1:A:2813:LEU:HG	1.93	0.50
1:B:1257:VAL:HG21	1:B:1597:VAL:HG11	1.94	0.50
1:C:4161:ARG:HE	1:C:4164:LEU:HD21	1.77	0.50
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.36	0.50
1:D:1422:ASP:OD2	1:D:1568:LYS:NZ	2.38	0.50
1:D:3203:VAL:HG12	1:D:3214:ASN:HD22	1.76	0.50
1:A:130:LYS:HD3	1:A:131:LEU:HG	1.93	0.50
1:A:168:ASP:OD1	1:A:201:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1547:LYS:NZ	1:A:1642:PRO:O	2.45	0.50
1:A:3226:GLU:HA	1:A:3229:ILE:HG12	1.94	0.50
1:B:110:ARG:NH1	1:B:115:ARG:O	2.45	0.50
1:B:1256:GLU:HB3	1:B:1275:ARG:HD2	1.93	0.50
1:B:1721:GLU:OE1	1:B:1725:ARG:NH2	2.45	0.50
1:B:2211:MET:HA	1:B:2214:VAL:HG12	1.94	0.50
1:B:4686:LEU:HA	1:B:4690:GLU:HG3	1.92	0.50
1:C:3607:GLU:HA	1:C:3610:GLU:HG2	1.93	0.50
1:C:4155:PRO:O	1:C:4161:ARG:NH1	2.45	0.50
1:D:110:ARG:NH1	1:D:115:ARG:O	2.45	0.50
1:D:2015:GLU:OE2	1:D:2032:GLN:NE2	2.45	0.50
1:D:2611:CYS:HA	1:D:2614:ILE:HG22	1.94	0.50
1:A:1106:ARG:NH2	1:A:1183:GLU:O	2.39	0.49
1:B:3592:ILE:HG13	1:B:3595:ARG:HE	1.76	0.49
1:C:1851:MET:HB2	1:C:1853:ILE:HG12	1.94	0.49
1:C:3690:VAL:HG13	1:C:3692:GLU:H	1.75	0.49
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.49
1:D:3888:LEU:HD23	1:D:3891:LEU:HD21	1.92	0.49
1:D:4161:ARG:HE	1:D:4164:LEU:HD21	1.77	0.49
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.45	0.49
1:A:1257:VAL:HG21	1:A:1597:VAL:HG11	1.94	0.49
1:A:2211:MET:HA	1:A:2214:VAL:HG12	1.94	0.49
1:C:1547:LYS:NZ	1:C:1642:PRO:O	2.45	0.49
1:C:2517:PHE:HA	1:C:2520:HIS:HB3	1.93	0.49
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.95	0.49
1:C:2695:LEU:O	1:C:2699:ALA:HB2	2.12	0.49
1:D:1257:VAL:HG21	1:D:1597:VAL:HG11	1.94	0.49
1:A:1721:GLU:OE1	1:A:1725:ARG:NH2	2.45	0.49
1:A:2695:LEU:O	1:A:2699:ALA:HB2	2.12	0.49
1:B:1225:PRO:HB2	1:B:1228:ILE:HB	1.94	0.49
1:B:3218:VAL:HB	1:B:3227:ARG:HD3	1.93	0.49
1:B:4161:ARG:HE	1:B:4164:LEU:HD21	1.77	0.49
1:C:110:ARG:NH1	1:C:115:ARG:O	2.45	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.49
1:C:1116:GLY:H	1:C:1121:ALA:HB3	1.77	0.49
1:C:1225:PRO:HB2	1:C:1228:ILE:HB	1.94	0.49
1:C:3206:LEU:HD13	1:C:3246:LEU:HD13	1.94	0.49
1:C:3226:GLU:HA	1:C:3229:ILE:HG12	1.94	0.49
1:C:3891:LEU:HD13	1:C:3899:PHE:HE1	1.77	0.49
1:C:4544:LEU:O	1:C:4548:ARG:HB2	2.12	0.49
1:D:653:ALA:HB3	1:D:656:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1547:LYS:NZ	1:D:1642:PRO:O	2.45	0.49
1:D:1870:VAL:HG11	1:D:2097:LEU:HD22	1.93	0.49
1:D:2755:ILE:HD12	1:D:2813:LEU:HG	1.93	0.49
1:A:2015:GLU:OE2	1:A:2032:GLN:NE2	2.45	0.49
1:A:3218:VAL:HB	1:A:3227:ARG:HD3	1.93	0.49
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.94	0.49
1:C:168:ASP:OD1	1:C:201:ASN:ND2	2.45	0.49
1:C:653:ALA:HB3	1:C:656:SER:HB2	1.94	0.49
1:C:1944:GLU:HB3	1:C:2123:LEU:HD21	1.94	0.49
1:D:130:LYS:HD3	1:D:131:LEU:HG	1.93	0.49
1:D:551:LEU:HD21	1:D:585:SER:HB3	1.95	0.49
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.95	0.49
1:D:2716:ASP:N	1:D:2716:ASP:OD1	2.46	0.49
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.95	0.49
1:A:551:LEU:HD21	1:A:585:SER:HB3	1.94	0.49
1:A:1421:ARG:O	1:A:1570:LYS:NZ	2.42	0.49
1:B:653:ALA:HB3	1:B:656:SER:HB2	1.94	0.49
1:B:1547:LYS:NZ	1:B:1642:PRO:O	2.45	0.49
1:B:1968:LYS:NZ	1:B:2030:ASP:OD2	2.44	0.49
1:B:2611:CYS:HA	1:B:2614:ILE:HG22	1.94	0.49
1:B:2695:LEU:O	1:B:2699:ALA:HB2	2.12	0.49
1:B:3203:VAL:HG12	1:B:3214:ASN:HD22	1.76	0.49
1:C:2015:GLU:OE2	1:C:2032:GLN:NE2	2.45	0.49
1:D:1116:GLY:H	1:D:1121:ALA:HB3	1.77	0.49
1:D:1443:GLN:NE2	1:D:1555:LEU:O	2.35	0.49
1:A:168:ASP:HB3	1:A:199:LEU:HD11	1.94	0.49
1:A:1650:ILE:HA	1:A:1653:LEU:HD13	1.95	0.49
1:B:3607:GLU:HA	1:B:3610:GLU:HG2	1.93	0.49
1:D:1225:PRO:HB2	1:D:1228:ILE:HB	1.94	0.49
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.94	0.49
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.95	0.49
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.36	0.49
1:A:1461:ASP:OD2	1:A:1468:LYS:NZ	2.40	0.49
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.95	0.49
1:B:4544:LEU:O	1:B:4548:ARG:HB2	2.12	0.49
1:C:3218:VAL:HB	1:C:3227:ARG:HD3	1.93	0.49
1:D:1650:ILE:HA	1:D:1653:LEU:HD13	1.95	0.49
1:D:1944:GLU:HB3	1:D:2123:LEU:HD21	1.94	0.49
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.78	0.49
1:D:3891:LEU:HD13	1:D:3899:PHE:HE1	1.77	0.49
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH1	1:A:115:ARG:O	2.45	0.49
1:A:1944:GLU:HB3	1:A:2123:LEU:HD21	1.94	0.49
1:A:3206:LEU:HD13	1:A:3246:LEU:HD13	1.94	0.49
1:B:3111:ARG:NH2	1:B:3174:SER:OG	2.46	0.49
1:B:3821:LYS:O	1:B:3824:LYS:NZ	2.39	0.49
1:B:4155:PRO:O	1:B:4161:ARG:NH1	2.45	0.49
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	1.95	0.49
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	1.95	0.49
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.94	0.49
1:A:867:LEU:HB3	1:A:929:LEU:HD13	1.94	0.49
1:A:2611:CYS:HA	1:A:2614:ILE:HG22	1.94	0.49
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	1.95	0.49
1:B:1650:ILE:HA	1:B:1653:LEU:HD13	1.95	0.49
1:B:2015:GLU:OE2	1:B:2032:GLN:NE2	2.45	0.49
1:B:2477:PRO:HG3	1:B:2546:MET:HE2	1.94	0.49
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.95	0.49
1:C:2211:MET:HA	1:C:2214:VAL:HG12	1.94	0.49
1:C:3037:GLU:HB3	1:C:3088:VAL:HG21	1.95	0.49
1:C:3203:VAL:HG12	1:C:3214:ASN:HD22	1.76	0.49
1:D:1106:ARG:NH2	1:D:1183:GLU:O	2.39	0.49
1:D:3111:ARG:NH2	1:D:3174:SER:OG	2.46	0.49
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.95	0.49
1:A:195:PHE:O	1:D:2359:ARG:NH1	2.46	0.49
1:A:497:TYR:O	1:A:553:ARG:NH2	2.41	0.49
1:A:3111:ARG:NH2	1:A:3174:SER:OG	2.46	0.49
1:A:3575:LEU:HD23	1:B:1219:LEU:HD22	1.94	0.49
1:A:4155:PRO:O	1:A:4161:ARG:NH1	2.45	0.49
1:A:4161:ARG:HE	1:A:4164:LEU:HD21	1.77	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.39	0.49
1:B:2013:LYS:NZ	1:B:3661:TRP:O	2.38	0.49
1:B:2971:GLN:HA	1:B:2974:ILE:HG12	1.95	0.49
1:C:1650:ILE:HA	1:C:1653:LEU:HD13	1.95	0.49
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.94	0.49
1:D:168:ASP:OD1	1:D:201:ASN:ND2	2.45	0.49
1:D:3202:PRO:O	1:D:3214:ASN:ND2	2.46	0.49
1:D:3206:LEU:HD13	1:D:3246:LEU:HD13	1.94	0.49
1:A:1225:PRO:HB2	1:A:1228:ILE:HB	1.94	0.48
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.94	0.48
1:A:2971:GLN:HA	1:A:2974:ILE:HG12	1.95	0.48
1:B:168:ASP:OD1	1:B:201:ASN:ND2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.94	0.48
1:C:637:LEU:HD13	1:C:1637:MET:HB3	1.95	0.48
1:C:1257:VAL:HG21	1:C:1597:VAL:HG11	1.94	0.48
1:C:3592:ILE:HG13	1:C:3595:ARG:HE	1.76	0.48
1:D:586:ILE:HA	1:D:589:LEU:HD23	1.96	0.48
1:D:1256:GLU:HB3	1:D:1275:ARG:HD2	1.93	0.48
1:D:2739:PRO:HG3	1:D:2888:ARG:HG2	1.95	0.48
1:C:1422:ASP:OD2	1:C:1568:LYS:NZ	2.38	0.48
1:C:3202:PRO:O	1:C:3214:ASN:ND2	2.46	0.48
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.95	0.48
1:D:3226:GLU:HA	1:D:3229:ILE:HG12	1.94	0.48
1:A:586:ILE:HA	1:A:589:LEU:HD23	1.96	0.48
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.48
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.95	0.48
1:B:3015:LEU:HD12	1:B:3025:LEU:HB3	1.95	0.48
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.94	0.48
1:C:3798:LEU:HD11	1:C:3884:LEU:HA	1.95	0.48
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.78	0.48
1:D:2211:MET:HA	1:D:2214:VAL:HG12	1.94	0.48
1:A:1068:ARG:HG2	1:A:1069:TRP:CD1	2.48	0.48
1:A:3566:SER:HB3	1:A:3569:LEU:HG	1.96	0.48
1:B:1068:ARG:HG2	1:B:1069:TRP:CD1	2.48	0.48
1:B:1116:GLY:H	1:B:1121:ALA:HB3	1.77	0.48
1:B:3053:ARG:HG3	1:B:3056:LEU:HD13	1.96	0.48
1:B:3206:LEU:HD13	1:B:3246:LEU:HD13	1.94	0.48
1:B:3226:GLU:HA	1:B:3229:ILE:HG12	1.94	0.48
1:C:168:ASP:HB3	1:C:199:LEU:HD11	1.94	0.48
1:C:586:ILE:HA	1:C:589:LEU:HD23	1.96	0.48
1:D:1077:ALA:HA	1:D:1236:THR:HG22	1.95	0.48
1:D:3607:GLU:HA	1:D:3610:GLU:HG2	1.93	0.48
1:A:1077:ALA:HA	1:A:1236:THR:HG22	1.95	0.48
1:A:3414:ARG:NH1	1:A:3469:PHE:O	2.45	0.48
1:A:3872:GLU:HG3	1:A:3874:VAL:H	1.78	0.48
1:A:3891:LEU:HD13	1:A:3899:PHE:HE1	1.78	0.48
1:B:3037:GLU:HB3	1:B:3088:VAL:HG21	1.95	0.48
1:C:497:TYR:O	1:C:553:ARG:NH2	2.41	0.48
1:C:2460:LEU:HA	1:D:131:LEU:HD21	1.96	0.48
1:C:3566:SER:HB3	1:C:3569:LEU:HG	1.96	0.48
1:D:867:LEU:HB3	1:D:929:LEU:HD13	1.94	0.48
1:D:3566:SER:HB3	1:D:3569:LEU:HG	1.96	0.48
1:D:3798:LEU:HD11	1:D:3884:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LEU:HD13	1:A:1637:MET:HB3	1.95	0.48
1:A:3202:PRO:O	1:A:3214:ASN:ND2	2.46	0.48
1:B:168:ASP:HB3	1:B:199:LEU:HD11	1.94	0.48
1:B:551:LEU:HD21	1:B:585:SER:HB3	1.95	0.48
1:B:637:LEU:HD13	1:B:1637:MET:HB3	1.95	0.48
1:B:867:LEU:HB3	1:B:929:LEU:HD13	1.94	0.48
1:C:639:ASN:HD21	1:C:676:THR:HG1	1.56	0.48
1:C:867:LEU:HB3	1:C:929:LEU:HD13	1.94	0.48
1:C:4865:LYS:HA	1:C:4865:LYS:HD2	1.66	0.48
1:D:775:GLY:H	1:D:848:HIS:CG	2.32	0.48
1:A:2677:LYS:HB3	1:A:2677:LYS:HE2	1.67	0.48
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	1.95	0.48
1:B:2460:LEU:HA	1:C:131:LEU:HD21	1.96	0.48
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.94	0.48
1:B:3891:LEU:HD13	1:B:3899:PHE:HE1	1.77	0.48
1:D:2971:GLN:HA	1:D:2974:ILE:HG12	1.95	0.48
1:A:1116:GLY:H	1:A:1121:ALA:HB3	1.77	0.48
1:A:3015:LEU:HD12	1:A:3025:LEU:HB3	1.95	0.48
1:B:3409:TYR:HE2	1:B:3510:ILE:HG12	1.78	0.48
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.95	0.48
1:C:3111:ARG:NH2	1:C:3174:SER:OG	2.46	0.48
1:D:182:LEU:HG	1:D:184:THR:HG23	1.96	0.48
1:A:1422:ASP:OD2	1:A:1568:LYS:NZ	2.38	0.48
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.34	0.48
1:A:2867:LEU:HB2	1:A:2928:LYS:HZ3	1.79	0.48
1:B:1422:ASP:OD2	1:B:1568:LYS:NZ	2.38	0.48
1:B:3872:GLU:HG3	1:B:3874:VAL:H	1.78	0.48
1:C:551:LEU:HD21	1:C:585:SER:HB3	1.95	0.48
1:C:775:GLY:H	1:C:848:HIS:CG	2.32	0.48
1:C:2971:GLN:HA	1:C:2974:ILE:HG12	1.95	0.48
1:C:3110:LEU:HB3	1:C:3175:LEU:HD11	1.96	0.48
1:D:497:TYR:O	1:D:553:ARG:NH2	2.41	0.48
1:D:637:LEU:HD13	1:D:1637:MET:HB3	1.95	0.48
1:D:758:ARG:HG2	1:D:763:PRO:HA	1.96	0.48
1:A:2739:PRO:HG3	1:A:2888:ARG:HG2	1.95	0.48
1:B:861:ILE:HG23	1:B:933:LEU:HD22	1.96	0.48
1:B:2465:ASP:O	1:B:2469:ILE:HG13	2.14	0.48
1:B:2467:VAL:HG23	1:B:2521:VAL:HG13	1.96	0.48
1:B:3566:SER:HB3	1:B:3569:LEU:HG	1.96	0.48
1:C:665:GLU:HB2	1:C:792:LEU:HB2	1.96	0.48
1:C:3015:LEU:HD12	1:C:3025:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:861:ILE:HG23	1:D:933:LEU:HD22	1.96	0.48
1:D:3053:ARG:HG3	1:D:3056:LEU:HD13	1.96	0.48
1:A:2465:ASP:O	1:A:2469:ILE:HG13	2.14	0.47
1:B:586:ILE:HA	1:B:589:LEU:HD23	1.96	0.47
1:B:775:GLY:H	1:B:848:HIS:CG	2.32	0.47
1:B:3798:LEU:HD11	1:B:3884:LEU:HA	1.95	0.47
1:B:4183:ILE:HG12	1:B:4193:ILE:HD11	1.96	0.47
1:C:2739:PRO:HG3	1:C:2888:ARG:HG2	1.95	0.47
1:C:3821:LYS:O	1:C:3824:LYS:NZ	2.39	0.47
1:D:1068:ARG:HG2	1:D:1069:TRP:CD1	2.48	0.47
1:D:2039:LEU:HD23	1:D:2044:ILE:HG21	1.96	0.47
1:D:2465:ASP:O	1:D:2469:ILE:HG13	2.14	0.47
1:D:3037:GLU:HB3	1:D:3088:VAL:HG21	1.95	0.47
1:D:3409:TYR:HE2	1:D:3510:ILE:HG12	1.78	0.47
1:D:4189:ARG:HG2	1:D:5031:GLN:HE22	1.79	0.47
1:A:878:ILE:HA	1:A:881:LEU:HB2	1.96	0.47
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	1.95	0.47
1:B:4861:LYS:H	1:B:4861:LYS:HG3	1.47	0.47
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.96	0.47
1:C:758:ARG:HG2	1:C:763:PRO:HA	1.96	0.47
1:C:861:ILE:HG23	1:C:933:LEU:HD22	1.96	0.47
1:C:1077:ALA:HA	1:C:1236:THR:HG22	1.95	0.47
1:C:2863:SER:HA	1:C:2928:LYS:HG3	1.96	0.47
1:C:4189:ARG:HG2	1:C:5031:GLN:HE22	1.79	0.47
1:D:168:ASP:HB3	1:D:199:LEU:HD11	1.94	0.47
1:D:3110:LEU:HB3	1:D:3175:LEU:HD11	1.96	0.47
1:A:775:GLY:H	1:A:848:HIS:CG	2.32	0.47
1:A:3037:GLU:HB3	1:A:3088:VAL:HG21	1.95	0.47
1:A:3209:GLN:HG2	1:A:3210:LEU:HG	1.96	0.47
1:B:1076:ARG:HD3	1:B:1109:LEU:HD21	1.96	0.47
1:B:2739:PRO:HG3	1:B:2888:ARG:HG2	1.95	0.47
1:B:3903:LEU:HB3	1:B:3915:ILE:HD11	1.96	0.47
1:C:2339:VAL:HG11	1:C:2353:VAL:HG11	1.96	0.47
1:C:2588:ARG:HE	1:C:2900:GLY:HA2	1.80	0.47
1:C:4183:ILE:HG12	1:C:4193:ILE:HD11	1.96	0.47
1:D:2624:ARG:HG3	1:D:2910:THR:HB	1.96	0.47
1:D:3015:LEU:HD12	1:D:3025:LEU:HB3	1.95	0.47
1:A:861:ILE:HG23	1:A:933:LEU:HD22	1.97	0.47
1:A:2457:LEU:HA	1:A:2460:LEU:HD12	1.97	0.47
1:B:2296:GLU:HA	1:B:2299:VAL:HG22	1.97	0.47
1:B:2457:LEU:HA	1:B:2460:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.43	0.47
1:C:1968:LYS:NZ	1:C:2030:ASP:OD2	2.44	0.47
1:C:2467:VAL:HG23	1:C:2521:VAL:HG13	1.96	0.47
1:C:3209:GLN:HG2	1:C:3210:LEU:HG	1.97	0.47
1:A:850:ASP:O	1:A:1025:ARG:NH2	2.45	0.47
1:A:1076:ARG:HD3	1:A:1109:LEU:HD21	1.96	0.47
1:A:3053:ARG:HG3	1:A:3056:LEU:HD13	1.96	0.47
1:B:2190:VAL:HA	1:B:2193:GLN:HB2	1.97	0.47
1:B:2863:SER:HA	1:B:2928:LYS:HG3	1.96	0.47
1:D:878:ILE:HA	1:D:881:LEU:HB2	1.97	0.47
1:D:1743[A]:ARG:HE	1:D:1743[A]:ARG:HB2	1.47	0.47
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	1.95	0.47
1:A:2460:LEU:HA	1:B:131:LEU:HD21	1.96	0.47
1:A:4183:ILE:HG12	1:A:4193:ILE:HD11	1.96	0.47
1:B:182:LEU:HG	1:B:184:THR:HG23	1.96	0.47
1:B:1077:ALA:HA	1:B:1236:THR:HG22	1.95	0.47
1:B:2339:VAL:HG11	1:B:2353:VAL:HG11	1.96	0.47
1:B:3110:LEU:HB3	1:B:3175:LEU:HD11	1.96	0.47
1:B:3202:PRO:O	1:B:3214:ASN:ND2	2.46	0.47
1:C:41:GLY:O	1:C:45:ARG:NH1	2.41	0.47
1:C:1068:ARG:HG2	1:C:1069:TRP:CD1	2.48	0.47
1:C:2457:LEU:HA	1:C:2460:LEU:HD12	1.97	0.47
1:C:2465:ASP:O	1:C:2469:ILE:HG13	2.14	0.47
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	1.95	0.47
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.32	0.47
1:D:276:TRP:NE1	1:D:346:CYS:SG	2.75	0.47
1:D:2457:LEU:HA	1:D:2460:LEU:HD12	1.97	0.47
2:H:55:VAL:HG21	2:H:59:PHE:HD2	1.80	0.47
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.96	0.47
1:A:2190:VAL:HA	1:A:2193:GLN:HB2	1.97	0.47
1:A:3110:LEU:HB3	1:A:3175:LEU:HD11	1.96	0.47
1:A:3821:LYS:O	1:A:3824:LYS:NZ	2.40	0.47
1:B:497:TYR:O	1:B:553:ARG:NH2	2.41	0.47
1:B:665:GLU:HB2	1:B:792:LEU:HB2	1.96	0.47
1:B:2039:LEU:HD23	1:B:2044:ILE:HG21	1.96	0.47
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.95	0.47
1:B:3209:GLN:HG2	1:B:3210:LEU:HG	1.97	0.47
1:C:232:THR:HG21	1:C:252:VAL:HG12	1.96	0.47
1:C:3409:TYR:HE2	1:C:3510:ILE:HG12	1.78	0.47
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.97	0.47
1:C:3903:LEU:HB3	1:C:3915:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:THR:HG21	1:D:252:VAL:HG12	1.96	0.47
1:D:2977:LEU:HG	1:D:3056:LEU:HD23	1.97	0.47
1:A:2039:LEU:HD23	1:A:2044:ILE:HG21	1.96	0.47
1:A:3003:LEU:O	1:A:3007:ASN:HB2	2.15	0.47
1:B:232:THR:HG21	1:B:252:VAL:HG12	1.96	0.47
1:B:639:ASN:HD21	1:B:676:THR:HG1	1.56	0.47
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.46	0.47
1:C:3019:SER:O	1:C:3036:LYS:NZ	2.46	0.47
1:C:3053:ARG:HG3	1:C:3056:LEU:HD13	1.96	0.47
1:D:850:ASP:O	1:D:1025:ARG:NH2	2.45	0.47
1:D:1455:PRO:HB3	1:D:1549:PHE:HE1	1.80	0.47
1:D:1653:LEU:HA	1:D:1656:ARG:HB2	1.97	0.47
2:G:55:VAL:HG21	2:G:59:PHE:HD2	1.80	0.47
1:A:131:LEU:HD21	1:D:2460:LEU:HA	1.97	0.47
1:A:232:THR:HG21	1:A:252:VAL:HG12	1.96	0.47
1:A:2737:PRO:HB2	1:A:2884:ASN:HB2	1.97	0.47
