



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 12:08 AM UTC

PDB ID : 6L54 / pdb_00006l54
EMDB ID : EMD-0837
Title : Structure of SMG189
Authors : Xu, Y.; Qi, Y.
Deposited on : 2019-10-22
Resolution : 3.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

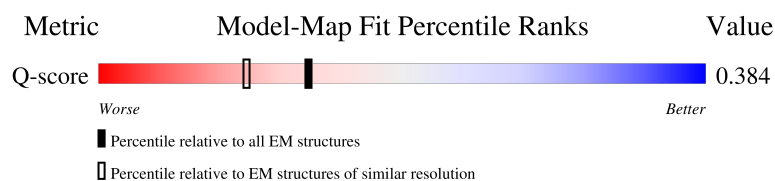
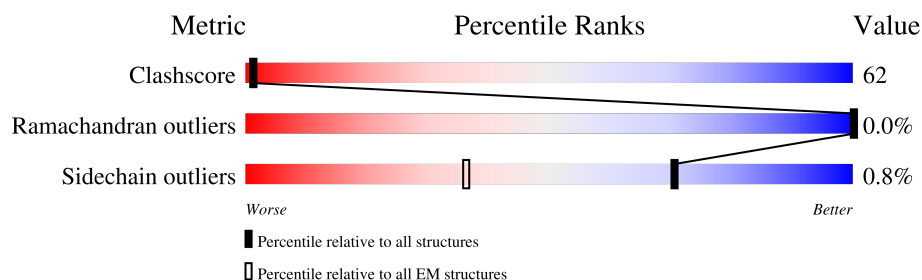
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13927 (2.93 - 3.93)

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	3661	 5% 19% 33% 48%
2	B	991	 13% 26% 61%
3	C	520	 19% 40% 41%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	C	601	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20387 atoms, of which 857 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 Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1911	Total	C	N	O	S	0	0
			13859	8742	2364	2681	72		

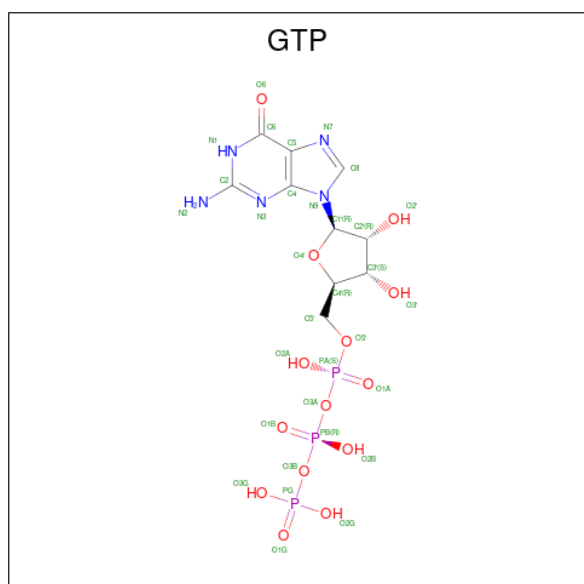
- Molecule 2 is a protein called Protein SMG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	389	Total	C	H	N	O	S	0	0
			3551	2036	393	548	554	20		

- Molecule 3 is a protein called Protein SMG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	308	Total	C	H	N	O	S	0	0
			2944	1591	464	423	449	17		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

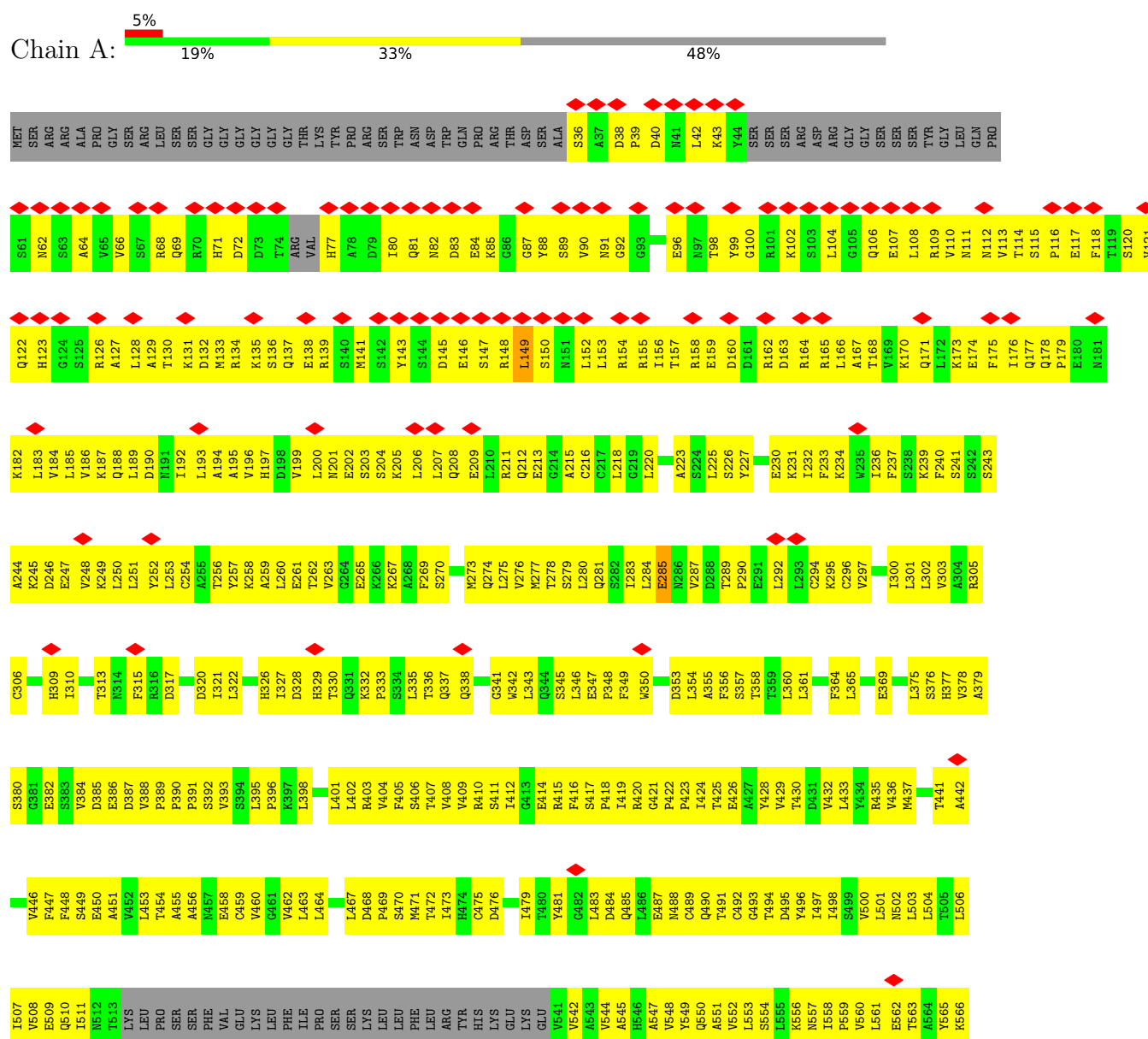
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

• Molecule 1: Serine/threonine-protein kinase SMG1

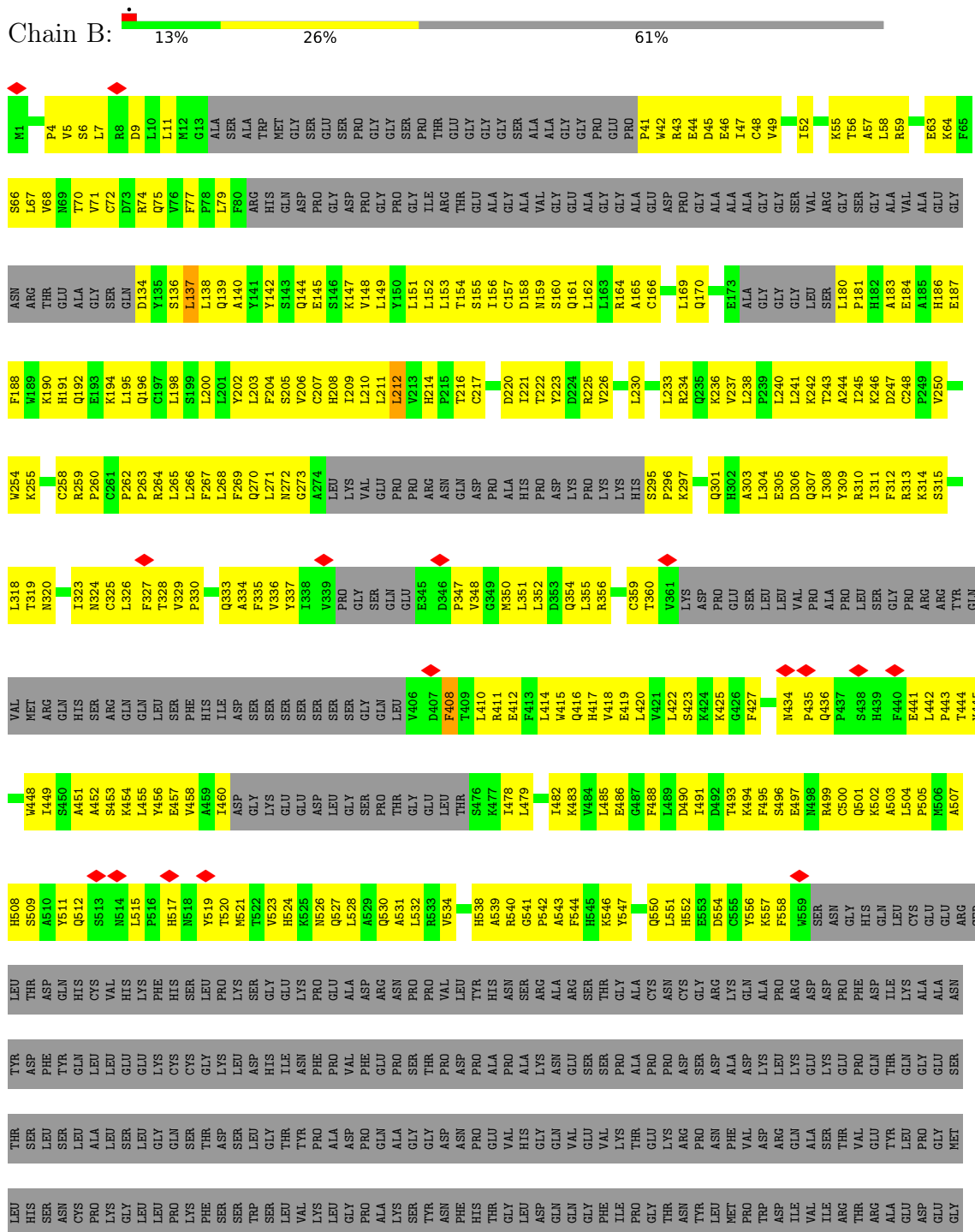




P2293	N2294	L2228	D2163	L2099	A2030	L1951	H1819	F1752	ASP	L1622	PHE	E1486
N2296	L2296	K2232	E2164	A2100	PRO	V1952	R1820	T1753	GLU	L1623	THR	K1487
A2297	L2296	A2101	R2165	A2101	ALA	E1953	G1821	F1754	ASP	L1624	GLY	T1488
K2298	L2296	T2102	L2166	GLN	GLU	E1954	I1822	L1755	ILE	S1624	LEU	K1489
E2299	L2296	T2103	Q2167	PRO	THR	L1955	I1823	K1756	THR	A1626	SER	
L2300	L2296	H2104	T2169	HIS	HIS	V1958	Q1824	L1757	GLN	Y1627	LEU	T1493
W2301	L2296	T2105	E2037	E2037	THR	T1959	Q1825		ILE	R1628	LEU	H1499
S2302	L2296	E2106	K2038	K2038	VAL	L1960	F1826	G1760	GLN	W1629	SER	A1500
C2304	L2296	T2107	W2039	SER	SER	L1961	F1827	ILE	THR	G1630	ASN	M1501
T2305	L2296	A2108	Q2041	CYS	CYS	E1964	H1832	LEU	GLU	R1631	ILE	E1502
T2306	L2296	L2109	D2042	GLY	GLY	L1971	E1833	LEU	GLU	K1632	THR	M1503
P2307	L2296	V2113	Y2044	GLY	GLY	Q1972	E1834	ASP	ASN	V1634	LEU	L1504
D2308	L2296	ALA	G2045	SER	SER	Q1973	Y1835	GLN	GLU	D1635	ILE	A1508
E2309	L2296	ARG	D2046	PRO	PRO	H1974	Y1836	ASP	GLU	N1636	GLU	I1509
W2310	L2296	ASP	A2047	ALA	ALA	Y1975	R1837	PRO	SER	A1637	LEU	S1510
W2311	L2296	THR	I2048	SER	SER	Y1976	R1838	LEU	THR	S1638	SER	F1511
R2312	L2296	T2119	E2053	GLN	GLN	V1977	I1841	HIS	VAL	Q1639	VAL	C1512
R2313	L2296	T2120	K2054	ASN	ASN	L1978	C1842	SER	GLU	G1640	ASN	K1513
T2314	L2296	H2121	L2055	SER	SER		L1844	HIS	THR	L1646	THR	S1514
Q2315	L2296	S2123	K2056	LYS	LYS	Q1983	L1845	ARG	GLU	P1647	MET	E1518
S2316	L2296	G2125	T2057	ASP	ASP	Q1986	V1848	VAL	GLU	E1648	GLU	Y1519
Y2317	L2296	G2126	P2058	GLY	GLY	D1987	A1849	GLN	GLU	E1649	GLU	A1520
A2318	L2296	K2134	L2059	LEU	LEU	E1987		SER	THR	S1651	THR	V1521
R2319	L2296	T2128	ASN	ASN	ASN	E1985	L1855	THR	ASP	E1652	GLU	E1518
S2320	L2296	T2129	ALA	LYS	LYS	D1986	I1856	ASP	ASP	S1713	GLU	Y1519
A2322	L2296	T2130	PRO	PRO	PRO	V1987	L1857	ASP	ASP	Q1714	GLU	A1522
Y2323	L2296	L2131	ALA	GLY	GLY	Y1988	Y1858	LEU	PRO	V1653	GLU	K1523
W2324	L2296	T2132	GLY	GLY	GLY	V1989	P1859	THR	THR	Q1654	GLU	S1524
S2325	L2296	T2133	S2067	ALA	ALA	K1989	A1860	M1786	LEU	N1655	THR	I1525
W2326	L2296	T2134	W2068	GLN	GLN	R1990	V1862	M1787	SER	L1656	THR	I1527
Y2327	L2296	K2134	L2069	MET	MET	V1991	G1863	T1789	GLU	P1658	THR	L1528
L2330	L2330	T2135	W2068	GLN	GLN			L1790	LEU	D1659	GLU	A1529
T2331	L2331	T2136	I2069	ASN	ASN	ASN	T1864	L1791	ASP	T1660	GLU	K1530
G2332	L2332	P2137	P2070	ASN	ASN	L1865	I1866	L1792	GLU	I1661	THR	W1531
L2333	L2333	K2138	F2071	ASN	ASN	D1928		L1793	SER	T1662	ASP	I1532
G2334	L2334	T2139	K2072	THR	THR	C1929		R1794	ALA	E1663	THR	A1534
D2335	L2335	L2140	E2073	LEU	LEU	Y1930		L1795	ALA	E1664	THR	E1535
R2336	L2336	L2141	L2076	ARG	ARG			V1797	THR	E1665	THR	W1536
H2337	L2337	G2144	S2077	LYS	LYS				ASP	K1666	THR	K1537
L2338	L2338	S2145	L2078	GLU	GLU			E1802	GLU	E1667	THR	E1538
D2339	L2339	ASP	L2078	GLU	GLU			L1803	THR	R1668	THR	I1539
N2340	L2340	GLY	K2084	LYS	LYS			L1807	THR	Y1604	THR	SER
V2341	L2341	LYS	R2085	ALA	ALA			E1808	GLY	Y1605	THR	GLN
L2342	L2342	LYS	A2086	ALA	ALA			H1809	GLY	H1606	THR	LEU
D2344	L2344	Y2150	S2087	ILE	ILE				LYS	L1607	THR	LYS
W2345	L2345	P2151	T2088	THR	THR			E1812	THR	S1608	THR	GLN
T2346	L2346	Y2152	I2089	ALA	ALA			T1813	THR	Q1611	THR	VAL
T2347	L2347	L2153	L2089	ILE	ILE			T1814	THR	Q1611	THR	VAL
Q2348	L2348	F2154	L2092	PRO	PRO			T1815	THR	A1612	THR	ARG
E2349	L2349	K2155	E2093	THR	THR			T1816	THR	Y1677	THR	ALA
W2350	L2350	E2158	I2095	LEU	LEU			A1817	THR	VAL	THR	GLN
V2351	L2351	D2159	E2096	LEU	LEU			A1750	THR	ALA	THR	HIS
H2352	L2352	L2160	S2096	GLY	GLY			Y1751	THR	A1616	THR	GLN
L2353	L2353	L2162	W2098						GLY	ILE	THR	ASN

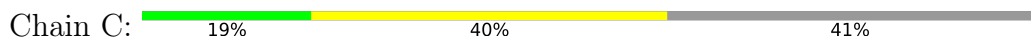


- Molecule 2: Protein SMG8



GLN	PRO	PRO	PRO	CYS	VAL	PHE	TYR	PRO	GLU	GLY	GLN	GLU	ILE	THR	LEU	PRO	PRO	ASP	GLY	LEU	TRP	VAL	LEU	ARG	PHE	PRO	TYR	ALA	TYR	VAL	THR	GLU	ARG	GLY	PRO	CYS	PHE	PRO	PRO	LYS	GLU	ASN	VAL	GLN	LEU	MET	SER	TYR	LYS	VAL	LEU	ARG	GLY	VAL	LEU	LYS	ALA	VAL	THR
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- Molecule 3: Protein SMG9

[illegible][illegible]

K182	L183	V184	D185	D186	Q187	M188	M189	V190	C191	D192	S193	A194	E195	L196	V197	L198	L199	Z200	Q201	T202	D203	V204	L205	L206	V207	G208	V209	L210	G211	L212	Q213	G214	T215	G216	K217	S218	M219	V220	M221	S222	S223	L223	L224		T228	T229	F230	E231	D232	Q233	R234	T235		F238	R239	A240	Q241		E244	W245
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K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644	K645	K646	K647	K648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713	K714	K715	K716	K717	K718	K719	K720	K721	K722	K723	K724	K725	K726	K727	K728	K729	K730	K731	K732	K733	K734	K735	K736	K737	K738	K739	K740	K741	K742	K743	K744	K745	K746	K747	K748	K749	K750	K751	K752	K753	K754	K755	K756	K757	K758	K759	K760	K761	K762	K763	K764	K765	K766	K767	K768	K769	K770	K771	K772	K773	K774	K775	K776	K777	K778	K779	K780	K781	K782	K783	K784	K785	K786	K787	K788	K789	K790	K791	K792	K793	K794	K795	K796	K797	K798	K799	K800	K801	K802	K803	K804	K805	K806	K807	K808	K809	K810	K811	K812	K813	K814	K815	K816	K817	K818	K819	K820	K821	K822	K823	K824	K825	K826	K827	K828	K829	K830	K831	K832	K833	K834	K835	K836	K837	K838	K839	K840	K841	K842	K843	K844	K845	K846	K847	K848	K849	K850	K851	K852	K853	K854	K855	K856	K857	K858	K859	K860	K861	K862	K863	K864	K865	K866	K867	K868	K869	K870	K871	K872	K873	K874	K875	K876	K877	K878	K879	K880	K881	K882	K883	K884	K885	K886	K887	K888	K889	K890	K891	K892	K893	K894	K895	K896	K897	K898	K899	K900	K901	K902	K903	K904	K905	K906	K907	K908	K909	K910	K911	K912	K913	K914	K915	K916	K917	K918	K919	K920	K921	K922	K923	K924	K925	K926	K927	K928	K929	K930	K931	K932	K933	K934	K935	K936	K937	K938	K939	K940	K941	K942	K943	K944	K945	K946	K947	K948	K949	K950	K951	K952	K953	K954	K955	K956	K957	K958	K959	K960	K961	K962	K963	K964	K965	K966	K967	K968	K969	K970	K971	K972	K973	K974	K975	K976	K977	K978	K979	K980	K981	K982	K983	K984	K985	K986	K987	K988	K989	K990	K991	K992	K993	K994	K995	K996	K997	K998	K999	K1000
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L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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E377	D378	D379	D380	D381	D382	D383	D384	D385	D386	D387	D388	D389	M390	I391	D392	D393	D394	M395	D396	D397	D398	H399	L400	R401	L402	K403	G404	T405	L406	S407	M408	L409	L410	C411	M412	V413	F414	F415	L417	P418	P419	D420	F421	L422	D423	M427	L428	P429	LEU	VAL	PRO	PRO	PHE	PHE	MET	ASP	SER	GLU	ALA	GLY	SER
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[illegible]

R507	K508	S509		L512		Y515		L518	L519	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	420000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	48.493	Depositor
Minimum map value	-23.751	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP

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	0.09	0/14051	0.30	1/19153 (0.0%)
2	B	0.09	0/3231	0.32	2/4367 (0.0%)
3	C	0.08	0/2539	0.39	4/3440 (0.1%)
All	All	0.09	0/19821	0.31	7/26960 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	325	PHE	CA-C-N	8.62	135.04	122.63
3	C	325	PHE	C-N-CA	8.62	135.04	122.63
3	C	399	HIS	CA-C-N	8.50	134.67	122.09
3	C	399	HIS	C-N-CA	8.50	134.67	122.09
2	B	137	LEU	CA-C-N	8.39	133.33	121.24
2	B	137	LEU	C-N-CA	8.39	133.33	121.24
1	A	3627	PRO	N-CA-CB	6.38	110.06	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13859	0	13122	1818	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3158	393	3174	340	0
3	C	2480	464	2469	314	0
4	C	32	0	11	10	0
5	C	1	0	0	0	0
All	All	19530	857	18776	2377	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 62.

