



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 08:24 am GMT

PDB ID : 6TA1
EMDB ID : EMD-10420
Title : Fatty acid synthase of *S. cerevisiae*
Authors : Vonck, J.; D'Imprima, E.; Joppe, M.; Grninger, M.
Deposited on : 2019-10-29
Resolution : 3.10 Å (reported)
Based on initial model : 3HMJ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

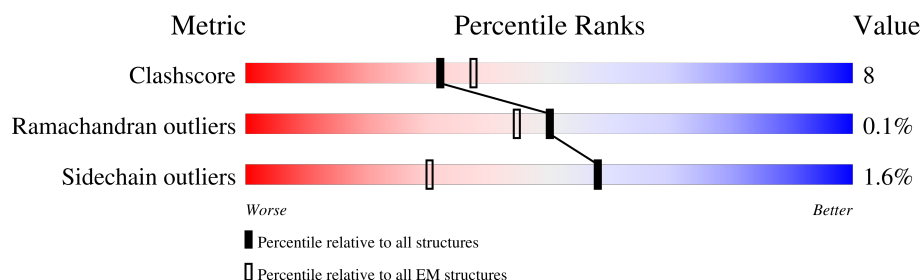
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1887	<div> <div>15%</div> <div>77%</div> <div>15%</div> <div>7%</div> </div>
1	B	1887	<div> <div>15%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	D	1887	<div> <div>15%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	F	1887	<div> <div>15%</div> <div>78%</div> <div>14%</div> <div>7%</div> </div>
1	I	1887	<div> <div>15%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	K	1887	<div> <div>15%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
2	C	2051	<div> <div>8%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
2	E	2051	<div> <div>8%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2051	<div><div>8%</div><div><div></div><div>81%</div><div>17%</div><div>..</div></div></div>
2	H	2051	<div><div>8%</div><div><div></div><div>81%</div><div>17%</div><div>..</div></div></div>
2	J	2051	<div><div>8%</div><div><div></div><div>81%</div><div>17%</div><div>..</div></div></div>
2	L	2051	<div><div>8%</div><div><div></div><div>81%</div><div>17%</div><div>..</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 178206 atoms, of which 156 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.

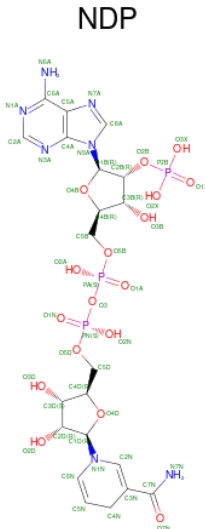
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1750	Total 13619	C 8620	N 2297	O 2650	P 1	S 51	0	0
1	B	1750	Total 13619	C 8620	N 2297	O 2650	P 1	S 51	0	0
1	D	1750	Total 13619	C 8620	N 2297	O 2650	P 1	S 51	0	0
1	K	1750	Total 13619	C 8620	N 2297	O 2650	P 1	S 51	0	0
1	F	1750	Total 13619	C 8620	N 2297	O 2650	P 1	S 51	0	0
1	I	1750	Total 13619	C 8620	N 2297	O 2650	P 1	S 51	0	0

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

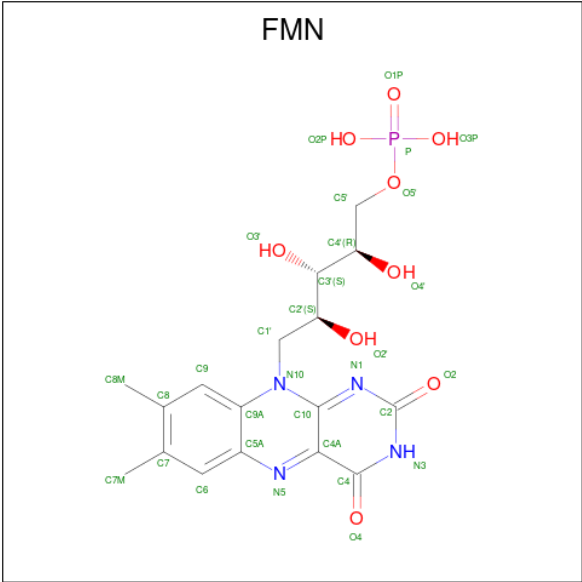
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	C	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	E	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	L	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	H	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	J	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