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.97	0.47
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.97	0.47
1:D:2588:ARG:HE	1:D:2900:GLY:HA2	1.80	0.47
1:D:3903:LEU:HB3	1:D:3915:ILE:HD11	1.96	0.47
1:A:294:THR:HG23	1:A:297:GLN:H	1.80	0.47
1:A:758:ARG:HG2	1:A:763:PRO:HA	1.96	0.47
1:A:2296:GLU:HA	1:A:2299:VAL:HG22	1.96	0.47
1:A:3214:ASN:HB3	1:A:3217:SER:HB2	1.97	0.47
1:A:3409:TYR:HE2	1:A:3510:ILE:HG12	1.78	0.47
1:B:758:ARG:HG2	1:B:763:PRO:HA	1.96	0.47
1:B:783:PHE:HB2	1:B:787:VAL:HG21	1.97	0.47
1:B:2977:LEU:HG	1:B:3056:LEU:HD23	1.97	0.47
1:C:1076:ARG:HD3	1:C:1109:LEU:HD21	1.96	0.47
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.96	0.47
1:D:2863:SER:HA	1:D:2928:LYS:HG3	1.96	0.47
1:D:3003:LEU:O	1:D:3007:ASN:HB2	2.15	0.47
1:A:76:ARG:HD2	1:D:3935:TRP:O	2.15	0.46
1:A:1091:GLU:HB2	1:A:1203:ASN:HB3	1.97	0.46
1:A:2624:ARG:HG3	1:A:2910:THR:HB	1.96	0.46
1:A:2863:SER:HA	1:A:2928:LYS:HG3	1.96	0.46
1:B:878:ILE:HA	1:B:881:LEU:HB2	1.97	0.46
1:B:2677:LYS:HE2	1:B:2677:LYS:HB3	1.67	0.46
1:B:2737:PRO:HB2	1:B:2884:ASN:HB2	1.97	0.46
1:B:3019:SER:O	1:B:3036:LYS:NZ	2.46	0.46
1:C:294:THR:HG23	1:C:297:GLN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:783:PHE:HB2	1:C:787:VAL:HG21	1.97	0.46
1:C:1091:GLU:HB2	1:C:1203:ASN:HB3	1.97	0.46
1:C:2039:LEU:HD23	1:C:2044:ILE:HG21	1.96	0.46
1:D:1091:GLU:HB2	1:D:1203:ASN:HB3	1.97	0.46
1:A:76:ARG:HH12	1:D:3938:SER:N	2.14	0.46
1:C:182:LEU:HG	1:C:184:THR:HG23	1.96	0.46
1:C:873:LYS:H	1:C:873:LYS:HG2	1.48	0.46
1:C:878:ILE:HA	1:C:881:LEU:HB2	1.97	0.46
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.98	0.46
1:C:2190:VAL:HA	1:C:2193:GLN:HB2	1.97	0.46
1:D:294:THR:HG23	1:D:297:GLN:H	1.80	0.46
1:D:665:GLU:HB2	1:D:792:LEU:HB2	1.96	0.46
1:D:783:PHE:HB2	1:D:787:VAL:HG21	1.97	0.46
1:D:1076:ARG:HD3	1:D:1109:LEU:HD21	1.96	0.46
1:D:2467:VAL:HG23	1:D:2521:VAL:HG13	1.96	0.46
1:D:3589:PRO:HA	1:D:3592:ILE:HG22	1.98	0.46
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.97	0.46
1:A:182:LEU:HG	1:A:184:THR:HG23	1.96	0.46
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.31	0.46
1:A:3589:PRO:HA	1:A:3592:ILE:HG22	1.98	0.46
1:B:4188:ARG:HA	1:B:4188:ARG:HD2	1.57	0.46
1:B:4189:ARG:HG2	1:B:5031:GLN:HE22	1.79	0.46
1:C:2624:ARG:HG3	1:C:2910:THR:HB	1.96	0.46
1:D:2190:VAL:HA	1:D:2193:GLN:HB2	1.97	0.46
1:A:1433:TYR:O	1:A:1519:LEU:HA	2.15	0.46
1:A:1653:LEU:HA	1:A:1656:ARG:HB2	1.97	0.46
1:A:2467:VAL:HG23	1:A:2521:VAL:HG13	1.96	0.46
1:A:2588:ARG:HE	1:A:2900:GLY:HA2	1.80	0.46
1:A:3798:LEU:HD11	1:A:3884:LEU:HA	1.96	0.46
1:A:4189:ARG:HG2	1:A:5031:GLN:HE22	1.79	0.46
1:A:4202:ARG:O	1:A:4206:GLU:HG2	2.16	0.46
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	1.95	0.46
1:B:3938:SER:OG	1:C:76:ARG:NH1	2.48	0.46
1:C:2737:PRO:HB2	1:C:2884:ASN:HB2	1.97	0.46
1:C:3003:LEU:O	1:C:3007:ASN:HB2	2.15	0.46
1:C:3938:SER:OG	1:D:76:ARG:NH1	2.48	0.46
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.97	0.46
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.97	0.46
1:D:3209:GLN:HG2	1:D:3210:LEU:HG	1.97	0.46
1:D:3214:ASN:HB3	1:D:3217:SER:HB2	1.97	0.46
1:B:1091:GLU:HB2	1:B:1203:ASN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4865:LYS:HA	1:B:4865:LYS:HD2	1.66	0.46
1:C:736:HIS:ND1	1:C:737:LEU:O	2.42	0.46
1:C:1455:PRO:HB3	1:C:1549:PHE:HE1	1.80	0.46
1:C:1653:LEU:HA	1:C:1656:ARG:HB2	1.97	0.46
1:C:1980:LEU:HD11	1:C:1994:ARG:HB3	1.98	0.46
1:C:2296:GLU:HA	1:C:2299:VAL:HG22	1.97	0.46
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.34	0.46
1:D:2339:VAL:HG11	1:D:2353:VAL:HG11	1.96	0.46
1:A:783:PHE:HB2	1:A:787:VAL:HG21	1.97	0.46
1:A:946:ALA:O	1:A:950:LEU:CB	2.64	0.46
1:A:1018:ASN:H	1:A:1021:LEU:HD12	1.81	0.46
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.34	0.46
1:A:1455:PRO:HB3	1:A:1549:PHE:HE1	1.80	0.46
1:A:2339:VAL:HG11	1:A:2353:VAL:HG11	1.96	0.46
1:A:2583:LEU:HA	1:A:2586:VAL:HG22	1.98	0.46
1:A:3903:LEU:HB3	1:A:3915:ILE:HD11	1.96	0.46
1:B:1433:TYR:O	1:B:1519:LEU:HA	2.15	0.46
1:B:1769:THR:N	1:B:1956:GLU:OE2	2.49	0.46
1:B:2624:ARG:HG3	1:B:2910:THR:HB	1.96	0.46
1:B:3003:LEU:O	1:B:3007:ASN:HB2	2.15	0.46
1:C:1291:LEU:HD12	1:C:1550:PRO:HG2	1.97	0.46
1:C:1769:THR:N	1:C:1956:GLU:OE2	2.49	0.46
1:D:2296:GLU:HA	1:D:2299:VAL:HG22	1.97	0.46
1:D:4183:ILE:HG12	1:D:4193:ILE:HD11	1.96	0.46
1:A:585:SER:O	1:A:588:SER:OG	2.27	0.46
1:A:2977:LEU:HG	1:A:3056:LEU:HD23	1.97	0.46
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.97	0.46
1:B:1291:LEU:HD12	1:B:1550:PRO:HG2	1.97	0.46
1:B:1980:LEU:HD11	1:B:1994:ARG:HB3	1.98	0.46
1:B:2583:LEU:HA	1:B:2586:VAL:HG22	1.98	0.46
1:B:3589:PRO:HA	1:B:3592:ILE:HG22	1.98	0.46
1:B:3705:PHE:HA	1:B:3708:THR:HG22	1.97	0.46
1:B:4204:GLN:HA	1:B:4207:MET:HG3	1.98	0.46
1:C:3214:ASN:HB3	1:C:3217:SER:HB2	1.97	0.46
1:D:2867:LEU:HB2	1:D:2928:LYS:HZ3	1.81	0.46
2:H:73:LYS:HZ3	2:H:75:THR:HG1	1.61	0.46
1:A:4204:GLN:HA	1:A:4207:MET:HG3	1.98	0.46
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.34	0.46
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.98	0.46
1:B:4202:ARG:O	1:B:4206:GLU:HG2	2.16	0.46
1:C:719:LEU:HD23	1:C:735:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2977:LEU:HG	1:C:3056:LEU:HD23	1.97	0.46
1:D:1018:ASN:H	1:D:1021:LEU:HD12	1.81	0.46
1:A:665:GLU:HB2	1:A:792:LEU:HB2	1.96	0.46
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.51	0.46
1:C:4718:LYS:H	1:C:4718:LYS:HG2	1.43	0.46
1:D:2703:LEU:HG	1:D:3005:LEU:HD13	1.98	0.46
1:D:3705:PHE:HA	1:D:3708:THR:HG22	1.97	0.46
1:D:4202:ARG:O	1:D:4206:GLU:HG2	2.16	0.46
1:A:299:LEU:HD22	1:A:378:LEU:HB2	1.98	0.46
1:A:1451:GLY:HA3	1:A:1494:MET:HA	1.98	0.46
1:A:3705:PHE:HA	1:A:3708:THR:HG22	1.97	0.46
1:B:719:LEU:HD23	1:B:735:GLN:HB2	1.98	0.46
1:B:1973:GLN:HE22	1:B:3640:PRO:HB2	1.81	0.46
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.49	0.46
1:B:3214:ASN:HB3	1:B:3217:SER:HB2	1.97	0.46
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.97	0.46
1:C:2003:GLN:O	1:C:2007:ASN:ND2	2.49	0.46
1:C:3589:PRO:HA	1:C:3592:ILE:HG22	1.98	0.46
1:C:4202:ARG:O	1:C:4206:GLU:HG2	2.16	0.46
1:D:719:LEU:HD23	1:D:735:GLN:HB2	1.98	0.46
1:D:1433:TYR:O	1:D:1519:LEU:HA	2.15	0.46
1:A:873:LYS:HE3	1:A:873:LYS:HB3	1.85	0.45
1:A:1694:LEU:HD12	1:A:1715:LEU:HB2	1.98	0.45
1:A:1828:ASP:N	1:A:1828:ASP:OD1	2.49	0.45
1:A:3523:ASN:OD1	1:A:3582:ARG:NH2	2.50	0.45
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.99	0.45
1:B:1455:PRO:HB3	1:B:1549:PHE:HE1	1.80	0.45
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.97	0.45
1:B:2588:ARG:HE	1:B:2900:GLY:HA2	1.80	0.45
1:B:3329:ILE:HD11	1:B:3332:ALA:HB2	1.98	0.45
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.34	0.45
1:C:1451:GLY:HA3	1:C:1494:MET:HA	1.98	0.45
1:C:1694:LEU:HD12	1:C:1715:LEU:HB2	1.98	0.45
1:D:299:LEU:HD22	1:D:378:LEU:HB2	1.98	0.45
1:D:1109:LEU:HA	1:D:1120:LEU:HD13	1.98	0.45
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.98	0.45
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.51	0.45
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.32	0.45
2:E:55:VAL:HG21	2:E:59:PHE:HD2	1.80	0.45
1:B:889:GLN:O	1:B:892:THR:OG1	2.25	0.45
1:C:629:ARG:NH1	2:G:90:VAL:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1018:ASN:H	1:C:1021:LEU:HD12	1.81	0.45
1:C:3705:PHE:HA	1:C:3708:THR:HG22	1.97	0.45
1:D:1291:LEU:HD12	1:D:1550:PRO:HG2	1.97	0.45
1:D:4188:ARG:HD2	1:D:4188:ARG:HA	1.57	0.45
1:B:299:LEU:HD22	1:B:378:LEU:HB2	1.98	0.45
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.36	0.45
1:C:1433:TYR:O	1:C:1519:LEU:HA	2.15	0.45
1:D:1782:PHE:O	2:H:82:TYR:OH	2.35	0.45
1:D:2737:PRO:HB2	1:D:2884:ASN:HB2	1.97	0.45
1:D:3132:THR:HG23	1:D:3136:LEU:HD23	1.98	0.45
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.99	0.45
2:G:2:VAL:HA	2:G:75:THR:O	2.17	0.45
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.97	0.45
1:A:719:LEU:HD23	1:A:735:GLN:HB2	1.98	0.45
1:A:1291:LEU:HD12	1:A:1550:PRO:HG2	1.97	0.45
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.96	0.45
1:B:294:THR:HG23	1:B:297:GLN:H	1.80	0.45
1:B:946:ALA:O	1:B:950:LEU:CB	2.64	0.45
1:B:1018:ASN:H	1:B:1021:LEU:HD12	1.81	0.45
1:B:1653:LEU:HA	1:B:1656:ARG:HB2	1.97	0.45
1:B:1694:LEU:HD12	1:B:1715:LEU:HB2	1.98	0.45
1:B:2765:LYS:HA	1:B:2765:LYS:HD3	1.71	0.45
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.99	0.45
1:C:873:LYS:HE3	1:C:873:LYS:HB3	1.85	0.45
1:C:2703:LEU:HG	1:C:3005:LEU:HD13	1.98	0.45
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.99	0.45
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.49	0.45
1:D:2583:LEU:HA	1:D:2586:VAL:HG22	1.98	0.45
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	1.99	0.45
2:F:55:VAL:HG21	2:F:59:PHE:HD2	1.80	0.45
1:A:1109:LEU:HA	1:A:1120:LEU:HD13	1.98	0.45
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.51	0.45
1:A:3938:SER:OG	1:B:76:ARG:NH1	2.49	0.45
1:B:1828:ASP:N	1:B:1828:ASP:OD1	2.49	0.45
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.99	0.45
1:B:4680:LYS:HB2	1:B:4680:LYS:HE3	1.72	0.45
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.97	0.45
1:C:1973:GLN:HE22	1:C:3640:PRO:HB2	1.81	0.45
1:C:4569:LEU:HD23	1:C:4650:HIS:HA	1.99	0.45
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.49	0.45
1:B:171:LEU:HD21	1:B:180:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:HIS:ND1	1:B:737:LEU:O	2.42	0.45
1:B:1100:MET:HE3	1:B:1198:GLN:HB3	1.98	0.45
1:B:2703:LEU:HG	1:B:3005:LEU:HD13	1.98	0.45
1:B:3147:ILE:HG23	1:B:3152:PHE:HB2	1.99	0.45
1:B:3414:ARG:NH1	1:B:3469:PHE:O	2.45	0.45
1:C:276:TRP:NE1	1:C:346:CYS:SG	2.75	0.45
1:C:400:ALA:O	1:C:404:ILE:HD12	2.17	0.45
1:C:3132:THR:HG23	1:C:3136:LEU:HD23	1.98	0.45
1:C:3523:ASN:OD1	1:C:3582:ARG:NH2	2.50	0.45
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.98	0.45
1:D:3523:ASN:OD1	1:D:3582:ARG:NH2	2.50	0.45
1:D:4204:GLN:HA	1:D:4207:MET:HG3	1.98	0.45
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.97	0.45
1:A:1973:GLN:HE22	1:A:3640:PRO:HB2	1.81	0.45
1:A:1980:LEU:HD11	1:A:1994:ARG:HB3	1.98	0.45
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.99	0.45
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.51	0.45
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.99	0.45
1:C:1109:LEU:HA	1:C:1120:LEU:HD13	1.98	0.45
1:D:1461:ASP:OD2	1:D:1468:LYS:NZ	2.40	0.45
1:D:1828:ASP:OD1	1:D:1828:ASP:N	2.49	0.45
1:D:3414:ARG:NH1	1:D:3469:PHE:O	2.45	0.45
1:A:400:ALA:O	1:A:404:ILE:HD12	2.17	0.45
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.97	0.45
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	1.98	0.45
1:A:4690:GLU:H	1:A:4690:GLU:HG2	1.53	0.45
1:B:1109:LEU:HA	1:B:1120:LEU:HD13	1.98	0.45
1:C:590:LEU:HG	1:C:631:LEU:HD22	1.99	0.45
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.99	0.45
1:C:3414:ARG:NH1	1:C:3469:PHE:O	2.45	0.45
1:D:1980:LEU:HD11	1:D:1994:ARG:HB3	1.98	0.45
1:D:3329:ILE:HD11	1:D:3332:ALA:HB2	1.98	0.45
1:A:873:LYS:H	1:A:873:LYS:HG2	1.47	0.45
1:B:1842:LEU:O	1:B:1846:SER:OG	2.30	0.45
1:C:171:LEU:HD21	1:C:180:LEU:HB2	1.98	0.45
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.99	0.45
1:C:1254:HIS:HA	1:C:1276:THR:HG22	1.99	0.45
1:C:1828:ASP:OD1	1:C:1828:ASP:N	2.49	0.45
1:C:2583:LEU:HA	1:C:2586:VAL:HG22	1.98	0.45
1:C:2765:LYS:HD3	1:C:2765:LYS:HA	1.71	0.45
1:C:4092:ASP:O	1:C:4096:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ASP:N	1:D:134:ASP:OD1	2.50	0.45
1:D:1254:HIS:HA	1:D:1276:THR:HG22	1.99	0.45
1:D:2004:GLU:HA	1:D:2007:ASN:HB2	1.99	0.45
1:A:3329:ILE:HD11	1:A:3332:ALA:HB2	1.98	0.45
1:B:590:LEU:HG	1:B:631:LEU:HD22	1.99	0.45
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.99	0.45
1:B:3523:ASN:OD1	1:B:3582:ARG:NH2	2.50	0.45
1:C:946:ALA:O	1:C:950:LEU:CB	2.64	0.45
1:C:1743[A]:ARG:HE	1:C:1743[A]:ARG:HB2	1.47	0.45
1:C:1782:PHE:O	2:G:82:TYR:OH	2.35	0.45
1:C:3147:ILE:HG23	1:C:3152:PHE:HB2	1.99	0.45
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.32	0.45
1:C:4204:GLN:HA	1:C:4207:MET:HG3	1.98	0.45
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.82	0.45
1:C:4848:VAL:O	1:C:4852:THR:OG1	2.34	0.45
1:D:171:LEU:HD21	1:D:180:LEU:HB2	1.98	0.45
2:F:2:VAL:HA	2:F:75:THR:O	2.17	0.45
1:A:590:LEU:HG	1:A:631:LEU:HD22	1.99	0.44
1:A:3556:ASN:HB3	1:A:3559:LEU:HD13	1.98	0.44
1:B:134:ASP:OD1	1:B:134:ASP:N	2.50	0.44
1:B:1451:GLY:HA3	1:B:1494:MET:HA	1.98	0.44
1:B:3132:THR:HG23	1:B:3136:LEU:HD23	1.98	0.44
1:B:4092:ASP:O	1:B:4096:ALA:HB2	2.17	0.44
1:C:2313:LEU:HG	1:C:2416:VAL:HG21	2.00	0.44
1:C:3329:ILE:HD11	1:C:3332:ALA:HB2	1.98	0.44
1:C:3995:VAL:O	1:C:3999:MET:HG2	2.17	0.44
1:D:2458:ARG:NH2	1:D:2510:TYR:O	2.50	0.44
1:D:4569:LEU:HD23	1:D:4650:HIS:HA	1.99	0.44
2:H:2:VAL:HA	2:H:75:THR:O	2.17	0.44
1:A:1769:THR:N	1:A:1956:GLU:OE2	2.49	0.44
1:A:4921:PHE:HE2	1:D:4891:VAL:HG12	1.81	0.44
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.99	0.44
1:B:400:ALA:O	1:B:404:ILE:HD12	2.17	0.44
1:B:873:LYS:HE3	1:B:873:LYS:HB3	1.85	0.44
1:B:1087:ARG:HA	1:B:1153:ILE:O	2.17	0.44
1:B:1727:ARG:NH2	1:B:1773:PRO:O	2.50	0.44
1:B:2313:LEU:HG	1:B:2416:VAL:HG21	2.00	0.44
1:C:294:THR:N	1:C:298:GLY:O	2.49	0.44
1:C:733:PRO:HG2	1:C:762:CYS:HB3	2.00	0.44
1:C:1087:ARG:HA	1:C:1153:ILE:O	2.17	0.44
1:D:629:ARG:NH1	2:H:90:VAL:O	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:733:PRO:HG2	1:D:762:CYS:HB3	2.00	0.44
1:D:1973:GLN:HE22	1:D:3640:PRO:HB2	1.81	0.44
1:D:2395:PRO:HG2	1:D:2397:VAL:HG12	2.00	0.44
1:D:3019:SER:O	1:D:3036:LYS:NZ	2.46	0.44
1:D:3821:LYS:O	1:D:3824:LYS:NZ	2.39	0.44
2:E:2:VAL:HA	2:E:75:THR:O	2.17	0.44
1:A:1219:LEU:HD22	1:D:3575:LEU:HD23	1.98	0.44
1:A:1727:ARG:NH2	1:A:1773:PRO:O	2.50	0.44
1:A:3147:ILE:HG23	1:A:3152:PHE:HB2	1.99	0.44
1:A:3995:VAL:O	1:A:3999:MET:HG2	2.17	0.44
1:B:733:PRO:HG2	1:B:762:CYS:HB3	2.00	0.44
1:B:3556:ASN:HB3	1:B:3559:LEU:HD13	1.98	0.44
1:C:299:LEU:HD22	1:C:378:LEU:HB2	1.98	0.44
1:C:2004:GLU:HA	1:C:2007:ASN:HB2	1.99	0.44
1:C:2458:ARG:NH2	1:C:2510:TYR:O	2.50	0.44
1:D:3995:VAL:O	1:D:3999:MET:HG2	2.17	0.44
1:A:171:LEU:HD21	1:A:180:LEU:HB2	1.98	0.44
1:A:2458:ARG:NH2	1:A:2510:TYR:O	2.51	0.44
1:D:1028:ASP:OD1	1:D:1028:ASP:N	2.51	0.44
1:D:1087:ARG:HA	1:D:1153:ILE:O	2.17	0.44
1:D:1088:TRP:HB2	1:D:1153:ILE:HG22	1.99	0.44
2:G:73:LYS:HZ3	2:G:75:THR:HG1	1.61	0.44
1:A:733:PRO:HG2	1:A:762:CYS:HB3	2.00	0.44
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	1.99	0.44
1:A:1443:GLN:NE2	1:A:1555:LEU:O	2.35	0.44
1:A:2395:PRO:HG2	1:A:2397:VAL:HG12	2.00	0.44
1:A:2703:LEU:HG	1:A:3005:LEU:HD13	1.98	0.44
1:A:3616:LYS:HD3	1:A:3616:LYS:HA	1.83	0.44
1:A:4092:ASP:O	1:A:4096:ALA:HB2	2.17	0.44
1:B:850:ASP:O	1:B:1025:ARG:NH2	2.45	0.44
1:B:1782:PHE:O	2:F:82:TYR:OH	2.35	0.44
1:B:2359:ARG:NH1	1:C:195:PHE:O	2.50	0.44
1:B:2867:LEU:HB2	1:B:2928:LYS:HZ3	1.82	0.44
1:B:3078:ARG:NH2	1:B:3151:GLN:O	2.51	0.44
1:C:3556:ASN:HB3	1:C:3559:LEU:HD13	1.98	0.44
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.99	0.44