All (2377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:GLU:HA	1:A:1503:MET:HB2	1.30	1.09
1:A:1338:SER:HB3	1:A:1401:MET:HE2	1.36	1.08
2:B:198:LEU:HD11	2:B:483:LYS:HE2	1.36	1.06
1:A:649:VAL:HG11	1:A:667:THR:HB	1.40	1.04
1:A:820:LEU:HD22	1:A:886:LEU:HB2	1.35	1.03
3:C:406:LEU:HB2	3:C:422:LEU:HA	1.40	1.03
1:A:276:VAL:HG11	1:A:280:LEU:HG	1.40	1.03
1:A:557:ASN:HB3	1:A:612:ILE:HG21	1.41	1.02
3:C:345:PRO:HG3	3:C:486:SER:HB2	1.38	1.02
1:A:811:THR:HA	1:A:814:ARG:HG2	1.39	1.02
1:A:163:ASP:HA	1:A:170:LYS:HE3	1.42	1.01
1:A:131:LYS:HE2	1:A:174:GLU:HG2	1.43	1.01
1:A:1525:ILE:HG13	1:A:1526:LEU:HD12	1.44	1.00
1:A:108:LEU:HD13	1:A:110:VAL:HG13	1.39	1.00
1:A:1410:ILE:HD13	1:A:1424:LEU:HD23	1.41	0.99
1:A:2390:GLY:H	1:A:2394:LEU:HD13	1.25	0.99
2:B:482:ILE:HG23	2:B:485:LEU:HD12	1.40	0.99
1:A:2277:LEU:H	1:A:2278:HIS:HB3	1.27	0.98
1:A:1086:PRO:HB2	1:A:1092:ILE:HG12	1.45	0.98
1:A:2069:ILE:HG13	1:A:2070:PRO:HD3	1.44	0.98
3:C:313:THR:HG22	3:C:341:LYS:HE2	1.43	0.97
1:A:215:ALA:HA	1:A:218:LEU:HD13	1.47	0.97
1:A:100:GLY:HA2	1:A:133:MET:HE2	1.46	0.97
1:A:1786:VAL:HG13	1:A:1823:ILE:HD11	1.47	0.97
1:A:751:LEU:HD22	3:C:174:PRO:HG3	1.43	0.97
1:A:433:LEU:HD21	1:A:471:MET:HG2	1.46	0.96
1:A:2037:GLU:HG3	1:A:2094:GLU:HA	1.47	0.96
1:A:114:THR:HG22	1:A:134:ARG:HG2	1.47	0.96
1:A:1753:THR:HG23	1:A:1788:ALA:HB1	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1786:VAL:HG11	1:A:2172:ILE:HD12	1.48	0.94
1:A:2296:LEU:HD22	1:A:2383:LEU:HD13	1.48	0.94
1:A:675:HIS:HB2	1:A:676:ASP:HB2	1.50	0.94
1:A:1336:ARG:HB3	1:A:1337:LEU:HA	1.50	0.93
1:A:866:ILE:HD12	1:A:1185:TYR:H	1.32	0.92
2:B:408:PHE:HB3	2:B:412:GLU:HB2	1.49	0.92
2:B:139:GLN:HE21	2:B:152:LEU:HD11	1.34	0.92
3:C:183:LEU:HD11	3:C:258:PHE:HB2	1.47	0.92
2:B:528:LEU:HD21	2:B:551:LEU:HD22	1.48	0.92
1:A:1306:PRO:HG2	1:A:2306:THR:HB	1.53	0.91
3:C:295:LEU:HD12	3:C:296:PRO:HD2	1.51	0.91
1:A:2195:VAL:HA	1:A:2205:ILE:HG22	1.53	0.91
1:A:2160:LEU:HD22	1:A:2203:GLY:HA3	1.49	0.91
1:A:2254:TYR:HA	1:A:2257:ILE:HG22	1.52	0.91
1:A:1038:GLY:HA3	1:A:1102:LYS:HE3	1.53	0.91
2:B:303:ALA:HB1	3:C:248:ARG:HA	1.53	0.89
1:A:1478:LYS:HE3	1:A:1532:ILE:HG12	1.53	0.89
1:A:2284:LEU:HD11	1:A:2288:MET:HE3	1.52	0.89
2:B:156:ILE:HG13	2:B:192:GLN:HB3	1.53	0.89
1:A:147:SER:H	1:A:149:LEU:HD23	1.37	0.88
1:A:769:LEU:HD13	3:C:265:ILE:HD11	1.55	0.88
1:A:2089:ILE:HG21	1:A:2129:THR:HA	1.56	0.88
1:A:1131:ALA:HB1	1:A:1206:TRP:HE1	1.38	0.88
1:A:983:LEU:HD23	1:A:992:LYS:HE2	1.54	0.87
3:C:406:LEU:HD12	3:C:422:LEU:HB3	1.55	0.87
1:A:2330:ILE:HD12	1:A:2404:ARG:HH11	1.39	0.87
1:A:1472:GLN:HG2	1:A:1525:ILE:HG23	1.57	0.86
1:A:2276:PRO:HB2	1:A:2279:VAL:H	1.39	0.86
1:A:1502:GLU:HB3	1:A:1504:LEU:HB2	1.58	0.86
3:C:209:VAL:HG12	3:C:319:ILE:HB	1.57	0.86
1:A:738:ALA:HB3	1:A:830:LEU:HD21	1.57	0.86
1:A:740:VAL:HA	1:A:751:LEU:HD12	1.57	0.86
1:A:1656:LEU:HB3	1:A:1657:LEU:HA	1.57	0.86
1:A:1521:VAL:HG22	1:A:1522:ALA:HA	1.57	0.86
1:A:1509:ILE:HD13	1:A:1598:ASP:HA	1.59	0.85
1:A:249:LYS:HE3	1:A:297:VAL:HG22	1.57	0.85
2:B:337:TYR:HE1	2:B:410:LEU:HD11	1.40	0.85
1:A:471:MET:HA	1:A:471:MET:HE3	1.58	0.84
1:A:409:VAL:HG13	1:A:453:LEU:HD22	1.59	0.84
1:A:1419:SER:HA	1:A:1422:MET:HE2	1.56	0.84
1:A:2277:LEU:N	1:A:2278:HIS:HB3	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:HD13	1:A:401:LEU:HD11	1.60	0.84
1:A:1325:LYS:HE2	1:A:1325:LYS:HA	1.60	0.84
1:A:80:ILE:HG21	1:A:106:GLN:HE22	1.43	0.84
1:A:2152:TYR:HA	1:A:2206:GLN:HA	1.60	0.84
2:B:504:LEU:HD13	2:B:550:GLN:HG2	1.59	0.83
1:A:2273:ARG:HB3	1:A:2274:ASP:HA	1.61	0.83
1:A:1938:SER:HA	1:A:1945:VAL:HG11	1.61	0.83
1:A:335:LEU:HB3	1:A:336:THR:HB	1.59	0.82
1:A:1856:ILE:HB	1:A:1859:PRO:HG3	1.61	0.82
1:A:618:LEU:HD11	1:A:648:ILE:HG23	1.61	0.82
1:A:2128:ILE:HG22	1:A:2140:LEU:HB3	1.57	0.82
1:A:2176:MET:HE3	1:A:2407:ARG:HB2	1.58	0.82
1:A:379:ALA:HB3	1:A:382:GLU:HG2	1.61	0.82
1:A:863:SER:HB3	1:A:869:ILE:HG12	1.60	0.82
3:C:244:GLU:HA	3:C:247:GLU:HG2	1.62	0.82
1:A:1075:MET:HE2	1:A:1075:MET:HA	1.60	0.82
1:A:2365:LEU:HA	1:A:2366:ARG:HB3	1.60	0.82
3:C:408:MET:HE2	3:C:408:MET:HA	1.60	0.81
2:B:56:THR:OG1	2:B:158:ASP:OD1	1.98	0.81
1:A:199:VAL:HG23	1:A:200:LEU:HD12	1.60	0.81
1:A:736:LEU:HD11	3:C:199:LEU:HD12	1.60	0.81
1:A:98:THR:O	1:A:102:LYS:HG3	1.80	0.81
1:A:742:MET:HA	1:A:742:MET:HE2	1.63	0.81
1:A:275:LEU:HB2	1:A:276:VAL:HA	1.62	0.80
1:A:895:LYS:HB3	1:A:2224:ARG:HD2	1.63	0.80
2:B:236:LYS:HD3	2:B:485:LEU:HD13	1.63	0.80
1:A:1475:VAL:HG23	1:A:1528:LEU:HD12	1.62	0.80
1:A:1818:PRO:HB2	1:A:1848:VAL:HG12	1.62	0.80
1:A:390:PRO:HB2	1:A:391:PRO:HD3	1.61	0.80
1:A:2247:PRO:CD	1:A:2248:ARG:HA	2.12	0.80
1:A:1090:GLN:NE2	1:A:1422:MET:SD	2.55	0.80
1:A:891:GLN:HE22	1:A:2298:LYS:HD2	1.46	0.80
1:A:1521:VAL:HG13	1:A:1522:ALA:HB2	1.62	0.80
1:A:638:VAL:HB	1:A:639:PHE:HA	1.64	0.80
1:A:976:ASN:HD21	1:A:1074:MET:HG2	1.47	0.79
1:A:1508:ALA:HB1	1:A:1600:ILE:HG13	1.65	0.79
1:A:1673:LEU:HD21	1:A:1708:TRP:HD1	1.47	0.79
1:A:2102:MET:HE3	1:A:2105:THR:HG21	1.63	0.79
1:A:2223:GLN:HG2	1:A:2245:ILE:HD12	1.62	0.79
1:A:1022:THR:HB	1:A:1415:VAL:H	1.46	0.79
1:A:2247:PRO:HD2	1:A:2248:ARG:HA	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:HG3	1:A:436:VAL:H	1.48	0.79
1:A:2153:LEU:HD13	1:A:2155:LYS:HE2	1.64	0.79
1:A:2391:VAL:HG12	1:A:2392:PHE:H	1.47	0.79
2:B:44:GLU:HA	2:B:444:THR:HB	1.64	0.79
1:A:1413:GLN:H	1:A:1415:VAL:HA	1.45	0.79
1:A:2276:PRO:HG2	1:A:2280:MET:HE2	1.65	0.79
1:A:651:SER:HA	1:A:1304:LEU:HD22	1.64	0.78
1:A:1071:VAL:HG11	1:A:1074:MET:HG3	1.64	0.78
1:A:2407:ARG:HB3	1:A:2410:LEU:HD13	1.65	0.78
2:B:505:PRO:O	2:B:509:SER:OG	2.00	0.78
1:A:322:LEU:H	1:A:322:LEU:HD12	1.47	0.78
1:A:1085:CYS:HB3	1:A:1086:PRO:HD2	1.63	0.78
1:A:1090:GLN:O	1:A:1120:LYS:NZ	2.13	0.78
1:A:231:LYS:HG3	1:A:232:ILE:HD12	1.66	0.78
1:A:1103:ASN:HD22	1:A:1109:SER:HB2	1.49	0.78
1:A:2038:LYS:HG3	1:A:2095:ILE:HD12	1.64	0.78
2:B:434:ASN:O	2:B:436:GLN:NE2	2.16	0.78
1:A:1324:LEU:HD11	1:A:1339:THR:HG22	1.66	0.78
1:A:656:HIS:H	1:A:660:ILE:HD11	1.48	0.77
1:A:1666:LYS:HZ1	1:A:1713:SER:H	1.31	0.77
1:A:733:THR:OG1	1:A:822:LYS:HB2	1.83	0.77
1:A:2295:LEU:HD12	1:A:2379:ILE:HD13	1.67	0.77
1:A:2336:ARG:HH21	1:A:2340:ASN:HB3	1.48	0.77
2:B:162:LEU:HD22	3:C:390:MET:HE3	1.64	0.77
1:A:995:TYR:HA	1:A:998:TYR:HB3	1.66	0.77
1:A:2277:LEU:HB2	1:A:2278:HIS:CB	2.14	0.77
1:A:2276:PRO:N	1:A:2277:LEU:HA	1.99	0.77
3:C:376:ARG:HG3	3:C:462:GLY:HA3	1.67	0.77
1:A:1184:ASN:ND2	1:A:1288:SER:OG	2.18	0.77
1:A:1320:VAL:O	1:A:1324:LEU:HG	1.85	0.77
1:A:361:LEU:HA	1:A:401:LEU:HD13	1.65	0.77
1:A:1502:GLU:HG3	1:A:1504:LEU:HD23	1.65	0.76
1:A:1303:ALA:O	1:A:1308:GLU:HB2	1.85	0.76
1:A:1424:LEU:HD22	1:A:1458:THR:HG22	1.68	0.76
1:A:2069:ILE:CG1	1:A:2070:PRO:HD3	2.15	0.76
3:C:417:LEU:HB2	3:C:418:PRO:HD3	1.66	0.76
3:C:410:GLN:HB2	3:C:472:LYS:HE2	1.67	0.76
1:A:1207:GLN:NE2	1:A:1288:SER:OG	2.18	0.76
3:C:485:LEU:HB3	3:C:490:LEU:HD12	1.67	0.76
1:A:115:SER:HA	1:A:155:ARG:HH12	1.51	0.76
1:A:675:HIS:HB2	1:A:676:ASP:CB	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:LYS:NZ	1:A:861:ASP:OD2	2.19	0.76
1:A:364:PHE:HD2	1:A:365:LEU:HD12	1.50	0.76
1:A:1048:VAL:HG13	1:A:1052:PHE:HE2	1.51	0.76
1:A:2191:ARG:HG3	1:A:2351:VAL:HG12	1.66	0.75
3:C:325:PHE:HE1	3:C:391:ILE:HD11	1.47	0.75
1:A:166:LEU:HG	1:A:167:ALA:H	1.52	0.75
1:A:730:LEU:HD23	1:A:730:LEU:H	1.50	0.75
1:A:1282:PRO:O	1:A:1286:GLN:NE2	2.19	0.75
1:A:675:HIS:CB	1:A:676:ASP:HB2	2.16	0.75
1:A:1960:VAL:N	1:A:1961:LEU:HA	2.02	0.75
1:A:1324:LEU:HD21	1:A:1339:THR:HB	1.67	0.75
2:B:295:SER:HB2	2:B:296:PRO:HD3	1.67	0.75
1:A:1832:HIS:O	1:A:1838:ARG:NH2	2.20	0.75
3:C:183:LEU:CD1	3:C:258:PHE:HB2	2.16	0.75
1:A:104:LEU:HD13	1:A:136:SER:HB2	1.69	0.74
1:A:1081:CYS:O	1:A:1085:CYS:N	2.18	0.74
1:A:1477:GLU:O	1:A:1481:PRO:HD3	1.86	0.74
2:B:512:GLN:HB2	2:B:557:LYS:HE3	1.68	0.74
1:A:72:ASP:HA	1:A:106:GLN:HG2	1.69	0.74
1:A:618:LEU:HD13	1:A:648:ILE:HD12	1.69	0.74
1:A:2037:GLU:N	1:A:2093:GLU:O	2.21	0.74
1:A:2300:LEU:HD21	1:A:2343:ILE:HD11	1.69	0.74
1:A:2247:PRO:N	1:A:2248:ARG:HA	2.01	0.74
1:A:502:ASN:O	1:A:506:LEU:HG	1.87	0.74
1:A:111:ASN:O	1:A:115:SER:OG	2.04	0.74
2:B:49:VAL:HG22	2:B:149:LEU:HB3	1.69	0.74
1:A:820:LEU:CD2	1:A:886:LEU:HB2	2.17	0.74
1:A:637:THR:N	1:A:638:VAL:HA	2.03	0.74
1:A:2164:GLU:OE1	1:A:2165:ARG:NH1	2.21	0.74
3:C:254:SER:O	3:C:271:GLN:NE2	2.20	0.74
2:B:527:GLN:HE22	2:B:554:ASP:HB3	1.52	0.74
1:A:895:LYS:HE3	1:A:2228:LEU:HD12	1.70	0.74
1:A:1346:LEU:HD13	1:A:1349:LEU:HD11	1.70	0.74
1:A:1842:CYS:HA	1:A:1933:ILE:HD11	1.70	0.74
1:A:237:PHE:HA	1:A:240:PHE:HB2	1.68	0.73
1:A:411:SER:OG	1:A:435:ARG:N	2.19	0.73
1:A:1086:PRO:HA	1:A:1090:GLN:HB3	1.69	0.73
3:C:216:GLY:HA3	4:C:601:GTP:HN22	1.53	0.73
1:A:1586:SER:CB	1:A:1590:VAL:HB	2.18	0.73
2:B:63:GLU:O	2:B:67:LEU:HG	1.88	0.73
2:B:312:PHE:HB3	2:B:318:LEU:HG	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2207:TRP:CD1	1:A:2208:VAL:HG12	2.23	0.73
2:B:190:LYS:HG2	2:B:194:LYS:HE3	1.71	0.73
3:C:229:PRO:HG2	3:C:467:GLN:HG3	1.71	0.73
1:A:770:VAL:O	1:A:771:GLU:HG3	1.87	0.73
1:A:1343:SER:HA	1:A:1344:GLN:CB	2.17	0.73
1:A:1462:LEU:O	1:A:1466:PHE:N	2.22	0.73
1:A:987:LEU:HG	1:A:988:GLU:H	1.53	0.73
1:A:1586:SER:HB2	1:A:1590:VAL:HB	1.71	0.73
1:A:1790:LEU:HD21	1:A:1823:ILE:HD12	1.70	0.73
1:A:432:VAL:HG13	1:A:433:LEU:HD12	1.71	0.73
3:C:211:GLY:HA3	3:C:215:THR:HG21	1.71	0.73
1:A:135:LYS:HZ3	1:A:177:GLN:HB2	1.52	0.72
1:A:1650:LYS:HE3	1:A:1654:GLN:HE21	1.54	0.72
1:A:300:ILE:HG23	1:A:302:LEU:HG	1.71	0.72
1:A:432:VAL:HG13	1:A:433:LEU:CD1	2.20	0.72
1:A:893:LEU:HA	1:A:911:VAL:HG22	1.71	0.72
1:A:2245:ILE:N	1:A:2246:VAL:HA	2.04	0.72
2:B:301:GLN:HG2	2:B:336:VAL:HG23	1.71	0.72
2:B:64:LYS:NZ	2:B:153:LEU:O	2.20	0.72
1:A:192:ILE:O	1:A:196:VAL:HG23	1.89	0.72
1:A:1818:PRO:CB	1:A:1848:VAL:HG12	2.19	0.72
1:A:100:GLY:HA2	1:A:133:MET:CE	2.20	0.72
1:A:2332:GLY:HA3	1:A:2360:GLU:H	1.54	0.72
2:B:136:SER:HB2	2:B:153:LEU:HD11	1.71	0.72
1:A:2185:THR:HB	1:A:2186:PRO:HD3	1.71	0.72
1:A:1412:GLU:O	1:A:1416:PRO:HD2	1.89	0.72
1:A:2245:ILE:HB	1:A:2246:VAL:C	2.15	0.72
3:C:403:LYS:HB3	3:C:421:PHE:HB2	1.72	0.72
1:A:649:VAL:O	1:A:653:LEU:HG	1.90	0.71
1:A:1346:LEU:HB2	1:A:1349:LEU:HD13	1.71	0.71
1:A:69:GLN:HB2	1:A:102:LYS:HZ2	1.54	0.71
1:A:858:HIS:HB2	1:A:859:PRO:HD2	1.73	0.71
1:A:1410:ILE:HD13	1:A:1424:LEU:CD2	2.17	0.71
1:A:346:LEU:HA	1:A:349:PHE:HD1	1.55	0.71
1:A:1407:LEU:HD11	1:A:1427:THR:HG21	1.72	0.71
1:A:432:VAL:HG11	1:A:479:ILE:HD11	1.70	0.71
1:A:503:LEU:O	1:A:507:ILE:HG12	1.91	0.71
1:A:1502:GLU:OE1	1:A:1502:GLU:N	2.23	0.71
1:A:1352:LEU:HD12	1:A:1353:GLN:HA	1.72	0.71
1:A:1657:LEU:HD12	1:A:1658:PRO:N	2.06	0.71
2:B:63:GLU:OE1	2:B:63:GLU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:MET:HE1	4:C:601:GTP:H2'	1.71	0.71
1:A:552:VAL:HG22	1:A:556:LYS:HE2	1.71	0.71
1:A:769:LEU:HD22	3:C:263:GLU:HB3	1.72	0.71
1:A:1502:GLU:HB3	1:A:1504:LEU:N	2.06	0.71
1:A:2276:PRO:CD	1:A:2277:LEU:HA	2.20	0.71
1:A:174:GLU:OE1	1:A:174:GLU:N	2.24	0.71
1:A:346:LEU:HD21	1:A:375:LEU:HD12	1.73	0.71
2:B:267:PHE:HD2	2:B:308:ILE:HD13	1.55	0.71
3:C:362:GLU:OE1	3:C:364:TYR:OH	2.06	0.71
1:A:1030:ILE:O	1:A:1034:ILE:HG13	1.90	0.71
1:A:1412:GLU:HA	1:A:1413:GLN:C	2.16	0.71
2:B:307:GLN:HE22	3:C:249:GLY:HA3	1.55	0.71
3:C:257:ASP:HB2	3:C:269:ASP:OD1	1.89	0.71
1:A:858:HIS:HD2	1:A:860:GLN:HB2	1.57	0.70
1:A:2247:PRO:HD2	1:A:2249:PRO:HD3	1.71	0.70
1:A:386:GLU:C	1:A:389:PRO:HD2	2.16	0.70
3:C:213:GLN:OE1	3:C:251:ASN:N	2.24	0.70
2:B:184:GLU:OE1	2:B:184:GLU:N	2.25	0.70
1:A:281:GLN:OE1	1:A:281:GLN:N	2.24	0.70
1:A:504:LEU:HD22	2:B:359:CYS:SG	2.32	0.70
1:A:2365:LEU:HA	1:A:2366:ARG:CB	2.21	0.70
2:B:211:LEU:HD23	2:B:266:LEU:HB2	1.73	0.70
1:A:154:ARG:O	1:A:157:THR:OG1	2.05	0.70
1:A:380:SER:HA	2:B:350:MET:HE1	1.74	0.70
1:A:675:HIS:H	1:A:676:ASP:HB2	1.56	0.70
1:A:897:ASP:OD1	1:A:2224:ARG:NH2	2.25	0.70
1:A:1816:THR:OG1	1:A:1817:ALA:HA	1.92	0.70
1:A:2223:GLN:HG2	1:A:2245:ILE:HG23	1.74	0.70
1:A:1511:PHE:O	1:A:1514:SER:OG	2.02	0.70
1:A:254:CYS:O	1:A:258:LYS:HG2	1.92	0.70
1:A:731:LEU:HD23	1:A:731:LEU:H	1.55	0.70
1:A:990:LEU:H	1:A:990:LEU:HD12	1.57	0.70
1:A:1324:LEU:CD2	1:A:1339:THR:HB	2.21	0.70
1:A:1338:SER:H	1:A:1339:THR:HA	1.53	0.70
1:A:557:ASN:HB3	1:A:612:ILE:CG2	2.20	0.70
1:A:1293:LEU:HD13	1:A:1322:LYS:HD2	1.72	0.70
1:A:1410:ILE:HG21	1:A:1424:LEU:HD21	1.73	0.70
2:B:234:ARG:HH12	2:B:238:LEU:HD13	1.56	0.70
2:B:267:PHE:CD2	2:B:308:ILE:HD13	2.27	0.70
1:A:571:GLU:HG2	3:C:457:LEU:HD21	1.73	0.69
1:A:2186:PRO:O	1:A:2319:ARG:HG2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:VAL:HG21	2:B:448:TRP:CE2	2.26	0.69
2:B:155:SER:HB2	2:B:196:GLN:HG3	1.72	0.69
1:A:454:THR:HB	1:A:501:LEU:CD1	2.23	0.69
1:A:742:MET:O	1:A:746:GLU:HG3	1.93	0.69
1:A:2246:VAL:HB	1:A:2247:PRO:C	2.17	0.69
2:B:137:LEU:N	2:B:154:THR:OG1	2.25	0.69
3:C:240:ALA:O	3:C:252:GLN:NE2	2.24	0.69
1:A:510:GLN:HG2	1:A:579:LEU:HD12	1.74	0.69
3:C:391:ILE:HD12	3:C:421:PHE:HZ	1.56	0.69
1:A:768:THR:O	3:C:479:SER:OG	2.11	0.69
1:A:2183:GLN:HA	1:A:2184:GLU:C	2.18	0.69
1:A:2388:VAL:HA	1:A:2393:ARG:HD3	1.74	0.69
1:A:104:LEU:HD13	1:A:136:SER:CB	2.22	0.69
1:A:976:ASN:HD22	1:A:1077:VAL:HG21	1.58	0.69
1:A:1413:GLN:N	1:A:1415:VAL:HA	2.07	0.69
1:A:2342:LEU:HB2	1:A:2351:VAL:CG2	2.23	0.69
2:B:495:PHE:HD2	3:C:339:MET:HE2	1.58	0.69
1:A:1334:PRO:O	1:A:1396:ALA:N	2.25	0.69
1:A:1650:LYS:O	1:A:1654:GLN:HG3	1.92	0.69
1:A:2274:ASP:O	1:A:2276:PRO:HD3	1.93	0.69
1:A:84:GLU:OE1	1:A:84:GLU:N	2.24	0.69
1:A:199:VAL:HG11	1:A:263:VAL:HG22	1.74	0.69
1:A:248:VAL:O	1:A:253:LEU:HD12	1.93	0.69
1:A:1591:HIS:HB2	1:A:1599:PHE:CZ	2.27	0.69
3:C:241:GLN:HB3	3:C:245:MET:HG3	1.75	0.69
3:C:241:GLN:NE2	4:C:601:GTP:O1G	2.26	0.69
1:A:990:LEU:HD23	1:A:2395:SER:HB2	1.73	0.69
1:A:2365:LEU:CA	1:A:2366:ARG:HB3	2.23	0.69
2:B:245:ILE:O	2:B:255:LYS:NZ	2.26	0.69
1:A:1637:ALA:HB1	1:A:1675:GLN:CB	2.24	0.68
1:A:2167:MET:HE3	1:A:2193:TYR:HB3	1.75	0.68
1:A:346:LEU:HB2	1:A:385:ASP:OD2	1.94	0.68
1:A:559:PRO:O	1:A:561:LEU:HG	1.94	0.68
2:B:495:PHE:O	2:B:499:ARG:HG2	1.93	0.68
3:C:229:PRO:CG	3:C:467:GLN:HG3	2.23	0.68
1:A:350:TRP:CE3	1:A:392:SER:HB3	2.28	0.68
1:A:1942:PRO:HA	1:A:1945:VAL:HG22	1.75	0.68
1:A:2153:LEU:HD23	1:A:2207:TRP:HA	1.75	0.68
3:C:202:THR:HB	3:C:489:ILE:HD11	1.73	0.68
1:A:1665:GLU:HG3	1:A:1668:ARG:HH21	1.57	0.68
1:A:1951:LEU:HD21	1:A:2102:MET:HE1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:TYR:CE1	2:B:410:LEU:HD11	2.28	0.68
1:A:458:GLU:HG2	1:A:501:LEU:HD22	1.75	0.68
1:A:2326:MET:HE2	1:A:2326:MET:HA	1.76	0.68
1:A:2171:SER:HA	1:A:2192:HIS:HE1	1.57	0.68
1:A:2335:ASP:O	1:A:2340:ASN:ND2	2.22	0.68
1:A:295:LYS:HD2	1:A:297:VAL:HG21	1.76	0.68
1:A:820:LEU:HD11	1:A:882:TRP:HA	1.74	0.68
1:A:1538:GLU:OE1	1:A:1538:GLU:N	2.27	0.68
1:A:305:ARG:HG2	1:A:332:LYS:HD3	1.76	0.68
1:A:722:ASN:HB2	1:A:2305:THR:HG21	1.74	0.68
1:A:2276:PRO:HD2	1:A:2277:LEU:HA	1.76	0.68
1:A:183:LEU:HD23	1:A:183:LEU:H	1.59	0.68
1:A:1074:MET:O	1:A:1078:GLU:HG2	1.93	0.68
1:A:1124:GLU:OE1	1:A:1124:GLU:N	2.27	0.68
1:A:2277:LEU:HB2	1:A:2278:HIS:HB2	1.75	0.68
1:A:259:ALA:O	1:A:263:VAL:HG23	1.93	0.67
1:A:983:LEU:CD2	1:A:992:LYS:HE2	2.24	0.67
1:A:1938:SER:HB2	1:A:1945:VAL:HG21	1.76	0.67
3:C:485:LEU:HD22	3:C:490:LEU:HB2	1.76	0.67
1:A:648:ILE:HD13	1:A:714:LEU:HG	1.75	0.67
1:A:1017:TYR:HB3	1:A:1026:TRP:CB	2.23	0.67
1:A:2326:MET:SD	1:A:2401:HIS:NE2	2.67	0.67
2:B:210:LEU:HB2	2:B:265:LEU:HD23	1.77	0.67
1:A:740:VAL:HG21	1:A:752:PHE:CE2	2.29	0.67
1:A:869:ILE:HB	1:A:1295:ARG:HH12	1.59	0.67
1:A:1844:LEU:O	1:A:1848:VAL:HG13	1.93	0.67
1:A:511:ILE:HD11	1:A:576:LEU:HD11	1.77	0.67
3:C:307:ILE:O	3:C:311:LEU:HD23	1.94	0.67
1:A:345:SER:C	1:A:348:PRO:HD2	2.20	0.67
1:A:2254:TYR:HA	1:A:2257:ILE:CG2	2.24	0.67
2:B:212:LEU:HD12	2:B:267:PHE:CE1	2.30	0.67
3:C:184:VAL:CG1	3:C:188:MET:HA	2.24	0.67
3:C:268:LEU:HD12	3:C:315:CYS:SG	2.35	0.67
1:A:637:THR:HB	1:A:638:VAL:O	1.95	0.67
1:A:1085:CYS:HB3	1:A:1086:PRO:CD	2.25	0.67
1:A:2365:LEU:HB3	1:A:2366:ARG:C	2.20	0.67
1:A:421:GLY:O	1:A:425:THR:N	2.26	0.67
1:A:767:ASN:ND2	1:A:806:LEU:HD22	2.10	0.67
2:B:203:LEU:O	2:B:207:CYS:HB2	1.95	0.67
1:A:645:ASN:HB3	1:A:666:TYR:HE2	1.60	0.67
1:A:1018:THR:HG21	1:A:1084:HIS:NE2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:VAL:O	1:A:1104:LEU:HG	1.95	0.67
1:A:1703:MET:O	1:A:1707:ILE:HG13	1.95	0.67
1:A:2092:LEU:HB2	1:A:2100:ALA:HB2	1.76	0.67
3:C:260:ILE:HG12	3:C:266:VAL:HG22	1.75	0.67
1:A:239:LYS:NZ	1:A:256:THR:OG1	2.28	0.66
1:A:356:PHE:CD2	1:A:360:LEU:HG	2.30	0.66
1:A:1086:PRO:HB2	1:A:1092:ILE:CG1	2.24	0.66
3:C:256:ILE:HG12	3:C:270:THR:HG22	1.76	0.66
1:A:2139:LYS:HA	1:A:2152:TYR:O	1.95	0.66
1:A:2277:LEU:HB2	1:A:2278:HIS:HB3	1.75	0.66
2:B:52:ILE:HG22	2:B:64:LYS:HG2	1.76	0.66
1:A:141:MET:HE1	1:A:146:GLU:H	1.60	0.66
1:A:337:GLN:HB2	1:A:338:GLN:CD	2.20	0.66
1:A:992:LYS:HB2	1:A:1016:PHE:CB	2.26	0.66
2:B:329:VAL:HB	2:B:330:PRO:HD3	1.78	0.66
1:A:131:LYS:HE2	1:A:174:GLU:CG	2.24	0.66
1:A:651:SER:HA	1:A:1304:LEU:CD2	2.24	0.66
1:A:2299:GLU:HG3	1:A:2345:MET:CE	2.25	0.66
3:C:311:LEU:HD13	3:C:315:CYS:SG	2.35	0.66
3:C:485:LEU:CB	3:C:490:LEU:HD12	2.25	0.66
1:A:376:SER:HB3	1:A:448:PHE:CE1	2.31	0.66
1:A:403:ARG:HH11	1:A:470:SER:HA	1.60	0.66
1:A:419:ILE:HG21	1:A:442:ALA:H	1.61	0.66
1:A:1419:SER:HA	1:A:1422:MET:CE	2.26	0.66
1:A:636:PRO:CB	1:A:638:VAL:HG22	2.26	0.66
1:A:2169:PHE:HA	1:A:2414:LEU:HD21	1.78	0.66
2:B:303:ALA:O	2:B:307:GLN:HG3	1.95	0.66
2:B:491:ILE:HD13	3:C:519:LEU:HD23	1.76	0.66
1:A:454:THR:HB	1:A:501:LEU:HD11	1.78	0.66
1:A:503:LEU:HD13	1:A:572:MET:HG3	1.77	0.66
1:A:1757:LEU:HB3	1:A:1816:THR:CG2	2.26	0.66
2:B:237:VAL:HG13	2:B:479:LEU:HG	1.78	0.66
1:A:320:ASP:HB3	1:A:322:LEU:CD1	2.26	0.66
1:A:497:ILE:HG13	2:B:355:LEU:HD11	1.77	0.66
1:A:581:HIS:NE2	1:A:636:PRO:HA	2.10	0.66
1:A:858:HIS:CD2	1:A:860:GLN:HB2	2.31	0.66
1:A:1086:PRO:CA	1:A:1090:GLN:HB3	2.24	0.66
1:A:114:THR:O	1:A:134:ARG:NH2	2.16	0.66
1:A:131:LYS:CE	1:A:174:GLU:HG2	2.25	0.66
1:A:384:VAL:O	1:A:388:VAL:HG23	1.96	0.66
1:A:387:ASP:C	1:A:390:PRO:HD2	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ASN:O	1:A:492:CYS:N	2.19	0.66
1:A:1459:ALA:O	1:A:1463:VAL:HG23	1.96	0.66
1:A:2045:GLY:HA2	1:A:2078:LEU:HD11	1.76	0.66
1:A:39:PRO:O	1:A:43:LYS:HG3	1.96	0.66
1:A:668:LEU:HD21	1:A:1319:ASN:ND2	2.11	0.66
1:A:1502:GLU:CA	1:A:1503:MET:HB2	2.17	0.66
1:A:826:LEU:HD22	1:A:909:ASP:OD2	1.96	0.65
3:C:406:LEU:HG	3:C:422:LEU:HD22	1.77	0.65
1:A:108:LEU:HD12	1:A:109:ARG:N	2.12	0.65
1:A:1124:GLU:HG2	1:A:1212:ASP:HB3	1.78	0.65
3:C:213:GLN:NE2	3:C:275:SER:HB2	2.12	0.65
1:A:1757:LEU:HB3	1:A:1816:THR:HG22	1.77	0.65
1:A:2340:ASN:HA	1:A:2353:ILE:CG1	2.25	0.65
1:A:738:ALA:HB1	1:A:830:LEU:HD11	1.78	0.65
1:A:820:LEU:O	1:A:824:ILE:HG12	1.96	0.65
1:A:1139:ILE:HD13	1:A:1207:GLN:HE21	1.61	0.65
2:B:420:LEU:HD23	2:B:425:LYS:HD2	1.77	0.65
2:B:507:ALA:HB1	2:B:534:VAL:HG13	1.79	0.65
3:C:263:GLU:OE1	3:C:263:GLU:N	2.30	0.65
1:A:1115:GLU:OE1	1:A:1115:GLU:N	2.30	0.65
1:A:2188:PHE:CE1	1:A:2319:ARG:HD2	2.31	0.65
2:B:43:ARG:O	2:B:445:TYR:HB3	1.96	0.65
2:B:55:LYS:HG2	2:B:157:CYS:HB3	1.79	0.65
1:A:415:ARG:O	1:A:419:ILE:HG13	1.96	0.65
1:A:637:THR:HB	1:A:638:VAL:C	2.22	0.65
1:A:673:THR:HG21	1:A:1342:VAL:O	1.97	0.65
1:A:2380:GLU:HA	1:A:2383:LEU:HG	1.77	0.65
2:B:303:ALA:CB	3:C:248:ARG:HA	2.26	0.65
1:A:104:LEU:HD21	1:A:133:MET:HA	1.79	0.65
1:A:2332:GLY:HA3	1:A:2360:GLU:N	2.12	0.65
1:A:463:LEU:HG	1:A:508:VAL:HB	1.77	0.65
1:A:552:VAL:HG22	1:A:556:LYS:CE	2.26	0.65
1:A:813:ILE:HD12	1:A:1306:PRO:HB2	1.77	0.65
1:A:1289:ILE:HG21	1:A:1326:GLN:HB3	1.78	0.65
1:A:1521:VAL:CG2	1:A:1522:ALA:HA	2.27	0.65
3:C:325:PHE:CE2	3:C:387:MET:HG2	2.32	0.65
1:A:247:GLU:H	1:A:253:LEU:HD11	1.60	0.65
1:A:1403:GLN:O	1:A:1407:LEU:HD13	1.97	0.65
1:A:2300:LEU:HD23	1:A:2345:MET:CE	2.26	0.65
2:B:508:HIS:NE2	2:B:550:GLN:OE1	2.29	0.65
1:A:653:LEU:HD22	1:A:664:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2342:LEU:HD11	1:A:2353:ILE:HD11	1.79	0.65
3:C:295:LEU:CD1	3:C:296:PRO:HD2	2.27	0.65
1:A:1346:LEU:HD22	1:A:1349:LEU:HD11	1.79	0.64
1:A:2196:THR:OG1	1:A:2204:LEU:O	2.06	0.64
2:B:159:ASN:ND2	3:C:325:PHE:O	2.30	0.64
3:C:205:LEU:HB2	3:C:482:ARG:HH12	1.62	0.64
1:A:636:PRO:HB2	1:A:638:VAL:HG22	1.79	0.64
1:A:736:LEU:HD11	3:C:199:LEU:CD1	2.25	0.64
1:A:1586:SER:OG	1:A:1590:VAL:HB	1.97	0.64
2:B:211:LEU:CD2	2:B:266:LEU:HB2	2.28	0.64
1:A:174:GLU:O	1:A:178:GLN:NE2	2.30	0.64
1:A:746:GLU:OE1	1:A:747:THR:HG23	1.97	0.64
1:A:1027:LEU:HD13	1:A:1084:HIS:HB2	1.80	0.64
1:A:472:THR:O	1:A:475:CYS:N	2.28	0.64
1:A:2181:ASN:C	1:A:2182:ARG:HD2	2.22	0.64
1:A:2295:LEU:HD12	1:A:2379:ILE:CD1	2.27	0.64
2:B:347:PRO:HB3	3:C:377:GLU:OE2	1.97	0.64
3:C:228:THR:HB	3:C:229:PRO:HD2	1.78	0.64
1:A:506:LEU:HB3	1:A:510:GLN:OE1	1.97	0.64
1:A:1022:THR:HB	1:A:1415:VAL:N	2.11	0.64
1:A:1114:ALA:HA	1:A:1117:ARG:HE	1.62	0.64
1:A:2128:ILE:HA	1:A:2139:LYS:O	1.97	0.64
1:A:2131:LEU:HD21	1:A:2139:LYS:H	1.63	0.64
1:A:167:ALA:O	1:A:168:THR:OG1	2.12	0.64
1:A:1089:ILE:O	1:A:1422:MET:HE1	1.98	0.64
1:A:1592:ILE:HB	1:A:1599:PHE:HE2	1.62	0.64
1:A:2367:VAL:HG13	1:A:2368:PRO:HD2	1.79	0.64
3:C:323:ASP:OD1	3:C:373:LYS:HD2	1.98	0.64
1:A:1032:LEU:HA	1:A:1035:MET:HE2	1.78	0.64
1:A:1930:TYR:O	1:A:1934:VAL:HG23	1.98	0.64
2:B:519:TYR:CE2	2:B:521:MET:HB2	2.33	0.64
2:B:500:CYS:HB3	2:B:546:LYS:HG3	1.79	0.64
3:C:327:ASP:OD1	3:C:329:SER:OG	2.07	0.64
1:A:1289:ILE:CG2	1:A:1326:GLN:HB3	2.27	0.64
1:A:990:LEU:HB2	1:A:2392:PHE:CD1	2.33	0.64
2:B:139:GLN:NE2	2:B:152:LEU:HD11	2.08	0.64
2:B:504:LEU:HB2	2:B:550:GLN:NE2	2.12	0.64
1:A:734:TRP:O	1:A:737:GLU:N	2.31	0.63
1:A:736:LEU:HD23	1:A:736:LEU:O	1.98	0.63
1:A:980:LEU:O	1:A:984:LEU:HD13	1.98	0.63
1:A:1054:LEU:HD13	1:A:1415:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD13	2:B:359:CYS:HB3	1.79	0.63
1:A:732:MET:O	1:A:733:THR:HG22	1.98	0.63
1:A:1086:PRO:HB3	1:A:1090:GLN:HB3	1.80	0.63
1:A:1673:LEU:HD23	1:A:1705:ASP:HA	1.79	0.63
1:A:153:LEU:CD1	1:A:156:ILE:HD12	2.29	0.63
1:A:207:LEU:HA	1:A:208:GLN:C	2.23	0.63
1:A:822:LYS:O	1:A:825:PRO:HD2	1.97	0.63
2:B:42:TRP:HB2	2:B:45:ASP:CG	2.24	0.63
2:B:220:ASP:OD2	2:B:222:THR:HB	1.97	0.63
3:C:421:PHE:CZ	3:C:423:ASP:HB2	2.33	0.63
1:A:42:LEU:HB3	1:A:64:ALA:HB1	1.81	0.63
1:A:893:LEU:HD22	1:A:914:GLN:OE1	1.99	0.63
1:A:1753:THR:CG2	1:A:1788:ALA:HB1	2.25	0.63
1:A:1095:TRP:NE1	1:A:1099:ILE:HD11	2.14	0.63
1:A:2337:HIS:O	1:A:2375:MET:HE1	1.98	0.63
2:B:238:LEU:CG	2:B:242:LYS:HE3	2.28	0.63
3:C:181:ILE:O	3:C:258:PHE:N	2.31	0.63
1:A:1038:GLY:HA3	1:A:1102:LYS:CE	2.26	0.63
1:A:1361:GLU:N	1:A:1361:GLU:OE1	2.31	0.63
1:A:1656:LEU:C	1:A:1658:PRO:HD2	2.24	0.63
3:C:208:GLY:HA3	3:C:311:LEU:HD12	1.80	0.63
1:A:148:ARG:C	1:A:153:LEU:HD22	2.23	0.63
1:A:766:ALA:O	1:A:770:VAL:HG23	1.98	0.63
1:A:1207:GLN:HB3	1:A:1289:ILE:HD11	1.81	0.63
1:A:1306:PRO:HG2	1:A:2306:THR:CB	2.26	0.63
1:A:2217:LEU:HD12	1:A:2218:TYR:N	2.14	0.63
1:A:1338:SER:N	1:A:1339:THR:HA	2.11	0.63
1:A:1475:VAL:HG23	1:A:1528:LEU:CD1	2.27	0.63
1:A:2215:PHE:HB3	1:A:2339:ASP:OD1	1.99	0.63
2:B:217:CYS:SG	2:B:271:LEU:HD23	2.38	0.63
2:B:458:VAL:O	2:B:479:LEU:HD22	1.98	0.63
1:A:249:LYS:HD3	1:A:297:VAL:HG13	1.81	0.63
1:A:447:PHE:CE1	1:A:491:THR:HG23	2.34	0.63
1:A:650:HIS:O	1:A:1304:LEU:HD22	1.99	0.63
1:A:740:VAL:HB	1:A:751:LEU:HB2	1.80	0.63
1:A:1521:VAL:HG22	1:A:1522:ALA:CA	2.28	0.63
1:A:1673:LEU:CD2	1:A:1705:ASP:HA	2.29	0.63
2:B:58:LEU:HD11	3:C:390:MET:SD	2.38	0.63
1:A:294:CYS:O	1:A:295:LYS:HD3	1.98	0.62
1:A:1186:LEU:HD13	1:A:1199:ASP:HB3	1.80	0.62
1:A:1669:ILE:O	1:A:1673:LEU:HD13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:GLU:OE1	1:A:773:VAL:HG13	1.99	0.62
1:A:1816:THR:CB	1:A:1817:ALA:HA	2.29	0.62
1:A:2038:LYS:HG3	1:A:2095:ILE:CD1	2.29	0.62
3:C:201:GLN:OE1	3:C:264:ARG:HG3	1.99	0.62
1:A:1073:ILE:O	1:A:1077:VAL:HG23	1.99	0.62
1:A:1509:ILE:HB	1:A:1598:ASP:CG	2.24	0.62
1:A:2040:PHE:O	1:A:2044:TYR:N	2.28	0.62
1:A:2191:ARG:CG	1:A:2351:VAL:HG12	2.29	0.62
1:A:2246:VAL:N	1:A:2247:PRO:HA	2.14	0.62
1:A:2387:GLY:C	1:A:2391:VAL:HG21	2.25	0.62
1:A:85:LYS:HD2	1:A:116:PRO:HG2	1.79	0.62
1:A:274:GLN:CB	1:A:275:LEU:HD23	2.29	0.62
1:A:280:LEU:HD23	1:A:283:ILE:HD12	1.81	0.62
1:A:769:LEU:HD22	3:C:263:GLU:CG	2.30	0.62
2:B:262:PRO:HB2	2:B:326:LEU:HD11	1.81	0.62
3:C:340:VAL:HG11	3:C:512:LEU:HD21	1.81	0.62
3:C:367:LEU:HD11	3:C:400:LEU:CD2	2.29	0.62
1:A:239:LYS:HE2	1:A:243:SER:HB3	1.82	0.62
1:A:566:LYS:HD2	1:A:625:LYS:NZ	2.14	0.62
1:A:675:HIS:N	1:A:676:ASP:HB2	2.13	0.62
1:A:1815:PRO:HB2	1:A:1819:TRP:CZ3	2.35	0.62
1:A:2020:ALA:O	1:A:2024:VAL:HG13	1.98	0.62
1:A:2037:GLU:HG3	1:A:2094:GLU:CA	2.25	0.62
1:A:2296:LEU:O	1:A:2296:LEU:HD23	1.99	0.62
2:B:162:LEU:HD22	3:C:390:MET:CE	2.29	0.62
2:B:238:LEU:HD11	2:B:242:LYS:HE3	1.82	0.62
3:C:208:GLY:HA3	3:C:311:LEU:CD1	2.29	0.62
1:A:190:ASP:HA	1:A:193:LEU:HG	1.80	0.62
1:A:893:LEU:HB3	1:A:910:ALA:O	2.00	0.62
1:A:999:GLU:OE1	1:A:999:GLU:N	2.32	0.62
1:A:1336:ARG:HB3	1:A:1337:LEU:HD23	1.81	0.62
1:A:2304:CYS:SG	1:A:2310:TRP:HA	2.39	0.62
3:C:205:LEU:HB2	3:C:482:ARG:HH22	1.64	0.62
1:A:295:LYS:HA	1:A:296:CYS:HB3	1.79	0.62
1:A:803:ARG:NH2	1:A:805:GLN:HB3	2.14	0.62
1:A:895:LYS:CD	1:A:907:LYS:HE2	2.30	0.62
1:A:2388:VAL:HG12	1:A:2393:ARG:HD3	1.82	0.62
1:A:813:ILE:HG13	1:A:881:ASN:HD21	1.65	0.62
1:A:920:ALA:HA	1:A:923:PHE:CE2	2.35	0.62
1:A:985:GLN:OE1	1:A:985:GLN:N	2.32	0.62
1:A:1786:VAL:HG11	1:A:2172:ILE:CD1	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1841:ILE:O	1:A:1845:LEU:HD23	2.00	0.62
2:B:42:TRP:HB2	2:B:45:ASP:OD2	2.00	0.62
1:A:223:ALA:HB3	1:A:270:SER:HB3	1.82	0.62
1:A:388:VAL:O	1:A:391:PRO:HD2	1.99	0.62
1:A:467:LEU:O	1:A:467:LEU:HD12	2.00	0.62
1:A:553:LEU:O	1:A:557:ASN:HB2	2.00	0.62
1:A:1027:LEU:HD11	1:A:1085:CYS:SG	2.39	0.62
1:A:1192:GLU:O	1:A:1195:ILE:HG22	2.00	0.62
1:A:1300:LEU:HD21	1:A:1316:ILE:HG13	1.82	0.62
1:A:1406:LEU:O	1:A:1410:ILE:HG13	2.00	0.62
1:A:1485:ILE:HG22	1:A:1488:THR:HG22	1.80	0.62
2:B:504:LEU:HD13	2:B:550:GLN:CG	2.29	0.62
1:A:261:GLU:OE1	1:A:303:VAL:HG13	2.00	0.62
1:A:558:ILE:N	1:A:559:PRO:HD3	2.15	0.62
3:C:410:GLN:HB2	3:C:472:LYS:CD	2.30	0.62
3:C:505:GLY:O	3:C:509:SER:HB2	2.00	0.62
1:A:379:ALA:HB3	1:A:382:GLU:CG	2.30	0.61
1:A:473:ILE:HA	1:A:476:ASP:HB3	1.82	0.61
1:A:746:GLU:CD	1:A:747:THR:HG23	2.25	0.61
1:A:2311:TRP:O	1:A:2315:GLN:HG2	2.00	0.61
1:A:2340:ASN:HA	1:A:2353:ILE:HG12	1.82	0.61
2:B:238:LEU:HG	2:B:242:LYS:HE3	1.82	0.61
3:C:410:GLN:HB2	3:C:472:LYS:CE	2.30	0.61
1:A:135:LYS:NZ	1:A:173:LYS:O	2.32	0.61
1:A:412:ILE:HG22	1:A:453:LEU:HD11	1.82	0.61
1:A:176:ILE:HG23	1:A:177:GLN:OE1	2.01	0.61
1:A:490:GLN:HA	3:C:381:PRO:HG2	1.81	0.61
1:A:891:GLN:HB3	1:A:894:ASP:HB3	1.82	0.61
2:B:221:ILE:HD13	3:C:279:LEU:HD22	1.82	0.61
3:C:312:PHE:HE1	3:C:318:VAL:HG11	1.65	0.61
1:A:360:LEU:HD13	1:A:361:LEU:N	2.16	0.61
1:A:554:SER:OG	1:A:608:LYS:HG2	1.99	0.61
1:A:571:GLU:OE2	3:C:453:LEU:HB3	2.01	0.61
1:A:920:ALA:HA	1:A:923:PHE:CD2	2.36	0.61
1:A:994:MET:HA	1:A:2390:GLY:O	2.00	0.61
1:A:646:LEU:HG	1:A:674:ARG:O	2.00	0.61
1:A:852:ALA:HB3	1:A:853:PRO:HD3	1.81	0.61
1:A:898:GLN:NE2	1:A:2212:THR:OG1	2.32	0.61
1:A:1336:ARG:CB	1:A:1337:LEU:HA	2.21	0.61
1:A:2099:LEU:HD13	1:A:2102:MET:SD	2.40	0.61
1:A:131:LYS:NZ	1:A:159:GLU:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LEU:CD1	1:A:648:ILE:HD12	2.30	0.61
1:A:720:LYS:HE3	1:A:2346:THR:HG21	1.81	0.61
1:A:897:ASP:HB2	1:A:2299:GLU:OE1	2.00	0.61
2:B:309:TYR:O	2:B:313:ARG:HG2	2.00	0.61
3:C:498:TYR:CZ	3:C:502:ILE:HD11	2.35	0.61
1:A:113:VAL:O	1:A:117:GLU:HG3	2.01	0.61
1:A:171:GLN:HG2	1:A:175:PHE:CE1	2.36	0.61
1:A:1086:PRO:CB	1:A:1090:GLN:HB3	2.31	0.61
1:A:1335:LEU:HD23	1:A:1335:LEU:H	1.64	0.61
1:A:1350:SER:O	1:A:1354:LEU:HB2	2.00	0.61
2:B:268:LEU:HD22	2:B:335:PHE:HB3	1.82	0.61
1:A:115:SER:HA	1:A:155:ARG:NH1	2.14	0.61
1:A:295:LYS:CA	1:A:296:CYS:HB3	2.31	0.61
1:A:2170:LEU:HD11	1:A:2355:TYR:HE2	1.65	0.61
2:B:456:TYR:O	2:B:460:ILE:N	2.31	0.61
1:A:411:SER:CB	1:A:435:ARG:H	2.13	0.61
1:A:769:LEU:CD1	3:C:265:ILE:HD11	2.30	0.61
1:A:803:ARG:HG2	1:A:804:VAL:H	1.66	0.61
1:A:1629:TRP:O	1:A:1633:VAL:HG23	2.00	0.61
1:A:1938:SER:CA	1:A:1945:VAL:HG11	2.29	0.61
1:A:2092:LEU:CB	1:A:2100:ALA:HB2	2.31	0.61
2:B:63:GLU:HG3	2:B:270:GLN:NE2	2.16	0.61
3:C:403:LYS:CB	3:C:421:PHE:HB2	2.31	0.61
1:A:275:LEU:HB2	1:A:276:VAL:CA	2.30	0.60
1:A:388:VAL:C	1:A:391:PRO:HD2	2.25	0.60
1:A:866:ILE:HA	1:A:1295:ARG:HH21	1.64	0.60
1:A:2055:LEU:HD13	1:A:2070:PRO:CD	2.31	0.60
2:B:497:GLU:O	2:B:501:GLN:HG2	2.01	0.60
1:A:91:ASN:OD1	1:A:92:GLY:N	2.30	0.60
1:A:251:LEU:HD23	1:A:251:LEU:H	1.65	0.60
1:A:294:CYS:O	1:A:296:CYS:HB3	2.01	0.60
1:A:1070:GLU:OE1	1:A:1070:GLU:N	2.33	0.60
1:A:2245:ILE:HB	1:A:2246:VAL:O	2.01	0.60
1:A:497:ILE:HG13	2:B:355:LEU:CD1	2.31	0.60
1:A:1468:LYS:O	1:A:1472:GLN:HG3	2.00	0.60
1:A:1502:GLU:CG	1:A:1504:LEU:HD23	2.29	0.60
1:A:1526:LEU:O	1:A:1530:LYS:HG2	2.01	0.60
1:A:1711:LEU:HD22	1:A:1712:ILE:HD12	1.83	0.60
1:A:1597:PRO:HG3	1:A:1629:TRP:CG	2.36	0.60
1:A:2125:GLY:HA3	1:A:2141:LEU:O	2.02	0.60
1:A:38:ASP:O	1:A:42:LEU:HD13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD12	1:A:185:LEU:O	2.01	0.60
1:A:455:ALA:HB2	2:B:355:LEU:HD21	1.82	0.60
1:A:822:LYS:HZ2	1:A:830:LEU:HG	1.65	0.60
1:A:1589:THR:HA	1:A:1593:GLY:HA3	1.83	0.60
1:A:2280:MET:HA	1:A:2283:VAL:HG12	1.83	0.60
3:C:221:MET:HE2	3:C:221:MET:HA	1.83	0.60
1:A:269:PHE:HE1	1:A:310:ILE:HG12	1.66	0.60
1:A:326:HIS:O	1:A:330:THR:N	2.29	0.60
1:A:2323:VAL:HA	1:A:2400:LEU:CD2	2.31	0.60
1:A:153:LEU:HD23	1:A:187:LYS:HZ1	1.67	0.60
1:A:571:GLU:HG2	3:C:457:LEU:CD2	2.32	0.60
1:A:739:ALA:N	1:A:830:LEU:HD22	2.16	0.60
1:A:740:VAL:HG11	1:A:752:PHE:CE1	2.36	0.60
1:A:820:LEU:HD22	1:A:886:LEU:CB	2.21	0.60
1:A:2180:ILE:CG2	1:A:2403:MET:HE3	2.31	0.60
2:B:202:TYR:OH	2:B:452:ALA:HB1	2.01	0.60
3:C:389:LEU:O	3:C:393:GLN:HG2	2.00	0.60
1:A:508:VAL:HG23	1:A:509:GLU:CD	2.27	0.60
1:A:573:THR:HB	1:A:613:PHE:CZ	2.36	0.60
1:A:751:LEU:HD22	3:C:174:PRO:CG	2.27	0.60
3:C:212:LEU:HD11	3:C:327:ASP:OD2	2.02	0.60
1:A:1025:ASP:OD1	1:A:1026:TRP:N	2.35	0.60
1:A:2296:LEU:HD13	1:A:2383:LEU:HD11	1.84	0.60
2:B:49:VAL:HG21	2:B:448:TRP:NE1	2.16	0.60
2:B:220:ASP:HB3	2:B:223:TYR:HD2	1.66	0.60
2:B:441:GLU:O	2:B:443:PRO:HD3	2.02	0.60
3:C:328:LEU:O	3:C:328:LEU:HD23	2.01	0.60
1:A:1816:THR:H	1:A:1817:ALA:HB2	1.67	0.59
1:A:2069:ILE:HG13	1:A:2070:PRO:CD	2.28	0.59
2:B:181:PRO:HG2	2:B:184:GLU:OE1	2.02	0.59
2:B:238:LEU:CD1	2:B:242:LYS:HE3	2.32	0.59
1:A:294:CYS:C	1:A:296:CYS:HB3	2.27	0.59
1:A:2043:ASN:O	1:A:2047:ALA:HB2	2.01	0.59
1:A:2092:LEU:O	1:A:2097:PRO:HA	2.03	0.59
1:A:2325:SER:CB	1:A:2374:ARG:HG3	2.32	0.59
3:C:216:GLY:HA2	4:C:601:GTP:PA	2.42	0.59
1:A:131:LYS:HE3	1:A:159:GLU:OE1	2.02	0.59
1:A:618:LEU:CD1	1:A:648:ILE:HG23	2.30	0.59
1:A:1074:MET:HA	1:A:1077:VAL:HB	1.83	0.59
1:A:2325:SER:OG	1:A:2374:ARG:HG3	2.02	0.59
2:B:301:GLN:O	2:B:305:GLU:HG3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:ALA:HB2	2:B:538:HIS:CD2	2.37	0.59
1:A:241:SER:O	1:A:245:LYS:HG2	2.03	0.59
1:A:675:HIS:HB2	1:A:676:ASP:CG	2.28	0.59
1:A:1502:GLU:HB3	1:A:1504:LEU:H	1.67	0.59
1:A:2167:MET:CE	1:A:2193:TYR:HB3	2.32	0.59
1:A:2169:PHE:O	1:A:2173:VAL:HG23	2.02	0.59
2:B:134:ASP:HB3	2:B:165:ALA:HA	1.83	0.59
2:B:220:ASP:HB3	2:B:223:TYR:CD2	2.37	0.59
2:B:546:LYS:O	2:B:550:GLN:HG3	2.01	0.59
3:C:183:LEU:O	3:C:191:CYS:N	2.34	0.59
3:C:345:PRO:CG	3:C:486:SER:HB2	2.21	0.59
1:A:112:ASN:OD1	1:A:113:VAL:N	2.35	0.59
1:A:261:GLU:HB3	1:A:303:VAL:HG22	1.85	0.59
1:A:269:PHE:CE1	1:A:310:ILE:HG12	2.38	0.59
2:B:512:GLN:CB	2:B:557:LYS:HE3	2.32	0.59
1:A:1942:PRO:O	1:A:1946:LEU:HD23	2.02	0.59
1:A:1945:VAL:O	1:A:1949:GLN:HG3	2.02	0.59
1:A:2195:VAL:CA	1:A:2205:ILE:HG22	2.31	0.59
2:B:155:SER:HB2	2:B:196:GLN:CG	2.32	0.59
3:C:410:GLN:NE2	3:C:464:PRO:HB3	2.17	0.59
1:A:511:ILE:CD1	1:A:576:LEU:HD11	2.33	0.59
1:A:1313:TRP:CB	1:A:1354:LEU:HD11	2.32	0.59
1:A:1648:ARG:HB2	1:A:1667:GLU:OE1	2.02	0.59
1:A:2420:ASP:N	1:A:2421:PRO:HD3	2.18	0.59
1:A:2421:PRO:HG2	1:A:2424:ASP:HB3	1.85	0.59
1:A:117:GLU:CD	1:A:134:ARG:HG3	2.27	0.59
1:A:503:LEU:HD13	1:A:572:MET:HE2	1.84	0.59
1:A:602:PHE:CB	1:A:603:ASN:HA	2.32	0.59
1:A:822:LYS:HZ3	1:A:829:VAL:N	2.01	0.59
1:A:2089:ILE:CG1	1:A:2128:ILE:HG13	2.33	0.59
2:B:234:ARG:NH1	2:B:238:LEU:HD13	2.17	0.59
2:B:503:ALA:HB2	2:B:538:HIS:HD2	1.67	0.59
1:A:193:LEU:HD12	1:A:194:ALA:N	2.18	0.59
1:A:715:GLY:O	1:A:719:LYS:HG3	2.03	0.59
1:A:838:ILE:HG23	1:A:918:TRP:CE2	2.38	0.59
1:A:893:LEU:HD12	1:A:894:ASP:N	2.17	0.59
1:A:207:LEU:CB	1:A:209:GLU:HG2	2.33	0.59
1:A:772:ASP:OD2	3:C:482:ARG:HG2	2.02	0.59
1:A:939:THR:HG23	1:A:2301:TRP:HE1	1.67	0.59
1:A:2285:GLU:O	1:A:2289:GLU:HG2	2.03	0.59
1:A:2390:GLY:N	1:A:2394:LEU:HD13	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:OE2	2:B:75:GLN:NE2	2.35	0.58
1:A:737:GLU:O	1:A:740:VAL:HG22	2.02	0.58
1:A:358:THR:O	1:A:398:LEU:HD22	2.02	0.58
1:A:360:LEU:O	1:A:401:LEU:HD22	2.04	0.58
1:A:496:TYR:CE2	3:C:460:TYR:HB2	2.37	0.58
1:A:656:HIS:N	1:A:660:ILE:HD11	2.16	0.58
1:A:719:LYS:HG2	1:A:1307:ILE:HG21	1.83	0.58
2:B:250:VAL:HB	2:B:254:TRP:CE3	2.38	0.58
2:B:296:PRO:HB3	3:C:246:LYS:HD2	1.84	0.58
1:A:720:LYS:HE3	1:A:2346:THR:CG2	2.33	0.58
1:A:1947:GLN:O	1:A:1951:LEU:HG	2.03	0.58
1:A:2276:PRO:CG	1:A:2280:MET:HG3	2.33	0.58
2:B:333:GLN:N	2:B:333:GLN:OE1	2.37	0.58
1:A:153:LEU:HD23	1:A:187:LYS:NZ	2.17	0.58
1:A:163:ASP:HA	1:A:170:LYS:CE	2.27	0.58
1:A:275:LEU:HD13	1:A:277:MET:HG2	1.85	0.58
1:A:503:LEU:HB2	1:A:572:MET:HE2	1.85	0.58
1:A:811:THR:CA	1:A:814:ARG:HG2	2.26	0.58
1:A:1787:MET:CB	1:A:2410:LEU:HG	2.34	0.58
3:C:298:THR:O	3:C:302:MET:HG2	2.03	0.58
3:C:476:GLN:O	3:C:480:MET:HG2	2.03	0.58
1:A:1021:GLN:NE2	1:A:1054:LEU:HB2	2.18	0.58
2:B:157:CYS:SG	2:B:196:GLN:NE2	2.73	0.58
3:C:312:PHE:HA	3:C:365:PRO:HG3	1.83	0.58
3:C:486:SER:HB3	3:C:498:TYR:OH	2.04	0.58
1:A:82:ASN:HA	1:A:85:LYS:HE2	1.86	0.58
1:A:131:LYS:HE3	1:A:159:GLU:HB3	1.85	0.58
1:A:634:LEU:HD23	1:A:634:LEU:O	2.02	0.58
1:A:1514:SER:OG	1:A:1530:LYS:HE3	2.03	0.58
1:A:2042:ASP:HA	1:A:2046:ASP:HB3	1.85	0.58
1:A:2342:LEU:HB2	1:A:2351:VAL:HG22	1.85	0.58
2:B:233:LEU:HD11	2:B:486:GLU:OE2	2.02	0.58
2:B:494:LYS:HD2	3:C:518:LEU:HD22	1.86	0.58
1:A:870:LEU:CB	1:A:1298:VAL:HG11	2.33	0.58
1:A:1292:GLN:HB3	1:A:1322:LYS:HD3	1.86	0.58
1:A:1753:THR:HB	1:A:1792:LEU:HD21	1.84	0.58
1:A:2180:ILE:HG21	1:A:2403:MET:HE3	1.85	0.58
1:A:1121:ALA:O	1:A:1122:SER:OG	2.18	0.58
1:A:1324:LEU:HD11	1:A:1339:THR:CG2	2.33	0.58
1:A:1338:SER:HB2	1:A:1339:THR:C	2.28	0.58
1:A:2129:THR:O	1:A:2138:LYS:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2284:LEU:CD1	1:A:2288:MET:HE3	2.31	0.58
1:A:2366:ARG:O	1:A:2367:VAL:HG23	2.03	0.58
2:B:59:ARG:HH12	3:C:375:ARG:HG3	1.68	0.58
1:A:769:LEU:HD22	3:C:263:GLU:CB	2.33	0.58
1:A:841:ILE:HD13	1:A:882:TRP:HZ3	1.69	0.58
1:A:2168:GLN:O	1:A:2172:ILE:HG12	2.02	0.58
1:A:2216:GLY:O	1:A:2220:ARG:HG2	2.04	0.58
2:B:547:TYR:O	2:B:551:LEU:HG	2.04	0.58
1:A:406:SER:HB3	1:A:410:ARG:CZ	2.34	0.58
1:A:675:HIS:H	1:A:676:ASP:CB	2.17	0.58
1:A:736:LEU:HD12	3:C:201:GLN:HB2	1.86	0.58
1:A:1323:TYR:O	1:A:1326:GLN:HG2	2.04	0.58
1:A:2248:ARG:CB	1:A:2251:GLU:HG2	2.34	0.58
2:B:540:ARG:NH1	3:C:364:TYR:OH	2.37	0.58
3:C:325:PHE:CE1	3:C:391:ILE:HD11	2.35	0.58
1:A:544:VAL:O	1:A:548:VAL:HG23	2.04	0.57
1:A:1856:ILE:HB	1:A:1859:PRO:CG	2.33	0.57
1:A:2128:ILE:HG22	1:A:2140:LEU:CB	2.32	0.57
1:A:2166:ILE:HG21	1:A:2355:TYR:HD2	1.68	0.57
1:A:2169:PHE:CE1	1:A:2411:LEU:HD22	2.39	0.57
2:B:491:ILE:HG23	3:C:518:LEU:HB3	1.86	0.57
1:A:633:ALA:C	1:A:636:PRO:HD2	2.29	0.57
1:A:805:GLN:HG3	1:A:806:LEU:H	1.69	0.57
1:A:2138:LYS:O	1:A:2153:LEU:HA	2.04	0.57