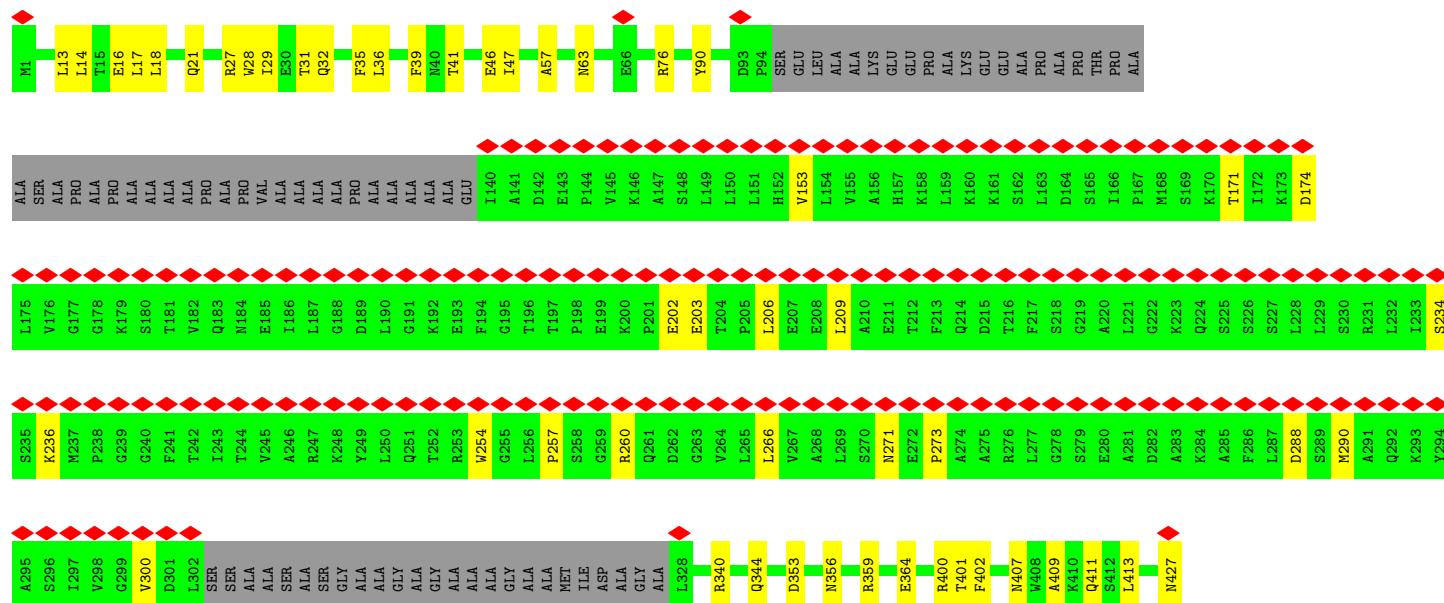


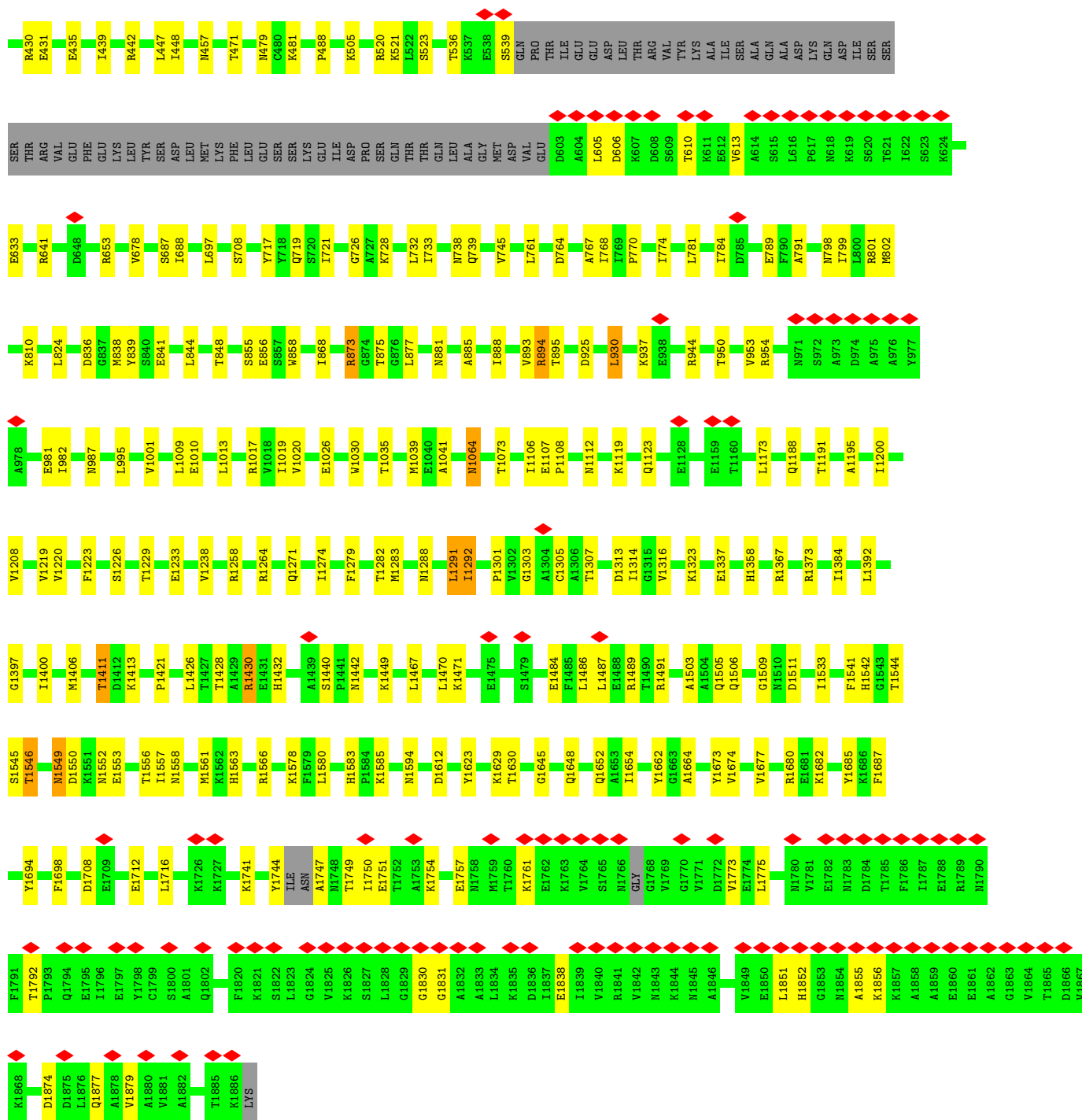
Id	Chain	Residues	Atoms						AltConf
3	A	1	Total 74	C 21	H 26	N 7	O 17	P 3	0
3	B	1	Total 74	C 21	H 26	N 7	O 17	P 3	0
3	D	1	Total 74	C 21	H 26	N 7	O 17	P 3	0
3	K	1	Total 74	C 21	H 26	N 7	O 17	P 3	0
3	F	1	Total 74	C 21	H 26	N 7	O 17	P 3	0
3	I	1	Total 74	C 21	H 26	N 7	O 17	P 3	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