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.99	0.44
1:A:3935:TRP:O	1:B:76:ARG:HD2	2.17	0.44
1:A:4569:LEU:HD23	1:A:4650:HIS:HA	1.99	0.44
1:B:3587:ASP:OD1	1:B:3595:ARG:NH2	2.51	0.44
1:C:3104:GLU:HA	1:C:3107:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1769:THR:N	1:D:1956:GLU:OE2	2.49	0.44
1:A:495:ASN:HD21	1:A:550:LYS:HG2	1.83	0.44
1:A:1254:HIS:HA	1:A:1276:THR:HG22	1.99	0.44
1:A:2121:PHE:O	1:A:3725:TYR:OH	2.28	0.44
1:A:2313:LEU:HG	1:A:2416:VAL:HG21	2.00	0.44
1:A:2359:ARG:NH1	1:B:195:PHE:O	2.51	0.44
1:B:2395:PRO:HG2	1:B:2397:VAL:HG12	2.00	0.44
1:B:2608:MET:HE2	1:B:2643:LEU:HD13	2.00	0.44
1:B:4569:LEU:HD23	1:B:4650:HIS:HA	1.99	0.44
1:C:2336:ARG:HG2	1:C:2435:ARG:HD2	2.00	0.44
1:D:894:GLY:H	1:D:903:LEU:HD13	1.83	0.44
1:D:1694:LEU:HD12	1:D:1715:LEU:HB2	1.98	0.44
1:D:3147:ILE:HG23	1:D:3152:PHE:HB2	1.99	0.44
1:D:3769:ARG:HG3	1:D:3773:ARG:HH12	1.83	0.44
1:D:4092:ASP:O	1:D:4096:ALA:HB2	2.17	0.44
1:A:134:ASP:OD1	1:A:134:ASP:N	2.50	0.44
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.99	0.44
1:A:708:GLY:HA3	1:A:722:TRP:HB3	2.00	0.44
1:A:3019:SER:O	1:A:3036:LYS:NZ	2.46	0.44
1:A:3760:LYS:HA	1:A:3760:LYS:HD3	1.88	0.44
1:B:894:GLY:H	1:B:903:LEU:HD13	1.83	0.44
1:B:3508:SER:HB3	1:B:3511:VAL:HG22	2.00	0.44
1:B:4580:TYR:HE2	1:B:4630:TYR:HB3	1.82	0.44
1:C:850:ASP:O	1:C:1025:ARG:NH2	2.45	0.44
1:C:894:GLY:H	1:C:903:LEU:HD13	1.83	0.44
1:C:1461:ASP:OD2	1:C:1468:LYS:NZ	2.40	0.44
1:C:3769:ARG:HG3	1:C:3773:ARG:HH12	1.83	0.44
1:D:436:LEU:HD23	1:D:436:LEU:HA	1.91	0.44
1:D:3508:SER:HB3	1:D:3511:VAL:HG22	2.00	0.44
1:A:1089:TYR:HE1	1:A:1211:LEU:HD22	1.83	0.44
1:A:4681:LEU:HD11	1:A:4706:LEU:HD22	2.00	0.44
1:B:871:ARG:HA	1:B:874:LEU:HB2	2.00	0.44
1:B:2336:ARG:HG2	1:B:2435:ARG:HD2	2.00	0.44
1:B:3844:LEU:HD23	1:B:3844:LEU:HA	1.85	0.44
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	1.99	0.44
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.34	0.44
1:C:3157:ILE:HB	1:C:3202:PRO:HG3	2.00	0.44
1:C:4680:LYS:HB2	1:C:4680:LYS:HE3	1.72	0.44
1:D:590:LEU:HG	1:D:631:LEU:HD22	1.99	0.44
1:D:2336:ARG:HG2	1:D:2435:ARG:HD2	2.00	0.44
1:A:894:GLY:H	1:A:903:LEU:HD13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2336:ARG:HG2	1:A:2435:ARG:HD2	2.00	0.43
1:A:3587:ASP:OD1	1:A:3595:ARG:NH2	2.51	0.43
1:B:1792:ALA:HA	1:B:2173:GLN:HA	2.00	0.43
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.50	0.43
1:B:3995:VAL:O	1:B:3999:MET:HG2	2.17	0.43
1:B:4247:ILE:HD11	1:B:4667:PRO:HB2	2.00	0.43
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.82	0.43
1:C:3301:PRO:HA	1:C:3302:PRO:HD3	1.92	0.43
1:C:3628:ARG:HG3	1:C:3631:ALA:HB3	2.00	0.43
1:C:4580:TYR:HE2	1:C:4630:TYR:HB3	1.82	0.43
1:D:3104:GLU:HA	1:D:3107:VAL:HG22	2.00	0.43
1:D:3301:PRO:HA	1:D:3302:PRO:HD3	1.92	0.43
1:D:3760:LYS:HA	1:D:3760:LYS:HD3	1.88	0.43
1:D:4580:TYR:HE2	1:D:4630:TYR:HB3	1.82	0.43
1:D:4681:LEU:HD11	1:D:4706:LEU:HD22	2.00	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.89	0.43
1:A:223:PHE:HD1	1:A:230:CYS:HB3	1.83	0.43
1:B:873:LYS:H	1:B:873:LYS:HG2	1.48	0.43
1:B:1254:HIS:HA	1:B:1276:THR:HG22	1.99	0.43
1:B:2245:GLN:NE2	1:B:3861:GLU:OE1	2.51	0.43
1:B:3628:ARG:HG3	1:B:3631:ALA:HB3	2.00	0.43
1:C:3587:ASP:OD1	1:C:3595:ARG:NH2	2.51	0.43
1:D:400:ALA:O	1:D:404:ILE:HD12	2.17	0.43
1:D:2245:GLN:NE2	1:D:3861:GLU:OE1	2.51	0.43
1:D:3556:ASN:HB3	1:D:3559:LEU:HD13	1.98	0.43
1:D:3587:ASP:OD1	1:D:3595:ARG:NH2	2.51	0.43
1:A:1087:ARG:HA	1:A:1153:ILE:O	2.17	0.43
1:A:3936:TYR:O	1:A:3940:LYS:NZ	2.48	0.43
1:B:223:PHE:HD1	1:B:230:CYS:HB3	1.83	0.43
1:B:417:GLY:O	1:B:420:SER:OG	2.32	0.43
1:B:647:ASN:OD1	1:B:647:ASN:N	2.51	0.43
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.46	0.43
1:C:415:ILE:HA	1:C:418:LEU:HD12	2.01	0.43
1:C:419:ASP:HA	1:C:422:SER:HB3	2.00	0.43
1:C:1089:TYR:HE1	1:C:1211:LEU:HD22	1.83	0.43
1:C:1792:ALA:HA	1:C:2173:GLN:HA	2.00	0.43
1:C:2395:PRO:HG2	1:C:2397:VAL:HG12	2.00	0.43
1:C:3078:ARG:NH2	1:C:3151:GLN:O	2.51	0.43
1:C:3844:LEU:HD23	1:C:3844:LEU:HA	1.85	0.43
1:C:4188:ARG:HA	1:C:4188:ARG:HD2	1.57	0.43
1:D:495:ASN:HD21	1:D:550:LYS:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:GLY:HA3	1:D:722:TRP:HB3	2.00	0.43
1:D:2313:LEU:HG	1:D:2416:VAL:HG21	2.00	0.43
1:D:4680:LYS:HB2	1:D:4680:LYS:HE3	1.72	0.43
1:A:1254:HIS:O	1:A:1275:ARG:N	2.43	0.43
1:A:1295:VAL:O	1:A:1547:LYS:HA	2.19	0.43
1:A:2245:GLN:NE2	1:A:3861:GLU:OE1	2.51	0.43
1:A:2911:LEU:HB2	1:A:2915:GLU:HG3	2.01	0.43
1:A:3078:ARG:NH2	1:A:3151:GLN:O	2.51	0.43
1:A:3875:MET:HB2	1:A:3953:LYS:HD3	2.01	0.43
1:A:4977:THR:O	1:A:4981:GLU:HB3	2.19	0.43
1:B:419:ASP:HA	1:B:422:SER:HB3	2.00	0.43
1:B:3915:ILE:O	1:B:3919:THR:OG1	2.34	0.43
1:B:3965:LEU:HD23	1:B:3965:LEU:HA	1.90	0.43
1:C:3508:SER:HB3	1:C:3511:VAL:HG22	2.00	0.43
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.99	0.43
1:D:601:ASP:OD1	1:D:1665:HIS:ND1	2.45	0.43
1:A:3157:ILE:HB	1:A:3202:PRO:HG3	2.00	0.43
1:B:1089:TYR:HE1	1:B:1211:LEU:HD22	1.83	0.43
1:B:3769:ARG:HG3	1:B:3773:ARG:HH12	1.83	0.43
1:C:495:ASN:HD21	1:C:550:LYS:HG2	1.83	0.43
1:C:661:LYS:HA	1:C:748:LEU:O	2.19	0.43
1:C:708:GLY:HA3	1:C:722:TRP:HB3	2.00	0.43
1:C:871:ARG:HA	1:C:874:LEU:HB2	2.00	0.43
1:C:1269:CYS:HA	1:C:1564:PHE:O	2.19	0.43
1:C:3256:LEU:O	1:C:3259:SER:OG	2.30	0.43
1:C:4247:ILE:HD11	1:C:4667:PRO:HB2	2.00	0.43
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.34	0.43
1:D:4977:THR:O	1:D:4981:GLU:HB3	2.19	0.43
1:A:2411:PRO:HD2	1:A:2415:ARG:HD2	2.00	0.43
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	1.99	0.43
1:B:2314:LEU:HD12	1:B:2314:LEU:HA	1.85	0.43
1:C:1028:ASP:OD1	1:C:1028:ASP:N	2.51	0.43
1:C:1295:VAL:O	1:C:1547:LYS:HA	2.19	0.43
1:C:2245:GLN:NE2	1:C:3861:GLU:OE1	2.51	0.43
1:C:2411:PRO:HD2	1:C:2415:ARG:HD2	2.00	0.43
1:C:3390:GLY:H	1:C:3392:LEU:HD23	1.84	0.43
1:D:946:ALA:O	1:D:950:LEU:CB	2.64	0.43
1:D:1089:TYR:HE1	1:D:1211:LEU:HD22	1.83	0.43
1:D:3354:LEU:O	1:D:3358:PHE:HB2	2.19	0.43
1:D:4718:LYS:H	1:D:4718:LYS:HG2	1.43	0.43
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1743[A]:ARG:HE	1:A:1743[A]:ARG:HB2	1.46	0.43
1:A:3508:SER:HB3	1:A:3511:VAL:HG22	2.00	0.43
1:B:495:ASN:HD21	1:B:550:LYS:HG2	1.83	0.43
1:B:708:GLY:HA3	1:B:722:TRP:HB3	2.00	0.43
1:B:2004:GLU:HA	1:B:2007:ASN:HB2	1.99	0.43
1:B:2458:ARG:NH2	1:B:2510:TYR:O	2.50	0.43
1:B:3354:LEU:O	1:B:3358:PHE:HB2	2.19	0.43
1:C:403:MET:O	1:C:407:THR:OG1	2.24	0.43
1:C:2911:LEU:HB2	1:C:2915:GLU:HG3	2.01	0.43
1:D:3915:ILE:O	1:D:3919:THR:OG1	2.34	0.43
1:D:4247:ILE:HD11	1:D:4667:PRO:HB2	2.00	0.43
1:B:415:ILE:HA	1:B:418:LEU:HD12	2.01	0.43
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.19	0.43
1:B:3104:GLU:HA	1:B:3107:VAL:HG22	2.00	0.43
1:B:3390:GLY:H	1:B:3392:LEU:HD23	1.84	0.43
1:B:4801:LEU:HD23	1:B:4801:LEU:HA	1.87	0.43
1:B:4977:THR:O	1:B:4981:GLU:HB3	2.19	0.43
1:C:2359:ARG:NH1	1:D:195:PHE:O	2.50	0.43
1:C:2387:SER:HB2	1:C:2419:GLY:HA3	2.00	0.43
1:C:3875:MET:HB2	1:C:3953:LYS:HD3	2.01	0.43
1:C:4977:THR:O	1:C:4981:GLU:HB3	2.19	0.43
1:D:415:ILE:HA	1:D:418:LEU:HD12	2.00	0.43
1:D:1254:HIS:O	1:D:1275:ARG:N	2.43	0.43
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.19	0.43
1:D:3390:GLY:H	1:D:3392:LEU:HD23	1.84	0.43
1:A:871:ARG:HA	1:A:874:LEU:HB2	2.00	0.43
1:A:4247:ILE:HD11	1:A:4667:PRO:HB2	2.00	0.43
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.91	0.43
1:B:4681:LEU:HD11	1:B:4706:LEU:HD22	2.00	0.43
1:C:1727:ARG:NH2	1:C:1773:PRO:O	2.50	0.43
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	2.01	0.43
1:C:3935:TRP:O	1:D:76:ARG:HD2	2.19	0.43
1:D:2411:PRO:HD2	1:D:2415:ARG:HD2	2.00	0.43
1:D:2911:LEU:HB2	1:D:2915:GLU:HG3	2.01	0.43
1:A:840:VAL:HG22	1:A:1199:VAL:HG22	2.01	0.43
1:A:1996:ARG:NH2	1:A:1999:ARG:O	2.52	0.43
1:A:2202:GLY:HA2	1:A:2204:HIS:CE1	2.54	0.43
1:A:2521:VAL:HG12	1:A:2526:PHE:HE2	1.84	0.43
1:C:1160:ILE:O	1:C:1178:ALA:N	2.52	0.43
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.84	0.43
1:C:3445:TRP:HA	1:C:3451:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4861:LYS:H	1:C:4861:LYS:HG3	1.47	0.43
1:D:417:GLY:O	1:D:420:SER:OG	2.32	0.43
1:D:661:LYS:HA	1:D:748:LEU:O	2.19	0.43
1:D:1685:LEU:HD23	1:D:1685:LEU:HA	1.91	0.43
1:D:1792:ALA:HA	1:D:2173:GLN:HA	2.00	0.43
1:D:3157:ILE:HB	1:D:3202:PRO:HG3	2.00	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.91	0.42
1:A:1160:ILE:O	1:A:1178:ALA:N	2.52	0.42
1:A:4580:TYR:HE2	1:A:4630:TYR:HB3	1.83	0.42
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.52	0.42
1:B:3157:ILE:HB	1:B:3202:PRO:HG3	2.00	0.42
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.32	0.42
1:B:4989:MET:HE2	1:B:4989:MET:HB2	1.96	0.42
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.52	0.42
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.91	0.42
1:C:4039:MET:SD	1:C:4043:GLN:NE2	2.92	0.42
1:C:4681:LEU:HD11	1:C:4706:LEU:HD22	2.00	0.42
1:D:2521:VAL:HG12	1:D:2526:PHE:HE2	1.84	0.42
1:D:3078:ARG:NH2	1:D:3151:GLN:O	2.51	0.42
1:D:4821:LYS:H	1:D:4821:LYS:HG2	1.53	0.42
2:E:73:LYS:HZ3	2:E:75:THR:HG1	1.62	0.42
1:A:417:GLY:O	1:A:420:SER:OG	2.32	0.42
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.51	0.42
1:A:1842:LEU:O	1:A:1846:SER:OG	2.30	0.42
1:A:3104:GLU:HA	1:A:3107:VAL:HG22	2.00	0.42
1:A:3390:GLY:H	1:A:3392:LEU:HD23	1.84	0.42
1:B:1254:HIS:O	1:B:1275:ARG:N	2.43	0.42
1:B:3445:TRP:HA	1:B:3451:PHE:HD2	1.84	0.42
1:B:3935:TRP:O	1:C:76:ARG:HD2	2.19	0.42
1:B:4039:MET:SD	1:B:4043:GLN:NE2	2.92	0.42
1:B:4690:GLU:H	1:B:4690:GLU:HG2	1.54	0.42
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.52	0.42
1:D:243:ARG:NH2	1:D:303:ASP:OD1	2.51	0.42
1:D:1295:VAL:O	1:D:1547:LYS:HA	2.19	0.42
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	2.01	0.42
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.33	0.42
1:A:736:HIS:ND1	1:A:737:LEU:O	2.42	0.42
1:A:872:GLU:HG2	1:A:873:LYS:HG2	2.01	0.42
1:A:2244:ARG:NH2	1:A:3861:GLU:OE2	2.53	0.42
1:B:411:TYR:HA	1:B:414:PHE:HB3	2.02	0.42
1:B:661:LYS:HA	1:B:748:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:GLY:HA2	1:B:2204:HIS:CE1	2.54	0.42
1:B:2387:SER:HB2	1:B:2419:GLY:HA3	2.00	0.42
1:B:4049:VAL:HG21	1:B:4159:ARG:HD2	2.02	0.42
1:C:12:GLN:HG3	1:C:165:VAL:HG22	2.02	0.42
1:C:2244:ARG:NH2	1:C:3861:GLU:OE2	2.53	0.42
1:D:223:PHE:HD1	1:D:230:CYS:HB3	1.83	0.42
1:A:1792:ALA:HA	1:A:2173:GLN:HA	2.00	0.42
1:A:2004:GLU:HA	1:A:2007:ASN:HB2	1.99	0.42
1:A:3354:LEU:O	1:A:3358:PHE:HB2	2.19	0.42
1:B:216:GLY:HA2	1:B:262:LEU:HD11	2.02	0.42
1:B:2244:ARG:NH2	1:B:3861:GLU:OE2	2.53	0.42
1:B:2254:LEU:O	1:B:2258:LEU:N	2.53	0.42
1:B:2411:PRO:HD2	1:B:2415:ARG:HD2	2.00	0.42
1:B:2810:LYS:HA	1:B:2810:LYS:HD3	1.89	0.42
1:B:3137:LEU:O	1:B:3141:THR:OG1	2.30	0.42
1:D:1205:GLY:HA2	1:D:1211:LEU:HD21	2.02	0.42
1:D:2765:LYS:HD3	1:D:2765:LYS:HA	1.71	0.42
1:D:3628:ARG:HG3	1:D:3631:ALA:HB3	2.00	0.42
1:D:4681:LEU:HD23	1:D:4681:LEU:HA	1.90	0.42
1:A:130:LYS:NZ	1:D:2460:LEU:O	2.52	0.42
1:A:661:LYS:HA	1:A:748:LEU:O	2.19	0.42
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	2.02	0.42
1:A:3769:ARG:HG3	1:A:3773:ARG:HH12	1.83	0.42
1:B:840:VAL:HG22	1:B:1199:VAL:HG22	2.01	0.42
1:B:1295:VAL:O	1:B:1547:LYS:HA	2.19	0.42
1:B:4112:LEU:O	1:B:4115:SER:OG	2.34	0.42
1:B:4190:ILE:H	1:B:4190:ILE:HG12	1.48	0.42
1:B:4227:GLU:H	1:B:4227:GLU:HG3	1.53	0.42
1:C:216:GLY:HA2	1:C:262:LEU:HD11	2.02	0.42
1:C:872:GLU:HG2	1:C:873:LYS:HG2	2.01	0.42
1:C:3354:LEU:O	1:C:3358:PHE:HB2	2.19	0.42
1:C:3670:GLU:OE1	1:C:3670:GLU:N	2.53	0.42
1:C:4049:VAL:HG21	1:C:4159:ARG:HD2	2.02	0.42
1:D:411:TYR:HA	1:D:414:PHE:HB3	2.02	0.42
1:D:871:ARG:HA	1:D:874:LEU:HB2	2.00	0.42
1:D:2387:SER:HB2	1:D:2419:GLY:HA3	2.00	0.42
1:D:2472:LEU:HD23	1:D:2472:LEU:HA	1.91	0.42
1:D:4049:VAL:HG21	1:D:4159:ARG:HD2	2.02	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.19	0.42
1:A:2110:TYR:HA	1:A:3700:GLN:HE21	1.85	0.42
1:A:3628:ARG:HG3	1:A:3631:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4049:VAL:HG21	1:A:4159:ARG:HD2	2.02	0.42
1:B:12:GLN:HG3	1:B:165:VAL:HG22	2.02	0.42
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.84	0.42
1:B:1849:LEU:HD23	1:B:1849:LEU:HA	1.88	0.42
1:B:2521:VAL:HG12	1:B:2526:PHE:HE2	1.84	0.42
1:B:3875:MET:HB2	1:B:3953:LYS:HD3	2.01	0.42
1:C:1205:GLY:HA2	1:C:1211:LEU:HD21	2.02	0.42
1:D:12:GLN:HG3	1:D:165:VAL:HG22	2.02	0.42
1:D:419:ASP:HA	1:D:422:SER:HB3	2.00	0.42
1:D:575:LEU:HD11	1:D:606:LEU:HA	2.02	0.42
1:D:2202:GLY:HA2	1:D:2204:HIS:CE1	2.54	0.42
1:D:2254:LEU:O	1:D:2258:LEU:N	2.53	0.42
1:D:2546:MET:N	1:D:2546:MET:SD	2.93	0.42
1:D:3875:MET:HB2	1:D:3953:LYS:HD3	2.01	0.42
1:A:216:GLY:HA2	1:A:262:LEU:HD11	2.02	0.42
1:A:419:ASP:HA	1:A:422:SER:HB3	2.00	0.42
1:A:1439:VAL:HB	1:A:1514:LEU:HB3	2.02	0.42
1:A:2387:SER:HB2	1:A:2419:GLY:HA3	2.00	0.42
1:A:3670:GLU:OE1	1:A:3670:GLU:N	2.53	0.42
1:A:4039:MET:SD	1:A:4043:GLN:NE2	2.92	0.42
1:B:2788:HIS:HB3	1:B:2791:LEU:HB2	2.02	0.42
1:B:2911:LEU:HB2	1:B:2915:GLU:HG3	2.01	0.42
1:C:223:PHE:HD1	1:C:230:CYS:HB3	1.83	0.42
1:C:1488:LYS:HE3	1:C:1488:LYS:HB2	1.85	0.42
1:C:2677:LYS:HE2	1:C:2677:LYS:HB3	1.67	0.42
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.85	0.42
1:D:3445:TRP:HA	1:D:3451:PHE:HD2	1.84	0.42
1:D:4865:LYS:HA	1:D:4865:LYS:HD2	1.66	0.42
1:A:415:ILE:HA	1:A:418:LEU:HD12	2.01	0.42
1:B:276:TRP:NE1	1:B:346:CYS:SG	2.75	0.42
1:B:1205:GLY:HA2	1:B:1211:LEU:HD21	2.02	0.42
1:B:2628:PHE:HE1	1:B:2725:LYS:HE3	1.85	0.42
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	2.01	0.42
1:B:3670:GLU:OE1	1:B:3670:GLU:N	2.53	0.42
1:C:411:TYR:HA	1:C:414:PHE:HB3	2.02	0.42
1:C:575:LEU:HD11	1:C:606:LEU:HA	2.02	0.42
1:C:1620:ALA:HB2	1:C:1627:ALA:HB2	2.02	0.42
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.85	0.42
1:D:736:HIS:ND1	1:D:737:LEU:O	2.42	0.42
1:A:411:TYR:HA	1:A:414:PHE:HB3	2.02	0.42
1:A:1205:GLY:HA2	1:A:1211:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.84	0.42
1:B:220:LEU:HD12	1:B:390:LEU:HB3	2.02	0.42
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.36	0.42
1:B:980:ALA:HB1	1:B:1055:PRO:HB3	2.02	0.42
1:B:2110:TYR:HA	1:B:3700:GLN:HE21	1.85	0.42
1:C:317:ARG:HG2	1:C:323:LEU:HG	2.01	0.42
1:C:909:ASN:OD1	1:C:911:HIS:ND1	2.53	0.42
1:C:2202:GLY:HA2	1:C:2204:HIS:CE1	2.54	0.42
1:C:2521:VAL:HG12	1:C:2526:PHE:HE2	1.84	0.42
1:C:2546:MET:N	1:C:2546:MET:SD	2.93	0.42
1:D:220:LEU:HD12	1:D:390:LEU:HB3	2.02	0.42
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.84	0.42
1:D:2244:ARG:NH2	1:D:3861:GLU:OE2	2.53	0.42
1:D:4039:MET:SD	1:D:4043:GLN:NE2	2.92	0.42
1:A:908:VAL:HG13	1:A:963:ASN:HB3	2.02	0.42
1:A:980:ALA:HB1	1:A:1055:PRO:HB3	2.02	0.42
1:A:2546:MET:N	1:A:2546:MET:SD	2.93	0.42
1:A:4578:LEU:HD23	1:A:4578:LEU:HA	1.89	0.42
1:B:281:ARG:NH1	1:B:309:THR:OG1	2.53	0.42
1:B:872:GLU:HG2	1:B:873:LYS:HG2	2.01	0.42
1:B:4802:GLY:HA2	1:B:4808:PHE:HB2	2.02	0.42
1:C:49:LEU:HD23	1:C:49:LEU:HA	1.89	0.42
1:C:601:ASP:OD1	1:C:1665:HIS:ND1	2.45	0.42