1:A:2365:LEU:HB3	1:A:2367:VAL:N	2.19	0.57
1:A:328:ASP:O	1:A:332:LYS:HG3	2.05	0.57
1:A:402:LEU:O	1:A:402:LEU:HD23	2.04	0.57
1:A:569:LEU:O	1:A:573:THR:HG23	2.05	0.57
1:A:1289:ILE:HG22	1:A:1293:LEU:CD2	2.35	0.57
1:A:1368:LEU:HD12	1:A:1368:LEU:O	2.05	0.57
1:A:1619:TRP:HB2	1:A:1756:LYS:HB2	1.84	0.57
1:A:1648:ARG:O	1:A:1652:GLU:HG3	2.04	0.57
1:A:2323:VAL:O	1:A:2327:VAL:HG23	2.04	0.57
2:B:48:CYS:SG	2:B:148:VAL:HG22	2.45	0.57
2:B:221:ILE:CG2	3:C:274:LEU:HB3	2.34	0.57
3:C:318:VAL:HB	3:C:367:LEU:HD23	1.86	0.57
1:A:69:GLN:HG3	1:A:102:LYS:HG2	1.86	0.57
1:A:675:HIS:CA	1:A:676:ASP:HB2	2.34	0.57
1:A:727:THR:HG22	1:A:899:SER:O	2.05	0.57
1:A:885:ARG:HA	1:A:888:TYR:CD2	2.39	0.57
1:A:2336:ARG:HB3	1:A:2375:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:312:PHE:CD1	3:C:318:VAL:HG21	2.39	0.57
1:A:1307:ILE:HB	1:A:2306:THR:HG21	1.86	0.57
1:A:1346:LEU:HD22	1:A:1349:LEU:CD1	2.34	0.57
1:A:1845:LEU:O	1:A:1848:VAL:HG22	2.05	0.57
3:C:383:LYS:O	3:C:387:MET:HG3	2.05	0.57
1:A:190:ASP:HA	1:A:193:LEU:CD2	2.35	0.57
1:A:660:ILE:O	1:A:664:VAL:HG23	2.04	0.57
1:A:2023:HIS:O	1:A:2027:ILE:HG12	2.04	0.57
1:A:2042:ASP:HA	1:A:2046:ASP:CB	2.35	0.57
3:C:244:GLU:HA	3:C:247:GLU:CG	2.33	0.57
3:C:427:ASN:OD1	3:C:469:LEU:HD12	2.04	0.57
1:A:295:LYS:HD2	1:A:297:VAL:CG2	2.34	0.57
1:A:309:HIS:O	1:A:313:THR:OG1	2.17	0.57
1:A:419:ILE:HD13	1:A:441:THR:H	1.70	0.57
1:A:449:SER:O	1:A:453:LEU:HG	2.05	0.57
1:A:978:LEU:O	1:A:982:LEU:HG	2.05	0.57
1:A:194:ALA:HA	1:A:197:HIS:CE1	2.40	0.57
1:A:220:LEU:HD23	1:A:270:SER:OG	2.05	0.57
1:A:290:PRO:HA	1:A:294:CYS:SG	2.44	0.57
1:A:566:LYS:NZ	1:A:620:THR:HG23	2.20	0.57
1:A:1827:PHE:CZ	1:A:1859:PRO:HB2	2.40	0.57
1:A:110:VAL:O	1:A:146:GLU:HG3	2.04	0.57
1:A:244:ALA:HB1	1:A:290:PRO:HB2	1.86	0.57
1:A:1296:SER:HB2	1:A:1322:LYS:HE3	1.87	0.57
1:A:1410:ILE:HG21	1:A:1424:LEU:CD2	2.33	0.57
1:A:1502:GLU:CB	1:A:1504:LEU:HB2	2.33	0.57
1:A:1751:TYR:O	1:A:1755:LEU:HG	2.04	0.57
1:A:2129:THR:HG22	1:A:2131:LEU:H	1.69	0.57
1:A:2277:LEU:CA	1:A:2278:HIS:HB3	2.34	0.57
1:A:2330:ILE:HD12	1:A:2404:ARG:NH1	2.16	0.57
2:B:546:LYS:O	2:B:550:GLN:N	2.37	0.57
3:C:244:GLU:HG3	3:C:248:ARG:HH22	1.70	0.57
3:C:386:GLN:O	3:C:390:MET:HG3	2.05	0.57
1:A:336:THR:HA	1:A:342:TRP:HZ2	1.69	0.57
1:A:1071:VAL:HG11	1:A:1074:MET:CG	2.31	0.57
1:A:1422:MET:O	1:A:1426:LEU:HG	2.05	0.57
1:A:1981:ILE:HG12	1:A:2067:SER:HA	1.87	0.57
1:A:2317:TYR:OH	1:A:2383:LEU:HD12	2.05	0.57
3:C:220:VAL:HG11	3:C:370:LEU:CD1	2.35	0.57
1:A:237:PHE:HA	1:A:240:PHE:CB	2.33	0.56
1:A:842:SER:HB2	1:A:918:TRP:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:TYR:O	1:A:1406:LEU:HD13	2.05	0.56
1:A:2342:LEU:O	1:A:2350:VAL:HG13	2.05	0.56
2:B:67:LEU:O	2:B:71:VAL:HG23	2.05	0.56
2:B:208:HIS:O	2:B:263:PRO:HA	2.05	0.56
3:C:188:MET:HE3	3:C:503:TRP:HH2	1.70	0.56
3:C:364:TYR:O	3:C:401:ARG:NH1	2.38	0.56
1:A:336:THR:HA	1:A:342:TRP:CZ2	2.41	0.56
1:A:494:THR:HA	1:A:497:ILE:HG22	1.87	0.56
1:A:496:TYR:O	1:A:500:VAL:HG23	2.06	0.56
1:A:645:ASN:HB3	1:A:666:TYR:CE2	2.41	0.56
1:A:1820:ARG:CB	1:A:1848:VAL:HB	2.34	0.56
1:A:1978:LEU:O	1:A:1982:GLN:HG3	2.05	0.56
2:B:311:ILE:HG12	3:C:279:LEU:HD23	1.87	0.56
1:A:131:LYS:CE	1:A:159:GLU:HB3	2.36	0.56
1:A:300:ILE:CG2	1:A:302:LEU:HG	2.35	0.56
1:A:412:ILE:CG2	1:A:453:LEU:HD11	2.35	0.56
1:A:817:PHE:CE2	1:A:821:LEU:HD11	2.40	0.56
1:A:982:LEU:HD12	1:A:992:LYS:HG2	1.87	0.56
1:A:989:ASN:OD1	1:A:990:LEU:HD12	2.04	0.56
1:A:1186:LEU:HD13	1:A:1199:ASP:CB	2.35	0.56
1:A:1673:LEU:HD21	1:A:1708:TRP:CD1	2.35	0.56
1:A:2408:GLU:O	1:A:2412:THR:HG23	2.04	0.56
2:B:254:TRP:CZ2	2:B:260:PRO:HG3	2.39	0.56
3:C:409:LEU:HD21	3:C:476:GLN:NE2	2.20	0.56
2:B:41:PRO:HB2	2:B:42:TRP:CE3	2.40	0.56
1:A:136:SER:HA	1:A:139:ARG:HG2	1.88	0.56
1:A:188:GLN:HG3	1:A:226:SER:HB2	1.86	0.56
1:A:851:LYS:HE3	1:A:856:THR:H	1.70	0.56
2:B:4:PRO:HA	2:B:140:ALA:O	2.05	0.56
1:A:1478:LYS:O	1:A:1481:PRO:HD2	2.05	0.56
2:B:159:ASN:CG	3:C:326:THR:HB	2.31	0.56
1:A:417:SER:O	1:A:420:ARG:HG2	2.06	0.56
1:A:1349:LEU:HD23	1:A:1355:TYR:CE1	2.40	0.56
1:A:1349:LEU:HB3	1:A:1355:TYR:HE1	1.70	0.56
1:A:2276:PRO:C	1:A:2279:VAL:HB	2.31	0.56
1:A:2301:TRP:HA	1:A:2310:TRP:CD1	2.40	0.56
1:A:2366:ARG:HA	1:A:2366:ARG:NE	2.21	0.56
2:B:248:CYS:HB2	2:B:255:LYS:HZ3	1.71	0.56
2:B:271:LEU:HG	2:B:336:VAL:HG12	1.87	0.56
2:B:445:TYR:CZ	2:B:449:ILE:HD11	2.41	0.56
3:C:409:LEU:HD21	3:C:476:GLN:CD	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:474:ARG:CG	3:C:478:MET:HE3	2.35	0.56
1:A:104:LEU:HD21	1:A:133:MET:CA	2.35	0.56
1:A:420:ARG:O	1:A:423:PRO:HG2	2.06	0.56
1:A:435:ARG:HG3	1:A:436:VAL:N	2.18	0.56
1:A:642:LEU:O	1:A:646:LEU:HD23	2.06	0.56
1:A:2176:MET:HE3	1:A:2407:ARG:CB	2.32	0.56
2:B:134:ASP:O	2:B:192:GLN:NE2	2.38	0.56
2:B:547:TYR:CZ	2:B:551:LEU:HD11	2.40	0.56
3:C:367:LEU:HD11	3:C:400:LEU:HD23	1.86	0.56
1:A:104:LEU:HD21	1:A:133:MET:CB	2.36	0.56
1:A:419:ILE:O	1:A:422:PRO:HD2	2.05	0.56
1:A:488:ASN:CB	1:A:495:ASP:HB2	2.36	0.56
1:A:772:ASP:O	1:A:774:ASN:HA	2.06	0.56
1:A:905:LEU:HD12	1:A:906:LEU:N	2.21	0.56
1:A:1026:TRP:O	1:A:1030:ILE:HG13	2.05	0.56
1:A:1086:PRO:CB	1:A:1092:ILE:HG12	2.29	0.56
1:A:1832:HIS:CD2	1:A:1837:VAL:HG21	2.40	0.56
1:A:2053:GLU:OE1	1:A:2057:THR:OG1	2.14	0.56
1:A:2320:SER:O	1:A:2323:VAL:HG22	2.05	0.56
2:B:139:GLN:HG3	2:B:152:LEU:HG	1.88	0.56
2:B:311:ILE:HG23	3:C:297:HIS:HE1	1.71	0.56
2:B:315:SER:HB2	3:C:297:HIS:NE2	2.20	0.56
3:C:380:CYS:O	3:C:384:LEU:HD23	2.06	0.56
1:A:404:VAL:O	1:A:408:VAL:HG23	2.06	0.56
1:A:433:LEU:CD2	1:A:471:MET:HG2	2.26	0.56
1:A:992:LYS:HD2	1:A:1016:PHE:CB	2.35	0.56
1:A:1054:LEU:HD13	1:A:1415:VAL:CG2	2.35	0.56
1:A:2073:GLU:OE1	1:A:2073:GLU:N	2.35	0.56
1:A:2277:LEU:CB	1:A:2278:HIS:HB3	2.36	0.56
3:C:278:ILE:O	3:C:282:LEU:HG	2.06	0.56
1:A:730:LEU:CD1	1:A:771:GLU:HB3	2.35	0.55
1:A:1655:ASN:HB2	1:A:1663:GLU:OE2	2.06	0.55
2:B:267:PHE:O	2:B:268:LEU:HD23	2.06	0.55
1:A:262:THR:N	1:A:303:VAL:HG21	2.20	0.55
1:A:506:LEU:HD22	1:A:549:TYR:CZ	2.41	0.55
1:A:1412:GLU:HA	1:A:1413:GLN:O	2.06	0.55
3:C:332:ARG:O	3:C:336:THR:HG23	2.07	0.55
3:C:408:MET:HA	3:C:408:MET:CE	2.32	0.55
1:A:230:GLU:O	1:A:234:LYS:HG3	2.06	0.55
1:A:346:LEU:HA	1:A:349:PHE:CD1	2.40	0.55
1:A:937:GLN:O	1:A:941:GLN:N	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:GLN:HG3	1:A:1091:GLY:H	1.71	0.55
3:C:302:MET:O	3:C:306:GLN:HG3	2.06	0.55
1:A:88:TYR:O	1:A:96:GLU:HG2	2.07	0.55
1:A:573:THR:HB	1:A:613:PHE:HZ	1.72	0.55
1:A:1082:GLU:O	1:A:1087:GLU:HB2	2.06	0.55
1:A:1532:ILE:HG13	1:A:1607:LEU:CD2	2.36	0.55
1:A:2323:VAL:HA	1:A:2400:LEU:HD22	1.86	0.55
1:A:2365:LEU:CA	1:A:2366:ARG:CB	2.84	0.55
2:B:247:ASP:O	2:B:454:LYS:NZ	2.39	0.55
3:C:212:LEU:CD2	3:C:330:LEU:HD21	2.36	0.55
1:A:386:GLU:O	1:A:389:PRO:HD2	2.06	0.55
1:A:2387:GLY:H	1:A:2391:VAL:HG11	1.71	0.55
2:B:311:ILE:HG23	3:C:297:HIS:CE1	2.41	0.55
1:A:85:LYS:NZ	1:A:113:VAL:HG13	2.22	0.55
1:A:199:VAL:CG1	1:A:263:VAL:HG22	2.36	0.55
1:A:213:GLU:OE1	1:A:213:GLU:N	2.35	0.55
1:A:390:PRO:HB3	1:A:456:ALA:HB1	1.89	0.55
1:A:645:ASN:O	1:A:649:VAL:HG23	2.06	0.55
1:A:1032:LEU:HA	1:A:1035:MET:CE	2.36	0.55
1:A:1704:VAL:HA	1:A:1707:ILE:HD12	1.88	0.55
1:A:2320:SER:O	1:A:2324:MET:HG2	2.06	0.55
2:B:161:GLN:OE1	2:B:164:ARG:NH2	2.33	0.55
1:A:159:GLU:HA	1:A:162:ARG:HG2	1.89	0.55
1:A:350:TRP:NE1	1:A:354:LEU:HD11	2.22	0.55
1:A:365:LEU:CD2	1:A:401:LEU:HG	2.36	0.55
1:A:1521:VAL:HG13	1:A:1522:ALA:CB	2.35	0.55
1:A:1600:ILE:O	1:A:1604:LEU:HG	2.07	0.55
1:A:2163:ASP:O	1:A:2167:MET:HG2	2.07	0.55
1:A:2165:ARG:HG3	1:A:2418:VAL:HG13	1.89	0.55
1:A:2300:LEU:HD23	1:A:2345:MET:HE1	1.88	0.55
1:A:2409:THR:HA	1:A:2412:THR:OG1	2.07	0.55
2:B:72:CYS:HB2	2:B:74:ARG:NH1	2.22	0.55
1:A:350:TRP:HE3	1:A:392:SER:HB3	1.70	0.55
1:A:1018:THR:HG21	1:A:1084:HIS:CE1	2.42	0.55
1:A:648:ILE:HD13	1:A:714:LEU:CG	2.36	0.55
1:A:1645:LEU:O	1:A:1648:ARG:HG2	2.07	0.55
1:A:1746:LEU:HD13	1:A:1795:LEU:CD1	2.37	0.55
3:C:209:VAL:HG22	3:C:269:ASP:HA	1.89	0.55
1:A:414:GLU:CD	1:A:433:LEU:HB2	2.31	0.54
1:A:489:CYS:HA	3:C:412:ASN:HD22	1.72	0.54
1:A:497:ILE:O	1:A:501:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2292:PRO:HG2	1:A:2295:LEU:HD21	1.88	0.54
1:A:2398:GLN:O	1:A:2402:ILE:HG13	2.07	0.54
2:B:259:ARG:HE	2:B:262:PRO:HA	1.71	0.54
3:C:188:MET:HB2	3:C:507:ARG:HH12	1.71	0.54
1:A:137:GLN:O	1:A:141:MET:HG3	2.07	0.54
1:A:389:PRO:HA	1:A:392:SER:OG	2.08	0.54
1:A:748:TYR:HA	1:A:875:HIS:HE1	1.72	0.54
1:A:1334:PRO:HG2	1:A:1335:LEU:HD23	1.88	0.54
1:A:2053:GLU:HB2	1:A:2057:THR:OG1	2.07	0.54
1:A:2141:LEU:HD13	1:A:2151:PRO:CA	2.38	0.54
1:A:2330:ILE:CD1	1:A:2404:ARG:HD2	2.37	0.54
2:B:72:CYS:SG	2:B:74:ARG:HG2	2.47	0.54
2:B:508:HIS:CE1	2:B:550:GLN:HB3	2.43	0.54
1:A:410:ARG:HH12	1:A:471:MET:H	1.54	0.54
1:A:476:ASP:HA	1:A:479:ILE:HG22	1.88	0.54
1:A:730:LEU:H	1:A:730:LEU:CD2	2.20	0.54
1:A:770:VAL:C	1:A:771:GLU:HG3	2.32	0.54
1:A:1184:ASN:N	1:A:1292:GLN:OE1	2.39	0.54
2:B:414:LEU:O	2:B:418:VAL:HG23	2.07	0.54
3:C:231:GLU:HG2	3:C:235:THR:OG1	2.07	0.54
3:C:313:THR:CG2	3:C:341:LYS:HG2	2.37	0.54
1:A:190:ASP:HA	1:A:193:LEU:CG	2.37	0.54
1:A:2414:LEU:O	1:A:2418:VAL:HG23	2.07	0.54
2:B:59:ARG:HA	3:C:377:GLU:OE1	2.06	0.54
2:B:552:HIS:HB3	2:B:556:TYR:CE2	2.43	0.54
3:C:212:LEU:HD21	3:C:330:LEU:HD21	1.90	0.54
3:C:473:LEU:O	3:C:477:VAL:HG23	2.07	0.54
1:A:117:GLU:OE1	1:A:134:ARG:HG3	2.07	0.54
1:A:216:CYS:O	1:A:220:LEU:HG	2.08	0.54
1:A:716:ILE:HG23	1:A:720:LYS:HZ3	1.71	0.54
1:A:822:LYS:C	1:A:825:PRO:HD2	2.32	0.54
1:A:994:MET:CB	1:A:2391:VAL:HA	2.38	0.54
3:C:218:SER:N	4:C:601:GTP:O1B	2.40	0.54
1:A:188:GLN:HE22	1:A:192:ILE:HD11	1.72	0.54
1:A:424:ILE:O	1:A:425:THR:OG1	2.21	0.54
1:A:869:ILE:HB	1:A:1295:ARG:NH1	2.23	0.54
1:A:1022:THR:HG23	1:A:1025:ASP:H	1.72	0.54
1:A:1103:ASN:ND2	1:A:1109:SER:HB2	2.20	0.54
1:A:1207:GLN:HG2	1:A:1289:ILE:CG1	2.37	0.54
1:A:1650:LYS:HG3	1:A:1654:GLN:NE2	2.22	0.54
1:A:1845:LEU:HA	1:A:1848:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1983:GLN:O	1:A:1987:GLU:HG3	2.07	0.54
2:B:491:ILE:CD1	3:C:519:LEU:HD23	2.38	0.54
1:A:135:LYS:HZ2	1:A:174:GLU:HA	1.73	0.54
1:A:1927:GLN:OE1	1:A:1927:GLN:N	2.33	0.54
1:A:2038:LYS:O	1:A:2041:GLN:HG3	2.07	0.54
1:A:117:GLU:HG2	1:A:130:THR:OG1	2.08	0.54
1:A:164:ARG:O	1:A:201:ASN:ND2	2.41	0.54
1:A:1753:THR:O	1:A:1757:LEU:HG	2.08	0.54
1:A:1824:PRO:HD2	1:A:2168:GLN:NE2	2.22	0.54
2:B:547:TYR:CE2	2:B:551:LEU:HD11	2.43	0.54
1:A:773:VAL:HG23	3:C:479:SER:HB3	1.89	0.54
1:A:1350:SER:OG	1:A:1354:LEU:HD23	2.08	0.54
1:A:1415:VAL:N	1:A:1416:PRO:HD3	2.22	0.54
1:A:2296:LEU:HD13	1:A:2383:LEU:CD1	2.38	0.54
2:B:244:ALA:CB	2:B:458:VAL:HG21	2.38	0.54
2:B:458:VAL:HG12	2:B:479:LEU:CD2	2.38	0.54
1:A:1984:LEU:O	1:A:1988:VAL:HG23	2.07	0.54
1:A:2099:LEU:HA	1:A:2102:MET:HG2	1.90	0.54
1:A:2228:LEU:O	1:A:2228:LEU:HD23	2.07	0.54
1:A:2292:PRO:HG2	1:A:2295:LEU:CD2	2.37	0.54
2:B:416:GLN:HG3	2:B:417:HIS:CD2	2.44	0.54
1:A:342:TRP:O	1:A:346:LEU:HG	2.08	0.53
1:A:550:GLN:HB2	1:A:605:ASP:HB3	1.90	0.53
1:A:1091:GLY:HA2	1:A:1120:LYS:NZ	2.22	0.53
1:A:1605:TYR:HB3	1:A:1622:LEU:HB2	1.88	0.53
1:A:1973:GLN:O	1:A:1977:VAL:HG12	2.07	0.53
1:A:2092:LEU:HD12	1:A:2099:LEU:CB	2.38	0.53
1:A:2214:LEU:HG	1:A:2341:VAL:O	2.07	0.53
2:B:149:LEU:HG	2:B:151:LEU:HD21	1.89	0.53
2:B:190:LYS:HG3	2:B:490:ASP:OD1	2.07	0.53
1:A:36:SER:HA	1:A:77:HIS:NE2	2.23	0.53
1:A:280:LEU:HB2	1:A:315:PHE:CE2	2.43	0.53
1:A:305:ARG:NH1	1:A:345:SER:HB2	2.23	0.53
1:A:982:LEU:HB2	1:A:992:LYS:HE3	1.88	0.53
1:A:1318:GLU:HA	1:A:1321:VAL:HG12	1.91	0.53
1:A:1862:VAL:HG11	1:A:2197:PRO:O	2.08	0.53
2:B:56:THR:HB	2:B:63:GLU:OE1	2.08	0.53
3:C:221:MET:HB3	3:C:238:PHE:HE2	1.74	0.53
3:C:381:PRO:HG3	3:C:414:PHE:CZ	2.44	0.53
1:A:283:ILE:O	1:A:287:VAL:HG23	2.08	0.53
1:A:904:ASN:HB3	1:A:906:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:SER:O	1:A:1100:VAL:HG23	2.08	0.53
1:A:1414:THR:OG1	1:A:1415:VAL:HB	2.08	0.53
1:A:1471:THR:O	1:A:1475:VAL:HG22	2.08	0.53
1:A:1929:CYS:O	1:A:1933:ILE:HG12	2.07	0.53
2:B:155:SER:HB2	2:B:196:GLN:CD	2.34	0.53
2:B:194:LYS:O	2:B:198:LEU:HG	2.07	0.53
1:A:43:LYS:O	1:A:99:TYR:OH	2.13	0.53
1:A:69:GLN:HB2	1:A:102:LYS:NZ	2.23	0.53
1:A:239:LYS:O	1:A:239:LYS:HD3	2.09	0.53
1:A:365:LEU:HD23	1:A:405:PHE:CB	2.39	0.53
1:A:1281:ASP:HB2	1:A:1282:PRO:HD3	1.89	0.53
1:A:2326:MET:SD	1:A:2397:GLU:HB3	2.48	0.53
1:A:2353:ILE:HG22	1:A:2354:ASP:N	2.24	0.53
3:C:515:TYR:CE2	3:C:519:LEU:HD21	2.43	0.53
1:A:220:LEU:HA	1:A:270:SER:OG	2.08	0.53
1:A:279:SER:O	1:A:283:ILE:HG13	2.07	0.53
1:A:1027:LEU:HD21	1:A:1085:CYS:HA	1.91	0.53
1:A:1353:GLN:O	1:A:1357:SER:HB3	2.08	0.53
1:A:1463:VAL:CG2	1:A:1470:SER:HB2	2.38	0.53
1:A:1636:ASN:O	1:A:1640:GLY:N	2.34	0.53
1:A:2045:GLY:CA	1:A:2078:LEU:HD11	2.38	0.53
2:B:190:LYS:CG	2:B:194:LYS:HE3	2.38	0.53
2:B:453:SER:O	2:B:457:GLU:HG3	2.09	0.53
2:B:523:VAL:HA	2:B:526:ASN:OD1	2.08	0.53
3:C:194:ALA:HB3	3:C:496:PHE:CE1	2.43	0.53
3:C:409:LEU:HD21	3:C:476:GLN:CG	2.38	0.53
1:A:379:ALA:CB	1:A:382:GLU:HG2	2.35	0.53
1:A:566:LYS:HD2	1:A:625:LYS:HZ2	1.71	0.53
1:A:625:LYS:O	1:A:629:ILE:HG12	2.07	0.53
1:A:1117:ARG:O	1:A:1120:LYS:HG2	2.09	0.53
1:A:2309:GLU:O	1:A:2313:VAL:HG23	2.08	0.53
1:A:2388:VAL:HG23	1:A:2389:GLU:H	1.72	0.53
3:C:261:THR:HG22	3:C:262:GLN:N	2.24	0.53
1:A:365:LEU:CD1	1:A:401:LEU:HD21	2.39	0.53
1:A:424:ILE:HG22	1:A:426:GLU:HG2	1.90	0.53
1:A:503:LEU:HG	3:C:454:PHE:CD1	2.44	0.53
1:A:716:ILE:HG23	1:A:720:LYS:NZ	2.24	0.53
1:A:845:LEU:HD11	1:A:883:LEU:HD11	1.90	0.53
1:A:974:GLY:O	1:A:978:LEU:HD13	2.08	0.53
1:A:1786:VAL:CG1	1:A:1823:ILE:HD11	2.30	0.53
1:A:1819:TRP:CZ2	1:A:1844:LEU:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1981:ILE:CD1	1:A:2067:SER:HA	2.39	0.53
1:A:2326:MET:HE2	1:A:2326:MET:CA	2.39	0.53
1:A:2391:VAL:HG12	1:A:2392:PHE:N	2.20	0.53
2:B:159:ASN:ND2	3:C:326:THR:HB	2.24	0.53
2:B:509:SER:HA	2:B:512:GLN:NE2	2.24	0.53
2:B:544:PHE:O	2:B:547:TYR:HB3	2.08	0.53
1:A:353:ASP:HB2	1:A:392:SER:HB2	1.90	0.53
1:A:378:VAL:N	2:B:79:LEU:HD21	2.24	0.53
1:A:566:LYS:HB2	1:A:625:LYS:HE2	1.90	0.53
1:A:653:LEU:HD22	1:A:664:VAL:CG2	2.39	0.53
1:A:770:VAL:HG12	1:A:771:GLU:N	2.24	0.53
1:A:1028:THR:O	1:A:1032:LEU:HG	2.08	0.53
1:A:1035:MET:HB3	1:A:1036:ARG:HA	1.91	0.53
1:A:1346:LEU:N	1:A:1347:PRO:HA	2.24	0.53
1:A:1478:LYS:CE	1:A:1532:ILE:HG12	2.34	0.53
1:A:1738:ASP:HA	1:A:1741:PHE:CE2	2.44	0.53
1:A:1988:VAL:HA	1:A:1991:VAL:HG22	1.89	0.53
1:A:2215:PHE:N	1:A:2338:LEU:HB3	2.24	0.53
2:B:478:ILE:O	2:B:482:ILE:HG12	2.09	0.53
3:C:211:GLY:O	3:C:273:ILE:HG12	2.09	0.53
3:C:270:THR:HG21	3:C:311:LEU:HD21	1.90	0.53
3:C:279:LEU:HD21	3:C:297:HIS:CE1	2.44	0.53
1:A:40:ASP:CG	1:A:80:ILE:HG12	2.33	0.53
1:A:605:ASP:O	1:A:609:PHE:N	2.34	0.53
1:A:1463:VAL:HG11	1:A:1499:HIS:CE1	2.44	0.53
3:C:313:THR:HG22	3:C:341:LYS:CE	2.29	0.53
1:A:183:LEU:HG	1:A:184:VAL:HG13	1.91	0.53
1:A:292:LEU:HD11	1:A:327:ILE:HG13	1.91	0.53
1:A:416:PHE:HA	1:A:419:ILE:HD12	1.90	0.53
1:A:839:GLN:O	1:A:843:LEU:HG	2.09	0.53
1:A:1071:VAL:O	1:A:1072:THR:OG1	2.16	0.53
1:A:1138:CYS:SG	1:A:1139:ILE:N	2.82	0.53
1:A:2169:PHE:CD2	1:A:2331:ILE:HD11	2.43	0.53
1:A:2326:MET:HB2	1:A:2400:LEU:HD23	1.90	0.53
1:A:2365:LEU:CB	1:A:2366:ARG:HB3	2.39	0.53
1:A:2389:GLU:O	1:A:2391:VAL:HG23	2.09	0.53
2:B:44:GLU:OE1	2:B:44:GLU:N	2.42	0.53
2:B:504:LEU:CD1	2:B:550:GLN:HG2	2.36	0.53
3:C:466:PHE:O	3:C:470:VAL:HG23	2.09	0.53
1:A:1837:VAL:O	1:A:1841:ILE:HG13	2.09	0.52
1:A:2153:LEU:N	1:A:2205:ILE:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2221:TRP:HA	1:A:2224:ARG:CZ	2.39	0.52
2:B:162:LEU:O	2:B:162:LEU:HD23	2.08	0.52
2:B:268:LEU:CD2	2:B:335:PHE:HB3	2.39	0.52
1:A:81:GLN:O	1:A:85:LYS:NZ	2.25	0.52
1:A:280:LEU:O	1:A:284:LEU:HD23	2.09	0.52
1:A:302:LEU:HD22	1:A:341:GLY:HA2	1.91	0.52
1:A:990:LEU:HD23	1:A:2395:SER:CB	2.38	0.52
1:A:1321:VAL:O	1:A:1325:LYS:HG2	2.09	0.52
1:A:1825:GLN:HE22	1:A:2165:ARG:HD2	1.73	0.52
2:B:155:SER:CB	2:B:196:GLN:HG3	2.37	0.52
2:B:297:LYS:HD2	2:B:336:VAL:HB	1.91	0.52
2:B:541:GLY:HA3	3:C:339:MET:HE3	1.91	0.52
3:C:209:VAL:HG21	3:C:217:LYS:O	2.09	0.52
1:A:239:LYS:CE	1:A:243:SER:HB3	2.39	0.52
1:A:414:GLU:OE1	1:A:433:LEU:HB2	2.09	0.52
1:A:471:MET:HG3	1:A:471:MET:O	2.09	0.52
1:A:556:LYS:HA	1:A:559:PRO:HG3	1.90	0.52
1:A:805:GLN:O	1:A:807:VAL:HG22	2.10	0.52
1:A:857:PHE:CE2	1:A:1190:ALA:HB2	2.44	0.52
1:A:1035:MET:CB	1:A:1036:ARG:HA	2.38	0.52
1:A:1424:LEU:HD22	1:A:1458:THR:CG2	2.36	0.52
1:A:1856:ILE:O	1:A:1859:PRO:HD3	2.09	0.52
1:A:2335:ASP:OD1	1:A:2337:HIS:NE2	2.43	0.52
1:A:337:GLN:HB2	1:A:338:GLN:NE2	2.24	0.52
1:A:772:ASP:OD1	3:C:481:ALA:HA	2.09	0.52
1:A:941:GLN:CB	1:A:978:LEU:HG	2.40	0.52
1:A:2342:LEU:HB2	1:A:2351:VAL:HG23	1.92	0.52
2:B:190:LYS:O	2:B:194:LYS:HG3	2.10	0.52
2:B:319:THR:HG22	2:B:320:ASN:H	1.74	0.52
2:B:540:ARG:HB3	3:C:339:MET:HA	1.91	0.52
3:C:171:LEU:C	3:C:172:LEU:HD12	2.34	0.52
1:A:377:HIS:HA	2:B:79:LEU:HD11	1.91	0.52
1:A:647:MET:CB	1:A:714:LEU:HD23	2.40	0.52
1:A:2169:PHE:HA	1:A:2414:LEU:CD2	2.38	0.52
1:A:2385:VAL:HG13	1:A:2386:THR:H	1.73	0.52
2:B:44:GLU:CA	2:B:444:THR:HB	2.37	0.52
2:B:237:VAL:CG1	2:B:479:LEU:HG	2.38	0.52
2:B:493:THR:O	2:B:497:GLU:HG3	2.09	0.52
1:A:289:THR:OG1	1:A:290:PRO:HD3	2.10	0.52
1:A:483:LEU:O	1:A:487:GLU:HG3	2.09	0.52
1:A:752:PHE:HB3	1:A:762:LYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:LYS:HD2	1:A:907:LYS:HE2	1.92	0.52
1:A:1713:SER:O	1:A:1714:SER:OG	2.27	0.52
1:A:1753:THR:HG21	1:A:1792:LEU:HG	1.91	0.52
1:A:1835:VAL:HG22	1:A:1836:TYR:H	1.74	0.52
1:A:2276:PRO:O	1:A:2279:VAL:HB	2.09	0.52
1:A:244:ALA:CB	1:A:290:PRO:HB2	2.38	0.52
1:A:356:PHE:CG	1:A:360:LEU:HG	2.44	0.52
1:A:1211:HIS:CE1	1:A:1285:LEU:HD13	2.45	0.52
1:A:1293:LEU:CD1	1:A:1322:LYS:HB3	2.40	0.52
1:A:2379:ILE:HG22	1:A:2379:ILE:O	2.09	0.52
1:A:2381:THR:HG22	1:A:2388:VAL:CG1	2.39	0.52
3:C:219:MET:O	3:C:223:LEU:HG	2.10	0.52
1:A:143:TYR:CE2	1:A:145:ASP:HB2	2.45	0.52
1:A:173:LYS:HA	1:A:176:ILE:HG22	1.90	0.52
1:A:240:PHE:CZ	1:A:257:TYR:HE1	2.28	0.52
1:A:332:LYS:N	1:A:333:PRO:HD2	2.25	0.52
1:A:547:ALA:HB1	1:A:605:ASP:OD2	2.10	0.52
1:A:740:VAL:HG12	1:A:751:LEU:HD12	1.92	0.52
1:A:1091:GLY:HA2	1:A:1120:LYS:HZ1	1.74	0.52
1:A:1463:VAL:HG23	1:A:1470:SER:HB2	1.91	0.52
1:A:1668:ARG:O	1:A:1672:ILE:HG13	2.10	0.52
3:C:188:MET:HE3	3:C:503:TRP:CH2	2.44	0.52
1:A:345:SER:O	1:A:348:PRO:HD2	2.09	0.52
1:A:820:LEU:HD21	1:A:882:TRP:CD2	2.45	0.52
1:A:866:ILE:HA	1:A:1295:ARG:NH2	2.25	0.52
1:A:1349:LEU:HD23	1:A:1355:TYR:OH	2.10	0.52
1:A:1412:GLU:N	1:A:1413:GLN:HB2	2.25	0.52
1:A:2021:LEU:O	1:A:2024:VAL:HG22	2.10	0.52
1:A:2219:LYS:O	1:A:2223:GLN:HG3	2.10	0.52
1:A:2223:GLN:CG	1:A:2245:ILE:HD12	2.38	0.52
2:B:499:ARG:HA	2:B:502:LYS:HZ3	1.75	0.52
3:C:265:ILE:CD1	3:C:478:MET:HG2	2.39	0.52
3:C:340:VAL:HG11	3:C:512:LEU:CD2	2.40	0.52
1:A:635:SER:HB2	1:A:636:PRO:HD3	1.92	0.52
1:A:1290:GLU:O	1:A:1294:LEU:HG	2.10	0.52
1:A:1332:ILE:HG22	1:A:1332:ILE:O	2.10	0.52
1:A:1529:ALA:O	1:A:1533:GLN:HG3	2.10	0.52
1:A:1623:ALA:HB2	1:A:1752:PHE:CB	2.40	0.52
3:C:183:LEU:H	3:C:183:LEU:HD12	1.74	0.52
1:A:153:LEU:HD12	1:A:156:ILE:HD12	1.92	0.51
1:A:232:ILE:O	1:A:236:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HA	1:A:342:TRP:CH2	2.44	0.51
1:A:1082:GLU:OE1	1:A:1112:GLN:HG2	2.10	0.51
1:A:1085:CYS:HG	1:A:1095:TRP:CG	2.28	0.51
1:A:1627:TYR:CG	1:A:1791:ARG:HD3	2.45	0.51
1:A:1860:ALA:O	1:A:1864:THR:HG23	2.10	0.51
1:A:2320:SER:HA	1:A:2323:VAL:HG22	1.91	0.51
2:B:166:CYS:HB3	3:C:393:GLN:HG3	1.92	0.51
3:C:232:ASP:OD1	3:C:233:GLN:N	2.42	0.51
3:C:244:GLU:CA	3:C:247:GLU:HG2	2.36	0.51
3:C:385:ARG:O	3:C:389:LEU:HG	2.10	0.51
1:A:81:GLN:HG3	1:A:112:ASN:ND2	2.25	0.51
1:A:258:LYS:O	1:A:262:THR:HG23	2.10	0.51
1:A:1412:GLU:CA	1:A:1413:GLN:HB2	2.40	0.51
1:A:1977:VAL:O	1:A:1981:ILE:HG13	2.10	0.51
1:A:2153:LEU:CD1	1:A:2155:LYS:HE2	2.39	0.51
1:A:2247:PRO:HD2	1:A:2249:PRO:CD	2.40	0.51
1:A:2324:MET:HE2	1:A:2352:HIS:CD2	2.45	0.51
1:A:2358:CYS:O	1:A:2361:LYS:HG3	2.11	0.51
3:C:216:GLY:HA2	4:C:601:GTP:O2A	2.10	0.51
1:A:463:LEU:HB3	1:A:464:LEU:HA	1.93	0.51
1:A:1040:LEU:HD23	1:A:1040:LEU:H	1.75	0.51
1:A:1054:LEU:HD22	1:A:1415:VAL:HG21	1.92	0.51
1:A:1090:GLN:HG3	1:A:1091:GLY:N	2.25	0.51
1:A:2246:VAL:H	1:A:2247:PRO:HA	1.75	0.51
2:B:272:ASN:OD1	2:B:273:GLY:N	2.43	0.51
1:A:147:SER:N	1:A:149:LEU:HD23	2.18	0.51
1:A:1858:TYR:CE1	1:A:1948:VAL:HB	2.45	0.51
1:A:2276:PRO:HD2	1:A:2277:LEU:O	2.10	0.51
3:C:313:THR:OG1	3:C:502:ILE:HG21	2.11	0.51
1:A:131:LYS:HE3	1:A:159:GLU:CD	2.35	0.51
1:A:186:VAL:HB	1:A:225:LEU:HD22	1.92	0.51
1:A:369:GLU:HB2	1:A:437:MET:HE2	1.93	0.51
1:A:578:ASN:O	1:A:582:SER:HB2	2.10	0.51
1:A:822:LYS:HZ3	1:A:829:VAL:H	1.58	0.51
1:A:1286:GLN:HG2	1:A:1330:ILE:HG12	1.93	0.51
1:A:1414:THR:CA	1:A:1415:VAL:HB	2.41	0.51
1:A:2120:THR:HB	1:A:2144:GLY:HA3	1.92	0.51
1:A:2131:LEU:HD23	1:A:2137:PRO:C	2.35	0.51
1:A:335:LEU:HA	1:A:342:TRP:HH2	1.75	0.51
1:A:672:CYS:HA	1:A:675:HIS:HE2	1.74	0.51
1:A:725:GLN:NE2	1:A:730:LEU:HD21	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:LEU:CD2	3:C:263:GLU:HB3	2.38	0.51
1:A:1293:LEU:HD12	1:A:1319:ASN:OD1	2.10	0.51
1:A:1311:GLN:CB	1:A:1312:LYS:HA	2.40	0.51
1:A:2296:LEU:HD21	1:A:2343:ILE:CD1	2.41	0.51
1:A:2300:LEU:HD21	1:A:2343:ILE:CD1	2.39	0.51
2:B:423:SER:OG	2:B:425:LYS:HG3	2.10	0.51
3:C:326:THR:HG21	3:C:390:MET:CE	2.41	0.51
1:A:278:THR:O	1:A:278:THR:HG22	2.11	0.51
1:A:1114:ALA:HB2	1:A:1117:ARG:HH21	1.75	0.51
1:A:1293:LEU:HD11	1:A:1322:LYS:HB3	1.93	0.51
1:A:1346:LEU:HB2	1:A:1349:LEU:CD1	2.38	0.51
1:A:1756:LYS:HZ2	1:A:1785:ILE:HG22	1.74	0.51
1:A:2171:SER:O	1:A:2175:THR:HG23	2.11	0.51
1:A:2215:PHE:HB2	1:A:2338:LEU:CB	2.41	0.51
1:A:2254:TYR:CA	1:A:2257:ILE:HG22	2.34	0.51
2:B:507:ALA:HB1	2:B:534:VAL:CG1	2.40	0.51
3:C:199:LEU:O	3:C:493:LYS:HG2	2.10	0.51
1:A:109:ARG:HA	1:A:112:ASN:OD1	2.11	0.51
1:A:249:LYS:CE	1:A:297:VAL:HG22	2.36	0.51
1:A:310:ILE:H	1:A:310:ILE:HD12	1.75	0.51
1:A:415:ARG:C	1:A:418:PRO:HD2	2.36	0.51
1:A:719:LYS:HE2	1:A:1307:ILE:CG2	2.41	0.51
2:B:359:CYS:HB3	3:C:454:PHE:CZ	2.46	0.51
1:A:305:ARG:HG2	1:A:332:LYS:CD	2.41	0.51
1:A:390:PRO:HB2	1:A:391:PRO:CD	2.39	0.51
1:A:630:GLY:O	1:A:634:LEU:HB2	2.10	0.51
1:A:837:GLU:O	1:A:841:ILE:HG13	2.10	0.51
1:A:939:THR:CG2	1:A:2301:TRP:HE1	2.23	0.51
1:A:1657:LEU:N	1:A:1658:PRO:HD2	2.26	0.51
2:B:209:ILE:N	2:B:209:ILE:HD12	2.26	0.51
3:C:270:THR:HB	3:C:307:ILE:HG21	1.93	0.51
1:A:290:PRO:O	1:A:294:CYS:HB2	2.10	0.51
1:A:558:ILE:HG23	1:A:612:ILE:HG23	1.93	0.51
1:A:674:ARG:HA	1:A:677:HIS:HB3	1.92	0.51
1:A:734:TRP:CE2	1:A:769:LEU:HG	2.46	0.51
1:A:1414:THR:HA	1:A:1415:VAL:HB	1.92	0.51
1:A:2072:LYS:O	1:A:2076:LEU:HD23	2.11	0.51
2:B:206:VAL:HB	2:B:455:LEU:CD1	2.41	0.51
2:B:262:PRO:CB	2:B:326:LEU:HD21	2.41	0.51
1:A:1293:LEU:CD2	1:A:1322:LYS:HG2	2.41	0.50
2:B:45:ASP:HB3	2:B:142:TYR:OH	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:ARG:HD3	2:B:488:PHE:O	2.11	0.50
2:B:244:ALA:O	2:B:454:LYS:HD3	2.11	0.50
2:B:515:LEU:HB3	2:B:517:HIS:CD2	2.46	0.50
1:A:40:ASP:OD2	1:A:80:ILE:HG12	2.11	0.50
1:A:353:ASP:CB	1:A:392:SER:HB2	2.41	0.50
1:A:652:ASP:O	1:A:655:VAL:HG23	2.10	0.50
1:A:886:LEU:O	1:A:890:CYS:N	2.40	0.50
1:A:1085:CYS:O	1:A:1087:GLU:N	2.44	0.50
1:A:1948:VAL:O	1:A:1952:VAL:HG23	2.10	0.50
2:B:259:ARG:HD2	2:B:263:PRO:HD3	1.92	0.50
2:B:540:ARG:HD2	3:C:339:MET:HA	1.94	0.50
3:C:180:SER:HB3	3:C:238:PHE:CD1	2.46	0.50
1:A:87:GLY:HA2	1:A:90:VAL:HG12	1.94	0.50
1:A:252:TYR:O	1:A:256:THR:HG22	2.11	0.50
1:A:664:VAL:O	1:A:668:LEU:HG	2.11	0.50
1:A:1086:PRO:HG2	1:A:1091:GLY:O	2.11	0.50
1:A:1418:ARG:O	1:A:1422:MET:HG3	2.11	0.50
1:A:1455:LYS:N	1:A:1455:LYS:HD2	2.27	0.50
1:A:1479:TRP:NE1	1:A:1535:GLU:OE2	2.44	0.50
1:A:1729:VAL:O	1:A:1732:VAL:HG22	2.11	0.50
1:A:2055:LEU:HD22	1:A:2068:TRP:HA	1.93	0.50
2:B:269:PHE:HD2	2:B:304:LEU:HD13	1.77	0.50
3:C:177:MET:HE2	3:C:197:TYR:CG	2.46	0.50
3:C:241:GLN:OE1	3:C:245:MET:HG2	2.12	0.50
1:A:249:LYS:CD	1:A:297:VAL:HG13	2.41	0.50
1:A:1401:MET:O	1:A:1405:GLN:HG2	2.11	0.50
1:A:2172:ILE:O	1:A:2176:MET:HG3	2.11	0.50
1:A:2283:VAL:O	1:A:2287:LEU:HG	2.12	0.50
3:C:210:LEU:HD23	3:C:270:THR:OG1	2.11	0.50
1:A:148:ARG:O	1:A:185:LEU:HD21	2.12	0.50
1:A:227:TYR:HA	1:A:273:MET:CE	2.41	0.50
1:A:549:TYR:O	1:A:552:VAL:HG12	2.11	0.50
1:A:731:LEU:H	1:A:731:LEU:CD2	2.24	0.50
1:A:1502:GLU:HA	1:A:1503:MET:CB	2.10	0.50
1:A:1606:HIS:HA	1:A:1622:LEU:HD22	1.94	0.50
2:B:55:LYS:HB3	3:C:324:TRP:CH2	2.47	0.50
3:C:271:GLN:HB2	3:C:272:PRO:HD2	1.94	0.50
1:A:503:LEU:HD13	1:A:572:MET:CG	2.41	0.50
1:A:1081:CYS:HB3	1:A:1085:CYS:SG	2.52	0.50
1:A:1411:LYS:C	1:A:1413:GLN:HB2	2.37	0.50
1:A:1533:GLN:HE22	1:A:1600:ILE:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2037:GLU:N	1:A:2094:GLU:HA	2.27	0.50
1:A:2421:PRO:CG	1:A:2424:ASP:HB3	2.41	0.50
2:B:265:LEU:O	2:B:333:GLN:HB2	2.12	0.50
3:C:306:GLN:HG2	3:C:512:LEU:CD1	2.41	0.50
1:A:447:PHE:CZ	1:A:491:THR:HG23	2.46	0.50
1:A:638:VAL:CB	1:A:639:PHE:HA	2.30	0.50
1:A:673:THR:HB	1:A:1344:GLN:CB	2.41	0.50
1:A:1463:VAL:HG21	1:A:1499:HIS:NE2	2.27	0.50
1:A:1666:LYS:O	1:A:1669:ILE:HG22	2.11	0.50
1:A:2195:VAL:HG12	1:A:2205:ILE:HG21	1.94	0.50
1:A:2301:TRP:HA	1:A:2310:TRP:HD1	1.76	0.50
1:A:2310:TRP:O	1:A:2314:THR:HG23	2.12	0.50
1:A:2326:MET:CB	1:A:2400:LEU:HD23	2.42	0.50
1:A:2379:ILE:O	1:A:2383:LEU:HD21	2.11	0.50
2:B:212:LEU:HB2	2:B:267:PHE:CD1	2.47	0.50
3:C:403:LYS:HA	3:C:422:LEU:H	1.76	0.50
1:A:68:ARG:HA	1:A:71:HIS:HD2	1.77	0.50
1:A:121:VAL:HG12	1:A:162:ARG:HH11	1.77	0.50
1:A:441:THR:OG1	1:A:446:VAL:HG22	2.11	0.50
1:A:549:TYR:O	1:A:553:LEU:HG	2.12	0.50
1:A:657:PHE:CB	1:A:658:PRO:HD2	2.41	0.50
1:A:2122:HIS:H	1:A:2144:GLY:HA2	1.77	0.50
2:B:254:TRP:CH2	2:B:260:PRO:HG3	2.47	0.50
3:C:199:LEU:O	3:C:492:GLU:HB2	2.11	0.50
3:C:279:LEU:O	3:C:283:ILE:HG13	2.12	0.50
1:A:108:LEU:HD13	1:A:110:VAL:CG1	2.27	0.50
1:A:301:LEU:O	1:A:305:ARG:HG3	2.12	0.50
1:A:558:ILE:N	1:A:559:PRO:CD	2.74	0.50
1:A:2098:TRP:O	1:A:2102:MET:N	2.42	0.50
1:A:2183:GLN:CA	1:A:2184:GLU:C	2.85	0.50
1:A:2191:ARG:HG3	1:A:2351:VAL:CG1	2.39	0.50
1:A:2299:GLU:HG3	1:A:2345:MET:HE1	1.93	0.50
1:A:2388:VAL:HG23	1:A:2389:GLU:N	2.27	0.50
3:C:239:ARG:HB3	3:C:252:GLN:OE1	2.12	0.50
3:C:244:GLU:HG3	3:C:248:ARG:NH2	2.27	0.50
3:C:251:ASN:ND2	3:C:251:ASN:O	2.45	0.50
1:A:150:SER:O	1:A:153:LEU:N	2.37	0.49
1:A:207:LEU:N	1:A:208:GLN:CB	2.75	0.49
1:A:343:LEU:O	1:A:347:GLU:HG3	2.12	0.49
1:A:551:ALA:HB2	1:A:605:ASP:OD1	2.12	0.49
1:A:1662:THR:O	1:A:1666:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1861:ILE:O	1:A:1865:ILE:HG12	2.11	0.49
1:A:2276:PRO:HG2	1:A:2280:MET:HG3	1.94	0.49
1:A:280:LEU:HB2	1:A:315:PHE:CZ	2.47	0.49
1:A:294:CYS:C	1:A:295:LYS:HD3	2.37	0.49
1:A:305:ARG:HG2	1:A:332:LYS:CE	2.42	0.49
1:A:671:HIS:O	1:A:675:HIS:NE2	2.42	0.49
1:A:813:ILE:HG13	1:A:881:ASN:ND2	2.27	0.49
1:A:1521:VAL:HG22	1:A:1522:ALA:CB	2.42	0.49
1:A:2319:ARG:O	1:A:2323:VAL:HG13	2.12	0.49
2:B:42:TRP:HB2	2:B:45:ASP:OD1	2.12	0.49
2:B:212:LEU:HD21	2:B:223:TYR:CE1	2.48	0.49
2:B:319:THR:HG22	2:B:320:ASN:N	2.27	0.49
3:C:251:ASN:HB3	3:C:277:SER:HB3	1.94	0.49
1:A:207:LEU:HG	1:A:209:GLU:OE2	2.12	0.49
1:A:320:ASP:HB3	1:A:322:LEU:HD12	1.92	0.49
1:A:365:LEU:HD22	1:A:401:LEU:HG	1.93	0.49
1:A:2055:LEU:HD23	1:A:2055:LEU:O	2.13	0.49
1:A:2092:LEU:HD12	1:A:2099:LEU:HB2	1.93	0.49
1:A:2214:LEU:O	1:A:2217:LEU:HG	2.12	0.49
2:B:47:ILE:HG22	2:B:142:TYR:HE1	1.77	0.49
2:B:204:PHE:HB3	2:B:324:ASN:OD1	2.11	0.49
1:A:742:MET:HE2	1:A:742:MET:CA	2.39	0.49
1:A:1399:TYR:O	1:A:1403:GLN:HG3	2.12	0.49
1:A:1415:VAL:HG13	1:A:1415:VAL:O	2.12	0.49
1:A:1463:VAL:HG21	1:A:1499:HIS:CD2	2.47	0.49
2:B:262:PRO:HB2	2:B:326:LEU:HD21	1.95	0.49
2:B:451:ALA:O	2:B:455:LEU:HG	2.12	0.49
1:A:553:LEU:HD21	1:A:572:MET:SD	2.53	0.49
1:A:1627:TYR:HB2	1:A:1749:SER:HB3	1.94	0.49
1:A:1732:VAL:O	1:A:1736:VAL:HG13	2.13	0.49
1:A:1809:HIS:O	1:A:1813:THR:OG1	2.26	0.49
1:A:1958:VAL:O	1:A:2138:LYS:NZ	2.45	0.49
1:A:2057:THR:HB	1:A:2058:PRO:HD3	1.93	0.49
1:A:2131:LEU:HD21	1:A:2139:LYS:N	2.27	0.49
1:A:2194:SER:HB3	1:A:2206:GLN:HG2	1.94	0.49
1:A:2215:PHE:N	1:A:2338:LEU:O	2.32	0.49
2:B:250:VAL:HB	2:B:254:TRP:CD2	2.47	0.49
3:C:241:GLN:O	4:C:601:GTP:O3'	2.30	0.49
3:C:326:THR:HG21	3:C:390:MET:HE2	1.94	0.49
3:C:377:GLU:O	3:C:383:LYS:HG3	2.11	0.49
1:A:81:GLN:NE2	1:A:107:GLU:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:THR:HG21	1:A:211:ARG:HD3	1.95	0.49
1:A:215:ALA:CA	1:A:218:LEU:HD13	2.30	0.49
1:A:305:ARG:HG2	1:A:332:LYS:NZ	2.28	0.49
1:A:503:LEU:HB2	1:A:572:MET:CE	2.43	0.49
1:A:1459:ALA:HB1	1:A:1474:GLN:CG	2.42	0.49
1:A:1478:LYS:HD2	1:A:1493:THR:HG22	1.93	0.49
3:C:212:LEU:O	3:C:217:LYS:NZ	2.41	0.49
1:A:127:ALA:O	1:A:130:THR:HG22	2.13	0.49
1:A:196:VAL:O	1:A:200:LEU:HD13	2.13	0.49
1:A:675:HIS:H	1:A:676:ASP:C	2.20	0.49
1:A:720:LYS:HE3	1:A:2346:THR:CB	2.43	0.49
1:A:720:LYS:HE3	1:A:2346:THR:HB	1.95	0.49
1:A:1125:TYR:CE2	1:A:1129:LEU:HD11	2.47	0.49
1:A:1323:TYR:HA	1:A:1326:GLN:HG2	1.95	0.49
1:A:1503:MET:O	1:A:1504:LEU:HD22	2.12	0.49
1:A:1627:TYR:HB3	1:A:1791:ARG:HD3	1.94	0.49
1:A:1631:ARG:O	1:A:1634:VAL:HG22	2.13	0.49
1:A:1656:LEU:CB	1:A:1657:LEU:HA	2.33	0.49
1:A:1659:ASP:OD1	1:A:1660:THR:N	2.45	0.49
1:A:2297:ALA:N	1:A:2383:LEU:HD22	2.28	0.49
1:A:2393:ARG:O	1:A:2397:GLU:HG3	2.13	0.49
2:B:509:SER:HA	2:B:512:GLN:HG2	1.95	0.49
3:C:248:ARG:HD3	3:C:248:ARG:N	2.28	0.49
3:C:406:LEU:HD12	3:C:422:LEU:CB	2.35	0.49
1:A:207:LEU:HB3	1:A:209:GLU:HG2	1.95	0.49
1:A:223:ALA:HB3	1:A:270:SER:CB	2.41	0.49
1:A:310:ILE:HD12	1:A:310:ILE:N	2.28	0.49
1:A:346:LEU:HD21	1:A:375:LEU:CD1	2.42	0.49
1:A:407:THR:OG1	1:A:435:ARG:NH2	2.46	0.49
1:A:982:LEU:CB	1:A:992:LYS:HE3	2.42	0.49
1:A:1054:LEU:HD13	1:A:1415:VAL:HG13	1.94	0.49
1:A:1292:GLN:CB	1:A:1322:LYS:HD3	2.43	0.49
1:A:1338:SER:HB2	1:A:1339:THR:CA	2.42	0.49
1:A:346:LEU:O	1:A:349:PHE:HB2	2.13	0.49
1:A:542:VAL:CG2	1:A:545:ALA:HB2	2.43	0.49
1:A:608:LYS:O	1:A:612:ILE:HG12	2.13	0.49
1:A:654:ALA:O	1:A:808:HIS:HB3	2.13	0.49
1:A:1285:LEU:O	1:A:1289:ILE:HG13	2.12	0.49
1:A:1304:LEU:O	1:A:1304:LEU:HG	2.12	0.49
1:A:1832:HIS:HB3	1:A:1837:VAL:HG21	1.95	0.49
2:B:134:ASP:HB3	2:B:165:ALA:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:LEU:CD2	2:B:325:CYS:HB2	2.43	0.49
3:C:202:THR:HB	3:C:489:ILE:CD1	2.41	0.49
3:C:395:MET:HE3	3:C:398:SER:HB3	1.95	0.49
3:C:409:LEU:HD21	3:C:476:GLN:HG2	1.94	0.49
1:A:62:ASN:O	1:A:66:VAL:HG23	2.12	0.49
1:A:287:VAL:C	1:A:290:PRO:HD2	2.38	0.49
1:A:328:ASP:O	1:A:332:LYS:HE3	2.13	0.49
1:A:391:PRO:HG3	1:A:459:CYS:SG	2.52	0.49
1:A:1292:GLN:HG3	1:A:1322:LYS:CE	2.42	0.49
1:A:1597:PRO:HG3	1:A:1629:TRP:CD1	2.48	0.49
1:A:1938:SER:CB	1:A:1945:VAL:HG11	2.43	0.49
3:C:372:ASN:OD1	4:C:601:GTP:N1	2.41	0.49
3:C:391:ILE:HD12	3:C:421:PHE:CZ	2.43	0.49
1:A:113:VAL:HG12	1:A:117:GLU:OE2	2.12	0.48
1:A:458:GLU:O	1:A:462:VAL:HG13	2.13	0.48
1:A:845:LEU:HD13	1:A:925:VAL:HG22	1.93	0.48
1:A:1960:VAL:N	1:A:1961:LEU:CA	2.75	0.48
1:A:2256:LYS:HD2	1:A:2287:LEU:CD2	2.42	0.48
2:B:142:TYR:HE2	2:B:144:GLN:HG2	1.77	0.48
2:B:307:GLN:O	2:B:311:ILE:HG13	2.13	0.48
2:B:415:TRP:O	2:B:419:GLU:HG3	2.11	0.48
2:B:496:SER:OG	2:B:543:ALA:HB2	2.13	0.48
3:C:502:ILE:O	3:C:506:VAL:HG12	2.13	0.48
1:A:1341:THR:HG22	1:A:1341:THR:O	2.14	0.48
1:A:1502:GLU:HB3	1:A:1504:LEU:CB	2.35	0.48
2:B:154:THR:CB	2:B:161:GLN:HE21	2.26	0.48
2:B:245:ILE:O	2:B:245:ILE:HG12	2.13	0.48
1:A:190:ASP:HA	1:A:193:LEU:HD21	1.95	0.48
1:A:738:ALA:CB	1:A:830:LEU:HD11	2.43	0.48
1:A:1018:THR:HA	1:A:1022:THR:O	2.12	0.48
1:A:2365:LEU:HD13	1:A:2367:VAL:CG2	2.44	0.48
2:B:511:TYR:HD2	2:B:531:ALA:HA	1.78	0.48
3:C:258:PHE:CE2	3:C:260:ILE:HG13	2.48	0.48
3:C:312:PHE:CE1	3:C:318:VAL:HG21	2.48	0.48
1:A:297:VAL:O	1:A:297:VAL:HG12	2.12	0.48
1:A:305:ARG:HA	1:A:332:LYS:HZ3	1.78	0.48
1:A:322:LEU:HD21	1:A:355:ALA:HB1	1.95	0.48
1:A:407:THR:CB	1:A:435:ARG:HH21	2.26	0.48
1:A:495:ASP:HB3	1:A:565:TYR:CE1	2.48	0.48
1:A:804:VAL:O	1:A:804:VAL:HG12	2.14	0.48
1:A:943:ILE:O	1:A:947:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1512:CYS:O	1:A:1515:VAL:HG23	2.13	0.48
1:A:1662:THR:HA	1:A:1665:GLU:OE1	2.12	0.48
1:A:2322:ALA:O	1:A:2326:MET:HG2	2.13	0.48
1:A:2380:GLU:HA	1:A:2383:LEU:CD1	2.43	0.48
2:B:58:LEU:HB3	3:C:383:LYS:HE3	1.95	0.48
2:B:248:CYS:SG	2:B:454:LYS:HD2	2.53	0.48
1:A:202:GLU:HA	1:A:205:LYS:HB2	1.94	0.48
1:A:721:ASP:OD1	1:A:802:CYS:HA	2.13	0.48
1:A:1125:TYR:O	1:A:1129:LEU:HG	2.14	0.48
1:A:1211:HIS:HE1	1:A:1285:LEU:HD13	1.77	0.48
1:A:1756:LYS:NZ	1:A:1785:ILE:HG22	2.28	0.48
1:A:1842:CYS:CA	1:A:1933:ILE:HD11	2.43	0.48
1:A:2169:PHE:CZ	1:A:2411:LEU:HD13	2.49	0.48
1:A:2388:VAL:HA	1:A:2393:ARG:CD	2.42	0.48
1:A:2388:VAL:CA	1:A:2393:ARG:HD3	2.42	0.48
2:B:411:ARG:HB3	2:B:411:ARG:NH1	2.28	0.48
1:A:395:LEU:HB3	1:A:396:PRO:HD3	1.96	0.48
2:B:318:LEU:HB3	2:B:327:PHE:CE2	2.49	0.48
3:C:248:ARG:O	3:C:248:ARG:HG2	2.13	0.48
3:C:330:LEU:O	3:C:334:LEU:HG	2.14	0.48
1:A:167:ALA:HB1	1:A:211:ARG:NH2	2.29	0.48
1:A:489:CYS:CA	3:C:412:ASN:HD22	2.26	0.48
1:A:507:ILE:HG13	3:C:454:PHE:CG	2.49	0.48
1:A:1022:THR:CB	1:A:1415:VAL:H	2.21	0.48
1:A:1203:VAL:HG12	1:A:1207:GLN:OE1	2.14	0.48
1:A:1407:LEU:CD1	1:A:1427:THR:HG21	2.43	0.48
1:A:1655:ASN:ND2	1:A:1663:GLU:OE2	2.45	0.48
1:A:2191:ARG:HD3	1:A:2349:GLU:OE1	2.14	0.48
2:B:269:PHE:CD2	2:B:304:LEU:HD13	2.48	0.48
3:C:485:LEU:HD22	3:C:490:LEU:CB	2.42	0.48
1:A:306:CYS:O	1:A:309:HIS:HB3	2.13	0.48
1:A:545:ALA:HB1	1:A:549:TYR:CZ	2.48	0.48
1:A:1324:LEU:HD13	1:A:1339:THR:N	2.28	0.48
1:A:1586:SER:HB3	1:A:1591:HIS:HD2	1.79	0.48
1:A:1605:TYR:HB2	1:A:1622:LEU:HD13	1.96	0.48
1:A:1657:LEU:N	1:A:1658:PRO:CD	2.77	0.48
1:A:2160:LEU:HD13	1:A:2202:SER:O	2.14	0.48
1:A:2183:GLN:HA	1:A:2185:THR:N	2.29	0.48
2:B:237:VAL:O	2:B:241:LEU:HG	2.13	0.48
1:A:36:SER:HA	1:A:77:HIS:CD2	2.49	0.48
1:A:40:ASP:HB3	1:A:83:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:LEU:HA	1:A:666:TYR:CD1	2.49	0.48
1:A:1204:GLN:HE21	1:A:1322:LYS:HZ3	1.61	0.48
1:A:1300:LEU:HD11	1:A:1316:ILE:HA	1.96	0.48
1:A:1802:GLU:HA	1:A:1803:LEU:HA	1.51	0.48
1:A:1959:THR:HA	1:A:1960:VAL:C	2.39	0.48
1:A:2276:PRO:CB	1:A:2279:VAL:HB	2.43	0.48
1:A:2276:PRO:CA	1:A:2279:VAL:HB	2.44	0.48
2:B:186:HIS:CD2	2:B:542:PRO:HG3	2.49	0.48
2:B:454:LYS:O	2:B:458:VAL:HG23	2.14	0.48
3:C:170:LYS:N	3:C:170:LYS:HD2	2.28	0.48
1:A:138:GLU:HB3	1:A:147:SER:OG	2.13	0.48
1:A:494:THR:O	1:A:498:ILE:HG13	2.14	0.48
1:A:646:LEU:HD11	1:A:675:HIS:CE1	2.49	0.48
1:A:852:ALA:HB3	1:A:853:PRO:CD	2.44	0.48
1:A:942:THR:O	1:A:946:ILE:HD12	2.14	0.48
1:A:1453:LEU:HD22	1:A:1453:LEU:H	1.79	0.48
1:A:2381:THR:HG22	1:A:2388:VAL:HG11	1.96	0.48
3:C:271:GLN:HG2	3:C:307:ILE:CD1	2.44	0.48
3:C:407:SER:HB3	3:C:420:ASP:OD1	2.14	0.48
1:A:108:LEU:HD12	1:A:109:ARG:H	1.78	0.47
1:A:320:ASP:HB3	1:A:322:LEU:HD11	1.95	0.47
1:A:728:ARG:NH1	1:A:801:VAL:HG22	2.29	0.47
1:A:770:VAL:O	1:A:771:GLU:CG	2.59	0.47
1:A:1107:ILE:HG12	1:A:1108:ASN:N	2.29	0.47
1:A:1849:ALA:HB2	1:A:1856:ILE:HD11	1.96	0.47
1:A:2380:GLU:CA	1:A:2383:LEU:HG	2.44	0.47
2:B:237:VAL:O	2:B:237:VAL:HG12	2.14	0.47
3:C:194:ALA:O	3:C:198:LEU:HG	2.14	0.47
3:C:378:ASP:CG	3:C:387:MET:HE1	2.39	0.47
1:A:195:ALA:O	1:A:199:VAL:HG22	2.14	0.47
1:A:295:LYS:HA	1:A:296:CYS:C	2.38	0.47
1:A:350:TRP:CE2	1:A:354:LEU:HD11	2.50	0.47
1:A:422:PRO:N	1:A:423:PRO:HD2	2.29	0.47
1:A:1530:LYS:NZ	1:A:1600:ILE:HD11	2.28	0.47
1:A:1627:TYR:CB	1:A:1791:ARG:HD3	2.44	0.47
1:A:1786:VAL:HG13	1:A:1823:ILE:CD1	2.30	0.47
1:A:2407:ARG:CB	1:A:2410:LEU:HD13	2.41	0.47
1:A:2419:TYR:CG	1:A:3609:ALA:HB1	2.49	0.47
2:B:43:ARG:HB3	2:B:44:GLU:OE1	2.13	0.47
2:B:315:SER:HB2	3:C:297:HIS:CE1	2.49	0.47
2:B:509:SER:HA	2:B:512:GLN:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:LEU:HD13	2:B:547:TYR:HE1	1.79	0.47
3:C:224:LEU:HD23	3:C:477:VAL:HG21	1.96	0.47