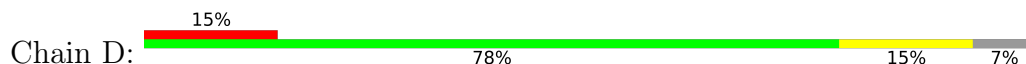


Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	L	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	H	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	J	1	Total	C	N	O	P	0
			31	17	4	9	1	

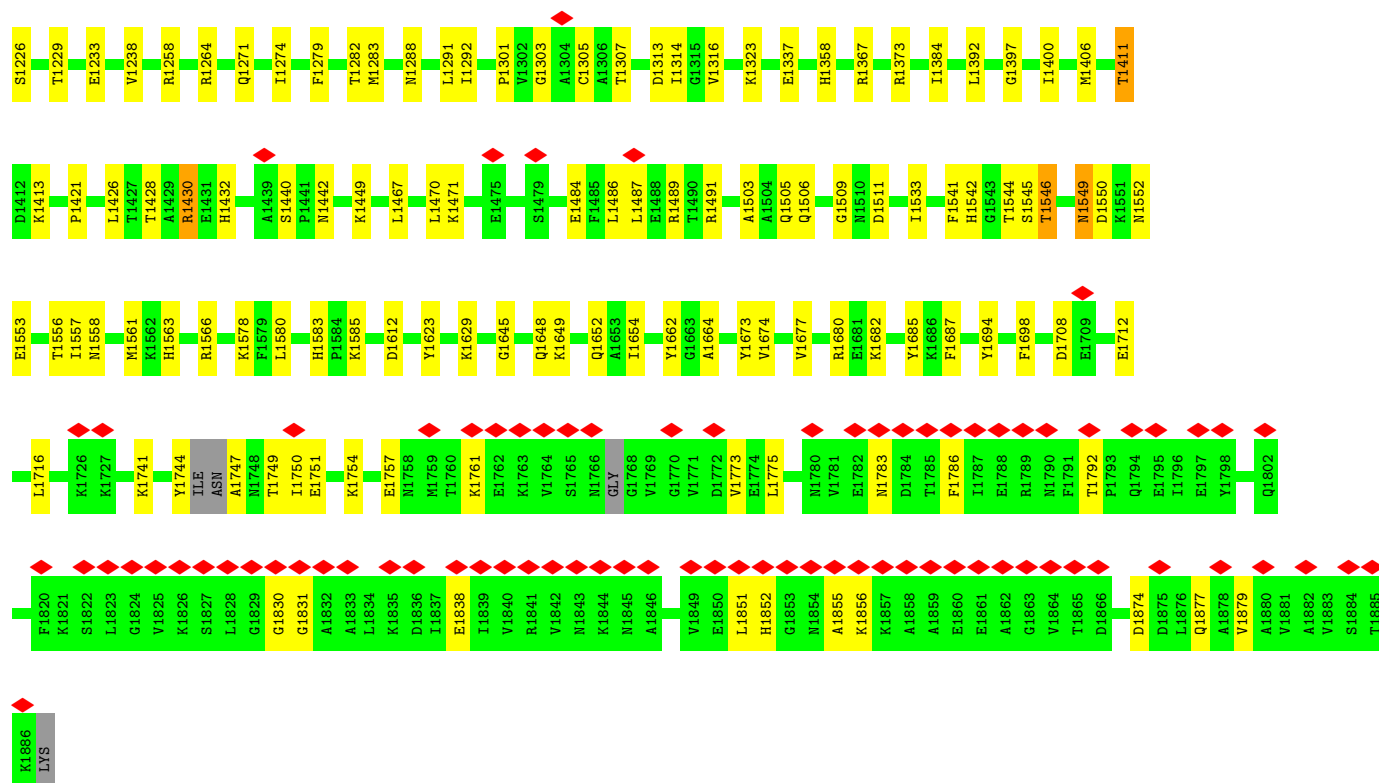