1:C:797:HIS:CE1	1:C:821:LEU:HD23	2.55	0.42
1:C:980:ALA:HB1	1:C:1055:PRO:HB3	2.02	0.42
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.30	0.42
1:C:4802:GLY:HA2	1:C:4808:PHE:HB2	2.02	0.42
1:D:216:GLY:HA2	1:D:262:LEU:HD11	2.02	0.42
1:D:872:GLU:HG2	1:D:873:LYS:HG2	2.01	0.42
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	2.02	0.42
1:D:3253:ILE:HD11	1:D:3273:THR:HG22	2.02	0.42
1:D:5006:GLN:H	1:D:5006:GLN:HG3	1.65	0.42
1:A:367:LEU:HD22	1:A:372:LEU:HA	2.02	0.41
1:A:3163:VAL:HG22	1:A:3232:LEU:HD21	2.02	0.41
1:A:3253:ILE:HD11	1:A:3273:THR:HG22	2.02	0.41
1:B:797:HIS:CE1	1:B:821:LEU:HD23	2.55	0.41
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.53	0.41
1:C:281:ARG:NH1	1:C:309:THR:OG1	2.53	0.41
1:C:356:TRP:N	1:C:379:HIS:O	2.53	0.41
1:C:2939:ARG:H	1:C:2939:ARG:HG3	1.70	0.41
1:C:3253:ILE:HD11	1:C:3273:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3936:TYR:O	1:C:3940:LYS:NZ	2.48	0.41
1:C:3949:ARG:O	1:C:3953:LYS:HG2	2.21	0.41
1:D:1727:ARG:NH2	1:D:1773:PRO:O	2.50	0.41
1:D:3844:LEU:HD23	1:D:3844:LEU:HA	1.85	0.41
1:D:4036:VAL:HG22	1:D:5032:TYR:HD2	1.86	0.41
1:A:243:ARG:NH2	1:A:303:ASP:OD1	2.51	0.41
1:A:317:ARG:HG2	1:A:323:LEU:HG	2.01	0.41
1:A:909:ASN:OD1	1:A:911:HIS:ND1	2.53	0.41
1:A:2314:LEU:HD12	1:A:2314:LEU:HA	1.85	0.41
1:A:2628:PHE:HE1	1:A:2725:LYS:HE3	1.85	0.41
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	2.01	0.41
1:B:170:ILE:HG23	1:B:197:GLN:HE21	1.85	0.41
1:B:1000:ARG:HD3	1:B:1000:ARG:HA	1.94	0.41
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	2.02	0.41
1:C:367:LEU:HD22	1:C:372:LEU:HA	2.02	0.41
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.91	0.41
1:C:3420:ARG:NH1	1:C:3516:LYS:O	2.43	0.41
1:D:786:GLY:N	1:D:1630:CYS:O	2.48	0.41
1:D:1160:ILE:O	1:D:1178:ALA:N	2.52	0.41
1:A:12:GLN:HG3	1:A:165:VAL:HG22	2.02	0.41
1:A:2090:LYS:HD3	1:A:2090:LYS:HA	1.96	0.41
1:A:2307:LEU:HD12	1:A:2308:GLN:HB3	2.02	0.41
1:A:3445:TRP:HA	1:A:3451:PHE:HD2	1.84	0.41
1:A:4036:VAL:HG22	1:A:5032:TYR:HD2	1.85	0.41
1:A:4802:GLY:HA2	1:A:4808:PHE:HB2	2.02	0.41
1:B:1160:ILE:O	1:B:1178:ALA:N	2.52	0.41
1:B:1461:ASP:OD2	1:B:1468:LYS:NZ	2.40	0.41
1:C:2254:LEU:O	1:C:2258:LEU:N	2.53	0.41
1:C:3163:VAL:HG22	1:C:3232:LEU:HD21	2.03	0.41
1:C:4036:VAL:HG22	1:C:5032:TYR:HD2	1.86	0.41
1:C:4150:LEU:HD23	1:C:4150:LEU:HA	1.89	0.41
1:D:170:ILE:HG23	1:D:197:GLN:HE21	1.85	0.41
1:D:367:LEU:HD22	1:D:372:LEU:HA	2.02	0.41
1:D:840:VAL:HG22	1:D:1199:VAL:HG22	2.01	0.41
1:D:1439:VAL:HB	1:D:1514:LEU:HB3	2.02	0.41
1:D:1759:ARG:HE	1:D:1760:HIS:H	1.69	0.41
1:D:2307:LEU:HD12	1:D:2308:GLN:HB3	2.02	0.41
1:D:3730:ALA:O	1:D:3803:SER:OG	2.31	0.41
1:A:592:LYS:HB3	1:A:1592:PRO:HB3	2.02	0.41
1:A:728:ARG:HA	1:A:729:PRO:HD3	1.96	0.41
1:A:2004:GLU:HA	1:A:2007:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3207:GLU:HG2	1:A:3209:GLN:HE22	1.86	0.41
1:B:909:ASN:OD1	1:B:911:HIS:ND1	2.53	0.41
1:B:1439:VAL:HB	1:B:1514:LEU:HB3	2.02	0.41
1:B:2004:GLU:HA	1:B:2007:ASN:HD22	1.85	0.41
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.91	0.41
1:C:134:ASP:OD1	1:C:134:ASP:N	2.50	0.41
1:C:840:VAL:HG22	1:C:1199:VAL:HG22	2.01	0.41
1:C:1759:ARG:HE	1:C:1760:HIS:H	1.69	0.41
1:C:2314:LEU:HD12	1:C:2314:LEU:HA	1.85	0.41
1:C:2365:GLY:H	1:C:2369[B]:ARG:HH21	1.69	0.41
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.89	0.41
1:D:294:THR:N	1:D:298:GLY:O	2.49	0.41
1:D:317:ARG:HG2	1:D:323:LEU:HG	2.01	0.41
1:D:797:HIS:CE1	1:D:821:LEU:HD23	2.55	0.41
1:D:2810:LYS:HA	1:D:2810:LYS:HD3	1.89	0.41
1:D:4690:GLU:H	1:D:4690:GLU:HG2	1.54	0.41
1:A:437:PRO:HB2	1:A:440:ALA:HB3	2.02	0.41
1:A:2365:GLY:H	1:A:2369[B]:ARG:HH21	1.69	0.41
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.85	0.41
1:A:2788:HIS:HB3	1:A:2791:LEU:HB2	2.02	0.41
1:A:3130:THR:HA	1:A:3133:THR:HG22	2.02	0.41
1:A:4172:GLU:HA	1:A:4175:ARG:HD3	2.03	0.41
1:A:4892:ARG:NH2	1:B:4899:ASP:OD1	2.54	0.41
1:B:592:LYS:HB3	1:B:1592:PRO:HB3	2.03	0.41
1:B:601:ASP:OD1	1:B:1665:HIS:ND1	2.45	0.41
1:B:622:THR:HG21	1:B:1681:VAL:HG22	2.03	0.41
1:B:908:VAL:HG13	1:B:963:ASN:HB3	2.02	0.41
1:B:3163:VAL:HG22	1:B:3232:LEU:HD21	2.03	0.41
1:B:3207:GLU:HG2	1:B:3209:GLN:HE22	1.86	0.41
1:C:592:LYS:HB3	1:C:1592:PRO:HB3	2.03	0.41
1:C:1254:HIS:O	1:C:1275:ARG:N	2.43	0.41
1:C:3878:ASP:OD1	1:C:3878:ASP:N	2.53	0.41
1:D:592:LYS:HB3	1:D:1592:PRO:HB3	2.03	0.41
1:D:909:ASN:OD1	1:D:911:HIS:ND1	2.53	0.41
1:D:1620:ALA:HB2	1:D:1627:ALA:HB2	2.02	0.41
1:D:3163:VAL:HG22	1:D:3232:LEU:HD21	2.03	0.41
1:D:3945:GLU:OE1	1:D:3949:ARG:NH1	2.54	0.41
1:A:356:TRP:N	1:A:379:HIS:O	2.53	0.41
1:A:622:THR:HG21	1:A:1681:VAL:HG22	2.03	0.41
1:A:3949:ARG:O	1:A:3953:LYS:HG2	2.20	0.41
1:A:4548:ARG:HE	1:A:4548:ARG:HB3	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4573:ILE:HG22	1:A:4577:LEU:HD22	2.03	0.41
1:B:317:ARG:HG2	1:B:323:LEU:HG	2.01	0.41
1:B:1854:PHE:HB3	1:B:1858:ASP:HB2	2.03	0.41
1:B:2546:MET:N	1:B:2546:MET:SD	2.93	0.41
1:C:207:SER:H	1:C:334:MET:HE1	1.86	0.41
1:C:622:THR:HG21	1:C:1681:VAL:HG22	2.03	0.41
1:C:2788:HIS:HB3	1:C:2791:LEU:HB2	2.02	0.41
1:C:4172:GLU:HA	1:C:4175:ARG:HD3	2.03	0.41
1:D:1616:GLU:HB2	1:D:1629:GLN:HB3	2.03	0.41
1:D:1854:PHE:HB3	1:D:1858:ASP:HB2	2.03	0.41
1:D:1996:ARG:NH2	1:D:1999:ARG:O	2.52	0.41
1:D:3949:ARG:O	1:D:3953:LYS:HG2	2.20	0.41
1:A:575:LEU:HD11	1:A:606:LEU:HA	2.02	0.41
1:A:2254:LEU:O	1:A:2258:LEU:N	2.53	0.41
1:A:4639:MET:HE3	1:A:4639:MET:HB3	1.93	0.41
1:A:4891:VAL:HG12	1:B:4921:PHE:HE2	1.85	0.41
1:B:865:PRO:HA	1:B:868:GLU:HG2	2.03	0.41
1:B:1784:ALA:HA	2:F:55:VAL:HA	2.03	0.41
1:B:2365:GLY:H	1:B:2369[B]:ARG:HH21	1.69	0.41
1:B:2816:MET:HG3	1:B:2878:LEU:HD22	2.03	0.41
1:B:3253:ILE:HD11	1:B:3273:THR:HG22	2.02	0.41
1:B:4172:GLU:HA	1:B:4175:ARG:HD3	2.03	0.41
1:B:4548:ARG:HE	1:B:4548:ARG:HB3	1.53	0.41
1:C:111:HIS:ND1	1:C:114:SER:OG	2.35	0.41
1:C:170:ILE:HG23	1:C:197:GLN:HE21	1.85	0.41
1:C:3112:LEU:HG	1:C:3180:ASN:HD21	1.86	0.41
1:C:3130:THR:HA	1:C:3133:THR:HG22	2.02	0.41
1:C:3537:LYS:HE2	1:C:3604:TYR:HB2	2.02	0.41
1:C:4639:MET:HE3	1:C:4639:MET:HB3	1.91	0.41
1:D:748:LEU:HD13	1:D:755:ILE:HG12	2.03	0.41
1:D:980:ALA:HB1	1:D:1055:PRO:HB3	2.02	0.41
1:D:2365:GLY:H	1:D:2369[B]:ARG:HH21	1.69	0.41
1:D:3416:VAL:HG23	1:D:3423:TRP:HZ3	1.86	0.41
1:D:3878:ASP:OD1	1:D:3878:ASP:N	2.53	0.41
1:D:4957:LYS:HB2	1:D:4957:LYS:HE2	1.82	0.41
2:F:38:SER:O	2:F:42:ARG:NH2	2.54	0.41
1:A:1759:ARG:HE	1:A:1760:HIS:H	1.69	0.41
1:A:2410:PRO:HA	1:A:2411:PRO:HD3	1.99	0.41
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.53	0.41
1:A:3420:ARG:NH1	1:A:3516:LYS:O	2.43	0.41
1:A:3652:MET:HE3	1:A:3652:MET:HB3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:LEU:HD11	1:B:606:LEU:HA	2.02	0.41
1:B:1620:ALA:HB2	1:B:1627:ALA:HB2	2.02	0.41
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.85	0.41
1:B:4639:MET:HE3	1:B:4639:MET:HB3	1.94	0.41
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.74	0.41
1:C:1784:ALA:HA	2:G:55:VAL:HA	2.03	0.41
1:C:2004:GLU:HA	1:C:2007:ASN:HD22	1.85	0.41
1:C:2816:MET:HG3	1:C:2878:LEU:HD22	2.03	0.41
1:D:437:PRO:HB2	1:D:440:ALA:HB3	2.02	0.41
1:D:622:THR:HG21	1:D:1681:VAL:HG22	2.03	0.41
1:D:2628:PHE:HE1	1:D:2725:LYS:HE3	1.85	0.41
1:D:3537:LYS:HE2	1:D:3604:TYR:HB2	2.02	0.41
1:D:4848:VAL:O	1:D:4852:THR:OG1	2.34	0.41
1:A:43:GLY:N	1:A:447:ASP:OD2	2.54	0.41
1:A:195:PHE:HA	1:D:2359:ARG:HH22	1.85	0.41
1:A:220:LEU:HD12	1:A:390:LEU:HB3	2.02	0.41
1:A:601:ASP:OD1	1:A:1665:HIS:ND1	2.45	0.41
1:A:1000:ARG:HA	1:A:1000:ARG:HD3	1.94	0.41
1:A:1153:ILE:H	1:A:1223:PHE:HE2	1.69	0.41
1:A:1620:ALA:HB2	1:A:1627:ALA:HB2	2.01	0.41
1:A:2203:MET:SD	1:A:2203:MET:N	2.92	0.41
1:A:2608:MET:HE2	1:A:2643:LEU:HD13	2.03	0.41
1:A:2816:MET:HG3	1:A:2878:LEU:HD22	2.03	0.41
1:A:3416:VAL:HG23	1:A:3423:TRP:HZ3	1.86	0.41
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.54	0.41
1:A:4718:LYS:H	1:A:4718:LYS:HG2	1.43	0.41
1:A:4725:LEU:HD12	1:A:4725:LEU:HA	1.95	0.41
1:A:4865:LYS:HD2	1:A:4865:LYS:HA	1.66	0.41
1:A:5006:GLN:H	1:A:5006:GLN:HG3	1.65	0.41
1:B:1442:GLY:H	1:B:1509:ILE:HG23	1.86	0.41
1:B:2585:THR:HG22	1:B:2588:ARG:HH22	1.86	0.41
1:B:2779:GLU:HG3	1:B:2792:ARG:HG2	2.03	0.41
1:B:3112:LEU:HG	1:B:3180:ASN:HD21	1.86	0.41
1:B:3949:ARG:O	1:B:3953:LYS:HG2	2.21	0.41
1:B:4036:VAL:HG22	1:B:5032:TYR:HD2	1.86	0.41
1:B:5006:GLN:H	1:B:5006:GLN:HG3	1.65	0.41
1:C:437:PRO:HB2	1:C:440:ALA:HB3	2.02	0.41
1:C:748:LEU:HD13	1:C:755:ILE:HG12	2.03	0.41
1:C:908:VAL:HG13	1:C:963:ASN:HB3	2.02	0.41
1:C:1442:GLY:H	1:C:1509:ILE:HG23	1.86	0.41
1:C:1616:GLU:HB2	1:C:1629:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	2.02	0.41
1:C:1854:PHE:HB3	1:C:1858:ASP:HB2	2.03	0.41
1:C:2287:ALA:O	1:C:2349:ASN:ND2	2.48	0.41
1:C:2307:LEU:HD12	1:C:2308:GLN:HB3	2.02	0.41
1:C:2585:THR:HG22	1:C:2588:ARG:HH22	1.86	0.41
1:C:3207:GLU:HG2	1:C:3209:GLN:HE22	1.86	0.41
1:C:3357:HIS:O	1:C:3361:THR:OG1	2.31	0.41
1:C:4573:ILE:HG22	1:C:4577:LEU:HD22	2.03	0.41
1:C:4989:MET:HE2	1:C:4989:MET:HB2	1.96	0.41
1:D:281:ARG:NH1	1:D:309:THR:OG1	2.53	0.41
1:D:356:TRP:N	1:D:379:HIS:O	2.53	0.41
1:D:873:LYS:HE3	1:D:873:LYS:HB3	1.85	0.41
1:D:952:LYS:HA	1:D:971:ASP:HB3	2.03	0.41
1:D:2090:LYS:HD3	1:D:2090:LYS:HA	1.96	0.41
1:D:2110:TYR:HA	1:D:3700:GLN:HE21	1.85	0.41
1:D:2816:MET:HG3	1:D:2878:LEU:HD22	2.03	0.41
1:D:2905:LEU:HD23	1:D:2905:LEU:HA	1.95	0.41
1:D:3936:TYR:O	1:D:3940:LYS:NZ	2.48	0.41
1:D:3965:LEU:HD23	1:D:3965:LEU:HA	1.90	0.41
1:D:4172:GLU:HA	1:D:4175:ARG:HD3	2.03	0.41
1:D:4802:GLY:HA2	1:D:4808:PHE:HB2	2.02	0.41
1:A:170:ILE:HG23	1:A:197:GLN:HE21	1.85	0.41
1:A:2094:LEU:O	1:A:2098:VAL:HG12	2.22	0.41
1:A:3537:LYS:HE2	1:A:3604:TYR:HB2	2.02	0.41
1:B:356:TRP:N	1:B:379:HIS:O	2.53	0.41
1:B:367:LEU:HD22	1:B:372:LEU:HA	2.02	0.41
1:B:437:PRO:HB2	1:B:440:ALA:HB3	2.02	0.41
1:B:3562:LYS:HA	1:B:3562:LYS:HD3	1.87	0.41
1:B:3945:GLU:OE1	1:B:3949:ARG:NH1	2.54	0.41
1:C:243:ARG:NH2	1:C:303:ASP:OD1	2.51	0.41
1:C:865:PRO:HA	1:C:868:GLU:HG2	2.03	0.41
1:C:897:ARG:HD2	1:C:897:ARG:HA	1.96	0.41
1:C:1439:VAL:HB	1:C:1514:LEU:HB3	2.02	0.41
1:C:2779:GLU:HG3	1:C:2792:ARG:HG2	2.03	0.41
1:C:5006:GLN:H	1:C:5006:GLN:HG3	1.65	0.41
1:D:2247:GLN:HG3	1:D:2279:SER:HA	2.03	0.41
1:D:4190:ILE:H	1:D:4190:ILE:HG12	1.48	0.41
1:A:2716:ASP:N	1:A:2716:ASP:OD1	2.46	0.40
1:A:3037:GLU:HG2	1:A:3080:VAL:HG13	2.03	0.40
1:B:1153:ILE:H	1:B:1223:PHE:HE2	1.69	0.40
1:B:1759:ARG:HE	1:B:1760:HIS:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3416:VAL:HG23	1:B:3423:TRP:HZ3	1.86	0.40
1:C:220:LEU:HD12	1:C:390:LEU:HB3	2.02	0.40
1:C:1634:LEU:HD23	1:C:1634:LEU:HA	1.87	0.40
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.54	0.40
1:D:43:GLY:N	1:D:447:ASP:OD2	2.54	0.40
1:D:144:GLU:HG3	1:D:175:SER:HB3	2.03	0.40
1:D:2094:LEU:O	1:D:2098:VAL:HG12	2.22	0.40
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.53	0.40
1:D:2608:MET:HE2	1:D:2643:LEU:HD13	2.03	0.40
1:D:3112:LEU:HG	1:D:3180:ASN:HD21	1.86	0.40
1:D:3670:GLU:OE1	1:D:3670:GLU:N	2.53	0.40
1:D:3940:LYS:O	1:D:4002:LYS:NZ	2.50	0.40
1:A:2585:THR:HG22	1:A:2588:ARG:HH22	1.86	0.40
1:A:4112:LEU:O	1:A:4115:SER:OG	2.34	0.40
1:A:4681:LEU:HD23	1:A:4681:LEU:HA	1.90	0.40
1:B:2307:LEU:HD12	1:B:2308:GLN:HB3	2.02	0.40
1:B:3256:LEU:O	1:B:3259:SER:OG	2.30	0.40
1:B:4869:GLU:H	1:B:4869:GLU:HG2	1.59	0.40
1:C:43:GLY:N	1:C:447:ASP:OD2	2.54	0.40
1:C:952:LYS:HA	1:C:971:ASP:HB3	2.03	0.40
1:C:1000:ARG:HD3	1:C:1000:ARG:HA	1.94	0.40
1:C:2094:LEU:O	1:C:2098:VAL:HG12	2.22	0.40
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.39	0.40
1:D:2996:LYS:HA	1:D:2996:LYS:HD3	1.91	0.40
1:D:3207:GLU:HG2	1:D:3209:GLN:HE22	1.86	0.40
1:D:4976:GLU:O	1:D:4980:LEU:HB2	2.22	0.40
1:A:125:ARG:H	1:A:125:ARG:HD3	1.86	0.40
1:A:1442:GLY:H	1:A:1509:ILE:HG23	1.86	0.40
1:A:1616:GLU:HB2	1:A:1629:GLN:HB3	2.03	0.40
1:A:4190:ILE:H	1:A:4190:ILE:HG12	1.48	0.40
1:A:4976:GLU:O	1:A:4980:LEU:HB2	2.21	0.40
1:B:897:ARG:HD2	1:B:897:ARG:HA	1.96	0.40
1:B:1685:LEU:HD23	1:B:1685:LEU:HA	1.91	0.40
1:B:2244:ARG:O	1:B:2248:ARG:N	2.46	0.40
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.54	0.40
1:B:3936:TYR:O	1:B:3940:LYS:NZ	2.48	0.40
1:C:1741:GLU:O	1:C:1745:ILE:HG13	2.22	0.40
1:C:2247:GLN:HG3	1:C:2279:SER:HA	2.03	0.40
1:C:2410:PRO:HA	1:C:2411:PRO:HD3	1.99	0.40
1:C:2628:PHE:HE1	1:C:2725:LYS:HE3	1.85	0.40
1:D:2788:HIS:HB3	1:D:2791:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3780:LEU:HD22	1:D:3820:LEU:HD21	2.03	0.40
1:D:4818:MET:H	1:D:4818:MET:HG2	1.67	0.40
1:A:151:HIS:HB2	1:A:170:ILE:HB	2.03	0.40
1:A:224:HIS:HB2	1:A:229:GLU:HB2	2.04	0.40
1:A:797:HIS:CE1	1:A:821:LEU:HD23	2.55	0.40
1:A:1249:PRO:HA	1:A:1250:PRO:HD3	2.00	0.40
1:A:1685:LEU:HD23	1:A:1685:LEU:HA	1.91	0.40
1:A:1741:GLU:O	1:A:1745:ILE:HG13	2.22	0.40
1:A:1854:PHE:HB3	1:A:1858:ASP:HB2	2.03	0.40
1:A:4818:MET:H	1:A:4818:MET:HG2	1.67	0.40
1:B:243:ARG:NH2	1:B:303:ASP:OD1	2.51	0.40
1:B:1634:LEU:HD23	1:B:1634:LEU:HA	1.87	0.40
1:B:1741:GLU:O	1:B:1745:ILE:HG13	2.22	0.40
1:B:2157:GLU:O	1:B:2161:GLN:HG2	2.21	0.40
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.55	0.40
1:B:3878:ASP:OD1	1:B:3878:ASP:N	2.53	0.40
1:B:3924:LEU:HD12	1:B:3924:LEU:HA	1.94	0.40
1:C:151:HIS:ND1	1:C:159:GLU:OE2	2.55	0.40
1:C:633:LEU:HD12	1:C:1639:LEU:HG	2.03	0.40
1:C:889:GLN:O	1:C:892:THR:OG1	2.25	0.40
1:C:1784:ALA:O	2:G:82:TYR:OH	2.33	0.40
1:C:2157:GLU:O	1:C:2161:GLN:HG2	2.21	0.40
1:C:2867:LEU:HB2	1:C:2928:LYS:HZ3	1.85	0.40
1:C:4567:LEU:HD12	1:C:4567:LEU:HA	1.94	0.40
1:C:4878:ASP:OD1	1:C:4879:MET:N	2.55	0.40
1:D:728:ARG:HA	1:D:729:PRO:HD3	1.96	0.40
1:D:2004:GLU:HA	1:D:2007:ASN:HD22	1.85	0.40
1:D:3037:GLU:HG2	1:D:3080:VAL:HG13	2.03	0.40
1:D:3130:THR:HA	1:D:3133:THR:HG22	2.02	0.40
1:D:4573:ILE:HG22	1:D:4577:LEU:HD22	2.03	0.40
1:D:4578:LEU:HD23	1:D:4578:LEU:HA	1.89	0.40
1:A:151:HIS:ND1	1:A:159:GLU:OE2	2.55	0.40
1:A:281:ARG:NH1	1:A:309:THR:OG1	2.53	0.40
1:A:889:GLN:O	1:A:892:THR:OG1	2.25	0.40
1:A:2443:ILE:HD13	1:A:2443:ILE:HA	1.94	0.40
1:A:3112:LEU:HG	1:A:3180:ASN:HD21	1.86	0.40
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.32	0.40
1:C:2163:ARG:HA	1:C:2166:LEU:HD13	2.04	0.40
1:C:3945:GLU:OE1	1:C:3949:ARG:NH1	2.54	0.40
1:D:908:VAL:HG13	1:D:963:ASN:HB3	2.02	0.40
1:D:2585:THR:HG22	1:D:2588:ARG:HH22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4582:VAL:HA	1:D:4629:TYR:O	2.22	0.40
2:G:38:SER:O	2:G:42:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4353/5037 (86%)	4217 (97%)	131 (3%)	5 (0%)	48	81
1	B	4353/5037 (86%)	4216 (97%)	132 (3%)	5 (0%)	48	81
1	C	4353/5037 (86%)	4216 (97%)	132 (3%)	5 (0%)	48	81
1	D	4353/5037 (86%)	4217 (97%)	131 (3%)	5 (0%)	48	81
2	E	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	F	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	G	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	H	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
All	All	17832/21548 (83%)	17266 (97%)	546 (3%)	20 (0%)	50	81