1:A:107:GLU:O	1:A:137:GLN:NE2	2.47	0.47
1:A:134:ARG:NH1	1:A:159:GLU:OE2	2.48	0.47
1:A:275:LEU:CD1	1:A:277:MET:HG2	2.44	0.47
1:A:329:HIS:CE1	1:A:348:PRO:HB3	2.49	0.47
1:A:638:VAL:HB	1:A:639:PHE:CA	2.41	0.47
1:A:740:VAL:CA	1:A:751:LEU:HD12	2.36	0.47
1:A:771:GLU:OE2	1:A:773:VAL:HG22	2.14	0.47
1:A:1021:GLN:HG2	1:A:1022:THR:HG22	1.96	0.47
1:A:2160:LEU:HD22	1:A:2203:GLY:CA	2.32	0.47
1:A:2374:ARG:HH11	1:A:2393:ARG:HH12	1.60	0.47
1:A:2385:VAL:HG13	1:A:2386:THR:N	2.29	0.47
3:C:172:LEU:HD12	3:C:172:LEU:N	2.30	0.47
3:C:313:THR:HG23	3:C:341:LYS:HG2	1.97	0.47
3:C:367:LEU:HD21	3:C:400:LEU:HD23	1.95	0.47
1:A:121:VAL:HG12	1:A:162:ARG:NH1	2.29	0.47
1:A:265:GLU:HG2	1:A:310:ILE:HD13	1.95	0.47
1:A:295:LYS:HB3	1:A:297:VAL:HG23	1.97	0.47
1:A:602:PHE:H	1:A:603:ASN:HA	1.79	0.47
1:A:674:ARG:CA	1:A:677:HIS:HB3	2.45	0.47
1:A:1790:LEU:CD2	1:A:1823:ILE:HD12	2.43	0.47
2:B:64:LYS:O	2:B:68:VAL:HG23	2.13	0.47
1:A:389:PRO:O	1:A:393:VAL:HG23	2.15	0.47
1:A:865:VAL:HG13	1:A:868:PHE:CB	2.44	0.47
1:A:2394:LEU:O	1:A:2394:LEU:HD23	2.15	0.47
1:A:38:ASP:N	1:A:39:PRO:HD2	2.29	0.47
1:A:246:ASP:HA	1:A:247:GLU:HA	1.58	0.47
1:A:247:GLU:HG2	1:A:248:VAL:HG13	1.96	0.47
1:A:337:GLN:HA	1:A:338:GLN:HA	1.60	0.47
1:A:403:ARG:O	1:A:407:THR:HG23	2.15	0.47
1:A:500:VAL:HG22	1:A:568:ILE:HD12	1.96	0.47
1:A:1627:TYR:HE2	1:A:1795:LEU:HB2	1.79	0.47
1:A:1753:THR:HG22	1:A:1792:LEU:HD11	1.96	0.47
1:A:1964:GLU:OE1	1:A:2078:LEU:HB3	2.15	0.47
1:A:2120:THR:C	1:A:2144:GLY:HA3	2.40	0.47
1:A:2195:VAL:HG12	1:A:2205:ILE:CG2	2.45	0.47
2:B:206:VAL:HG13	2:B:206:VAL:O	2.15	0.47
2:B:312:PHE:HD2	2:B:318:LEU:HD11	1.79	0.47
2:B:500:CYS:SG	2:B:543:ALA:HB1	2.55	0.47
3:C:251:ASN:CB	3:C:277:SER:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:282:LEU:HD13	3:C:299:TYR:HD2	1.80	0.47
1:A:122:GLN:HG2	1:A:123:HIS:N	2.30	0.47
1:A:131:LYS:HD2	1:A:162:ARG:HH21	1.80	0.47
1:A:233:PHE:CZ	1:A:267:LYS:HG3	2.50	0.47
1:A:379:ALA:HB3	1:A:382:GLU:CD	2.39	0.47
1:A:937:GLN:CB	1:A:981:VAL:HG21	2.44	0.47
1:A:1195:ILE:O	1:A:1195:ILE:HG12	2.15	0.47
1:A:1351:THR:HG21	1:A:1416:PRO:HG2	1.95	0.47
1:A:1523:LYS:HB3	1:A:1526:LEU:HD13	1.97	0.47
1:A:1816:THR:H	1:A:1817:ALA:CB	2.27	0.47
1:A:2099:LEU:O	1:A:2124:VAL:HG21	2.14	0.47
1:A:2153:LEU:C	1:A:2153:LEU:HD12	2.40	0.47
1:A:2181:ASN:OD1	1:A:2188:PHE:HB2	2.14	0.47
1:A:2191:ARG:CB	1:A:2351:VAL:HG12	2.45	0.47
1:A:2393:ARG:HA	1:A:2396:CYS:SG	2.55	0.47
1:A:2407:ARG:N	1:A:2407:ARG:HD2	2.29	0.47
2:B:268:LEU:HB3	2:B:337:TYR:CE2	2.50	0.47
2:B:307:GLN:HG2	3:C:280:ASP:OD2	2.15	0.47
2:B:419:GLU:O	2:B:423:SER:OG	2.12	0.47
2:B:552:HIS:O	2:B:556:TYR:N	2.48	0.47
3:C:198:LEU:CD1	3:C:496:PHE:HB2	2.45	0.47
3:C:205:LEU:HB2	3:C:482:ARG:NH1	2.30	0.47
3:C:382:ARG:O	3:C:386:GLN:HG3	2.13	0.47
1:A:156:ILE:O	1:A:159:GLU:HB2	2.15	0.47
1:A:422:PRO:HD3	1:A:428:TYR:HE1	1.80	0.47
1:A:1324:LEU:HD22	1:A:1337:LEU:CB	2.45	0.47
1:A:1343:SER:CA	1:A:1344:GLN:CB	2.91	0.47
1:A:1532:ILE:HG13	1:A:1607:LEU:HD23	1.96	0.47
1:A:1657:LEU:HD12	1:A:1658:PRO:CA	2.44	0.47
1:A:2193:TYR:CE1	1:A:2205:ILE:HD12	2.49	0.47
2:B:188:PHE:O	2:B:192:GLN:HG2	2.14	0.47
2:B:359:CYS:HB3	3:C:454:PHE:CE2	2.49	0.47
3:C:184:VAL:HG13	3:C:188:MET:HA	1.96	0.47
3:C:198:LEU:O	3:C:493:LYS:HE3	2.15	0.47
3:C:244:GLU:OE1	3:C:252:GLN:HB2	2.14	0.47
3:C:467:GLN:OE1	3:C:467:GLN:N	2.43	0.47
1:A:136:SER:HA	1:A:139:ARG:CG	2.44	0.47
1:A:468:ASP:N	1:A:469:PRO:HD3	2.30	0.47
1:A:740:VAL:HG21	1:A:752:PHE:CZ	2.49	0.47
1:A:1360:LEU:HB3	1:A:1361:GLU:OE1	2.15	0.47
1:A:1645:LEU:O	1:A:1649:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1655:ASN:OD1	1:A:1727:GLU:HG3	2.15	0.47
1:A:1712:ILE:HD12	1:A:1712:ILE:N	2.30	0.47
2:B:313:ARG:HD3	2:B:327:PHE:HE2	1.78	0.47
3:C:187:GLN:HG2	3:C:187:GLN:O	2.15	0.47
3:C:229:PRO:HG3	3:C:467:GLN:HA	1.97	0.47
3:C:232:ASP:O	3:C:235:THR:OG1	2.31	0.47
1:A:606:ASN:O	1:A:610:VAL:HG22	2.15	0.47
1:A:2336:ARG:NE	1:A:2336:ARG:HA	2.30	0.47
2:B:140:ALA:HB2	2:B:151:LEU:HD22	1.97	0.47
2:B:243:THR:O	2:B:246:LYS:NZ	2.48	0.47
2:B:479:LEU:H	2:B:479:LEU:HD12	1.79	0.47
1:A:232:ILE:HD12	1:A:232:ILE:N	2.30	0.46
1:A:492:CYS:HA	1:A:565:TYR:OH	2.16	0.46
1:A:672:CYS:HA	1:A:675:HIS:NE2	2.29	0.46
1:A:1945:VAL:HG23	1:A:1946:LEU:HD22	1.96	0.46
1:A:2303:SER:OG	1:A:2345:MET:HB3	2.15	0.46
1:A:2370:LYS:HB2	1:A:2372:PRO:HD3	1.97	0.46
1:A:262:THR:HA	1:A:265:GLU:OE1	2.15	0.46
1:A:622:GLY:O	1:A:623:ASN:HB3	2.15	0.46
1:A:735:ALA:HB1	1:A:822:LYS:HE3	1.97	0.46
1:A:1293:LEU:HD22	1:A:1322:LYS:HG2	1.97	0.46
1:A:1407:LEU:HD23	1:A:1453:LEU:HB2	1.96	0.46
1:A:1413:GLN:N	1:A:1414:THR:HA	2.27	0.46
2:B:314:LYS:O	3:C:295:LEU:HD11	2.16	0.46
2:B:495:PHE:CD2	3:C:339:MET:HE2	2.42	0.46
3:C:219:MET:CE	4:C:601:GTP:H2'	2.43	0.46
1:A:120:SER:O	1:A:127:ALA:HB2	2.15	0.46
1:A:127:ALA:HA	1:A:130:THR:HG22	1.97	0.46
1:A:134:ARG:O	1:A:138:GLU:HG3	2.16	0.46
1:A:192:ILE:N	1:A:192:ILE:HD12	2.30	0.46
1:A:335:LEU:HG	1:A:342:TRP:CH2	2.50	0.46
1:A:419:ILE:HG21	1:A:441:THR:OG1	2.14	0.46
1:A:450:GLU:OE2	1:A:454:THR:HG21	2.15	0.46
1:A:509:GLU:O	1:A:509:GLU:HG2	2.15	0.46
1:A:846:ARG:NH2	1:A:921:ALA:O	2.48	0.46
1:A:1207:GLN:HG2	1:A:1289:ILE:HG13	1.98	0.46
1:A:1934:VAL:C	1:A:1938:SER:HG	2.21	0.46
1:A:1961:LEU:N	1:A:1961:LEU:HD12	2.30	0.46
3:C:319:ILE:HG23	3:C:370:LEU:HG	1.97	0.46
1:A:491:THR:HG22	1:A:493:GLY:H	1.81	0.46
1:A:1289:ILE:O	1:A:1293:LEU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:PRO:HG2	1:A:2306:THR:CG2	2.45	0.46
1:A:1307:ILE:HB	1:A:2306:THR:CG2	2.45	0.46
1:A:1793:LEU:HG	1:A:2417:PHE:CE2	2.51	0.46
1:A:1989:LYS:HD2	1:A:1989:LYS:C	2.41	0.46
1:A:2098:TRP:O	1:A:2102:MET:HG2	2.15	0.46
1:A:2131:LEU:CD2	1:A:2139:LYS:H	2.28	0.46
1:A:2160:LEU:O	1:A:2197:PRO:HB3	2.15	0.46
1:A:2214:LEU:HD22	1:A:2296:LEU:HD12	1.97	0.46
2:B:318:LEU:HD23	2:B:325:CYS:HB2	1.97	0.46
3:C:248:ARG:HD3	3:C:248:ARG:H	1.81	0.46
1:A:190:ASP:O	1:A:193:LEU:HG	2.16	0.46
1:A:420:ARG:O	1:A:424:ILE:HG13	2.15	0.46
1:A:656:HIS:HA	1:A:660:ILE:HD11	1.97	0.46
1:A:805:GLN:HG3	1:A:806:LEU:N	2.30	0.46
1:A:1209:ALA:O	1:A:1213:LEU:HG	2.15	0.46
1:A:1673:LEU:O	1:A:1677:VAL:HG22	2.15	0.46
1:A:1981:ILE:O	1:A:1985:GLU:HG3	2.15	0.46
1:A:2276:PRO:HB2	1:A:2279:VAL:N	2.18	0.46
2:B:191:HIS:O	2:B:195:LEU:HG	2.15	0.46
2:B:420:LEU:HA	2:B:425:LYS:HB2	1.97	0.46
1:A:141:MET:HE1	1:A:146:GLU:N	2.28	0.46
1:A:380:SER:CA	2:B:350:MET:HE1	2.42	0.46
1:A:441:THR:HG1	1:A:446:VAL:HG22	1.81	0.46
1:A:1131:ALA:HB1	1:A:1206:TRP:NE1	2.18	0.46
1:A:1199:ASP:O	1:A:1203:VAL:HG23	2.16	0.46
1:A:1664:GLU:HB3	1:A:1668:ARG:HH12	1.80	0.46
1:A:2055:LEU:HD23	1:A:2055:LEU:C	2.41	0.46
1:A:2376:THR:HG23	1:A:2388:VAL:HG11	1.98	0.46
3:C:472:LYS:O	3:C:476:GLN:HG2	2.15	0.46
1:A:611:VAL:O	1:A:615:LEU:HD23	2.15	0.46
1:A:931:THR:HB	1:A:932:PRO:HD3	1.97	0.46
1:A:1286:GLN:NE2	1:A:1286:GLN:H	2.14	0.46
1:A:1597:PRO:HG3	1:A:1629:TRP:CD2	2.51	0.46
1:A:2087:SER:OG	1:A:2132:PRO:HG3	2.15	0.46
1:A:2332:GLY:O	1:A:2358:CYS:HA	2.16	0.46
2:B:265:LEU:HD11	2:B:325:CYS:SG	2.55	0.46
2:B:309:TYR:OH	2:B:313:ARG:NH1	2.49	0.46
3:C:390:MET:O	3:C:394:LEU:HG	2.16	0.46
1:A:80:ILE:HB	1:A:106:GLN:OE1	2.15	0.46
1:A:1027:LEU:CD2	1:A:1085:CYS:HA	2.45	0.46
1:A:1521:VAL:CG1	1:A:1522:ALA:HB2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2103:THR:O	1:A:2103:THR:HG22	2.16	0.46
2:B:154:THR:O	2:B:161:GLN:HG3	2.16	0.46
2:B:504:LEU:HD22	2:B:550:GLN:HG2	1.98	0.46
1:A:173:LYS:HA	1:A:176:ILE:CG2	2.46	0.46
1:A:508:VAL:HG23	1:A:509:GLU:OE1	2.14	0.46
1:A:1793:LEU:HG	1:A:2417:PHE:CZ	2.51	0.46
2:B:137:LEU:N	2:B:154:THR:HG1	2.13	0.46
2:B:226:VAL:O	2:B:230:LEU:HG	2.16	0.46
1:A:436:VAL:HG23	1:A:436:VAL:O	2.16	0.46
1:A:624:ALA:O	1:A:628:LEU:HG	2.16	0.46
1:A:636:PRO:HB3	1:A:638:VAL:HG22	1.98	0.46
1:A:2089:ILE:HG13	1:A:2128:ILE:HG13	1.97	0.46
1:A:2380:GLU:HA	1:A:2383:LEU:CG	2.44	0.46
2:B:5:VAL:O	2:B:9:ASP:HB2	2.15	0.46
2:B:151:LEU:HD11	2:B:448:TRP:CZ2	2.49	0.46
2:B:326:LEU:CD1	2:B:427:PHE:HB3	2.46	0.46
2:B:523:VAL:O	2:B:523:VAL:HG12	2.14	0.46
3:C:185:ASP:HB2	3:C:189:ASN:HB2	1.98	0.46
1:A:114:THR:HG22	1:A:134:ARG:CG	2.34	0.45
1:A:424:ILE:O	1:A:424:ILE:HG22	2.16	0.45
1:A:503:LEU:CB	1:A:572:MET:HE2	2.46	0.45
1:A:558:ILE:HG23	1:A:612:ILE:CG2	2.46	0.45
1:A:559:PRO:O	1:A:560:VAL:C	2.59	0.45
1:A:730:LEU:HG	1:A:730:LEU:O	2.17	0.45
1:A:1206:TRP:O	1:A:1210:ILE:HG13	2.16	0.45
1:A:1597:PRO:HG2	1:A:1625:TRP:CZ2	2.51	0.45
1:A:2055:LEU:HD23	1:A:2059:LEU:HB2	1.98	0.45
1:A:2365:LEU:CD1	1:A:2367:VAL:HB	2.45	0.45
2:B:45:ASP:O	2:B:147:LYS:HD3	2.16	0.45
2:B:47:ILE:HD13	2:B:445:TYR:HA	1.98	0.45
3:C:205:LEU:HD23	3:C:265:ILE:HG23	1.98	0.45
1:A:165:ARG:NE	1:A:165:ARG:HA	2.32	0.45
1:A:256:THR:O	1:A:260:LEU:HG	2.16	0.45
1:A:313:THR:O	1:A:313:THR:HG22	2.16	0.45
1:A:460:VAL:HB	1:A:473:ILE:HD13	1.97	0.45
1:A:633:ALA:O	1:A:636:PRO:HD2	2.16	0.45
1:A:748:TYR:O	1:A:750:PRO:HD3	2.16	0.45
1:A:826:LEU:HD22	1:A:909:ASP:CG	2.40	0.45
1:A:1281:ASP:HB2	1:A:1282:PRO:CD	2.46	0.45
1:A:1349:LEU:HB3	1:A:1355:TYR:CE1	2.50	0.45
1:A:2099:LEU:O	1:A:2102:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2102:MET:CE	1:A:2105:THR:HG21	2.41	0.45
1:A:2213:PRO:HG3	1:A:2342:LEU:HD22	1.97	0.45
1:A:2215:PHE:CA	1:A:2338:LEU:HB3	2.45	0.45
1:A:2369:GLU:HG3	1:A:2369:GLU:O	2.16	0.45
3:C:417:LEU:HB2	3:C:418:PRO:CD	2.43	0.45
1:A:170:LYS:O	1:A:174:GLU:HB2	2.16	0.45
1:A:249:LYS:O	1:A:250:LEU:HD23	2.16	0.45
1:A:251:LEU:H	1:A:251:LEU:CD2	2.28	0.45
1:A:335:LEU:HA	1:A:336:THR:HA	1.61	0.45
1:A:504:LEU:HD13	2:B:359:CYS:CB	2.46	0.45
1:A:1596:GLU:CB	1:A:1597:PRO:HD2	2.47	0.45
1:A:1605:TYR:CB	1:A:1622:LEU:HD13	2.47	0.45
1:A:1664:GLU:HB3	1:A:1668:ARG:NH1	2.31	0.45
1:A:2388:VAL:HG12	1:A:2393:ARG:CD	2.46	0.45
2:B:47:ILE:HG22	2:B:142:TYR:CE1	2.51	0.45
1:A:150:SER:O	1:A:152:LEU:N	2.50	0.45
1:A:199:VAL:CB	1:A:263:VAL:HG22	2.46	0.45
1:A:247:GLU:H	1:A:253:LEU:CD1	2.27	0.45
1:A:249:LYS:HG2	1:A:297:VAL:CG2	2.46	0.45
1:A:408:VAL:O	1:A:412:ILE:HG12	2.17	0.45
1:A:458:GLU:CG	1:A:501:LEU:HD22	2.45	0.45
1:A:653:LEU:HD23	1:A:663:ALA:HB3	1.98	0.45
1:A:1034:ILE:HG22	1:A:1102:LYS:NZ	2.31	0.45
1:A:1197:ILE:HG23	1:A:1318:GLU:OE2	2.16	0.45
1:A:1858:TYR:HB3	1:A:1862:VAL:HG23	1.97	0.45
1:A:1954:GLU:O	1:A:1958:VAL:HG13	2.17	0.45
1:A:2155:LYS:HB3	1:A:2158:GLU:OE1	2.17	0.45
1:A:2171:SER:HA	1:A:2192:HIS:CE1	2.45	0.45
1:A:2353:ILE:HG22	1:A:2354:ASP:H	1.79	0.45
2:B:169:LEU:CD1	2:B:180:LEU:HD12	2.46	0.45
3:C:326:THR:HG22	3:C:326:THR:O	2.16	0.45
3:C:391:ILE:HG21	3:C:421:PHE:CE1	2.52	0.45
1:A:148:ARG:HA	1:A:153:LEU:HD22	1.99	0.45
1:A:484:ASP:OD2	1:A:498:ILE:HD11	2.17	0.45
1:A:934:GLY:O	1:A:981:VAL:HG13	2.17	0.45
1:A:1307:ILE:CB	1:A:2306:THR:HG21	2.46	0.45
1:A:1486:GLU:OE1	1:A:1611:GLN:HB2	2.16	0.45
1:A:1711:LEU:HD22	1:A:1712:ILE:CD1	2.46	0.45
1:A:2141:LEU:HD13	1:A:2151:PRO:HA	1.99	0.45
2:B:310:ARG:NH1	3:C:284:ASN:HD21	2.15	0.45
3:C:490:LEU:HD13	3:C:498:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:N	1:A:207:LEU:HD12	2.31	0.45
1:A:903:ARG:N	1:A:903:ARG:HD2	2.31	0.45
1:A:1086:PRO:HB3	1:A:1090:GLN:C	2.42	0.45
1:A:1710:GLN:HA	1:A:1714:SER:HA	1.99	0.45
1:A:1796:LEU:HB2	1:A:1807:LEU:HD23	1.98	0.45
1:A:1951:LEU:HD21	1:A:2102:MET:CE	2.45	0.45
1:A:2325:SER:HB3	1:A:2374:ARG:HG3	1.98	0.45
1:A:2326:MET:HG3	1:A:2400:LEU:HD23	1.99	0.45
1:A:2410:LEU:H	1:A:2410:LEU:HD12	1.82	0.45
2:B:458:VAL:HG12	2:B:479:LEU:HD21	1.99	0.45
1:A:148:ARG:CA	1:A:153:LEU:HD22	2.47	0.45
1:A:148:ARG:CB	1:A:182:LYS:HG2	2.47	0.45
1:A:199:VAL:HG12	1:A:212:GLN:HE22	1.81	0.45
1:A:295:LYS:HB3	1:A:297:VAL:CG2	2.47	0.45
1:A:857:PHE:CZ	1:A:1190:ALA:HB2	2.52	0.45
1:A:1413:GLN:HE22	1:A:1460:GLN:HB2	1.82	0.45
1:A:1414:THR:CB	1:A:1415:VAL:HB	2.46	0.45
1:A:1462:LEU:CB	1:A:1470:SER:HB3	2.47	0.45
1:A:1655:ASN:HD22	1:A:1663:GLU:CD	2.24	0.45
1:A:2023:HIS:HA	1:A:2026:SER:OG	2.17	0.45
2:B:225:ARG:HH22	3:C:519:LEU:HB3	1.80	0.45
2:B:237:VAL:CG2	2:B:482:ILE:HG21	2.47	0.45
2:B:521:MET:O	2:B:523:VAL:HG23	2.16	0.45
3:C:421:PHE:CE2	3:C:423:ASP:HB2	2.52	0.45
1:A:129:ALA:O	1:A:132:ASP:HB2	2.17	0.45
1:A:135:LYS:O	1:A:139:ARG:HG2	2.17	0.45
1:A:596:ALA:HA	1:A:597:PHE:HA	1.77	0.45
1:A:740:VAL:HG12	1:A:751:LEU:CD1	2.47	0.45
1:A:1352:LEU:HD12	1:A:1353:GLN:CA	2.43	0.45
1:A:2247:PRO:HB2	1:A:2248:ARG:C	2.42	0.45
1:A:2295:LEU:HB2	1:A:2379:ILE:HG21	1.99	0.45
3:C:335:GLN:NE2	3:C:394:LEU:O	2.50	0.45
1:A:274:GLN:CB	1:A:275:LEU:HA	2.47	0.45
1:A:275:LEU:H	1:A:276:VAL:HA	1.81	0.45
1:A:562:GLU:HG2	1:A:563:THR:N	2.32	0.45
1:A:809:SER:O	1:A:813:ILE:HG22	2.17	0.45
1:A:983:LEU:HD12	1:A:1015:PHE:CE1	2.50	0.45
1:A:1816:THR:HG23	1:A:1819:TRP:HE3	1.82	0.45
1:A:1835:VAL:HG22	1:A:1836:TYR:N	2.31	0.45
1:A:2089:ILE:HD11	1:A:2128:ILE:CD1	2.46	0.45
1:A:2137:PRO:HA	1:A:2154:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2162:LEU:O	1:A:2166:ILE:HG13	2.17	0.45
1:A:2317:TYR:HA	1:A:2348:GLY:O	2.17	0.45
2:B:315:SER:HB2	3:C:297:HIS:CD2	2.52	0.45
3:C:258:PHE:HZ	3:C:260:ILE:HD11	1.82	0.45
1:A:275:LEU:N	1:A:276:VAL:HA	2.32	0.45
1:A:376:SER:OG	1:A:386:GLU:OE1	2.24	0.45
1:A:481:TYR:O	1:A:485:GLN:HB2	2.17	0.45
1:A:556:LYS:O	1:A:569:LEU:HD13	2.16	0.45
1:A:1048:VAL:HG13	1:A:1052:PHE:CE2	2.42	0.45
1:A:1467:LYS:O	1:A:1471:THR:HG23	2.17	0.45
1:A:1610:VAL:HA	1:A:1611:GLN:HA	1.47	0.45
1:A:1646:LEU:HD23	1:A:1646:LEU:C	2.42	0.45
1:A:2169:PHE:CD1	1:A:2414:LEU:HD23	2.53	0.45
2:B:312:PHE:CB	2:B:318:LEU:HG	2.45	0.45
3:C:260:ILE:CG2	3:C:264:ARG:HA	2.46	0.45
1:A:134:ARG:HH22	1:A:155:ARG:HD3	1.82	0.44
1:A:365:LEU:HD22	1:A:401:LEU:CD1	2.47	0.44
1:A:982:LEU:C	1:A:992:LYS:HE3	2.42	0.44
1:A:1338:SER:CB	1:A:1401:MET:HE2	2.26	0.44
1:A:1645:LEU:HA	1:A:1648:ARG:HG2	1.99	0.44
1:A:2025:ARG:NH1	1:A:2053:GLU:HG2	2.32	0.44
3:C:311:LEU:O	3:C:315:CYS:HB2	2.17	0.44
1:A:471:MET:O	1:A:472:THR:OG1	2.30	0.44
1:A:656:HIS:CA	1:A:660:ILE:HD11	2.48	0.44
1:A:820:LEU:HD13	1:A:885:ARG:CB	2.47	0.44
1:A:1054:LEU:HD13	1:A:1415:VAL:CG1	2.46	0.44
1:A:1077:VAL:O	1:A:1080:LEU:HD23	2.17	0.44
1:A:1088:ALA:O	1:A:1089:ILE:C	2.60	0.44
1:A:1334:PRO:HG2	1:A:1335:LEU:CD2	2.46	0.44
1:A:1856:ILE:O	1:A:1856:ILE:HG13	2.17	0.44
1:A:1958:VAL:O	1:A:1961:LEU:HD12	2.17	0.44
2:B:48:CYS:HG	2:B:148:VAL:HG22	1.80	0.44
2:B:152:LEU:HD12	2:B:152:LEU:O	2.17	0.44
2:B:205:SER:O	2:B:259:ARG:HA	2.17	0.44
2:B:208:HIS:C	2:B:209:ILE:HD12	2.42	0.44
2:B:296:PRO:HB3	3:C:246:LYS:CD	2.46	0.44
3:C:205:LEU:HB2	3:C:482:ARG:NH2	2.31	0.44
1:A:575:ALA:HA	3:C:453:LEU:HD12	1.99	0.44
1:A:638:VAL:H	1:A:639:PHE:HA	1.82	0.44
1:A:987:LEU:HG	1:A:988:GLU:N	2.27	0.44
1:A:1054:LEU:HB3	1:A:1415:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:LEU:CD1	1:A:1349:LEU:HD11	2.45	0.44
1:A:1348:VAL:O	1:A:1349:LEU:C	2.60	0.44
1:A:1955:LEU:O	1:A:1958:VAL:HG22	2.18	0.44
2:B:48:CYS:SG	2:B:418:VAL:HG13	2.57	0.44
2:B:323:ILE:HG13	2:B:324:ASN:N	2.32	0.44
3:C:221:MET:HB3	3:C:238:PHE:CE2	2.52	0.44
3:C:413:VAL:HG12	3:C:413:VAL:O	2.17	0.44
1:A:276:VAL:CG1	1:A:280:LEU:HG	2.29	0.44
1:A:1318:GLU:O	1:A:1321:VAL:HG12	2.18	0.44
1:A:2212:THR:O	1:A:2343:ILE:HG22	2.16	0.44
1:A:2371:VAL:N	1:A:2372:PRO:CD	2.80	0.44
1:A:2406:GLY:C	1:A:2407:ARG:HD2	2.42	0.44
2:B:66:SER:O	2:B:70:THR:HG23	2.16	0.44
1:A:602:PHE:N	1:A:603:ASN:HA	2.32	0.44
1:A:770:VAL:HG11	1:A:814:ARG:HH12	1.82	0.44
1:A:1521:VAL:HG13	1:A:1522:ALA:N	2.31	0.44
3:C:224:LEU:CD2	3:C:477:VAL:HG21	2.47	0.44
1:A:227:TYR:HA	1:A:273:MET:HE3	2.00	0.44
1:A:451:ALA:HB3	2:B:351:LEU:CD1	2.47	0.44
1:A:716:ILE:O	1:A:720:LYS:HG2	2.17	0.44
1:A:2055:LEU:HD13	1:A:2070:PRO:CG	2.48	0.44
1:A:2334:GLY:N	1:A:2357:VAL:O	2.47	0.44
1:A:2366:ARG:HA	1:A:2366:ARG:HE	1.81	0.44
2:B:49:VAL:HG22	2:B:149:LEU:HD23	2.00	0.44
2:B:541:GLY:N	3:C:339:MET:HG2	2.32	0.44
3:C:341:LYS:C	3:C:341:LYS:HD3	2.42	0.44
1:A:302:LEU:CD2	1:A:341:GLY:HA2	2.48	0.44
1:A:619:THR:HA	1:A:620:THR:HA	1.61	0.44
1:A:675:HIS:N	1:A:676:ASP:C	2.75	0.44
1:A:1664:GLU:O	1:A:1667:GLU:HG2	2.17	0.44
1:A:1756:LYS:C	1:A:1756:LYS:HD2	2.43	0.44
1:A:2423:VAL:HG22	1:A:2423:VAL:O	2.16	0.44
2:B:162:LEU:HD13	3:C:326:THR:CG2	2.47	0.44
3:C:301:GLU:O	3:C:305:LEU:HG	2.17	0.44
1:A:141:MET:CE	1:A:146:GLU:H	2.28	0.44
1:A:176:ILE:HG23	1:A:177:GLN:CD	2.43	0.44
1:A:285:GLU:O	1:A:289:THR:HG23	2.18	0.44
1:A:1341:THR:HB	1:A:1405:GLN:HE22	1.83	0.44
1:A:1727:GLU:OE1	1:A:1731:LYS:N	2.51	0.44
1:A:1827:PHE:CE2	1:A:1859:PRO:HB2	2.52	0.44
2:B:264:ARG:CG	2:B:326:LEU:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:VAL:HG13	3:C:376:ARG:HH22	1.82	0.44
3:C:215:THR:HA	3:C:323:ASP:HB2	2.00	0.44
3:C:407:SER:O	3:C:408:MET:HE3	2.18	0.44
1:A:336:THR:HG23	1:A:336:THR:O	2.18	0.44
1:A:419:ILE:CG2	1:A:442:ALA:H	2.29	0.44
1:A:455:ALA:O	1:A:458:GLU:HG3	2.17	0.44
1:A:607:ALA:O	1:A:611:VAL:HG23	2.17	0.44
1:A:638:VAL:N	1:A:639:PHE:HA	2.33	0.44
1:A:671:HIS:CD2	1:A:672:CYS:H	2.35	0.44
1:A:734:TRP:HE3	3:C:201:GLN:HE22	1.64	0.44
1:A:866:ILE:CD1	1:A:1291:VAL:HG12	2.48	0.44
1:A:1207:GLN:HG2	1:A:1289:ILE:HG12	2.00	0.44
1:A:1610:VAL:HG23	1:A:1610:VAL:O	2.18	0.44
1:A:2170:LEU:HD11	1:A:2355:TYR:CE2	2.51	0.44
1:A:2228:LEU:HD23	1:A:2228:LEU:C	2.42	0.44
1:A:2376:THR:CG2	1:A:2388:VAL:HG11	2.48	0.44
2:B:7:LEU:O	2:B:11:LEU:HG	2.18	0.44
1:A:420:ARG:HA	1:A:423:PRO:CG	2.48	0.43
1:A:471:MET:HE3	1:A:471:MET:CA	2.40	0.43
1:A:713:LEU:N	1:A:713:LEU:HD12	2.33	0.43
1:A:1292:GLN:CG	1:A:1322:LYS:HD3	2.48	0.43
1:A:1612:ALA:O	1:A:1619:TRP:NE1	2.44	0.43
1:A:1627:TYR:HD1	1:A:1791:ARG:HH11	1.66	0.43
1:A:2140:LEU:N	1:A:2140:LEU:HD23	2.33	0.43
2:B:63:GLU:HG3	2:B:270:GLN:HE22	1.83	0.43
2:B:260:PRO:O	2:B:441:GLU:HB3	2.18	0.43
1:A:85:LYS:HZ1	1:A:113:VAL:HG13	1.81	0.43
1:A:160:ASP:CG	1:A:178:GLN:HE22	2.26	0.43
1:A:729:LYS:CB	1:A:901:ILE:HD11	2.49	0.43
1:A:1092:ILE:H	1:A:1120:LYS:HZ3	1.65	0.43
1:A:1204:GLN:NE2	1:A:1322:LYS:HB2	2.32	0.43
1:A:1335:LEU:HG	1:A:1336:ARG:N	2.33	0.43
1:A:1711:LEU:HD23	1:A:1711:LEU:C	2.44	0.43
1:A:1793:LEU:O	1:A:1797:VAL:HG22	2.17	0.43
1:A:1844:LEU:HD23	1:A:1848:VAL:HG13	2.01	0.43
1:A:2023:HIS:CD2	1:A:2027:ILE:HG23	2.53	0.43
1:A:2180:ILE:HG23	1:A:2403:MET:HE3	1.99	0.43
2:B:305:GLU:HG3	2:B:334:ALA:HB3	1.99	0.43
2:B:323:ILE:HG13	2:B:324:ASN:H	1.83	0.43
2:B:348:VAL:HG13	2:B:348:VAL:O	2.19	0.43
1:A:305:ARG:HA	1:A:332:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ALA:CA	3:C:453:LEU:HD12	2.48	0.43
1:A:649:VAL:HG11	1:A:667:THR:CB	2.29	0.43
1:A:895:LYS:HD3	1:A:907:LYS:HE2	2.00	0.43
1:A:1015:PHE:CZ	1:A:1080:LEU:HG	2.53	0.43
2:B:152:LEU:HD12	2:B:152:LEU:C	2.42	0.43
3:C:322:GLN:HG2	3:C:330:LEU:CD1	2.48	0.43
1:A:104:LEU:HD21	1:A:133:MET:HB3	1.99	0.43
1:A:128:LEU:C	1:A:128:LEU:HD23	2.43	0.43
1:A:262:THR:CG2	1:A:303:VAL:HG21	2.49	0.43
1:A:1521:VAL:HA	1:A:1522:ALA:HA	1.85	0.43
1:A:1757:LEU:HB3	1:A:1816:THR:HG23	1.99	0.43
1:A:1816:THR:N	1:A:1817:ALA:HB2	2.32	0.43
1:A:1832:HIS:CD2	1:A:1834:GLU:H	2.36	0.43
1:A:2055:LEU:CB	1:A:2070:PRO:HG2	2.48	0.43
1:A:2281:LYS:O	1:A:2285:GLU:HG2	2.18	0.43
1:A:2388:VAL:CB	1:A:2393:ARG:HD3	2.47	0.43
1:A:2393:ARG:NH2	1:A:2397:GLU:OE2	2.51	0.43
1:A:637:THR:HB	1:A:638:VAL:CA	2.49	0.43
1:A:1454:GLY:O	1:A:1458:THR:HG23	2.17	0.43
1:A:1530:LYS:HZ1	1:A:1600:ILE:HD11	1.84	0.43
1:A:1827:PHE:HZ	1:A:1859:PRO:HB2	1.84	0.43
1:A:1838:ARG:HD3	1:A:1929:CYS:SG	2.58	0.43
1:A:2058:PRO:HG2	1:A:2059:LEU:CD1	2.49	0.43
1:A:2059:LEU:N	1:A:2059:LEU:HD12	2.33	0.43
2:B:57:ALA:HA	2:B:159:ASN:HD22	1.84	0.43
2:B:267:PHE:CE2	2:B:308:ILE:HG21	2.54	0.43
2:B:352:LEU:HD13	3:C:460:TYR:CD2	2.53	0.43
3:C:295:LEU:HG	3:C:297:HIS:H	1.83	0.43
1:A:89:SER:O	1:A:126:ARG:NE	2.51	0.43
1:A:130:THR:O	1:A:133:MET:HB2	2.18	0.43
1:A:317:ASP:OD1	1:A:357:SER:HB2	2.18	0.43
1:A:365:LEU:HD11	1:A:401:LEU:HD21	1.99	0.43
1:A:420:ARG:NH2	1:A:446:VAL:HG12	2.33	0.43
1:A:489:CYS:CB	3:C:412:ASN:HD22	2.32	0.43
1:A:613:PHE:CD1	1:A:629:ILE:HD12	2.53	0.43
1:A:1027:LEU:HD22	1:A:1084:HIS:O	2.18	0.43
1:A:1305:ASN:HA	1:A:1306:PRO:HA	1.74	0.43
1:A:1934:VAL:O	1:A:1938:SER:OG	2.34	0.43
1:A:2067:SER:OG	1:A:2069:ILE:HG23	2.19	0.43
1:A:2102:MET:HE3	1:A:2105:THR:CG2	2.43	0.43
2:B:351:LEU:O	2:B:355:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:GLN:HB2	3:C:276:PRO:HD2	2.00	0.43
1:A:892:ARG:N	1:A:903:ARG:HE	2.16	0.43
1:A:1501:MET:O	1:A:1503:MET:HB2	2.19	0.43
1:A:1935:ASP:O	1:A:1939:SER:N	2.51	0.43
2:B:186:HIS:CD2	2:B:493:THR:HG22	2.53	0.43
2:B:328:THR:O	2:B:328:THR:HG22	2.19	0.43
3:C:207:VAL:HG21	3:C:477:VAL:HG13	2.01	0.43
1:A:81:GLN:HB3	1:A:113:VAL:HG22	2.01	0.43
1:A:285:GLU:OE1	1:A:285:GLU:N	2.51	0.43
1:A:463:LEU:HD21	1:A:509:GLU:OE1	2.19	0.43
1:A:554:SER:OG	1:A:608:LYS:HE3	2.17	0.43
1:A:1306:PRO:HB2	1:A:2306:THR:HG22	2.00	0.43
1:A:2166:ILE:O	1:A:2170:LEU:HG	2.18	0.43
1:A:2273:ARG:H	1:A:2274:ASP:HB3	1.82	0.43
1:A:2342:LEU:CD1	1:A:2353:ILE:HD11	2.47	0.43
1:A:2385:VAL:HG22	1:A:2386:THR:HG23	2.00	0.43
2:B:46:GLU:HB3	2:B:442:LEU:HD21	2.00	0.43
2:B:154:THR:HB	2:B:161:GLN:HE21	1.82	0.43
2:B:240:LEU:HD11	2:B:478:ILE:HG22	2.00	0.43
2:B:271:LEU:HG	2:B:336:VAL:CG1	2.49	0.43
2:B:441:GLU:O	2:B:441:GLU:HG3	2.18	0.43
1:A:552:VAL:HG22	1:A:556:LYS:CD	2.49	0.43
1:A:739:ALA:CA	3:C:172:LEU:HD23	2.48	0.43
1:A:932:PRO:O	1:A:933:LEU:HD23	2.19	0.43
1:A:1523:LYS:HG3	1:A:1524:SER:N	2.33	0.43
1:A:1955:LEU:HA	1:A:1958:VAL:HG22	2.01	0.43
1:A:2055:LEU:HD13	1:A:2070:PRO:HG2	2.01	0.43
3:C:456:LEU:HD12	3:C:456:LEU:N	2.34	0.43
1:A:206:LEU:HD12	1:A:206:LEU:N	2.34	0.43
1:A:429:VAL:O	1:A:430:THR:OG1	2.32	0.43
1:A:767:ASN:HD22	1:A:806:LEU:HD22	1.81	0.43
1:A:866:ILE:HD13	1:A:1291:VAL:CG1	2.49	0.43
1:A:881:ASN:HD22	1:A:1306:PRO:HB3	1.84	0.43
1:A:903:ARG:HD2	1:A:903:ARG:H	1.83	0.43
1:A:1410:ILE:HD11	1:A:1423:GLU:C	2.44	0.43
1:A:1478:LYS:NZ	1:A:1532:ILE:HG21	2.33	0.43
1:A:1981:ILE:CG1	1:A:2067:SER:HA	2.49	0.43
1:A:2388:VAL:CG1	1:A:2393:ARG:HD3	2.48	0.43
2:B:48:CYS:SG	2:B:422:LEU:HD21	2.59	0.43
3:C:205:LEU:CB	3:C:482:ARG:HH22	2.32	0.43
3:C:454:PHE:O	3:C:457:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:HG2	1:A:126:ARG:HD2	2.00	0.42
1:A:556:LYS:C	1:A:559:PRO:HD3	2.43	0.42
1:A:1037:VAL:O	1:A:1037:VAL:HG12	2.19	0.42
1:A:1040:LEU:H	1:A:1040:LEU:CD2	2.32	0.42
1:A:1526:LEU:HD12	1:A:1526:LEU:N	2.34	0.42
1:A:1834:GLU:O	1:A:1837:VAL:HG22	2.18	0.42
1:A:2069:ILE:N	1:A:2070:PRO:CD	2.82	0.42
1:A:2215:PHE:HB2	1:A:2338:LEU:HB2	2.01	0.42
2:B:6:SER:HB3	2:B:138:LEU:O	2.19	0.42
2:B:238:LEU:CD1	2:B:258:CYS:HB2	2.49	0.42
1:A:389:PRO:N	1:A:390:PRO:CD	2.83	0.42
1:A:718:LEU:HD12	1:A:718:LEU:N	2.33	0.42
1:A:863:SER:HB3	1:A:869:ILE:CG1	2.41	0.42
1:A:1349:LEU:HD23	1:A:1355:TYR:CZ	2.54	0.42
1:A:1483:LEU:HD23	1:A:1484:ASP:N	2.33	0.42
1:A:406:SER:O	1:A:407:THR:C	2.61	0.42
1:A:807:VAL:HA	1:A:808:HIS:HA	1.55	0.42
1:A:1086:PRO:HB3	1:A:1090:GLN:CB	2.49	0.42
1:A:1414:THR:HA	1:A:1415:VAL:CB	2.48	0.42
1:A:1844:LEU:O	1:A:1844:LEU:HD23	2.18	0.42
1:A:2141:LEU:HD13	1:A:2151:PRO:HB3	2.01	0.42
1:A:2207:TRP:NE1	1:A:2208:VAL:HG12	2.34	0.42
1:A:2312:ARG:HD2	1:A:2312:ARG:C	2.44	0.42
1:A:2410:LEU:HD12	1:A:2410:LEU:N	2.34	0.42
2:B:49:VAL:HG13	2:B:149:LEU:O	2.19	0.42
3:C:178:LYS:O	3:C:179:HIS:ND1	2.49	0.42
3:C:204:VAL:O	3:C:204:VAL:HG13	2.20	0.42
3:C:213:GLN:HE21	3:C:276:PRO:HD2	1.84	0.42
1:A:332:LYS:N	1:A:333:PRO:CD	2.82	0.42
1:A:388:VAL:N	1:A:389:PRO:CD	2.82	0.42
1:A:422:PRO:HG3	1:A:428:TYR:OH	2.19	0.42
1:A:552:VAL:O	1:A:556:LYS:HG3	2.20	0.42
1:A:881:ASN:ND2	1:A:1306:PRO:HB3	2.35	0.42
1:A:1417:ILE:O	1:A:1421:LEU:HG	2.18	0.42
1:A:1650:LYS:O	1:A:1653:VAL:HG12	2.19	0.42
1:A:2055:LEU:CD2	1:A:2059:LEU:HB2	2.50	0.42
2:B:233:LEU:O	2:B:237:VAL:HB	2.18	0.42
2:B:479:LEU:HD12	2:B:479:LEU:N	2.33	0.42
1:A:202:GLU:HA	1:A:205:LYS:HE3	2.00	0.42
1:A:295:LYS:CA	1:A:296:CYS:CB	2.95	0.42
1:A:365:LEU:HD13	1:A:401:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:HG23	1:A:621:ILE:O	2.20	0.42
1:A:762:LYS:HD2	1:A:763:GLY:N	2.34	0.42
1:A:931:THR:HB	1:A:932:PRO:CD	2.49	0.42
1:A:1316:ILE:O	1:A:1320:VAL:HG23	2.20	0.42
1:A:1483:LEU:HD23	1:A:1485:ILE:HG13	2.01	0.42
1:A:1586:SER:HB3	1:A:1591:HIS:CD2	2.55	0.42
1:A:1807:LEU:N	1:A:1807:LEU:HD12	2.34	0.42
1:A:1832:HIS:CG	1:A:1837:VAL:HG21	2.54	0.42
1:A:2169:PHE:HZ	1:A:2411:LEU:HD13	1.84	0.42
1:A:2177:PHE:CZ	1:A:2400:LEU:HD11	2.54	0.42
1:A:2194:SER:H	1:A:2206:GLN:HE21	1.67	0.42
1:A:2277:LEU:CB	1:A:2278:HIS:CB	2.92	0.42
2:B:162:LEU:HD23	2:B:162:LEU:C	2.44	0.42
2:B:272:ASN:O	3:C:428:LEU:HD11	2.19	0.42
3:C:188:MET:HB2	3:C:507:ARG:NH1	2.33	0.42
3:C:198:LEU:HD23	3:C:260:ILE:CD1	2.50	0.42
3:C:395:MET:HE3	3:C:398:SER:CB	2.49	0.42
1:A:347:GLU:HB2	1:A:348:PRO:HD3	2.01	0.42
1:A:566:LYS:HZ1	1:A:620:THR:HG23	1.83	0.42
1:A:1293:LEU:HD22	1:A:1322:LYS:CD	2.50	0.42
1:A:1415:VAL:HG22	1:A:1415:VAL:O	2.18	0.42
1:A:1638:SER:HA	1:A:1676:ALA:HA	2.01	0.42
1:A:2167:MET:HG3	1:A:2193:TYR:O	2.19	0.42
3:C:341:LYS:HE3	3:C:363:TYR:O	2.19	0.42
1:A:80:ILE:HG21	1:A:106:GLN:NE2	2.21	0.42
1:A:131:LYS:HE3	1:A:159:GLU:CB	2.50	0.42
1:A:410:ARG:NH1	1:A:471:MET:H	2.16	0.42
1:A:554:SER:CB	1:A:608:LYS:HE3	2.50	0.42
1:A:1832:HIS:CB	1:A:1837:VAL:HG21	2.49	0.42
1:A:2166:ILE:HD11	1:A:2358:CYS:SG	2.60	0.42
1:A:2177:PHE:O	1:A:2181:ASN:N	2.53	0.42
1:A:2356:ASN:OD1	1:A:2357:VAL:N	2.53	0.42
1:A:118:PHE:CE1	1:A:158:ARG:HG2	2.54	0.42
1:A:141:MET:HE3	1:A:143:TYR:CZ	2.54	0.42
1:A:163:ASP:HB3	1:A:171:GLN:HG3	2.02	0.42
1:A:473:ILE:HA	1:A:476:ASP:CB	2.47	0.42
1:A:812:ARG:HA	1:A:812:ARG:HE	1.84	0.42
1:A:1324:LEU:HD22	1:A:1337:LEU:HB2	2.01	0.42
1:A:1489:LYS:O	1:A:1493:THR:HG23	2.20	0.42
1:A:2099:LEU:HA	1:A:2102:MET:SD	2.59	0.42
1:A:2212:THR:HG22	1:A:2345:MET:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2394:LEU:HD23	1:A:2394:LEU:C	2.45	0.42
2:B:268:LEU:HB3	2:B:337:TYR:CZ	2.53	0.42
2:B:520:THR:HG22	2:B:558:PHE:CD2	2.54	0.42
3:C:379:PHE:CD2	3:C:463:HIS:HB3	2.54	0.42
1:A:190:ASP:CA	1:A:193:LEU:HG	2.48	0.42
1:A:364:PHE:CD2	1:A:365:LEU:HD12	2.41	0.42
1:A:906:LEU:C	1:A:906:LEU:HD12	2.45	0.42
1:A:1462:LEU:HB2	1:A:1470:SER:HB3	2.02	0.42
1:A:1961:LEU:HD12	1:A:1961:LEU:H	1.85	0.42
1:A:2340:ASN:O	1:A:2352:HIS:HA	2.19	0.42
2:B:138:LEU:HD23	2:B:138:LEU:C	2.44	0.42
3:C:270:THR:CG2	3:C:311:LEU:HD21	2.49	0.42
3:C:477:VAL:HA	3:C:480:MET:HG2	2.02	0.42
1:A:138:GLU:HG2	1:A:147:SER:HA	2.01	0.42
1:A:329:HIS:NE2	1:A:348:PRO:HB3	2.35	0.42
1:A:386:GLU:O	1:A:390:PRO:HD3	2.20	0.42
1:A:387:ASP:O	1:A:390:PRO:HD2	2.20	0.42
1:A:1139:ILE:HD13	1:A:1207:GLN:NE2	2.32	0.42
1:A:1514:SER:O	1:A:1519:TYR:HB3	2.19	0.42
1:A:1750:ALA:O	1:A:1754:PHE:HD2	2.03	0.42
1:A:1816:THR:CG2	1:A:1819:TRP:HE3	2.33	0.42
1:A:2153:LEU:CD1	1:A:2205:ILE:HG12	2.50	0.42
1:A:2195:VAL:HA	1:A:2205:ILE:CG2	2.36	0.42
1:A:2256:LYS:HD2	1:A:2287:LEU:HD21	2.00	0.42
1:A:2273:ARG:H	1:A:2274:ASP:HA	1.83	0.42
3:C:220:VAL:O	3:C:224:LEU:HD13	2.20	0.42
3:C:427:ASN:HD21	3:C:466:PHE:HB2	1.85	0.42
3:C:464:PRO:HB2	3:C:469:LEU:HD21	2.01	0.42
1:A:69:GLN:CB	1:A:102:LYS:HZ2	2.29	0.41
1:A:156:ILE:HA	1:A:159:GLU:CD	2.45	0.41
1:A:503:LEU:HD13	1:A:572:MET:CE	2.50	0.41
1:A:573:THR:HB	1:A:609:PHE:HZ	1.84	0.41
1:A:714:LEU:N	1:A:714:LEU:HD22	2.35	0.41
1:A:1021:GLN:NE2	1:A:1025:ASP:OD2	2.53	0.41
1:A:1462:LEU:C	1:A:1470:SER:HB3	2.45	0.41
1:A:2089:ILE:HD11	1:A:2128:ILE:HD12	2.02	0.41
1:A:2158:GLU:C	1:A:2201:ARG:HA	2.45	0.41
1:A:2376:THR:O	1:A:2376:THR:HG22	2.20	0.41
2:B:496:SER:HG	2:B:543:ALA:HB2	1.85	0.41
2:B:524:HIS:O	2:B:527:GLN:HG3	2.19	0.41
1:A:141:MET:HE3	1:A:143:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD11	1:A:327:ILE:CG1	2.50	0.41
1:A:542:VAL:O	1:A:542:VAL:HG13	2.19	0.41
1:A:566:LYS:HB2	1:A:625:LYS:CE	2.49	0.41
1:A:1083:LEU:HD12	1:A:1083:LEU:N	2.36	0.41
1:A:1339:THR:OG1	1:A:1340:LEU:N	2.53	0.41
1:A:1352:LEU:HA	1:A:1353:GLN:HA	1.50	0.41
1:A:2296:LEU:HD21	1:A:2343:ILE:HD12	2.02	0.41
2:B:7:LEU:C	2:B:7:LEU:HD23	2.45	0.41
2:B:313:ARG:HD3	2:B:327:PHE:CE2	2.55	0.41
2:B:482:ILE:O	2:B:482:ILE:HG22	2.19	0.41
1:A:402:LEU:HD23	1:A:402:LEU:C	2.45	0.41
1:A:409:VAL:HG13	1:A:453:LEU:CD2	2.40	0.41
1:A:712:ASN:O	1:A:716:ILE:HG13	2.19	0.41
1:A:893:LEU:HD23	1:A:910:ALA:O	2.20	0.41
1:A:1207:GLN:NE2	1:A:1288:SER:HG	2.16	0.41
1:A:1360:LEU:HD23	1:A:1360:LEU:C	2.45	0.41
1:A:1942:PRO:HA	1:A:1945:VAL:CG2	2.47	0.41
1:A:2176:MET:CE	1:A:2407:ARG:HB2	2.40	0.41
3:C:177:MET:HE1	3:C:258:PHE:CD2	2.55	0.41
1:A:115:SER:HB2	1:A:116:PRO:HD3	2.02	0.41
1:A:338:GLN:NE2	2:B:145:GLU:OE2	2.54	0.41
1:A:389:PRO:HB2	1:A:390:PRO:HD3	2.03	0.41
1:A:492:CYS:O	3:C:460:TYR:OH	2.28	0.41
1:A:503:LEU:CD1	1:A:572:MET:HG3	2.48	0.41
1:A:634:LEU:HD23	1:A:634:LEU:C	2.45	0.41
1:A:866:ILE:HD13	1:A:1291:VAL:HG12	2.01	0.41
1:A:1133:THR:O	1:A:1133:THR:HG22	2.20	0.41
1:A:1459:ALA:HB1	1:A:1474:GLN:HG2	2.02	0.41
1:A:1943:THR:HG23	1:A:1944:MET:N	2.35	0.41
1:A:2057:THR:HB	1:A:2058:PRO:CD	2.51	0.41
1:A:2135:THR:HA	1:A:2136:LYS:HA	1.68	0.41
1:A:2330:ILE:HD12	1:A:2404:ARG:HD2	2.02	0.41
1:A:2365:LEU:HB3	1:A:2366:ARG:HB3	2.02	0.41
1:A:2371:VAL:N	1:A:2372:PRO:HD3	2.35	0.41
1:A:2374:ARG:NH1	1:A:3641:ILE:HA	2.35	0.41
2:B:170:GLN:OE1	3:C:389:LEU:HD22	2.20	0.41
2:B:350:MET:O	2:B:354:GLN:HG3	2.20	0.41
3:C:322:GLN:HG2	3:C:330:LEU:HD13	2.01	0.41
3:C:340:VAL:O	3:C:340:VAL:HG12	2.20	0.41
1:A:295:LYS:HB3	1:A:297:VAL:HB	2.02	0.41
1:A:771:GLU:OE1	1:A:773:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:LYS:NZ	1:A:830:LEU:HG	2.35	0.41
1:A:976:ASN:ND2	1:A:1077:VAL:HG11	2.36	0.41
1:A:1078:GLU:OE1	1:A:1078:GLU:HA	2.20	0.41
1:A:1816:THR:HG1	1:A:1819:TRP:HE3	1.65	0.41
1:A:2365:LEU:CB	1:A:2367:VAL:HB	2.50	0.41
2:B:214:HIS:CE1	2:B:216:THR:HB	2.56	0.41
2:B:216:THR:O	2:B:217:CYS:HB2	2.19	0.41
2:B:356:ARG:O	2:B:360:THR:HG23	2.21	0.41
3:C:405:THR:O	3:C:406:LEU:HG	2.20	0.41
1:A:130:THR:HG23	1:A:131:LYS:N	2.34	0.41
1:A:136:SER:HA	1:A:139:ARG:HD3	2.02	0.41
1:A:154:ARG:C	1:A:157:THR:HG1	2.16	0.41
1:A:189:LEU:N	1:A:189:LEU:HD23	2.36	0.41
1:A:253:LEU:O	1:A:256:THR:HG22	2.21	0.41
1:A:617:ALA:C	1:A:618:LEU:HD12	2.45	0.41
1:A:1308:GLU:HG3	1:A:2308:ASP:CG	2.46	0.41
1:A:1453:LEU:HD22	1:A:1453:LEU:N	2.35	0.41
2:B:221:ILE:CD1	3:C:279:LEU:HD22	2.50	0.41
3:C:205:LEU:CA	3:C:482:ARG:HH22	2.33	0.41
3:C:279:LEU:HD21	3:C:297:HIS:ND1	2.35	0.41
3:C:428:LEU:HD23	3:C:428:LEU:C	2.45	0.41
1:A:85:LYS:CD	1:A:116:PRO:HG2	2.47	0.41
1:A:171:GLN:HA	1:A:175:PHE:HD1	1.86	0.41
1:A:275:LEU:HB2	1:A:277:MET:N	2.36	0.41
1:A:292:LEU:HD23	1:A:292:LEU:C	2.46	0.41
1:A:494:THR:O	1:A:497:ILE:HG22	2.21	0.41
1:A:510:GLN:OE1	1:A:510:GLN:HA	2.20	0.41
1:A:1040:LEU:HD23	1:A:1040:LEU:N	2.35	0.41
1:A:1341:THR:HB	1:A:1405:GLN:NE2	2.36	0.41
1:A:1511:PHE:CB	1:A:1526:LEU:HD23	2.51	0.41
2:B:183:ALA:O	2:B:187:GLU:HG3	2.21	0.41
2:B:539:ALA:O	2:B:540:ARG:HD3	2.21	0.41
1:A:203:SER:HB2	1:A:259:ALA:HB2	2.03	0.41
1:A:237:PHE:O	1:A:240:PHE:HB3	2.21	0.41
1:A:350:TRP:O	1:A:354:LEU:HG	2.20	0.41
1:A:566:LYS:HZ2	1:A:620:THR:HG23	1.84	0.41
1:A:1204:GLN:HE21	1:A:1322:LYS:HB2	1.86	0.41
1:A:1609:SER:HB2	1:A:1619:TRP:CH2	2.55	0.41
2:B:208:HIS:CB	2:B:209:ILE:HD12	2.50	0.41
2:B:305:GLU:CG	2:B:334:ALA:HB3	2.51	0.41
1:A:40:ASP:OD1	1:A:80:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:H	1:A:122:GLN:CD	2.28	0.41
1:A:122:GLN:HG3	1:A:126:ARG:HH11	1.85	0.41
1:A:472:THR:OG1	1:A:475:CYS:HB2	2.20	0.41
1:A:510:GLN:NE2	1:A:576:LEU:HD13	2.35	0.41
1:A:926:LEU:HD21	1:A:941:GLN:N	2.36	0.41
1:A:978:LEU:HD12	1:A:978:LEU:N	2.36	0.41
1:A:982:LEU:CD1	1:A:992:LYS:HG2	2.50	0.41
1:A:990:LEU:HB2	1:A:2392:PHE:HD1	1.81	0.41
1:A:1071:VAL:CG1	1:A:1074:MET:H	2.34	0.41
1:A:1529:ALA:HA	1:A:1532:ILE:HG22	2.03	0.41
1:A:1657:LEU:HD12	1:A:1658:PRO:HA	2.03	0.41
1:A:2275:TRP:CB	1:A:2277:LEU:HD23	2.51	0.41
2:B:68:VAL:HG11	2:B:77:PHE:HE2	1.84	0.41
3:C:177:MET:HE2	3:C:197:TYR:CD2	2.56	0.41
3:C:182:LYS:HA	3:C:257:ASP:HA	2.02	0.41
1:A:178:GLN:N	1:A:179:PRO:HD2	2.36	0.41
1:A:215:ALA:HA	1:A:218:LEU:CD1	2.34	0.41
1:A:343:LEU:HD12	1:A:343:LEU:N	2.36	0.41
1:A:361:LEU:CA	1:A:401:LEU:HD13	2.43	0.41
1:A:467:LEU:HD12	1:A:467:LEU:C	2.45	0.41
1:A:1034:ILE:HG22	1:A:1102:LYS:HZ1	1.85	0.41
1:A:1526:LEU:HD12	1:A:1526:LEU:H	1.85	0.41
1:A:1529:ALA:O	1:A:1532:ILE:HG22	2.20	0.41
1:A:1945:VAL:HA	1:A:1948:VAL:HG22	2.03	0.41
1:A:2178:ALA:HA	1:A:2181:ASN:HB2	2.03	0.41
1:A:2273:ARG:H	1:A:2274:ASP:CA	2.34	0.41
1:A:2294:ASN:HB2	1:A:2298:LYS:HG2	2.02	0.41
2:B:200:LEU:HG	2:B:204:PHE:CE2	2.56	0.41
1:A:184:VAL:HG23	1:A:185:LEU:N	2.37	0.40
1:A:338:GLN:OE1	2:B:74:ARG:NE	2.41	0.40
1:A:468:ASP:N	1:A:469:PRO:CD	2.84	0.40
1:A:495:ASP:HB3	1:A:565:TYR:HE1	1.85	0.40
1:A:736:LEU:HD23	1:A:736:LEU:C	2.46	0.40
1:A:888:TYR:HE1	1:A:2301:TRP:CE2	2.39	0.40
1:A:1818:PRO:HB3	1:A:1848:VAL:HG12	1.99	0.40
1:A:2042:ASP:HA	1:A:2046:ASP:HB2	2.02	0.40
1:A:193:LEU:HD12	1:A:193:LEU:C	2.45	0.40
1:A:262:THR:HG23	1:A:303:VAL:HG21	2.03	0.40
1:A:387:ASP:O	1:A:391:PRO:CD	2.70	0.40
1:A:510:GLN:HG2	1:A:579:LEU:CD1	2.48	0.40
1:A:770:VAL:HG11	1:A:814:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:LEU:HD23	1:A:995:TYR:OH	2.21	0.40
1:A:1071:VAL:HG12	1:A:1073:ILE:H	1.85	0.40
1:A:1794:ARG:HA	1:A:1797:VAL:HG22	2.03	0.40
1:A:2141:LEU:HD22	1:A:2141:LEU:N	2.35	0.40
1:A:2153:LEU:CD2	1:A:2207:TRP:HE3	2.34	0.40
1:A:2248:ARG:H	1:A:2251:GLU:CG	2.34	0.40
2:B:304:LEU:O	2:B:308:ILE:HG13	2.21	0.40
2:B:306:ASP:O	2:B:310:ARG:HG3	2.21	0.40
1:A:204:SER:O	1:A:206:LEU:HD12	2.21	0.40
1:A:275:LEU:CB	1:A:276:VAL:HA	2.31	0.40
1:A:320:ASP:CG	1:A:321:ILE:H	2.30	0.40
1:A:378:VAL:H	2:B:79:LEU:HD21	1.85	0.40
1:A:1986:ASP:O	1:A:1990:ARG:HG3	2.20	0.40
1:A:2169:PHE:HE1	1:A:2411:LEU:HB3	1.85	0.40
1:A:2191:ARG:HB3	1:A:2351:VAL:HG12	2.04	0.40
1:A:2221:TRP:HA	1:A:2224:ARG:NH2	2.37	0.40
1:A:2376:THR:HG22	1:A:2381:THR:CG2	2.51	0.40
2:B:270:GLN:HA	2:B:337:TYR:HB2	2.02	0.40
2:B:511:TYR:CE2	2:B:530:GLN:HG3	2.56	0.40
2:B:540:ARG:HB3	3:C:339:MET:CB	2.52	0.40
3:C:412:ASN:C	3:C:414:PHE:H	2.30	0.40
1:A:108:LEU:C	1:A:137:GLN:HE21	2.30	0.40
1:A:200:LEU:HD12	1:A:200:LEU:N	2.35	0.40
1:A:295:LYS:N	1:A:296:CYS:HB3	2.37	0.40
1:A:305:ARG:HG2	1:A:332:LYS:HZ2	1.86	0.40
1:A:360:LEU:HD13	1:A:360:LEU:C	2.47	0.40
1:A:554:SER:HB3	1:A:608:LYS:HE3	2.03	0.40
1:A:734:TRP:CB	1:A:737:GLU:HB3	2.51	0.40
1:A:739:ALA:HA	3:C:172:LEU:HD23	2.03	0.40
1:A:762:LYS:HD2	1:A:762:LYS:C	2.46	0.40
1:A:1114:ALA:CB	1:A:1117:ARG:HH21	2.34	0.40
1:A:1324:LEU:HD13	1:A:1339:THR:H	1.87	0.40
1:A:1325:LYS:HE2	1:A:1325:LYS:CA	2.40	0.40
2:B:234:ARG:HH21	2:B:259:ARG:NH1	2.19	0.40
2:B:268:LEU:HD13	2:B:337:TYR:OH	2.22	0.40
3:C:192:ASP:OD1	3:C:195:ILE:HD13	2.22	0.40
4:C:601:GTP:HO3'	4:C:601:GTP:HO2'	1.60	0.40
1:A:189:LEU:HD23	1:A:189:LEU:H	1.86	0.40
1:A:361:LEU:HA	1:A:401:LEU:CD1	2.43	0.40
1:A:405:PHE:O	1:A:409:VAL:HG23	2.21	0.40
1:A:576:LEU:O	1:A:580:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ASN:CB	1:A:836:THR:HG21	2.52	0.40
1:A:1027:LEU:O	1:A:1031:ARG:HG3	2.21	0.40
1:A:1844:LEU:HD23	1:A:1844:LEU:C	2.46	0.40
1:A:1861:ILE:CD1	1:A:1948:VAL:HG23	2.51	0.40
1:A:2295:LEU:HB2	1:A:2379:ILE:CG2	2.52	0.40
2:B:158:ASP:OD2	2:B:160:SER:HB3	2.20	0.40
2:B:181:PRO:HG2	2:B:184:GLU:CD	2.45	0.40
2:B:264:ARG:HG3	2:B:326:LEU:HD12	2.03	0.40
2:B:297:LYS:HD2	2:B:336:VAL:O	2.21	0.40
2:B:348:VAL:O	3:C:376:ARG:NH2	2.55	0.40
2:B:434:ASN:HB3	2:B:435:PRO:CD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1853/3661 (51%)	1684 (91%)	168 (9%)	1 (0%)	48	78
2	B	373/991 (38%)	345 (92%)	28 (8%)	0	100	100
3	C	300/520 (58%)	274 (91%)	26 (9%)	0	100	100
All	All	2526/5172 (49%)	2303 (91%)	222 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1086	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	1398/3224 (43%)	1385 (99%)	13 (1%)	70	76
2	B	351/847 (41%)	349 (99%)	2 (1%)	78	80
3	C	279/450 (62%)	278 (100%)	1 (0%)	84	82
All	All	2028/4521 (45%)	2012 (99%)	16 (1%)	70	77