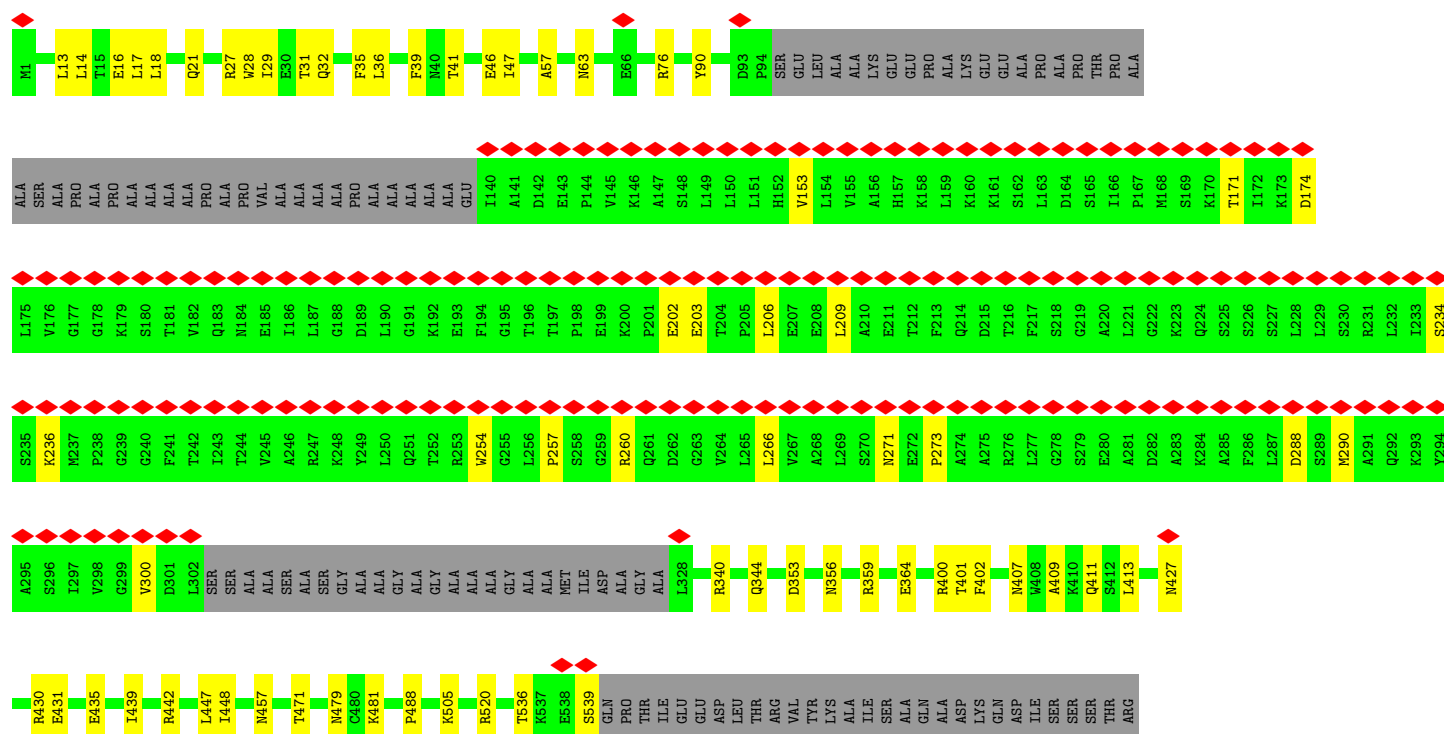
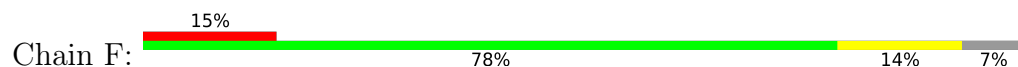
• Molecule 1: Fatty acid synthase subunit alpha



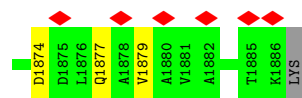




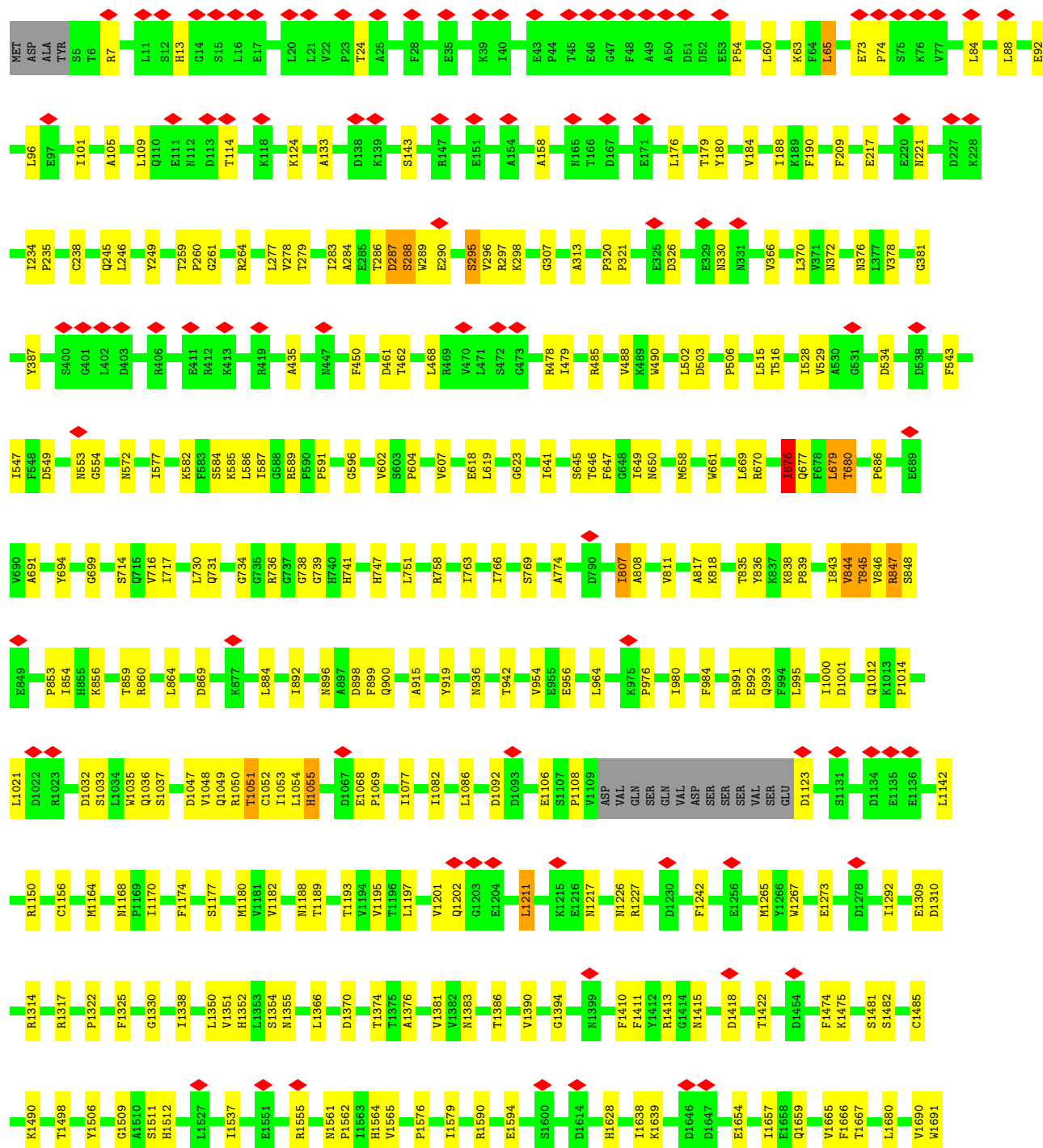
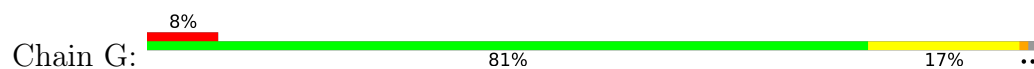
• Molecule 1: Fatty acid synthase subunit alpha