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3616	LYS
1	B	3616	LYS
1	C	3616	LYS
1	D	3616	LYS
1	A	4694	ASP
1	B	4694	ASP
1	C	4694	ASP
1	D	4694	ASP

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Mol	Chain	Res	Type
1	A	4691	GLN
1	B	4691	GLN
1	C	4691	GLN
1	D	4691	GLN
1	A	4712	PRO
1	B	4712	PRO
1	C	4712	PRO
1	D	4712	PRO
1	A	3612	PRO
1	B	3612	PRO
1	C	3612	PRO
1	D	3612	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
1	B	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
1	C	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
1	D	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15572/18320 (85%)	14972 (96%)	600 (4%)	30	51

All (600) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ARG
1	A	373	LYS
1	A	830	ARG

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Mol	Chain	Res	Type
1	A	873	LYS
1	A	1068	ARG
1	A	1128	ARG
1	A	1534	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	1752	ARG
1	A	1758	ARG
1	A	1993	ARG
1	A	2203	MET
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2584[A]	HIS
1	A	2584[B]	HIS
1	A	2612[A]	ARG
1	A	2612[B]	ARG
1	A	2786	LYS
1	A	2827	ARG
1	A	2914	LYS
1	A	3023	LYS
1	A	3034	LYS
1	A	3053	ARG
1	A	3225	ARG
1	A	3515	LYS
1	A	3570	ARG
1	A	3614	LYS
1	A	3622	LYS
1	A	3731	LYS
1	A	4178	LEU
1	A	4184	MET
1	A	4187	SER
1	A	4188	ARG
1	A	4189	ARG
1	A	4190	ILE
1	A	4193	ILE
1	A	4196	GLU
1	A	4198	SER
1	A	4199	GLU
1	A	4200	THR
1	A	4202	ARG
1	A	4204	GLN
1	A	4206	GLU

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Mol	Chain	Res	Type
1	A	4207	MET
1	A	4211	LYS
1	A	4212	GLU
1	A	4213	SER
1	A	4224	GLU
1	A	4227	GLU
1	A	4245	MET
1	A	4246	GLN
1	A	4252	SER
1	A	4544	LEU
1	A	4545	GLU
1	A	4548	ARG
1	A	4550	LYS
1	A	4552	LEU
1	A	4556	SER
1	A	4561	THR
1	A	4577	LEU
1	A	4580	TYR
1	A	4583	SER
1	A	4584	ASP
1	A	4585	SER
1	A	4627	MET
1	A	4628	VAL
1	A	4632	LEU
1	A	4634	GLU
1	A	4635	SER
1	A	4636	THR
1	A	4639	MET
1	A	4651	THR
1	A	4653	VAL
1	A	4655	PHE
1	A	4658	ILE
1	A	4673	ARG
1	A	4676	GLU
1	A	4680	LYS
1	A	4684	ASP
1	A	4689	THR
1	A	4690	GLU
1	A	4691	GLN
1	A	4692	PRO
1	A	4694	ASP
1	A	4696	ASP

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Mol	Chain	Res	Type
1	A	4698	LYS
1	A	4716	TRP
1	A	4718	LYS
1	A	4722	ARG
1	A	4727	LYS
1	A	4728	HIS
1	A	4730	ASP
1	A	4731	ILE
1	A	4735	GLU
1	A	4736	ARG
1	A	4737	ILE
1	A	4739	GLU
1	A	4743	MET
1	A	4773	VAL
1	A	4774	LYS
1	A	4777	ILE
1	A	4779	LYS
1	A	4788	SER
1	A	4796	MET
1	A	4804	TYR
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR
1	A	4824	ARG
1	A	4825	THR
1	A	4826	ILE
1	A	4835	LYS
1	A	4836	GLN
1	A	4844	LEU
1	A	4861	LYS
1	A	4863	TYR
1	A	4865	LYS
1	A	4867	GLU
1	A	4868	ASP
1	A	4869	GLU
1	A	4870	ASP
1	A	4871	GLU
1	A	4889	VAL
1	A	4899	ASP
1	A	4903	ASP
1	A	4911	LEU
1	A	4913	ARG

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Mol	Chain	Res	Type
1	A	4920	PHE
1	A	4933	GLN
1	A	4951	LYS
1	A	4952	GLU
1	A	4954	MET
1	A	4955	GLU
1	A	4957	LYS
1	A	4971	THR
1	A	4980	LEU
1	A	4989	MET
1	A	4997	ASN
1	A	5006	GLN
1	A	5008	SER
1	A	5012	LYS
1	A	5015	GLN
1	A	5018	CYS
1	A	5027	CYS
1	A	5029	ARG
1	A	5034	ASP
1	A	5035	GLN
1	A	5037	SER
1	B	125	ARG
1	B	373	LYS
1	B	830	ARG
1	B	873	LYS
1	B	1068	ARG
1	B	1128	ARG
1	B	1534	LYS
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG
1	B	1758	ARG
1	B	1993	ARG
1	B	2203	MET
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2584[A]	HIS
1	B	2584[B]	HIS
1	B	2612[A]	ARG
1	B	2612[B]	ARG
1	B	2786	LYS
1	B	2827	ARG

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Mol	Chain	Res	Type
1	B	2914	LYS
1	B	3023	LYS
1	B	3034	LYS
1	B	3053	ARG
1	B	3225	ARG
1	B	3515	LYS
1	B	3570	ARG
1	B	3614	LYS
1	B	3622	LYS
1	B	3731	LYS
1	B	4178	LEU
1	B	4184	MET
1	B	4187	SER
1	B	4188	ARG
1	B	4189	ARG
1	B	4190	ILE
1	B	4193	ILE
1	B	4196	GLU
1	B	4198	SER
1	B	4199	GLU
1	B	4200	THR
1	B	4202	ARG
1	B	4204	GLN
1	B	4206	GLU
1	B	4207	MET
1	B	4211	LYS
1	B	4212	GLU
1	B	4213	SER
1	B	4224	GLU
1	B	4227	GLU
1	B	4245	MET
1	B	4246	GLN
1	B	4252	SER
1	B	4544	LEU
1	B	4545	GLU
1	B	4548	ARG
1	B	4550	LYS
1	B	4552	LEU
1	B	4556	SER
1	B	4561	THR
1	B	4577	LEU
1	B	4580	TYR

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Mol	Chain	Res	Type
1	B	4583	SER
1	B	4584	ASP
1	B	4585	SER
1	B	4627	MET
1	B	4628	VAL
1	B	4632	LEU
1	B	4634	GLU
1	B	4635	SER
1	B	4636	THR
1	B	4639	MET
1	B	4651	THR
1	B	4653	VAL
1	B	4655	PHE
1	B	4658	ILE
1	B	4673	ARG
1	B	4676	GLU
1	B	4680	LYS
1	B	4684	ASP
1	B	4689	THR
1	B	4690	GLU
1	B	4691	GLN
1	B	4692	PRO
1	B	4694	ASP
1	B	4696	ASP
1	B	4698	LYS
1	B	4716	TRP
1	B	4718	LYS
1	B	4722	ARG
1	B	4727	LYS
1	B	4728	HIS
1	B	4730	ASP
1	B	4731	ILE
1	B	4735	GLU
1	B	4736	ARG
1	B	4737	ILE
1	B	4739	GLU
1	B	4743	MET
1	B	4773	VAL
1	B	4774	LYS
1	B	4777	ILE
1	B	4779	LYS
1	B	4788	SER

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Mol	Chain	Res	Type
1	B	4796	MET
1	B	4804	TYR
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4824	ARG
1	B	4825	THR
1	B	4826	ILE
1	B	4835	LYS
1	B	4836	GLN
1	B	4844	LEU
1	B	4861	LYS
1	B	4863	TYR
1	B	4865	LYS
1	B	4867	GLU
1	B	4868	ASP
1	B	4869	GLU
1	B	4870	ASP
1	B	4871	GLU
1	B	4889	VAL
1	B	4899	ASP
1	B	4903	ASP
1	B	4911	LEU
1	B	4913	ARG
1	B	4920	PHE
1	B	4933	GLN
1	B	4951	LYS
1	B	4952	GLU
1	B	4954	MET
1	B	4955	GLU
1	B	4957	LYS
1	B	4971	THR
1	B	4980	LEU
1	B	4989	MET
1	B	4997	ASN
1	B	5006	GLN
1	B	5008	SER
1	B	5012	LYS
1	B	5015	GLN
1	B	5018	CYS
1	B	5027	CYS
1	B	5029	ARG

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Mol	Chain	Res	Type
1	B	5034	ASP
1	B	5035	GLN
1	B	5037	SER
1	C	125	ARG
1	C	373	LYS
1	C	830	ARG
1	C	873	LYS
1	C	1068	ARG
1	C	1128	ARG
1	C	1534	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	1752	ARG
1	C	1758	ARG
1	C	1993	ARG
1	C	2203	MET
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2584[A]	HIS
1	C	2584[B]	HIS
1	C	2612[A]	ARG
1	C	2612[B]	ARG
1	C	2786	LYS
1	C	2827	ARG
1	C	2914	LYS
1	C	3023	LYS
1	C	3034	LYS
1	C	3053	ARG
1	C	3225	ARG
1	C	3515	LYS
1	C	3570	ARG
1	C	3614	LYS
1	C	3622	LYS
1	C	3731	LYS
1	C	4178	LEU
1	C	4184	MET
1	C	4187	SER
1	C	4188	ARG
1	C	4189	ARG
1	C	4190	ILE
1	C	4193	ILE
1	C	4196	GLU

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Mol	Chain	Res	Type
1	C	4198	SER
1	C	4199	GLU
1	C	4200	THR
1	C	4202	ARG
1	C	4204	GLN
1	C	4206	GLU
1	C	4207	MET
1	C	4211	LYS
1	C	4212	GLU
1	C	4213	SER
1	C	4224	GLU
1	C	4227	GLU
1	C	4245	MET
1	C	4246	GLN
1	C	4252	SER
1	C	4544	LEU
1	C	4545	GLU
1	C	4548	ARG
1	C	4550	LYS
1	C	4552	LEU
1	C	4556	SER
1	C	4561	THR
1	C	4577	LEU
1	C	4580	TYR
1	C	4583	SER
1	C	4584	ASP
1	C	4585	SER
1	C	4627	MET
1	C	4628	VAL
1	C	4632	LEU
1	C	4634	GLU
1	C	4635	SER
1	C	4636	THR
1	C	4639	MET
1	C	4651	THR
1	C	4653	VAL
1	C	4655	PHE
1	C	4658	ILE
1	C	4673	ARG
1	C	4676	GLU
1	C	4680	LYS
1	C	4684	ASP

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Mol	Chain	Res	Type
1	C	4689	THR
1	C	4690	GLU
1	C	4691	GLN
1	C	4692	PRO
1	C	4694	ASP
1	C	4696	ASP
1	C	4698	LYS
1	C	4716	TRP
1	C	4718	LYS
1	C	4722	ARG
1	C	4727	LYS
1	C	4728	HIS
1	C	4730	ASP
1	C	4731	ILE
1	C	4735	GLU
1	C	4736	ARG
1	C	4737	ILE
1	C	4739	GLU
1	C	4743	MET
1	C	4773	VAL
1	C	4774	LYS
1	C	4777	ILE
1	C	4779	LYS
1	C	4788	SER
1	C	4796	MET
1	C	4804	TYR
1	C	4818	MET
1	C	4821	LYS
1	C	4822	THR
1	C	4824	ARG
1	C	4825	THR
1	C	4826	ILE
1	C	4835	LYS
1	C	4836	GLN
1	C	4844	LEU
1	C	4861	LYS
1	C	4863	TYR
1	C	4865	LYS
1	C	4867	GLU
1	C	4868	ASP
1	C	4869	GLU
1	C	4870	ASP

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Mol	Chain	Res	Type
1	C	4871	GLU
1	C	4889	VAL
1	C	4899	ASP
1	C	4903	ASP
1	C	4911	LEU
1	C	4913	ARG
1	C	4920	PHE
1	C	4933	GLN
1	C	4951	LYS
1	C	4952	GLU
1	C	4954	MET
1	C	4955	GLU
1	C	4957	LYS
1	C	4971	THR
1	C	4980	LEU
1	C	4989	MET
1	C	4997	ASN
1	C	5006	GLN
1	C	5008	SER
1	C	5012	LYS
1	C	5015	GLN
1	C	5018	CYS
1	C	5027	CYS
1	C	5029	ARG
1	C	5034	ASP
1	C	5035	GLN
1	C	5037	SER
1	D	125	ARG
1	D	373	LYS
1	D	830	ARG
1	D	873	LYS
1	D	1068	ARG
1	D	1128	ARG
1	D	1534	LYS
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	1752	ARG
1	D	1758	ARG
1	D	1993	ARG
1	D	2203	MET
1	D	2369[A]	ARG
1	D	2369[B]	ARG