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LEU
1	A	285	GLU
1	A	613	PHE
1	A	773	VAL
1	A	985	GLN
1	A	1368	LEU
1	A	1464	GLN
1	A	1521	VAL
1	A	1603	GLN
1	A	1727	GLU
1	A	1816	THR
1	A	1964	GLU
1	A	2279	VAL
2	B	212	LEU
2	B	408	PHE
3	C	408	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	171	GLN
1	A	197	HIS
1	A	212	GLN
1	A	314	ASN

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Mol	Chain	Res	Type
1	A	502	ASN
1	A	577	ASN
1	A	600	HIS
1	A	606	ASN
1	A	645	ASN
1	A	671	HIS
1	A	677	HIS
1	A	767	ASN
1	A	808	HIS
1	A	858	HIS
1	A	881	ASN
1	A	891	GLN
1	A	898	GLN
1	A	976	ASN
1	A	1090	GLN
1	A	1103	ASN
1	A	1113	GLN
1	A	1184	ASN
1	A	1204	GLN
1	A	1211	HIS
1	A	1286	GLN
1	A	1305	ASN
1	A	1405	GLN
1	A	1464	GLN
1	A	1472	GLN
1	A	1474	GLN
1	A	1499	HIS
1	A	1533	GLN
1	A	1591	HIS
1	A	1654	GLN
1	A	1825	GLN
1	A	1832	HIS
1	A	2168	GLN
1	A	2189	HIS
1	A	2192	HIS
1	A	2206	GLN
1	A	2229	GLN
2	B	139	GLN
2	B	192	GLN
2	B	196	GLN
2	B	257	ASN
2	B	270	GLN