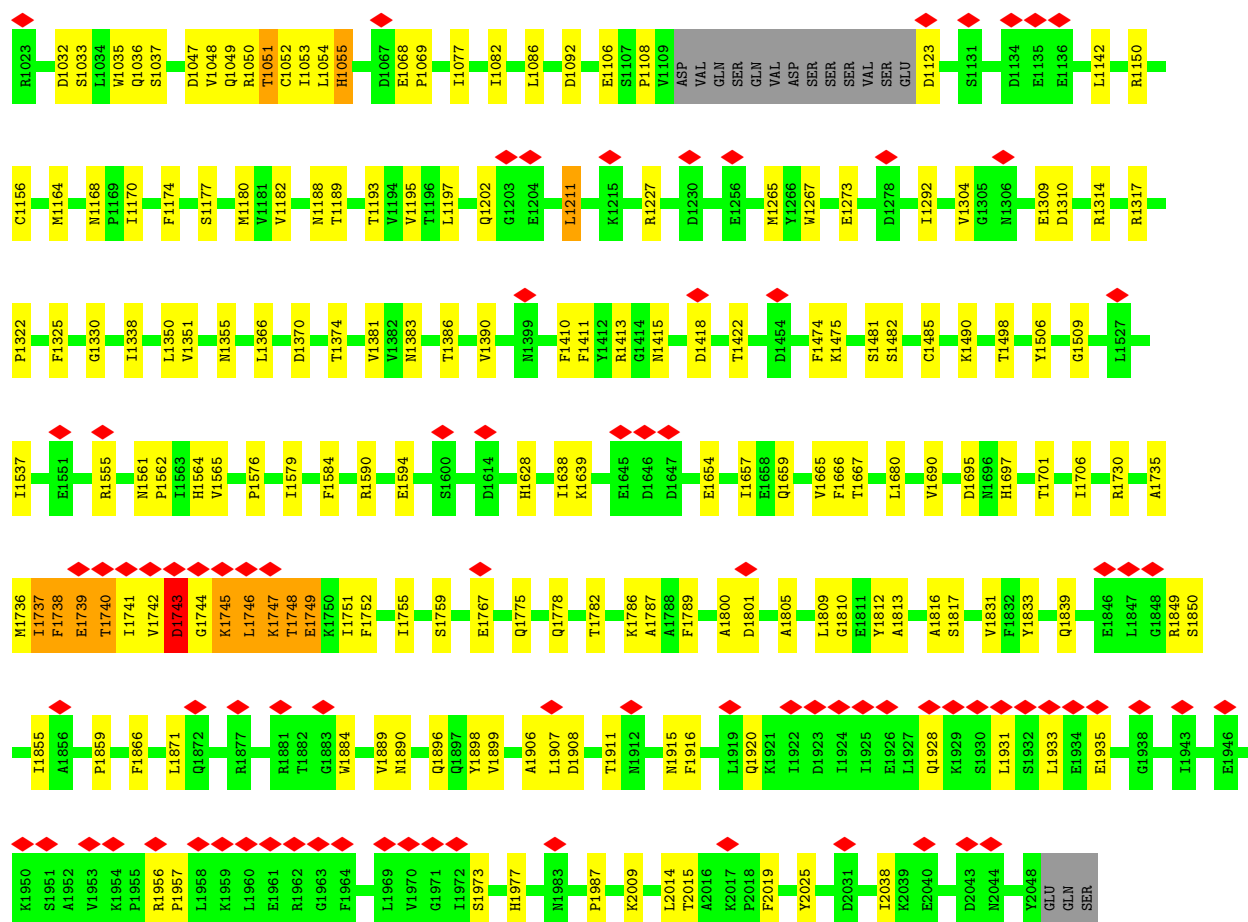


L175	V176	G177	G178	K179	S180	T181	V182	Q183	N184	E185	I186	L187	G188	D189	L190	G191	K192	E193	F194	G195	T196	T197	P198	E199	K200	P201	E202	E203	T204	P205	L206	E207	E208	L209	A210	E211	T212	F213	Q214	D215	T216	F217	G218	G219	A220	L221	G222	K223	Q224	S225	S226	S227	L228	L229	R230	R231	L232	I233	S234			
S235	K236	M237	P238	G239	G240	F241	T242	L243	T244	V245	A246	R247	K248	Y249	L250	Q251	T252	R253	V254	G255	L256	P257	S258	G259	R260	Q261	D262	G263	V264	L265	L266	V267	A268	L269	S270	N271	E272	P273	A274	R275	R276	L277	G278	S279	K410	Q411	S412	L413	A281	D282	A283	K284	A285	F286	L287	D288	S289	M290	A291	Q292	K293	Y294
A295	S296	I297	V298	G299	V300	D301	L302	SER	ALA	ALA	SER	ALA	SER	ALA	GLY	ALA	GLY	ALA	ALA	ALA	GLY	ALA	GLY	ILE	ASP	ALA	GLY	L328	R340	Q344	D353	N356	R359	E364	R400	T401	F402	N407	W408	A409	K410	Q411	S412	L413	A281	D282	A283	K284	A285	F286	L287	D288	S289	M290	A291	Q292	K293	Y294				
R430	E431	E435	I439	R442	L447	I448	N457	T471	M479	C480	K481	P488	G498	K505	R520	K521	L522	S523	T536	K537	E538	S539	GLN	PRO	THR	ILE	GLU	GLU	L605	ASP	LEU	THR	ARG	VAL	TTR	LYS	ALA	ILE	SER	ALA	GLN	ALA	ASP	GLN	LYS	S615	L616	P617	N618	K619	S620	T621	I622	S623								
SER	SER	THR	ARG	VAL	GLU	PHE	GLU	LYS	TYR	SER	ASP	LEU	MET	LYS	PHE	LEU	GLU	SER	LYS	GLY	ILE	ASP	PRO	SER	GLN	THR	GLN	LEU	ALA	GLY	MET	ASP	VAL	GLU	D603	A604	L605	D606	K607	D608	S609	T610	K611	E612	V613	A614	S615	L616	P617	N618	K619	S620	T621	I622	S623							
K624	E633	R641	D648	R653	V678	S687	I688	L697	S708	Y717	Q718	Q719	S720	I721	G726	A727	K728	L732	I733	N738	Q739	V745	L761	D764	A767	I768	I769	P770	I774	L781	I784	D785	E789	F790	A791	N798	I799	L800																								
R801	R802	K810	L824	D836	G837	R838	Y839	S840	E841	L844	T848	S855	T869	R873	G874	S875	G876	L877	N881	A885	T888	V893	R894	T895	D925	L930	K937	E938	R944	T950	V953	R954	N971	S972	A973	D974	A975	A976	Y977	A978																						