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Mol	Chain	Res	Type
1	D	2584[A]	HIS
1	D	2584[B]	HIS
1	D	2612[A]	ARG
1	D	2612[B]	ARG
1	D	2786	LYS
1	D	2827	ARG
1	D	2914	LYS
1	D	3023	LYS
1	D	3034	LYS
1	D	3053	ARG
1	D	3225	ARG
1	D	3515	LYS
1	D	3570	ARG
1	D	3614	LYS
1	D	3622	LYS
1	D	3731	LYS
1	D	4178	LEU
1	D	4184	MET
1	D	4187	SER
1	D	4188	ARG
1	D	4189	ARG
1	D	4190	ILE
1	D	4193	ILE
1	D	4196	GLU
1	D	4198	SER
1	D	4199	GLU
1	D	4200	THR
1	D	4202	ARG
1	D	4204	GLN
1	D	4206	GLU
1	D	4207	MET
1	D	4211	LYS
1	D	4212	GLU
1	D	4213	SER
1	D	4224	GLU
1	D	4227	GLU
1	D	4245	MET
1	D	4246	GLN
1	D	4252	SER
1	D	4544	LEU
1	D	4545	GLU
1	D	4548	ARG

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Mol	Chain	Res	Type
1	D	4550	LYS
1	D	4552	LEU
1	D	4556	SER
1	D	4561	THR
1	D	4577	LEU
1	D	4580	TYR
1	D	4583	SER
1	D	4584	ASP
1	D	4585	SER
1	D	4627	MET
1	D	4628	VAL
1	D	4632	LEU
1	D	4634	GLU
1	D	4635	SER
1	D	4636	THR
1	D	4639	MET
1	D	4651	THR
1	D	4653	VAL
1	D	4655	PHE
1	D	4658	ILE
1	D	4673	ARG
1	D	4676	GLU
1	D	4680	LYS
1	D	4684	ASP
1	D	4689	THR
1	D	4690	GLU
1	D	4691	GLN
1	D	4692	PRO
1	D	4694	ASP
1	D	4696	ASP
1	D	4698	LYS
1	D	4716	TRP
1	D	4718	LYS
1	D	4722	ARG
1	D	4727	LYS
1	D	4728	HIS
1	D	4730	ASP
1	D	4731	ILE
1	D	4735	GLU
1	D	4736	ARG
1	D	4737	ILE
1	D	4739	GLU

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Mol	Chain	Res	Type
1	D	4743	MET
1	D	4773	VAL
1	D	4774	LYS
1	D	4777	ILE
1	D	4779	LYS
1	D	4788	SER
1	D	4796	MET
1	D	4804	TYR
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4824	ARG
1	D	4825	THR
1	D	4826	ILE
1	D	4835	LYS
1	D	4836	GLN
1	D	4844	LEU
1	D	4861	LYS
1	D	4863	TYR
1	D	4865	LYS
1	D	4867	GLU
1	D	4868	ASP
1	D	4869	GLU
1	D	4870	ASP
1	D	4871	GLU
1	D	4889	VAL
1	D	4899	ASP
1	D	4903	ASP
1	D	4911	LEU
1	D	4913	ARG
1	D	4920	PHE
1	D	4933	GLN
1	D	4951	LYS
1	D	4952	GLU
1	D	4954	MET
1	D	4955	GLU
1	D	4957	LYS
1	D	4971	THR
1	D	4980	LEU
1	D	4989	MET
1	D	4997	ASN
1	D	5006	GLN

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Mol	Chain	Res	Type
1	D	5008	SER
1	D	5012	LYS
1	D	5015	GLN
1	D	5018	CYS
1	D	5027	CYS
1	D	5029	ARG
1	D	5034	ASP
1	D	5035	GLN
1	D	5037	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	197	GLN
1	A	201	ASN
1	A	479	GLN
1	A	533	ASN
1	A	581	ASN
1	A	1052	ASN
1	A	1563	GLN
1	A	2003	GLN
1	A	2007	ASN
1	A	2283	ASN
1	A	2551	ASN
1	A	2620	GLN
1	A	3180	ASN
1	A	3214	ASN
1	A	3851	ASN
1	A	4109	GLN
1	A	4691	GLN
1	A	4836	GLN
1	A	5031	GLN
1	A	5035	GLN
1	B	54	ASN
1	B	197	GLN
1	B	201	ASN
1	B	479	GLN
1	B	533	ASN
1	B	1052	ASN
1	B	1563	GLN
1	B	2003	GLN

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Mol	Chain	Res	Type
1	B	2007	ASN
1	B	2283	ASN
1	B	2551	ASN
1	B	2620	GLN
1	B	3180	ASN
1	B	3214	ASN
1	B	3851	ASN
1	B	4109	GLN
1	B	4691	GLN
1	B	4836	GLN
1	B	5031	GLN
1	B	5035	GLN
1	C	54	ASN
1	C	197	GLN
1	C	201	ASN
1	C	479	GLN
1	C	533	ASN
1	C	1052	ASN
1	C	1563	GLN
1	C	2003	GLN
1	C	2007	ASN
1	C	2283	ASN
1	C	2551	ASN
1	C	2620	GLN
1	C	3180	ASN
1	C	3214	ASN
1	C	3851	ASN
1	C	4109	GLN
1	C	4691	GLN
1	C	4836	GLN
1	C	5031	GLN
1	C	5035	GLN
1	D	54	ASN
1	D	197	GLN
1	D	201	ASN
1	D	479	GLN
1	D	533	ASN
1	D	581	ASN
1	D	1052	ASN
1	D	1563	GLN
1	D	2003	GLN
1	D	2007	ASN

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Mol	Chain	Res	Type
1	D	2283	ASN
1	D	2551	ASN
1	D	2620	GLN
1	D	3180	ASN
1	D	3214	ASN
1	D	3851	ASN
1	D	4109	GLN
1	D	4691	GLN
1	D	4836	GLN
1	D	5031	GLN
1	D	5035	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	AGS	B	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (16%)
3	AGS	C	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	A	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (16%)
3	AGS	D	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (16%)

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
3	AGS	B	5101	-	-	6/17/38/38	0/3/3/3
3	AGS	C	5101	-	-	6/17/38/38	0/3/3/3
3	AGS	A	5101	-	-	6/17/38/38	0/3/3/3
3	AGS	D	5101	-	-	6/17/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	AGS	PG-S1G	2.09	1.95	1.90
3	B	5101	AGS	PG-S1G	2.09	1.95	1.90
3	C	5101	AGS	PG-S1G	2.09	1.95	1.90
3	D	5101	AGS	PG-S1G	2.09	1.95	1.90

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	A	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	B	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	C	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	C	5101	AGS	O5'-C5'-C4'	3.12	119.63	108.99
3	A	5101	AGS	O5'-C5'-C4'	3.12	119.63	108.99
3	D	5101	AGS	O5'-C5'-C4'	3.12	119.63	108.99
3	B	5101	AGS	O5'-C5'-C4'	3.12	119.62	108.99
3	B	5101	AGS	C1'-N9-C4	2.55	131.12	126.64
3	C	5101	AGS	C1'-N9-C4	2.55	131.12	126.64
3	D	5101	AGS	C1'-N9-C4	2.55	131.12	126.64
3	A	5101	AGS	C1'-N9-C4	2.55	131.12	126.64
3	B	5101	AGS	C5-C6-N6	2.25	123.74	120.31
3	C	5101	AGS	C5-C6-N6	2.25	123.74	120.31
3	D	5101	AGS	C5-C6-N6	2.25	123.74	120.31
3	A	5101	AGS	C5-C6-N6	2.25	123.74	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5101	AGS	O4'-C1'-N9	2.01	111.41	108.75
3	C	5101	AGS	O4'-C1'-N9	2.01	111.41	108.75
3	B	5101	AGS	O4'-C1'-N9	2.01	111.41	108.75
3	D	5101	AGS	O4'-C1'-N9	2.01	111.41	108.75

There are no chirality outliers.

All (24) torsion outliers are listed below:

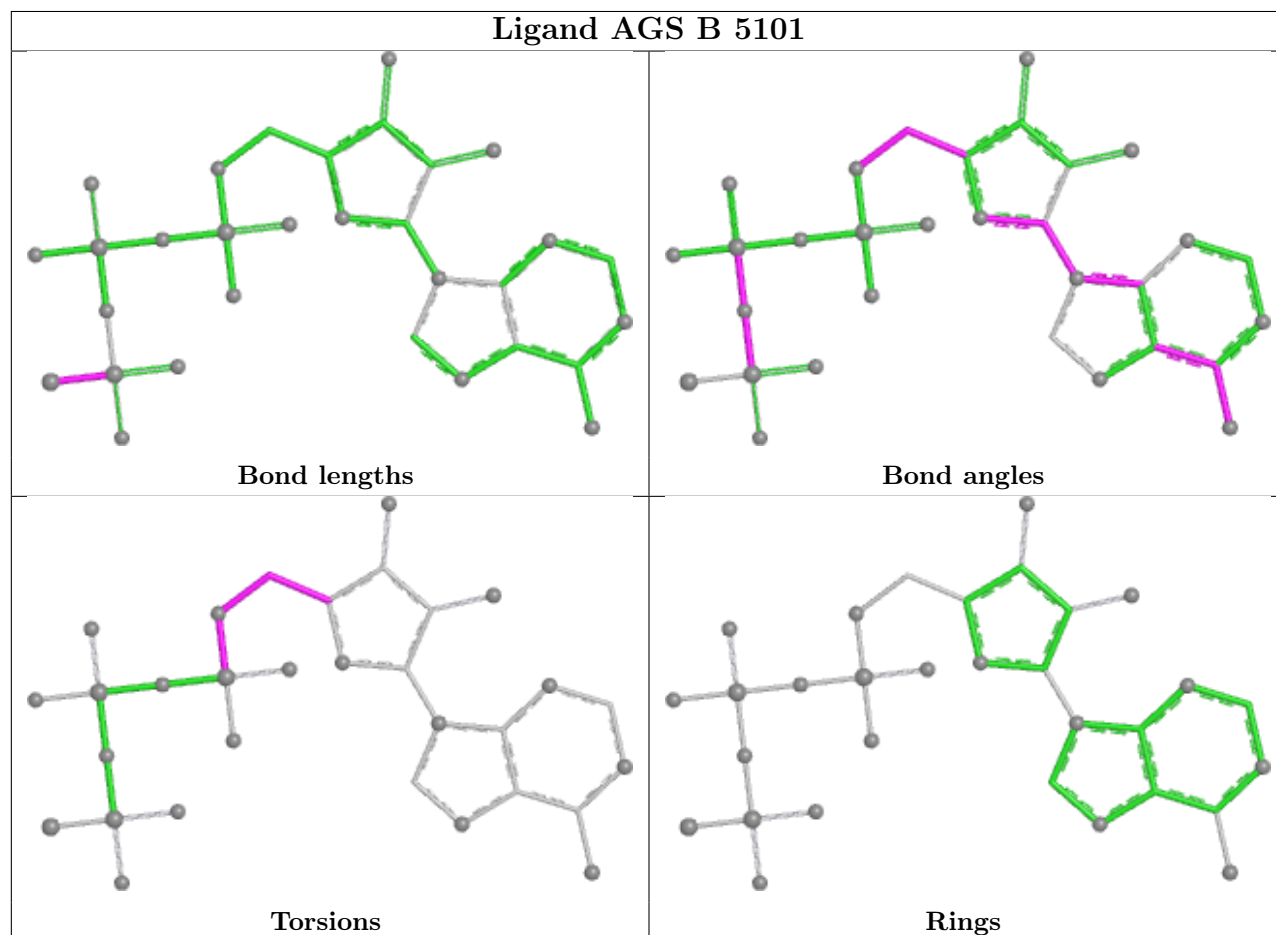
Mol	Chain	Res	Type	Atoms
3	A	5101	AGS	C5'-O5'-PA-O3A
3	A	5101	AGS	C4'-C5'-O5'-PA
3	A	5101	AGS	O4'-C4'-C5'-O5'
3	B	5101	AGS	C5'-O5'-PA-O3A
3	B	5101	AGS	C4'-C5'-O5'-PA
3	B	5101	AGS	O4'-C4'-C5'-O5'
3	C	5101	AGS	C5'-O5'-PA-O3A
3	C	5101	AGS	C4'-C5'-O5'-PA
3	C	5101	AGS	O4'-C4'-C5'-O5'
3	D	5101	AGS	C5'-O5'-PA-O3A
3	D	5101	AGS	C4'-C5'-O5'-PA
3	D	5101	AGS	O4'-C4'-C5'-O5'
3	A	5101	AGS	C3'-C4'-C5'-O5'
3	B	5101	AGS	C3'-C4'-C5'-O5'
3	C	5101	AGS	C3'-C4'-C5'-O5'
3	D	5101	AGS	C3'-C4'-C5'-O5'
3	A	5101	AGS	C5'-O5'-PA-O1A
3	A	5101	AGS	C5'-O5'-PA-O2A
3	B	5101	AGS	C5'-O5'-PA-O1A
3	B	5101	AGS	C5'-O5'-PA-O2A
3	C	5101	AGS	C5'-O5'-PA-O1A
3	C	5101	AGS	C5'-O5'-PA-O2A
3	D	5101	AGS	C5'-O5'-PA-O1A
3	D	5101	AGS	C5'-O5'-PA-O2A

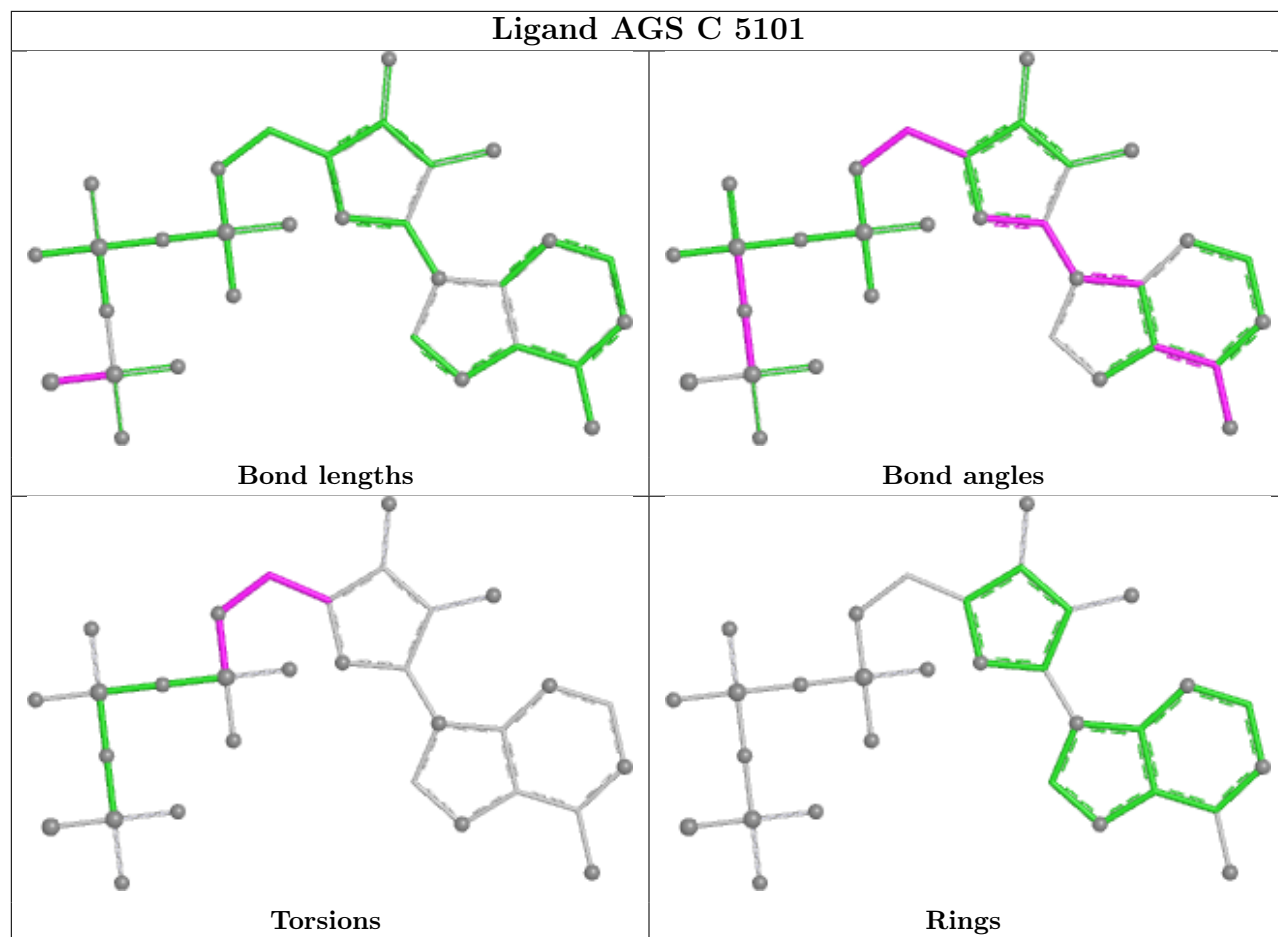
There are no ring outliers.

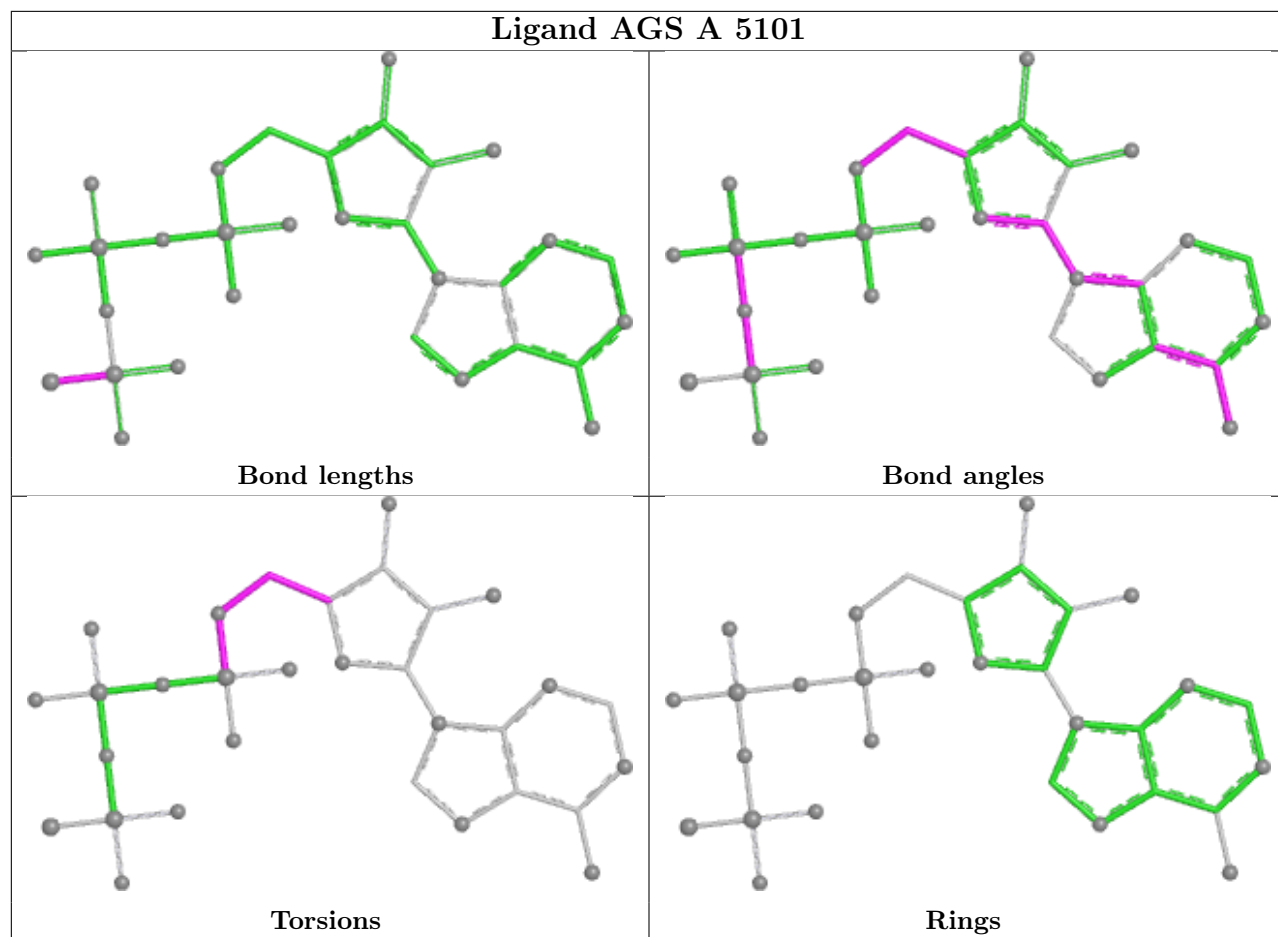
No monomer is involved in short contacts.

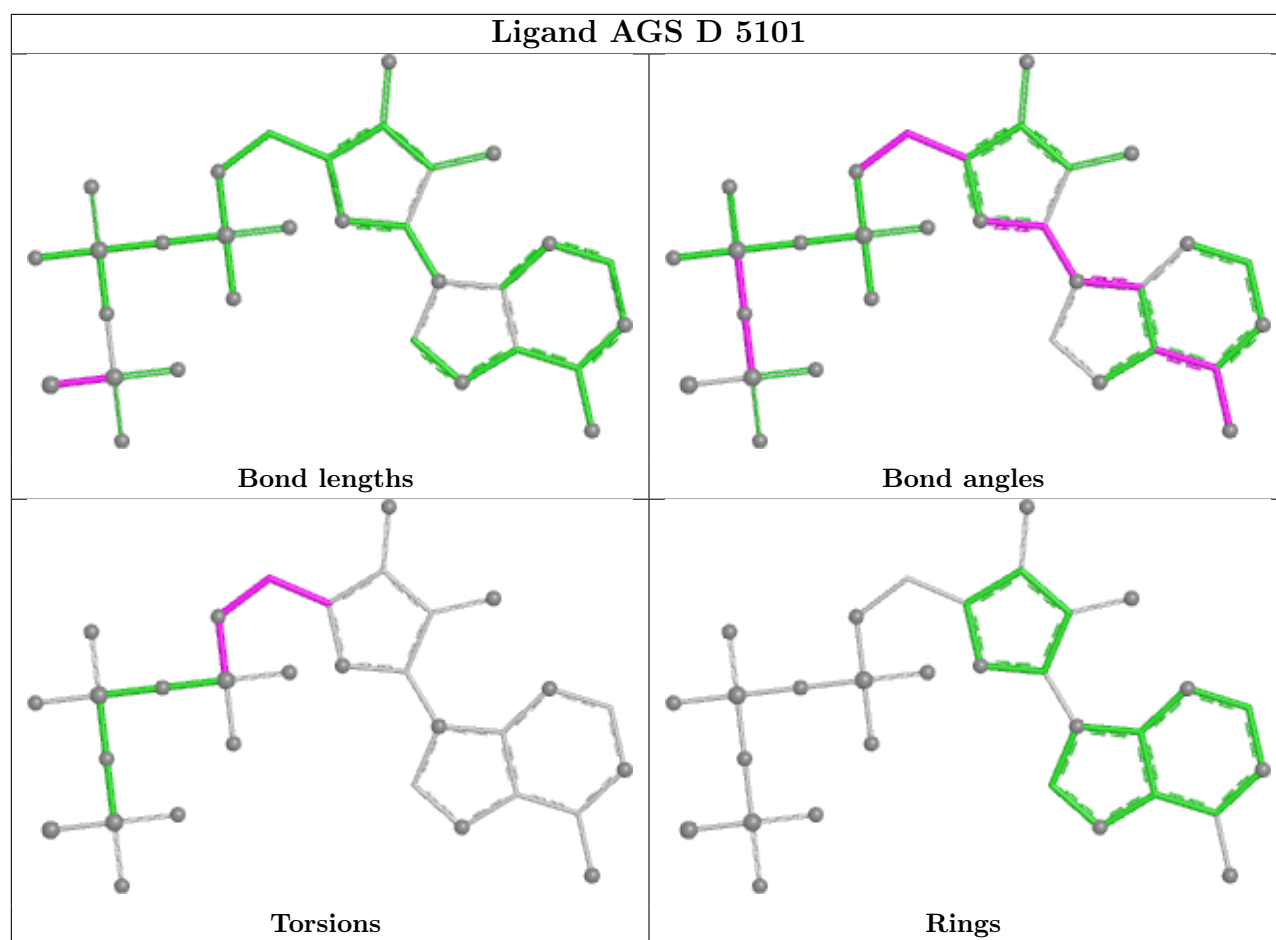
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.