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Mol	Chain	Res	Type
2	B	307	GLN
2	B	320	ASN
2	B	321	GLN
2	B	354	GLN
2	B	436	GLN
2	B	514	ASN
2	B	527	GLN
2	B	530	GLN
2	B	538	HIS
2	B	545	HIS
3	C	271	GLN
3	C	281	HIS
3	C	284	ASN
3	C	294	ASN
3	C	303	GLN
3	C	322	GLN
3	C	393	GLN
3	C	412	ASN
3	C	463	HIS
3	C	484	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
4	GTP	C	601	5	33,34,34	0.96	1 (3%)	50,54,54	1.62	9 (18%)

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
4	GTP	C	601	5	-	7/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	GTP	C2-N3	2.21	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	GTP	C5-C4-N3	-5.10	120.27	128.39
4	C	601	GTP	C2-N3-C4	4.66	120.32	112.30
4	C	601	GTP	N9-C4-N3	3.33	132.61	125.95
4	C	601	GTP	C2-N1-C6	-2.85	119.94	125.11
4	C	601	GTP	N9-C8-N7	-2.58	108.61	113.40
4	C	601	GTP	C5-C6-N1	2.48	119.58	113.25
4	C	601	GTP	C8-N7-C5	2.47	108.66	104.26
4	C	601	GTP	O6-C6-C5	-2.40	120.21	126.53
4	C	601	GTP	C3'-C2'-C1'	2.02	105.29	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	GTP	C5'-O5'-PA-O3A
4	C	601	GTP	C3'-C4'-C5'-O5'
4	C	601	GTP	O4'-C1'-N9-C4
4	C	601	GTP	O4'-C4'-C5'-O5'
4	C	601	GTP	O4'-C1'-N9-C8