E981	I982	N987	L995	V1001	L1009	E1010	L1013	R1017	I1018	I1019	V1020	E1026	W1030	T1035	M1039	N1064	T1073	I1106	E1107	N1112	K1119	Q1123	E1128	E1159	T1160	L1173	Q1188	T1191	A1195	I1200	V1208	V1219	V1220																													
F1223	S1226	T1229	E1233	V1238	R1258	R1264	Q1271	I1274	F1279	T1282	M1283	N1288	L1291	I1292	P1301	V1302	G1303	A1304	C1305	A1306	T1307	D1313	I1314	G1315	V1316	K1323	E1337	F1341	H1358	R1367	R1373	I1384	L1392	G1397																												
I1400	M1406	T1411	D1412	K1413	P1421	G1422	K1423	L1426	T1427	A1428	R1430	E1431	H1432	S1440	P1441	N1442	K1449	L1467	L1470	K1471	E1475	S1479	E1484	F1485	L1486	L1487	E1488	R1489	T1490	R1491	A1503	Q1505	Q1506	G1509	M1510	D1511	I1533	F1541	H1542	G1543	T1544	S1545																				
T1546	M1549	D1550	K1551	N1552	E1553	T1556	I1557	N1558	E1559	M1560	M1561	K1562	H1563	R1566	K1578	F1579	L1580	H1583	P1584	K1585	M1594	D1612	Y1623	K1629	G1645	Q1648	K1649	Q1652	A1653	I1654	Y1662	G1663	A1664	Y1673	V1674	V1677	R1680	E1681	K1682	Y1685	K1686	F1687																				
Y1694	F1698	D1708	E1709	L1716	K1726	K1727	K1741	D1742	S1743	Y1744	ILE	ASN	A1747	N1748	T1749	I1750	E1751	T1752	A1753	K1754	E1757	N1758	M1759	T1760	K1761	E1762	K1763	V1764	S1765	N1766	GLY	G1768	V1769	G1770	V1771	D1772	V1773	L1775	N1780	V1781	E1782	N1783	D1784	T1785	F1786	I1787	E1788	R1789	E1860	E1861	A1862	G1863	V1864	T1865	D1866	V1867	K1868					
T1792	P1793	Q1794	E1795	I1796	E1797	Y1798	G1799	S1800	A1801	Q1802	F1820	K1821	S1822	L1823	G1824	V1825	K1826	S1827	L1828	G1829	G1830	G1831	A1832	A1833	K1835	D1836	I1837	E1838	T1839	V1840	R1841	V1842	N1843	K1844	N1845	A1846	V1849	L1851	H1852	G1853	N1854	A1855	K1856	K1857	A1858	A1859	E1860	E1861	A1862	G1863	V1864	T1865	D1866	V1867	K1868							