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.

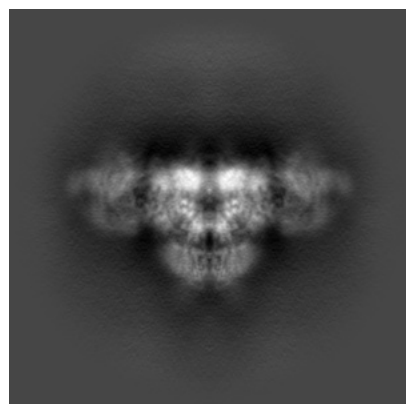
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40423. These allow visual inspection of the internal detail of the map and identification of artifacts.

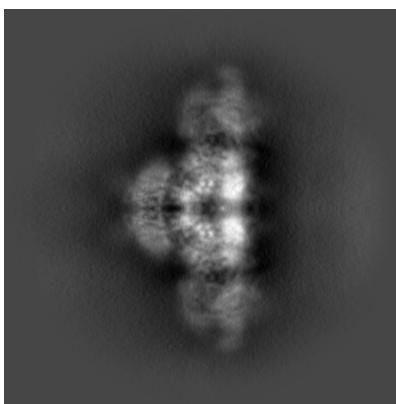
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

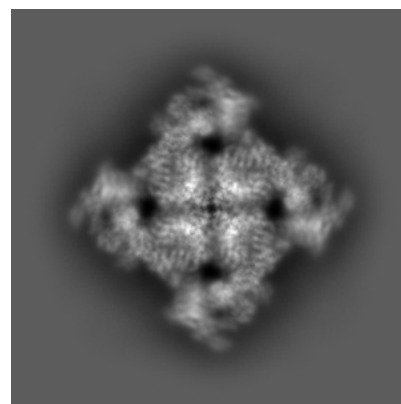
6.1.1 Primary map



X

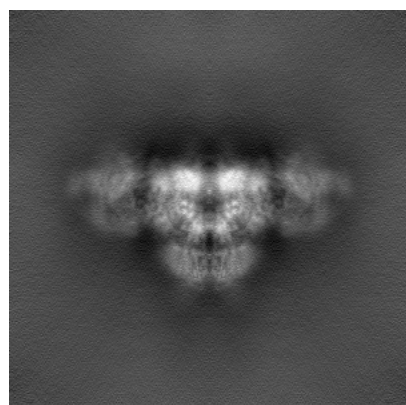


Y

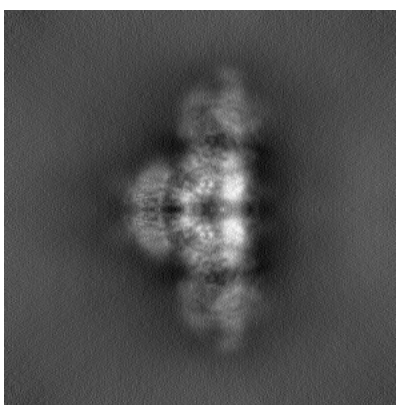


Z

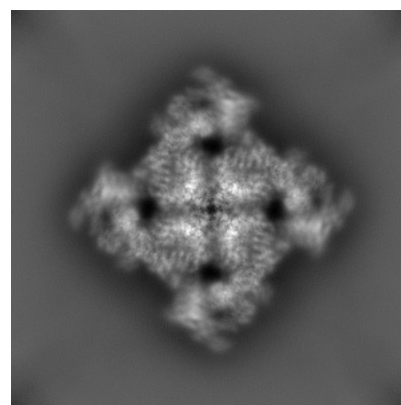
6.1.2 Raw map



X



Y

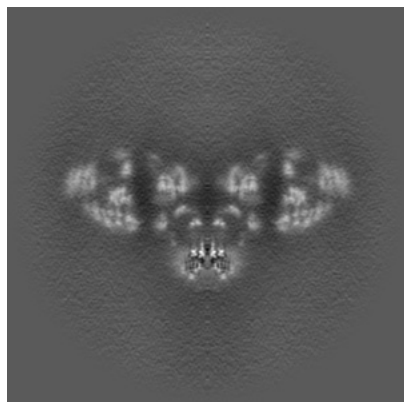


Z

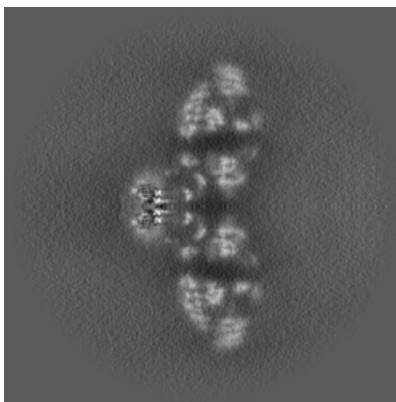
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

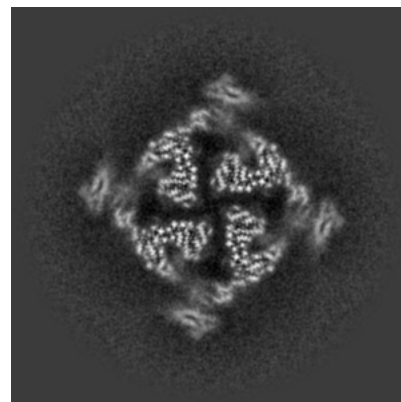
6.2.1 Primary map



X Index: 200

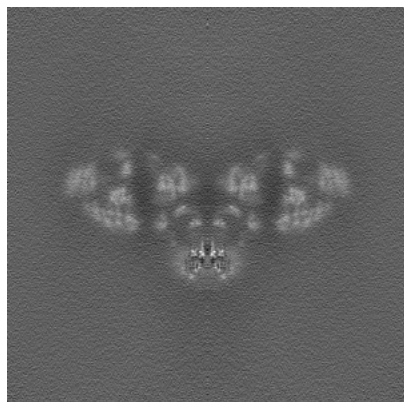


Y Index: 200

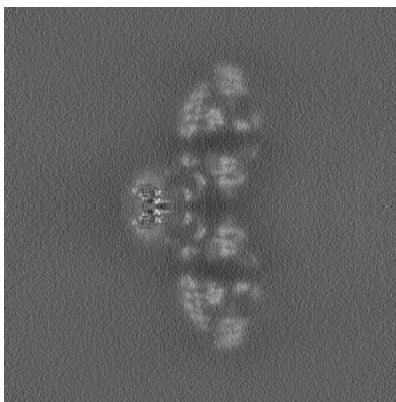


Z Index: 200

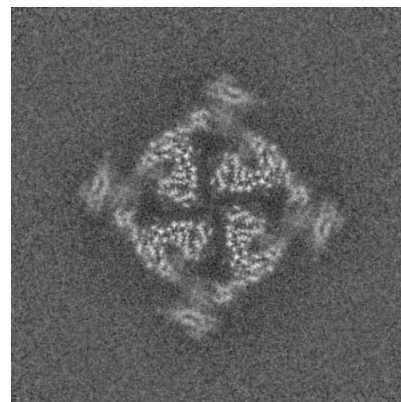
6.2.2 Raw map



X Index: 200



Y Index: 200

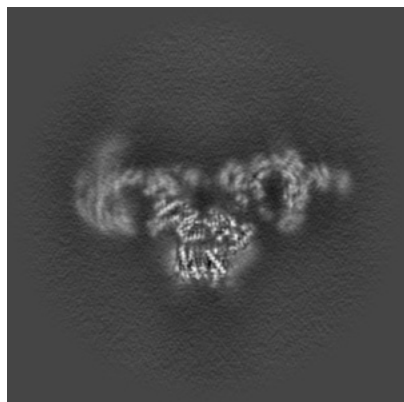


Z Index: 200

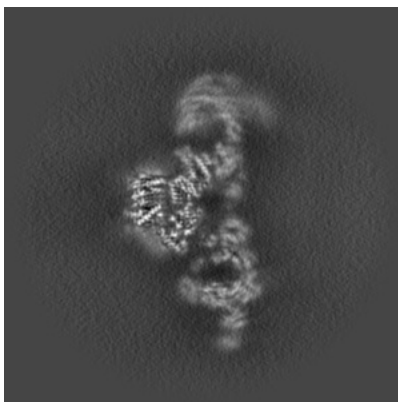
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

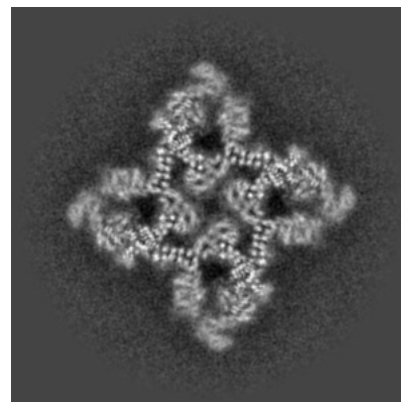
6.3.1 Primary map



X Index: 186

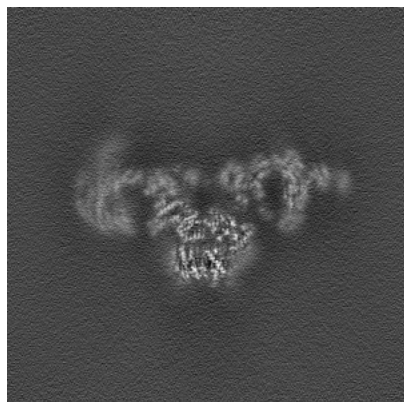


Y Index: 186

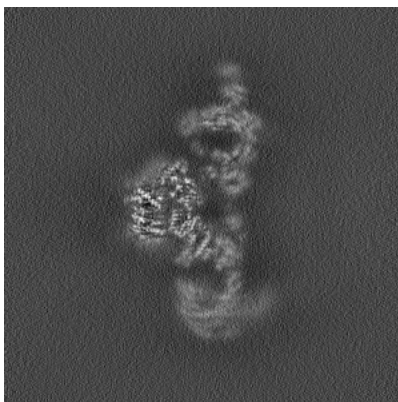


Z Index: 225

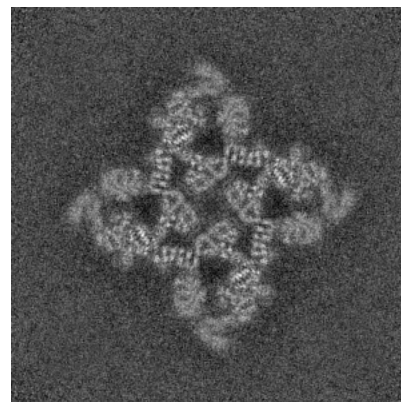
6.3.2 Raw map



X Index: 186



Y Index: 214

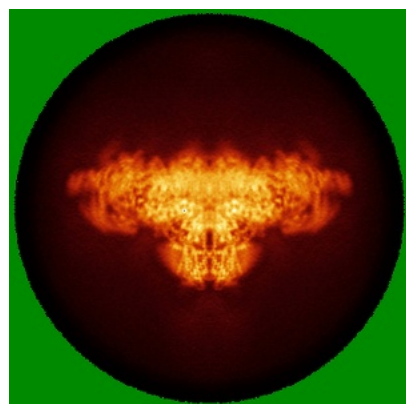


Z Index: 223

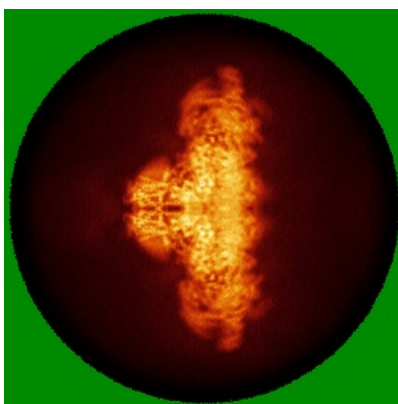
The images above show the largest variance slices of the map in three orthogonal directions.

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

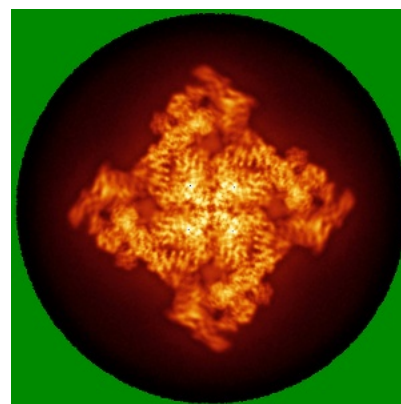
6.4.1 Primary map



X

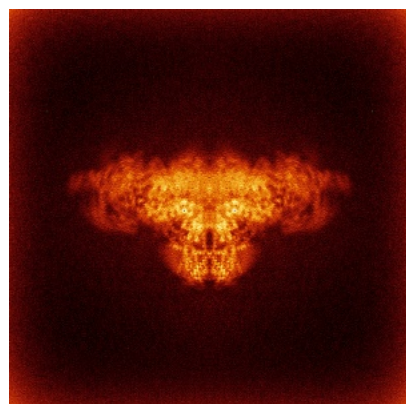


Y

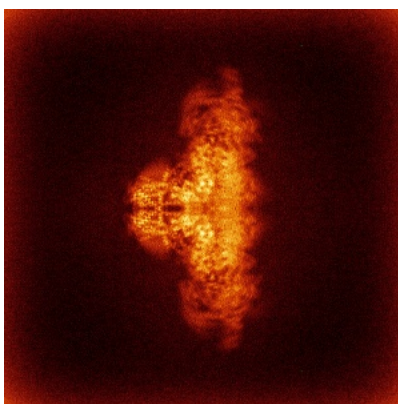


Z

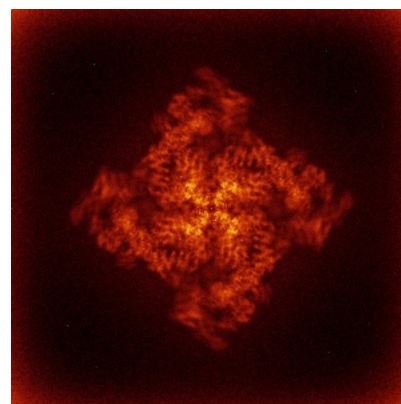
6.4.2 Raw map



X



Y

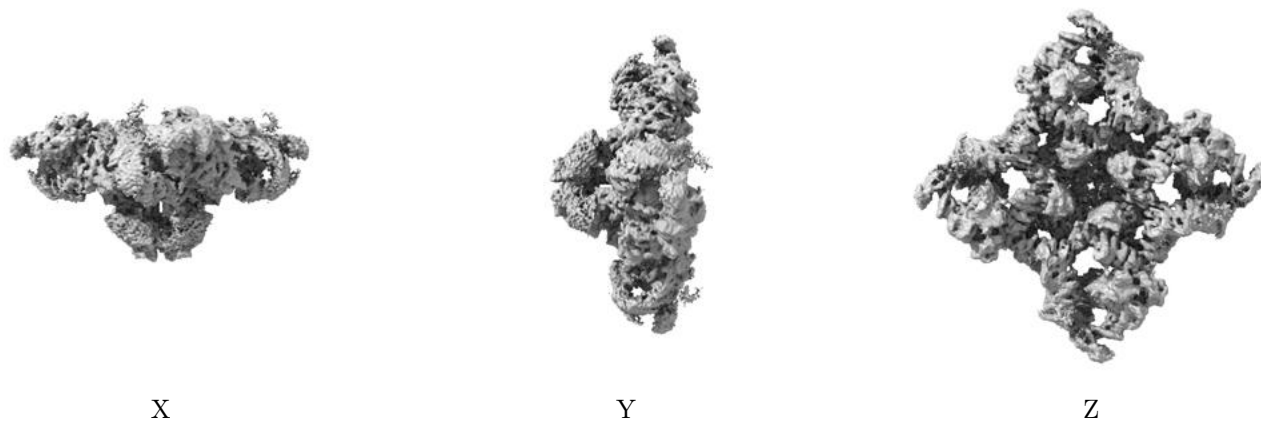


Z

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

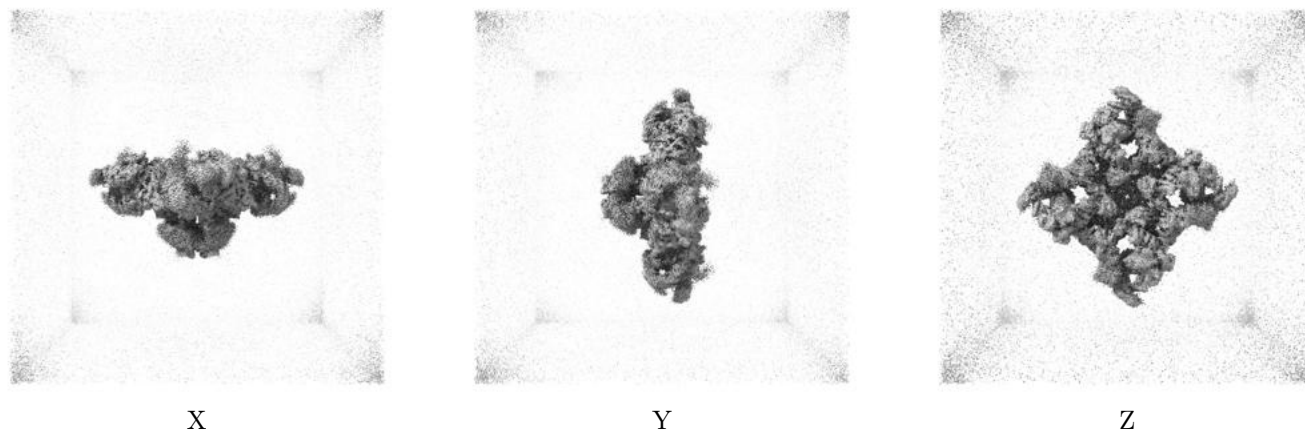
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.287. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

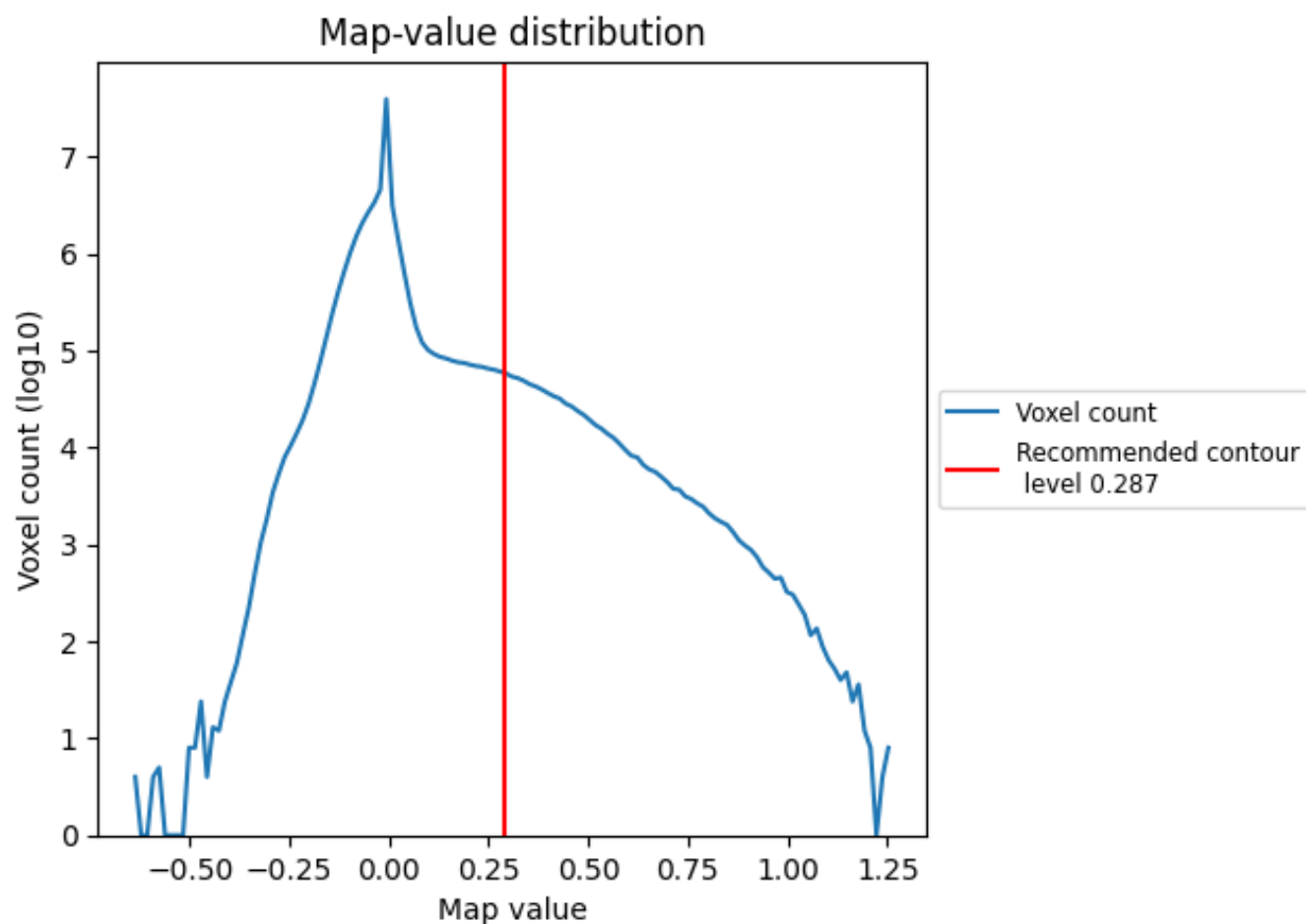
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