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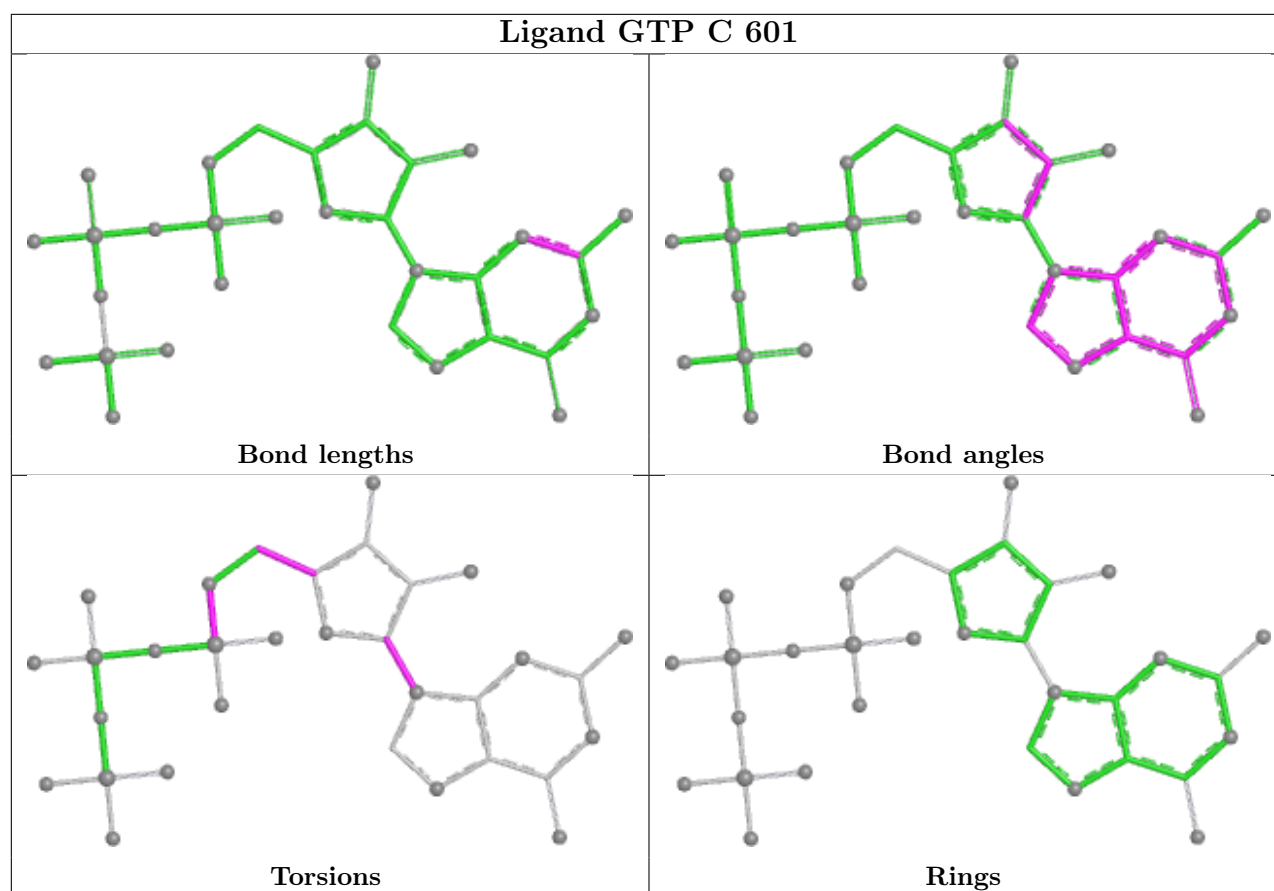
Mol	Chain	Res	Type	Atoms
4	C	601	GTP	C5'-O5'-PA-O1A
4	C	601	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	GTP	10	0

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



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.