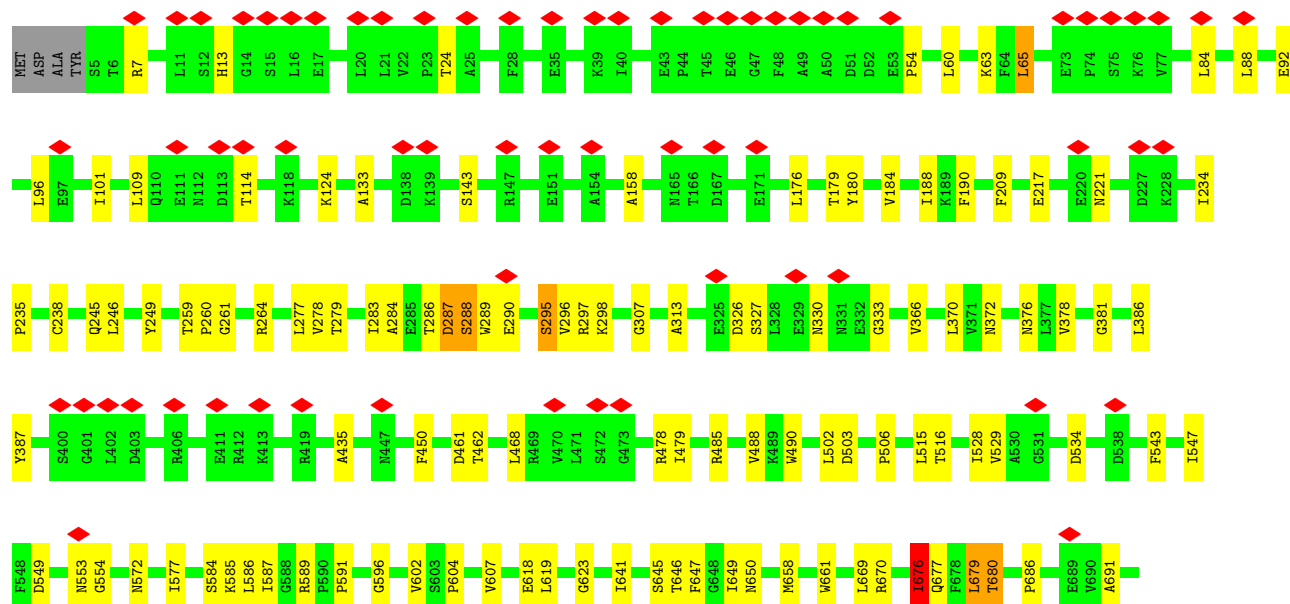
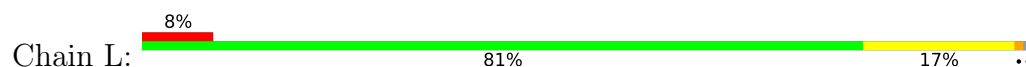


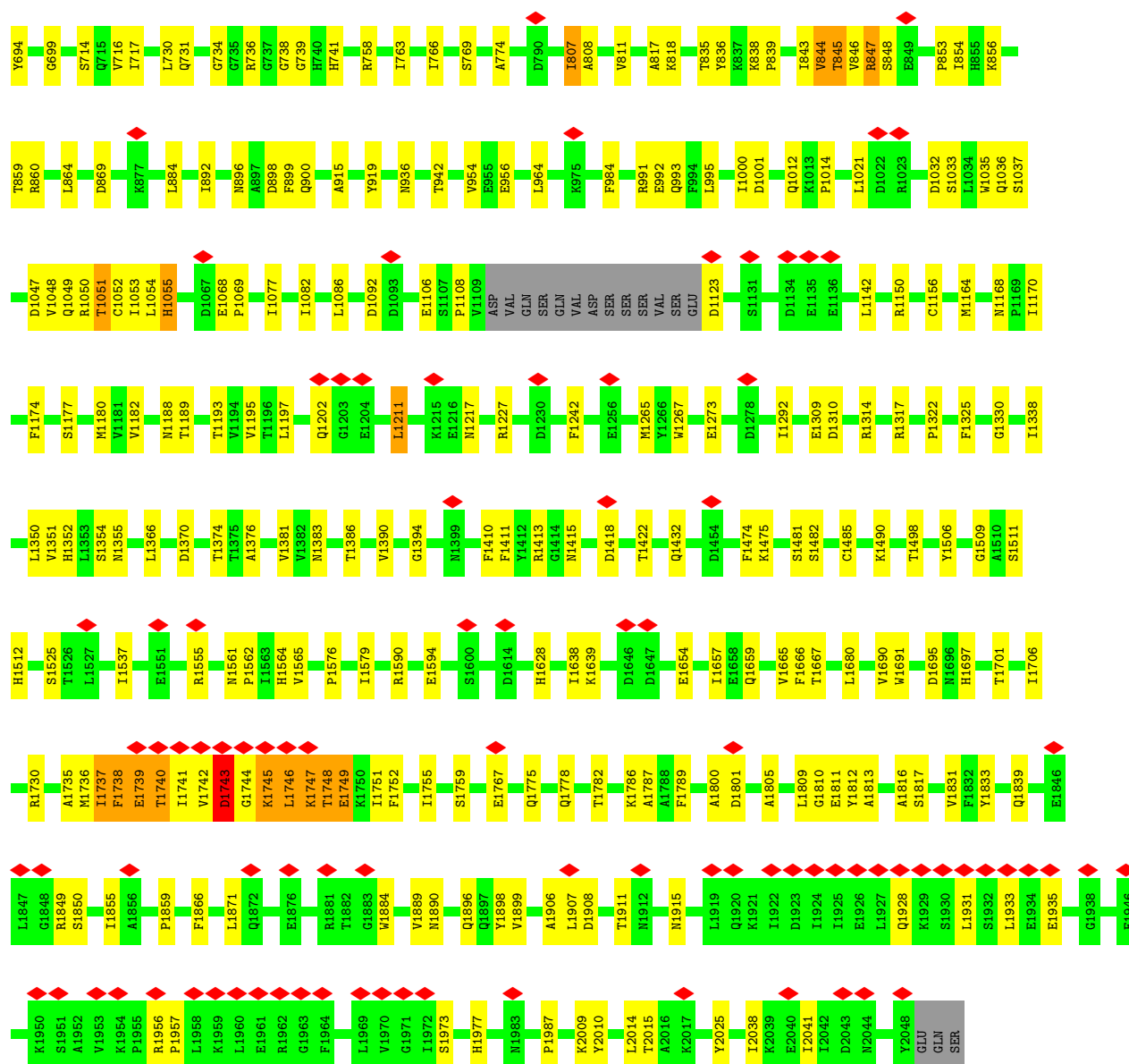
• Molecule 2: Fatty acid synthase subunit beta