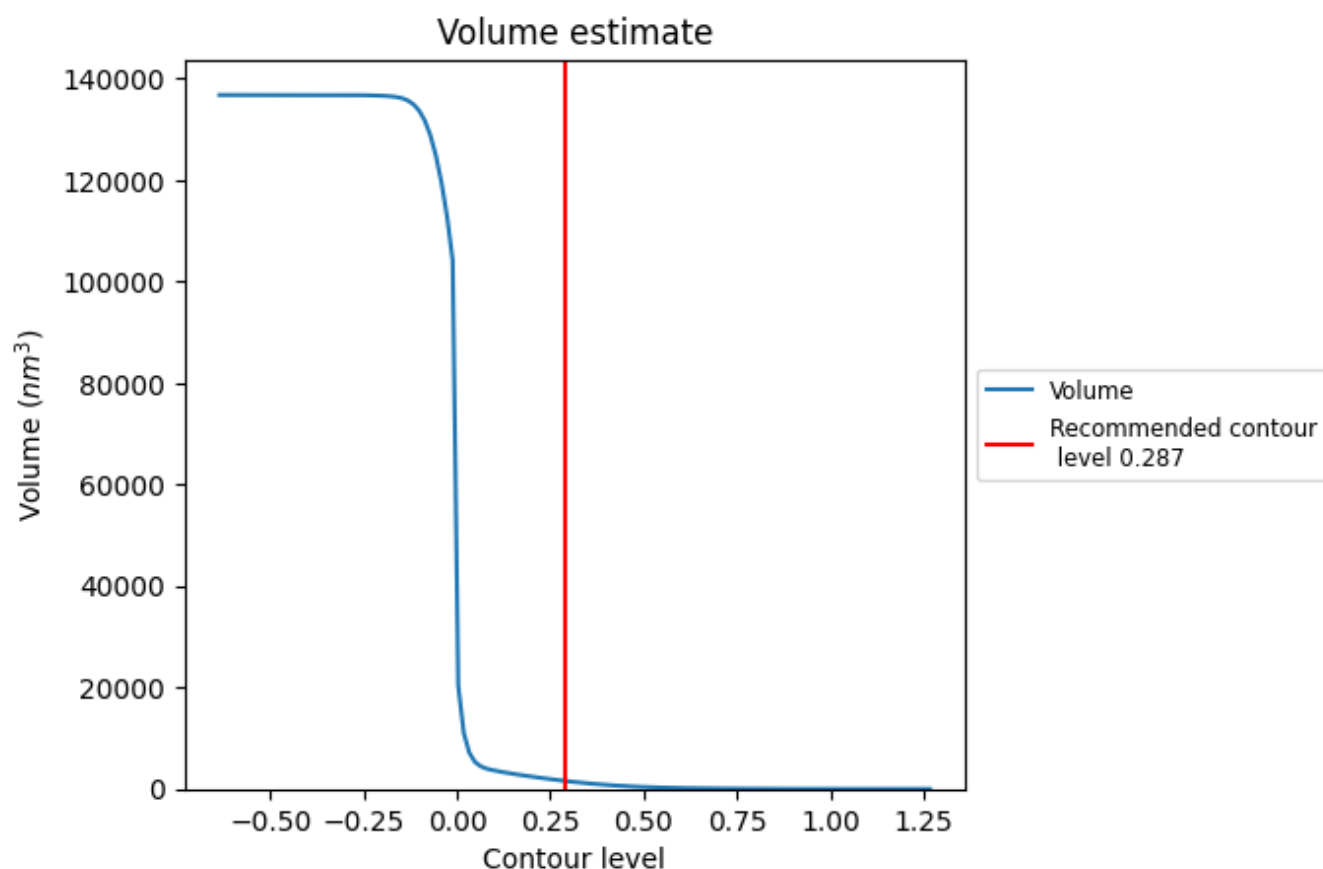
This section contains the results of statistical analysis of the map.

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.

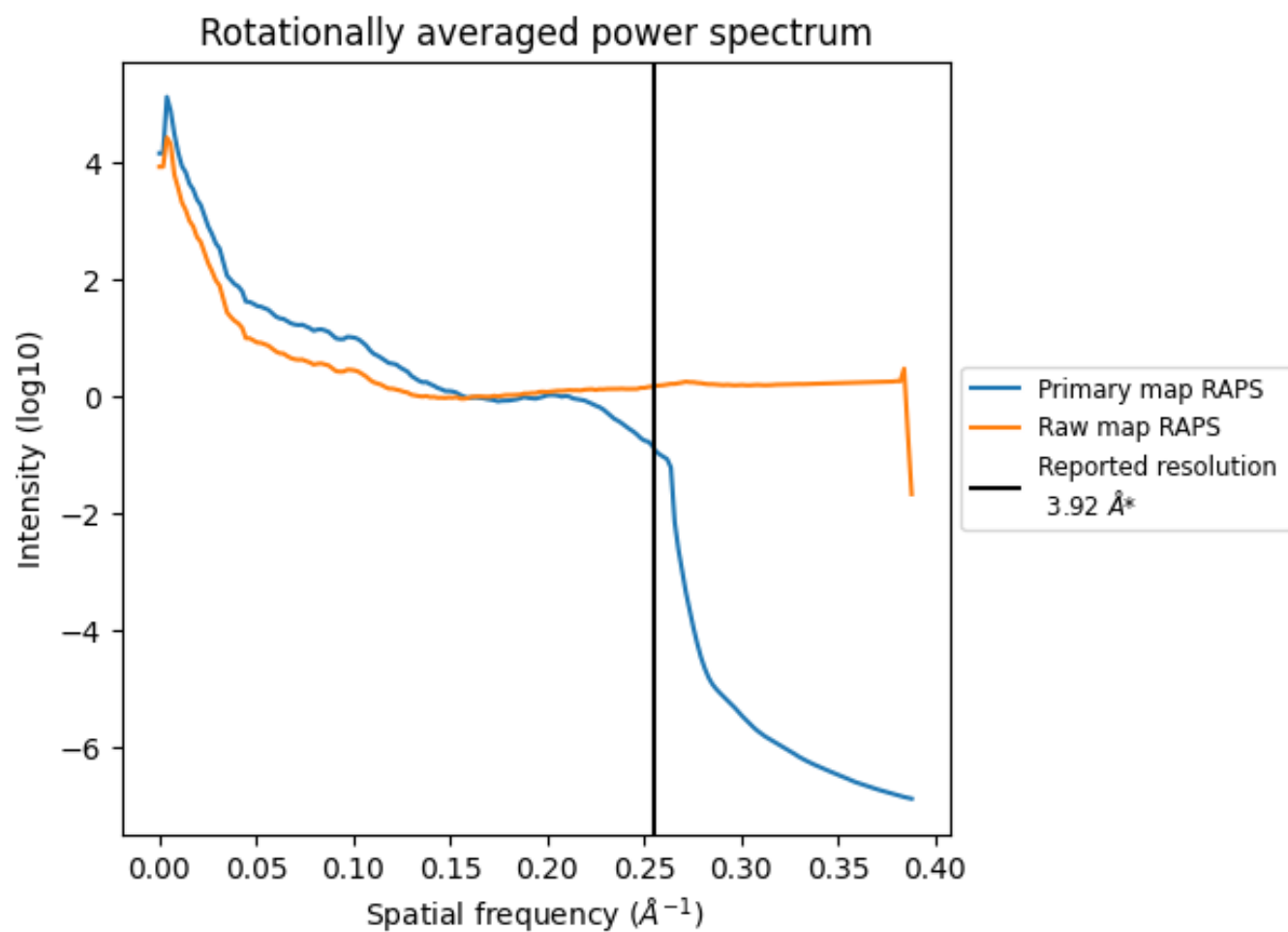
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1594 nm³; this corresponds to an approximate mass of 1440 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 ⓘ

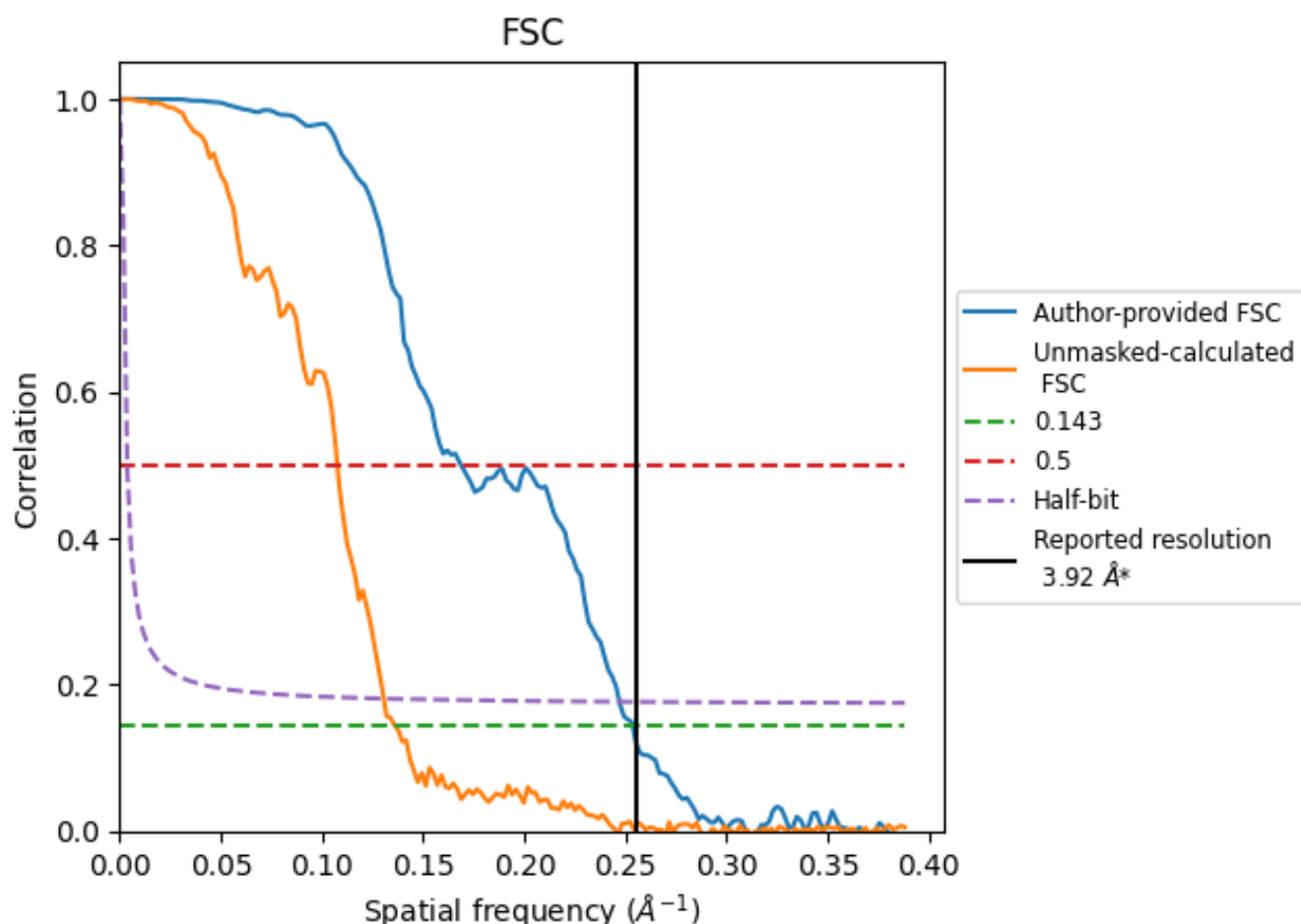


*Reported resolution corresponds to spatial frequency of 0.255 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.255 Å⁻¹

8.2 Resolution estimates [i](#)

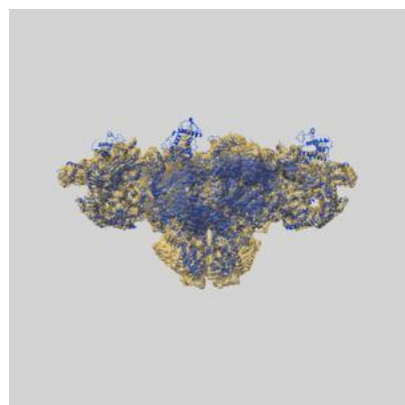
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.92	-	-
Author-provided FSC curve	3.94	5.92	4.05
Unmasked-calculated*	7.34	9.29	7.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.34 differs from the reported value 3.92 by more than 10 %

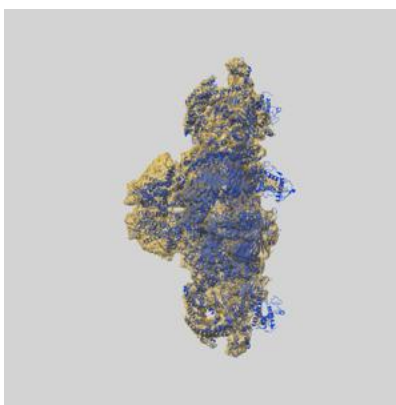
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40423 and PDB model 8SEO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

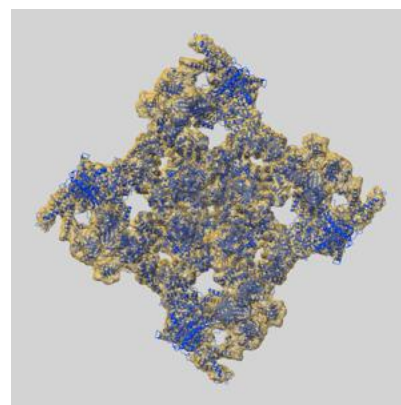
9.1 Map-model overlay [i](#)



X



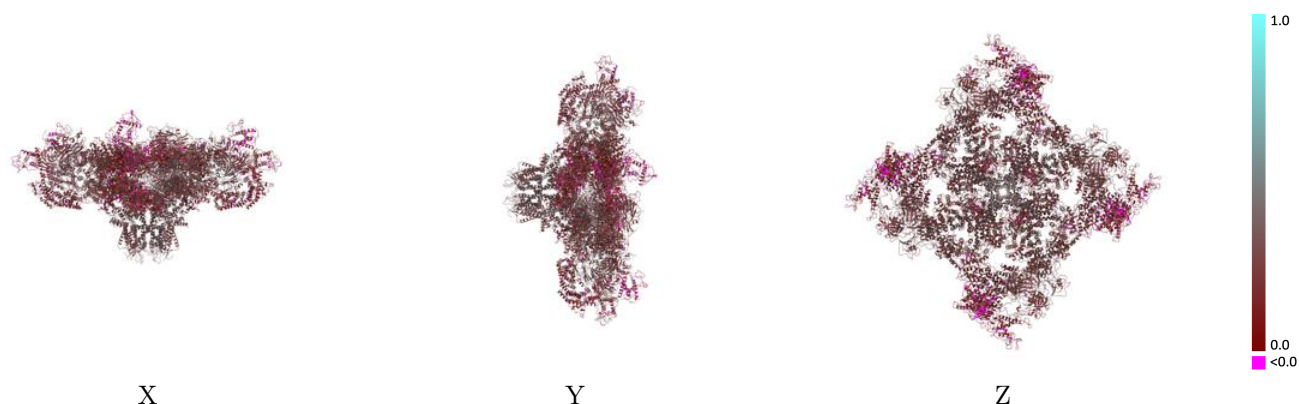
Y



Z

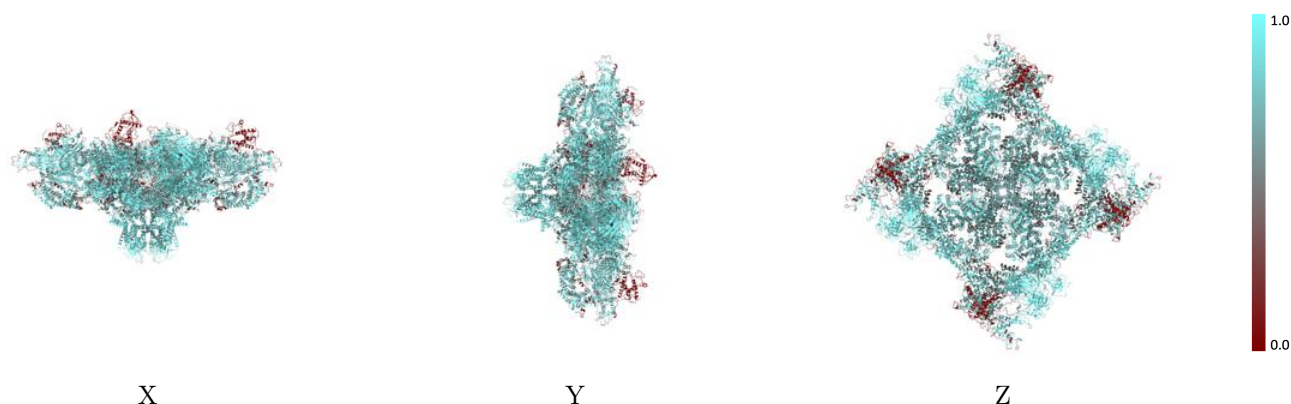
The images above show the 3D surface view of the map at the recommended contour level 0.287 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



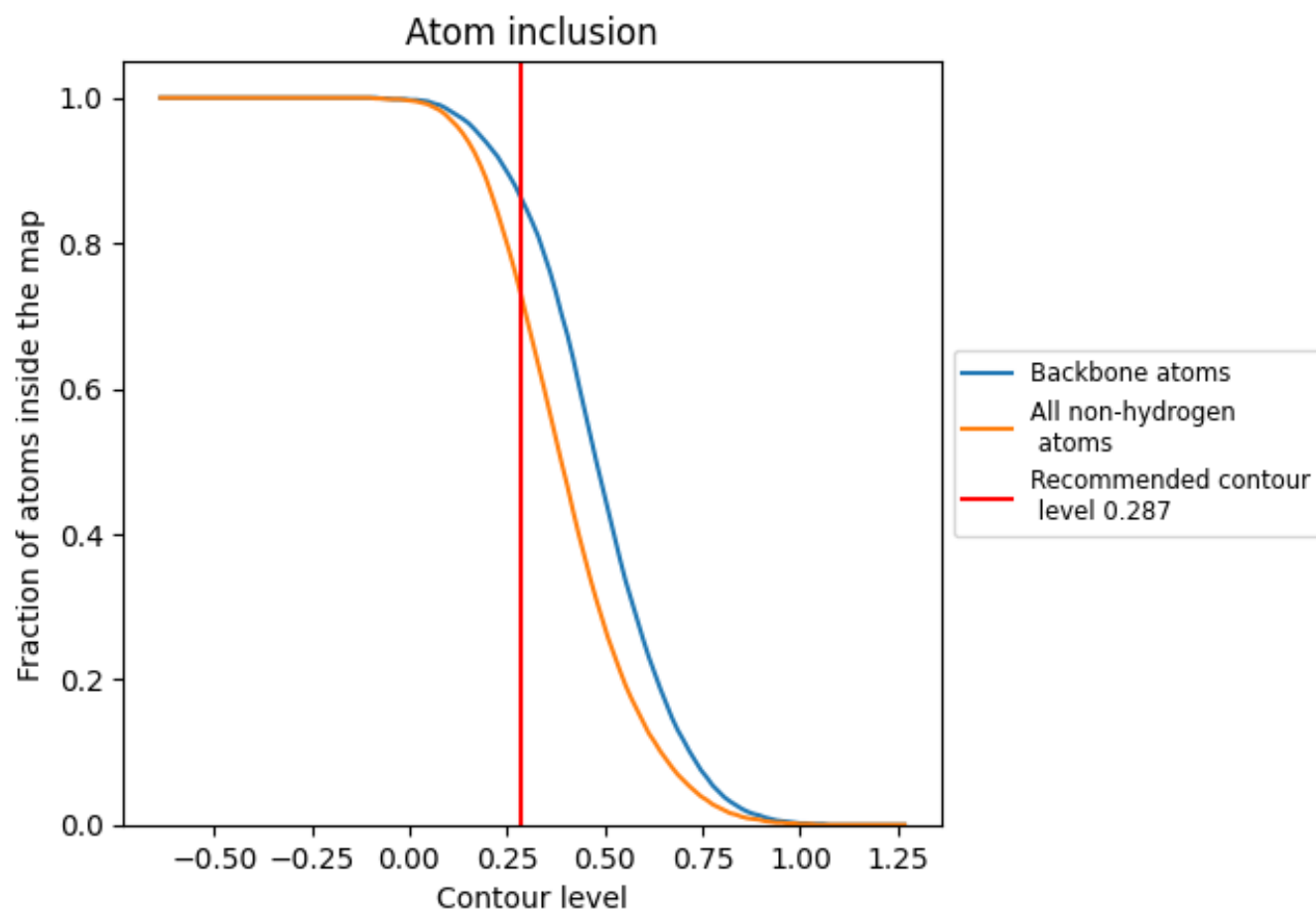
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.287).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.287) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7270	<div><div></div></div> 0.2530
A	<div><div></div></div> 0.7230	<div><div></div></div> 0.2520
B	<div><div></div></div> 0.7230	<div><div></div></div> 0.2530
C	<div><div></div></div> 0.7230	<div><div></div></div> 0.2520
D	<div><div></div></div> 0.7230	<div><div></div></div> 0.2520
E	<div><div></div></div> 0.8870	<div><div></div></div> 0.3060
F	<div><div></div></div> 0.8870	<div><div></div></div> 0.3060
G	<div><div></div></div> 0.8870	<div><div></div></div> 0.3060
H	<div><div></div></div> 0.8870	<div><div></div></div> 0.3080

1.0

0.0

<0.0