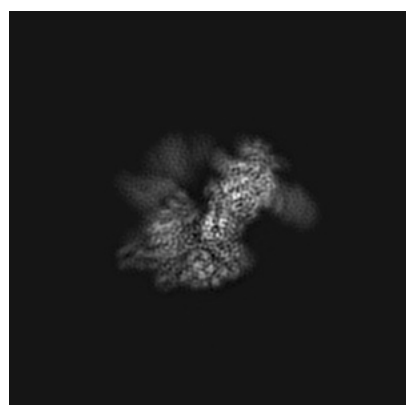
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0837. These allow visual inspection of the internal detail of the map and identification of artifacts.

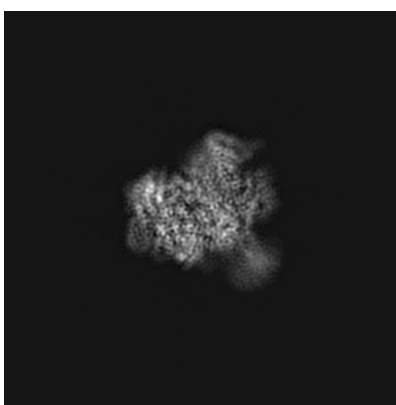
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

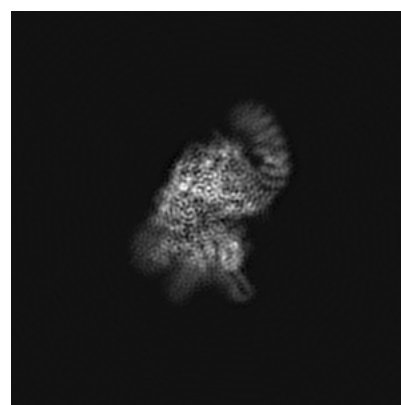
6.1.1 Primary map



X



Y

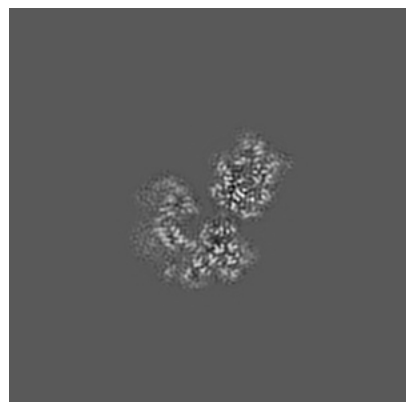


Z

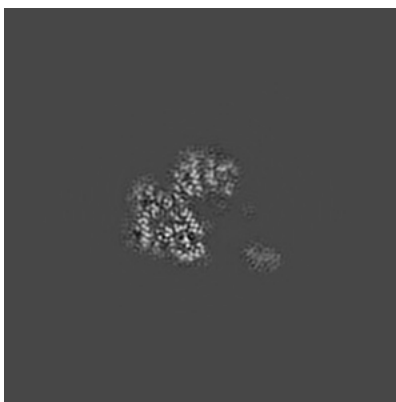
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

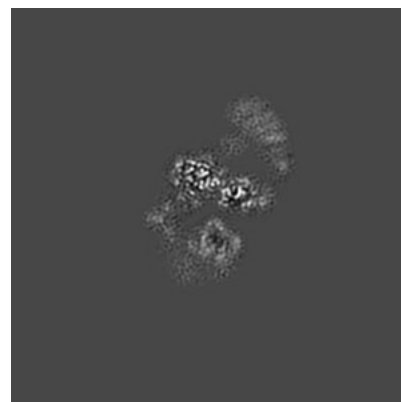
6.2.1 Primary map



X Index: 160



Y Index: 160

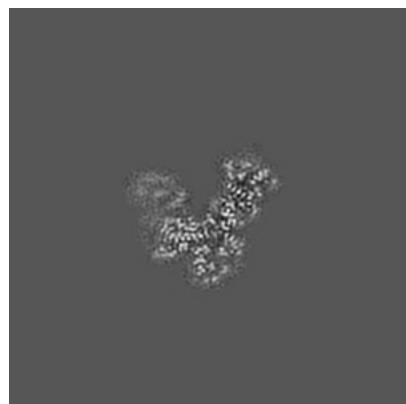


Z Index: 160

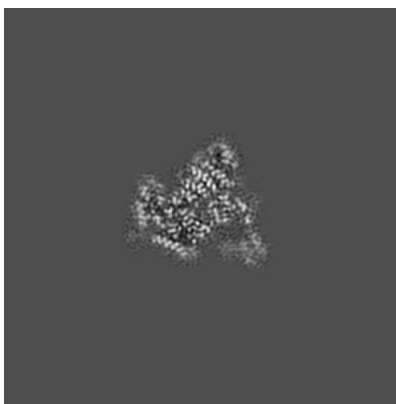
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

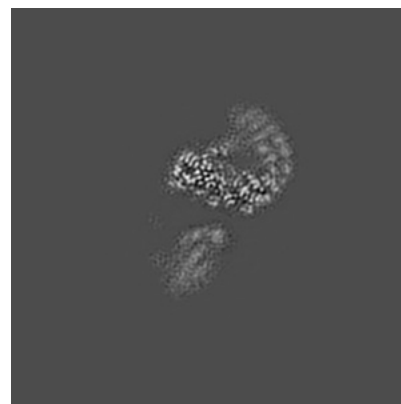
6.3.1 Primary map



X Index: 147



Y Index: 172

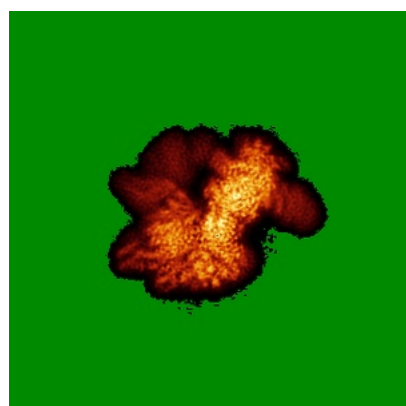


Z Index: 171

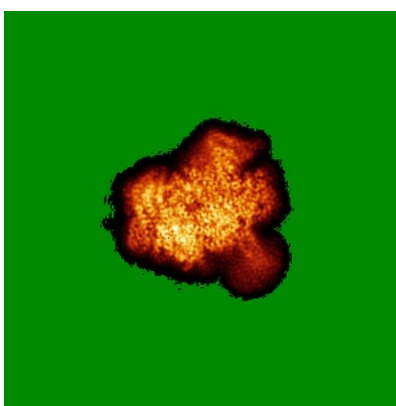
The images above show the largest variance slices of the map in three orthogonal directions.

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

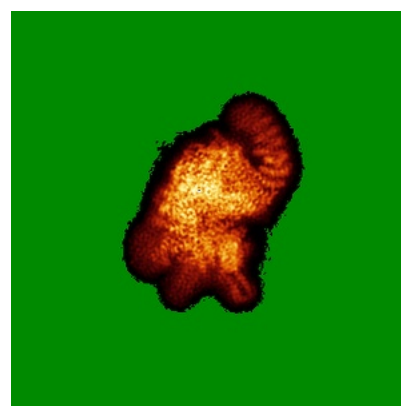
6.4.1 Primary map



X



Y

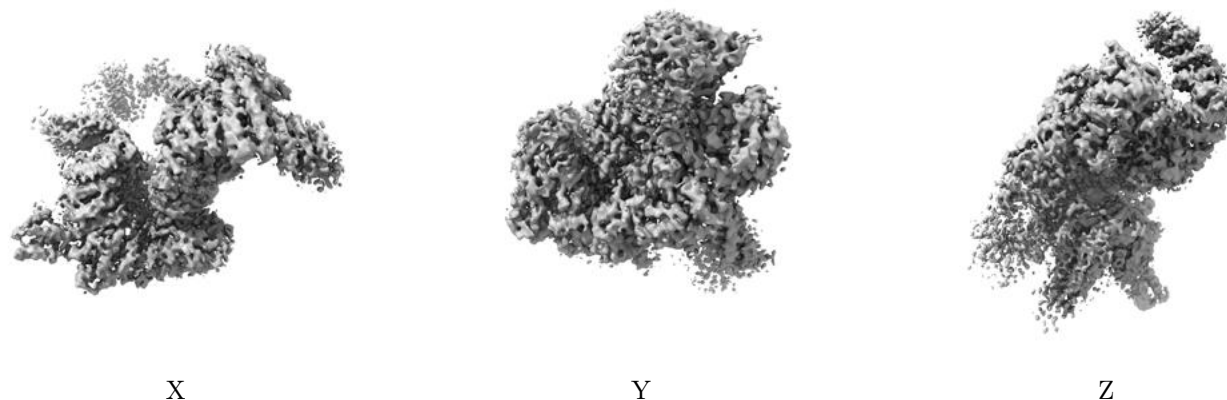


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

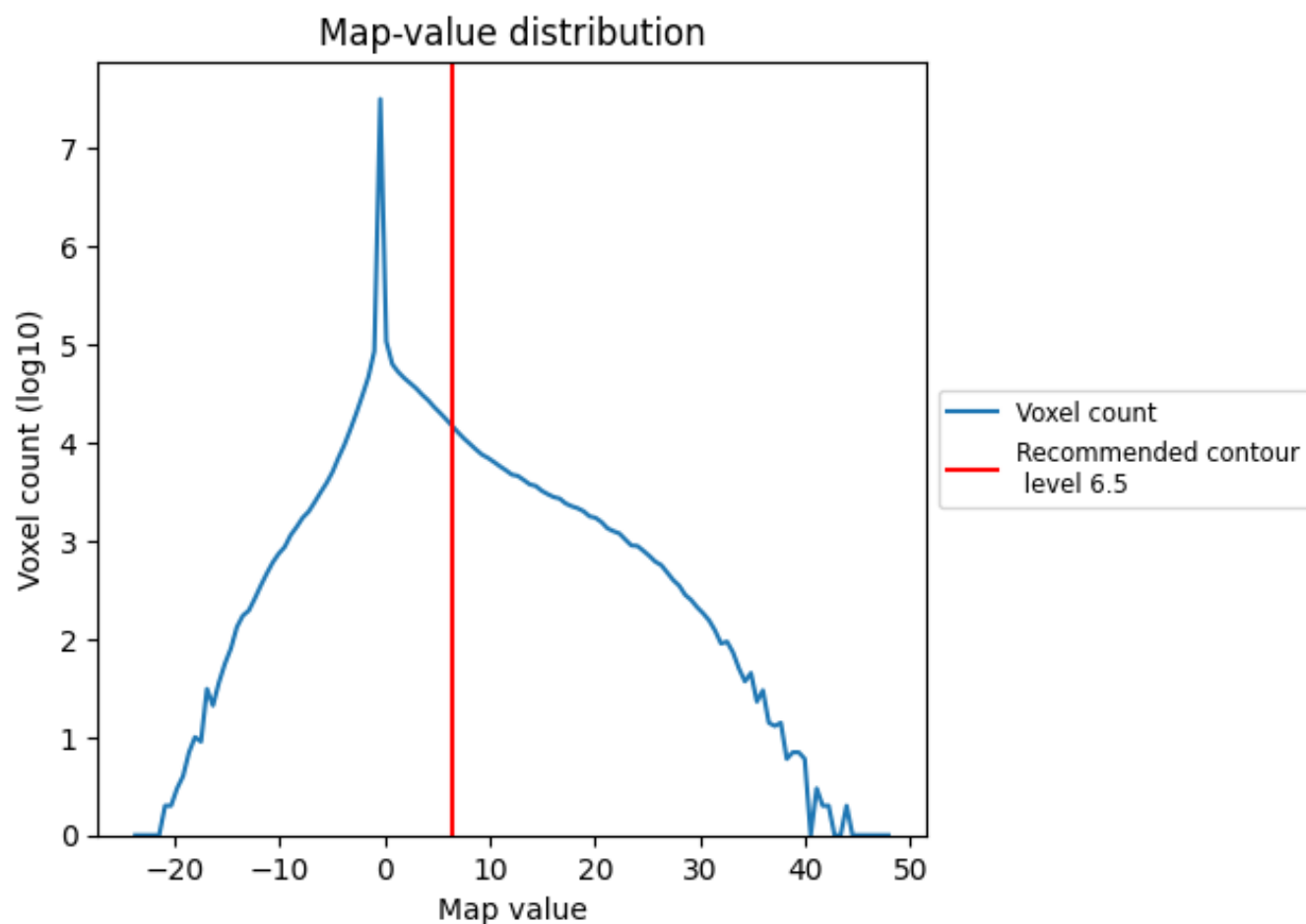
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

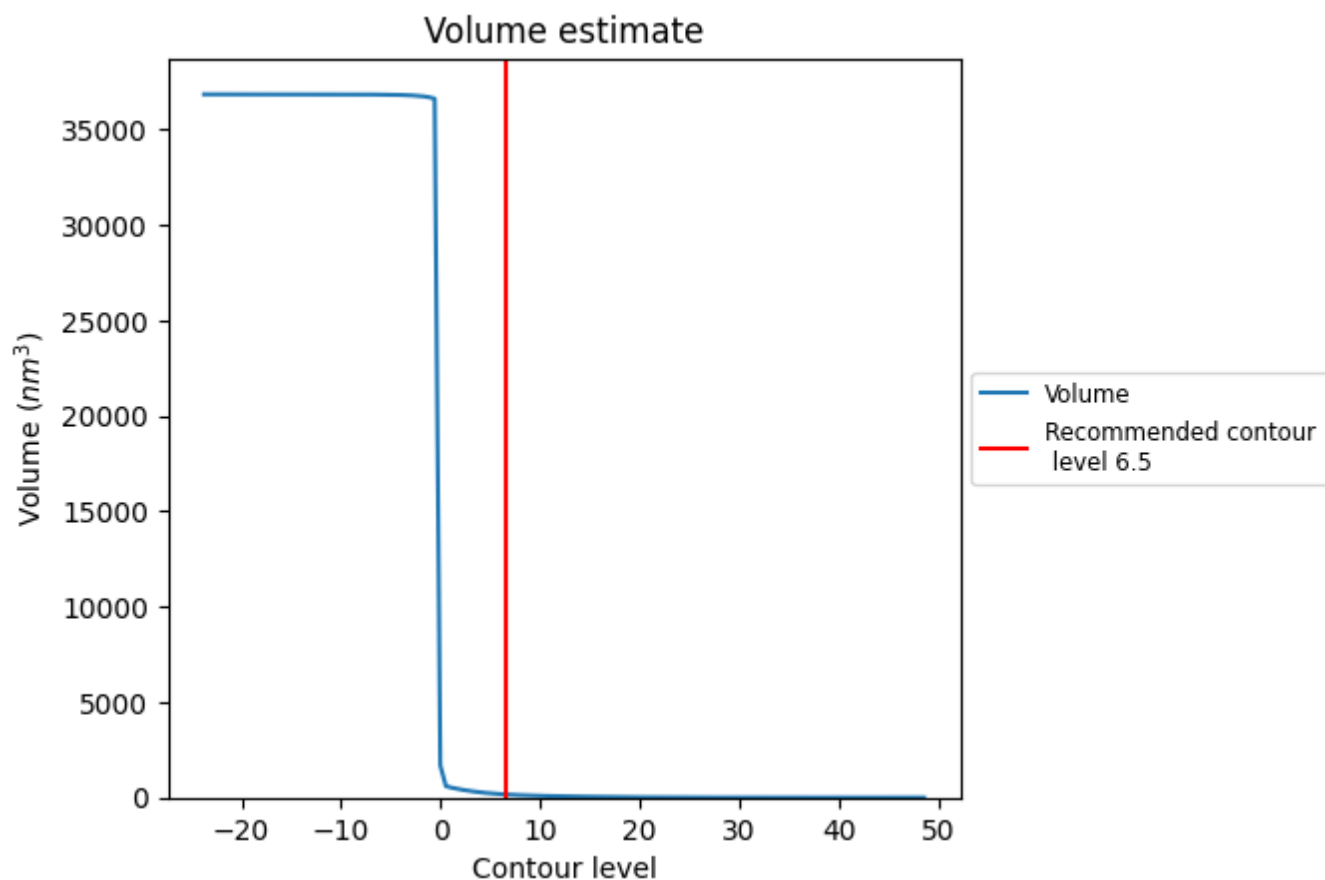
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

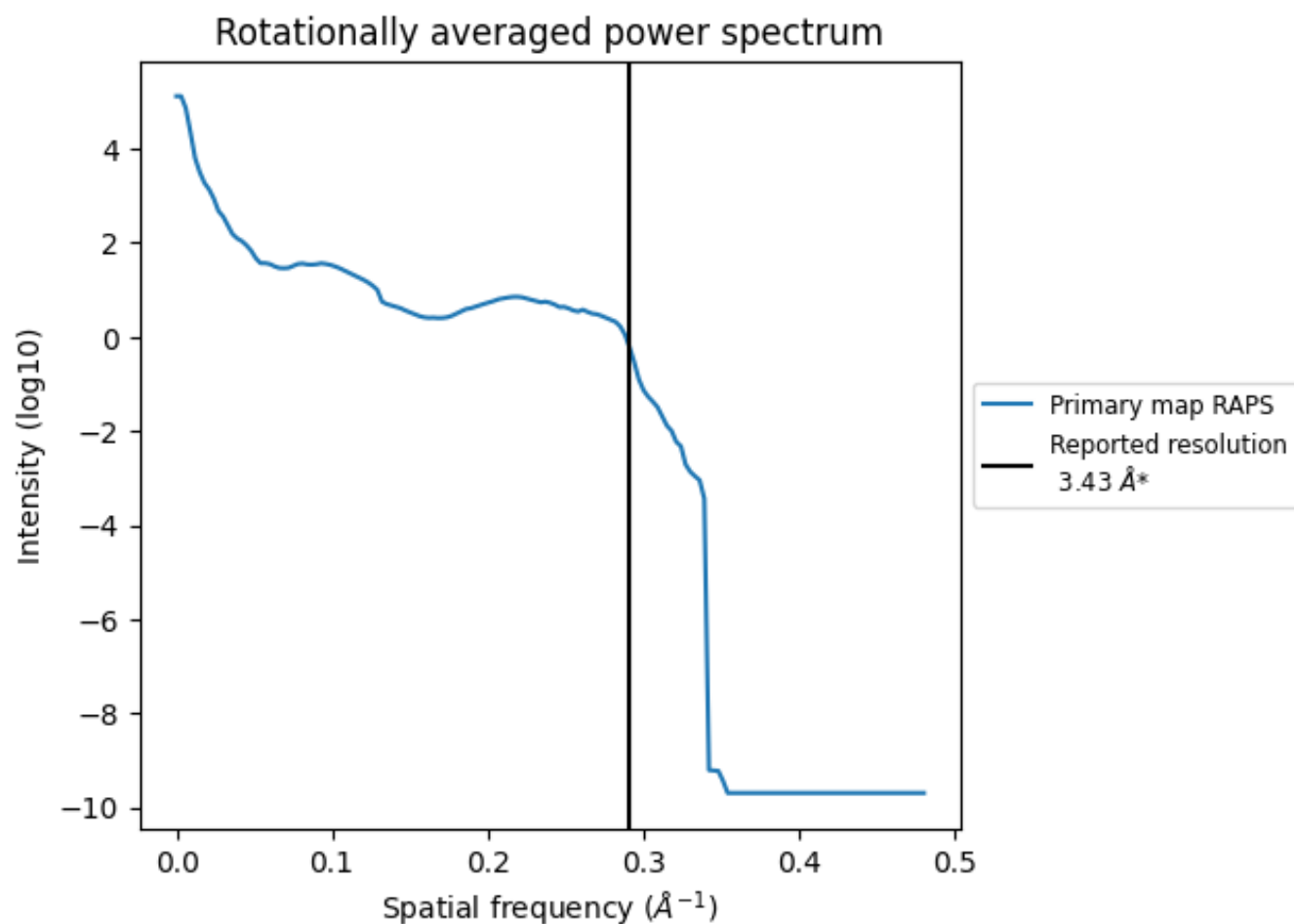
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm^3 ; this corresponds to an approximate mass of 148 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 0.292 Å⁻¹

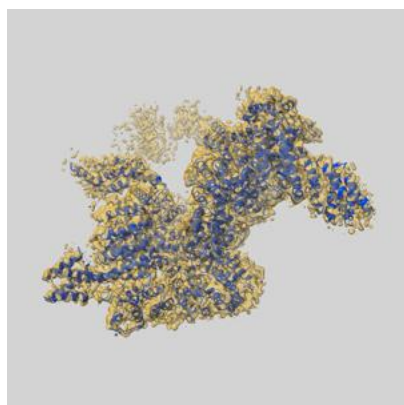
8 Fourier-Shell correlation ⓘ

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

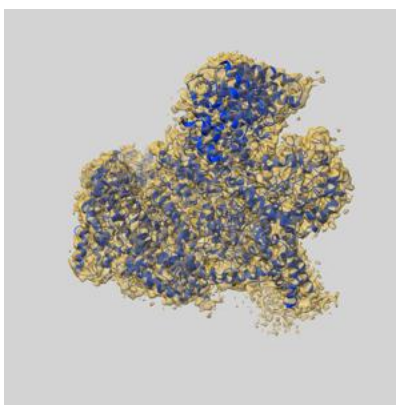
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0837 and PDB model 6L54. Per-residue inclusion information can be found in section 3 on page 6.

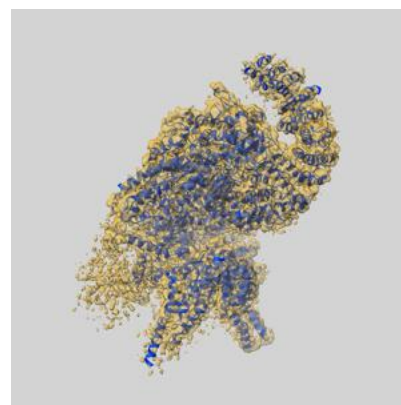
9.1 Map-model overlay [i](#)



X



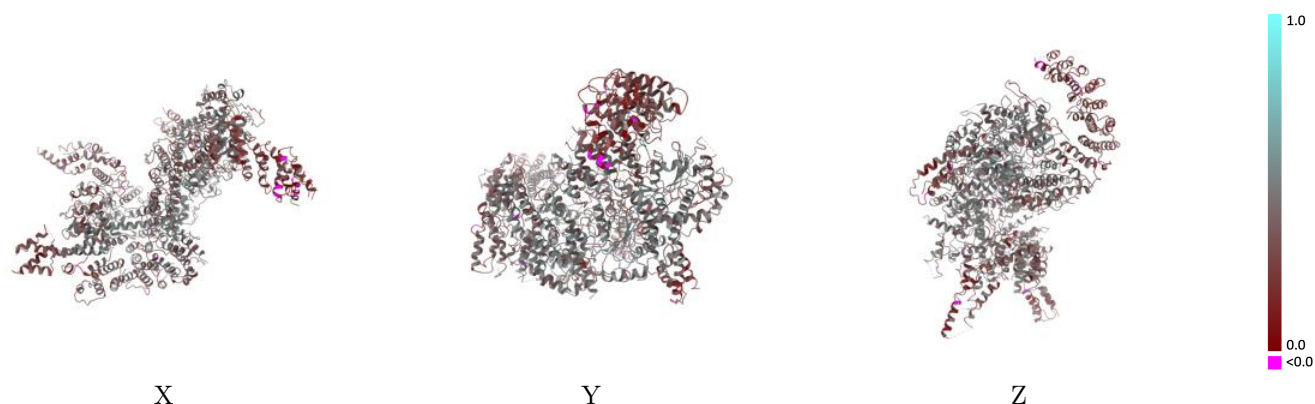
Y



Z

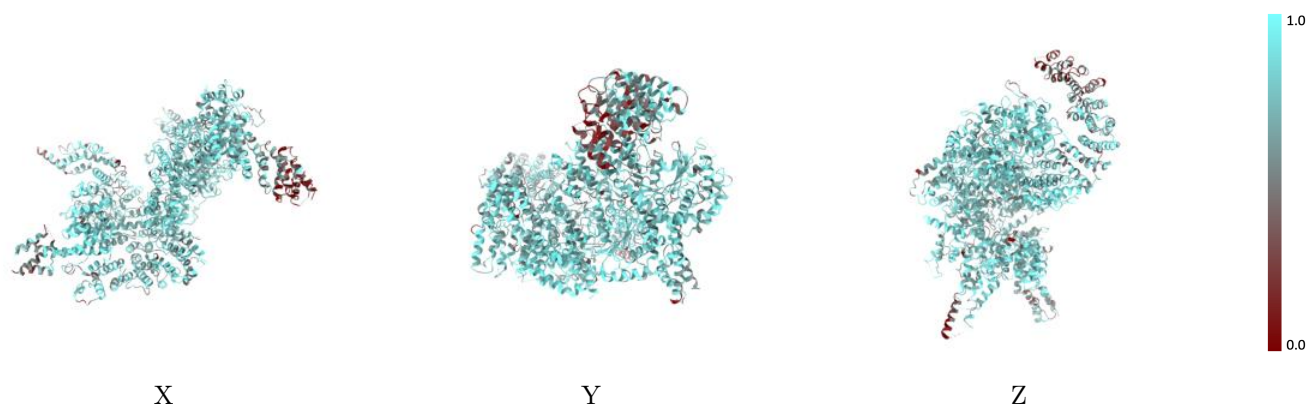
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



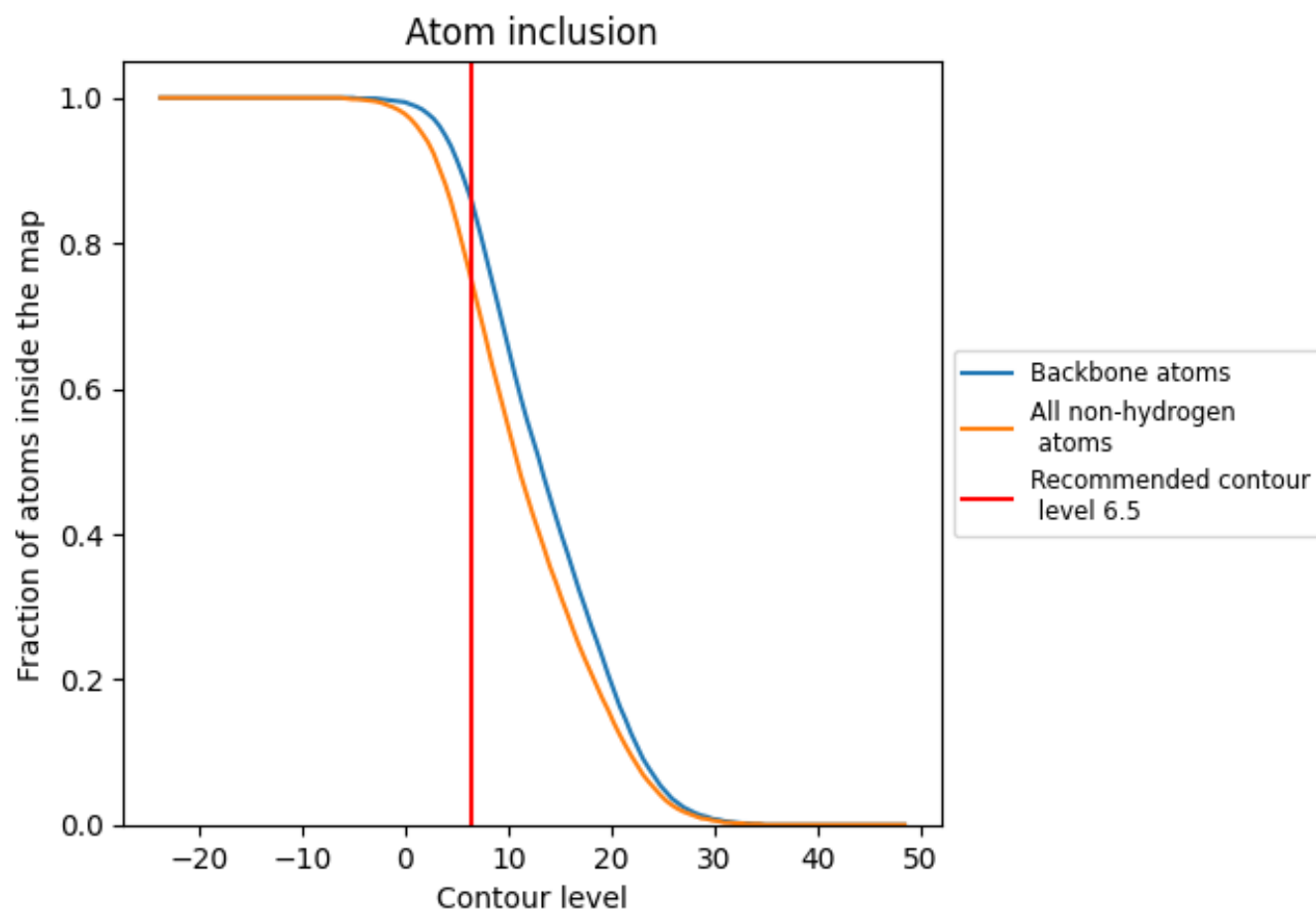
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.3840
A	0.7330	0.3640
B	0.7740	0.4080
C	0.8350	0.4640