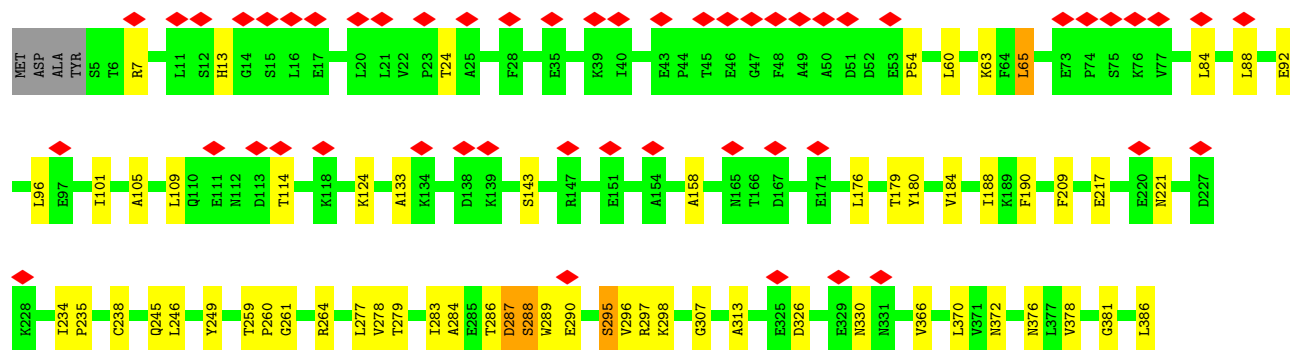
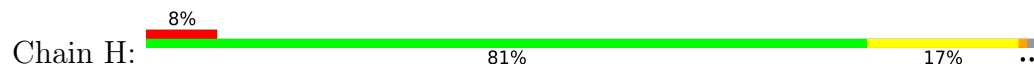


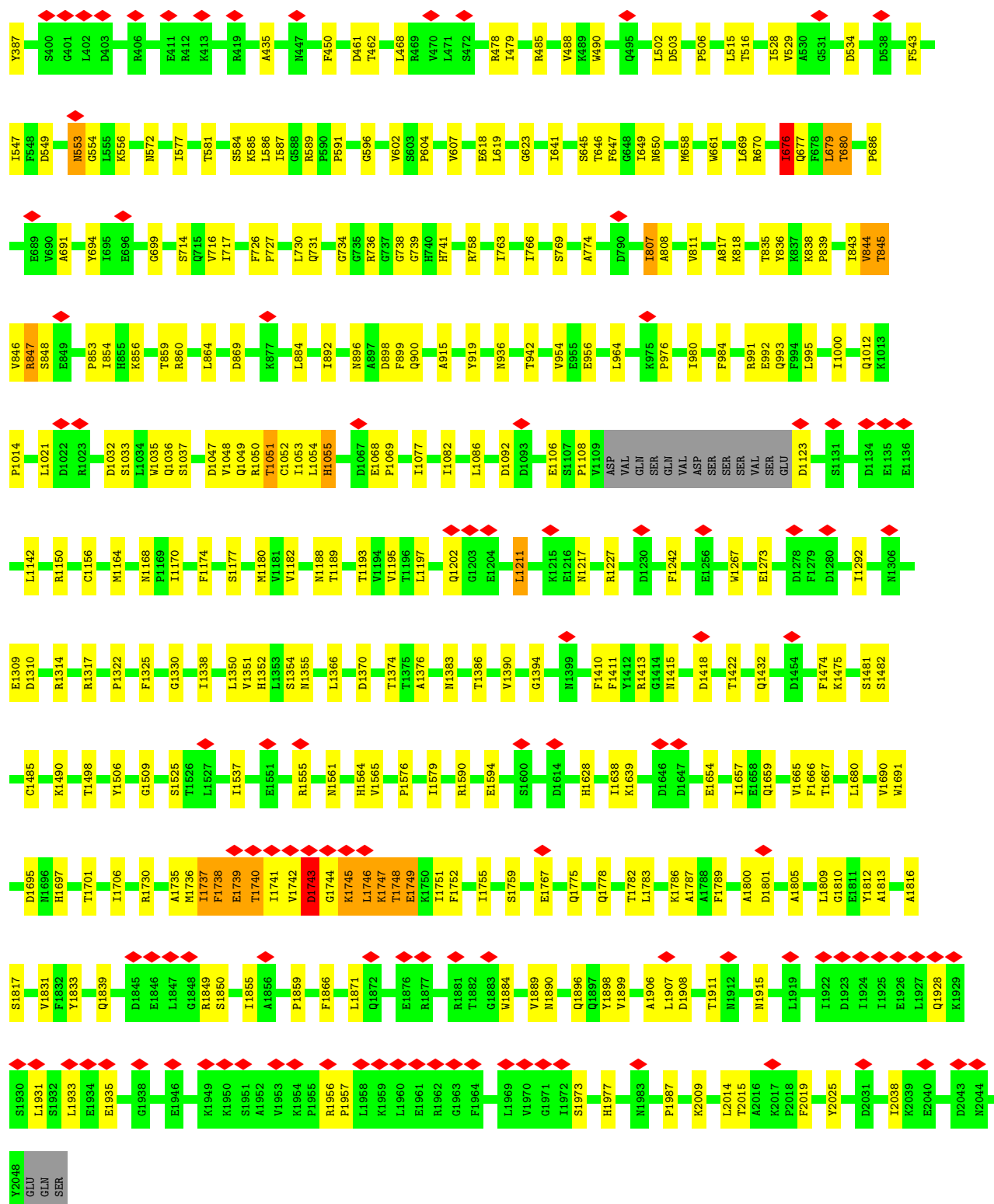
• Molecule 2: Fatty acid synthase subunit beta



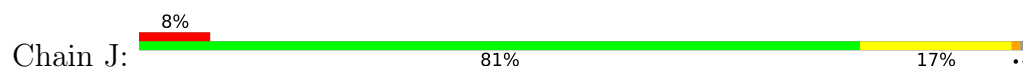


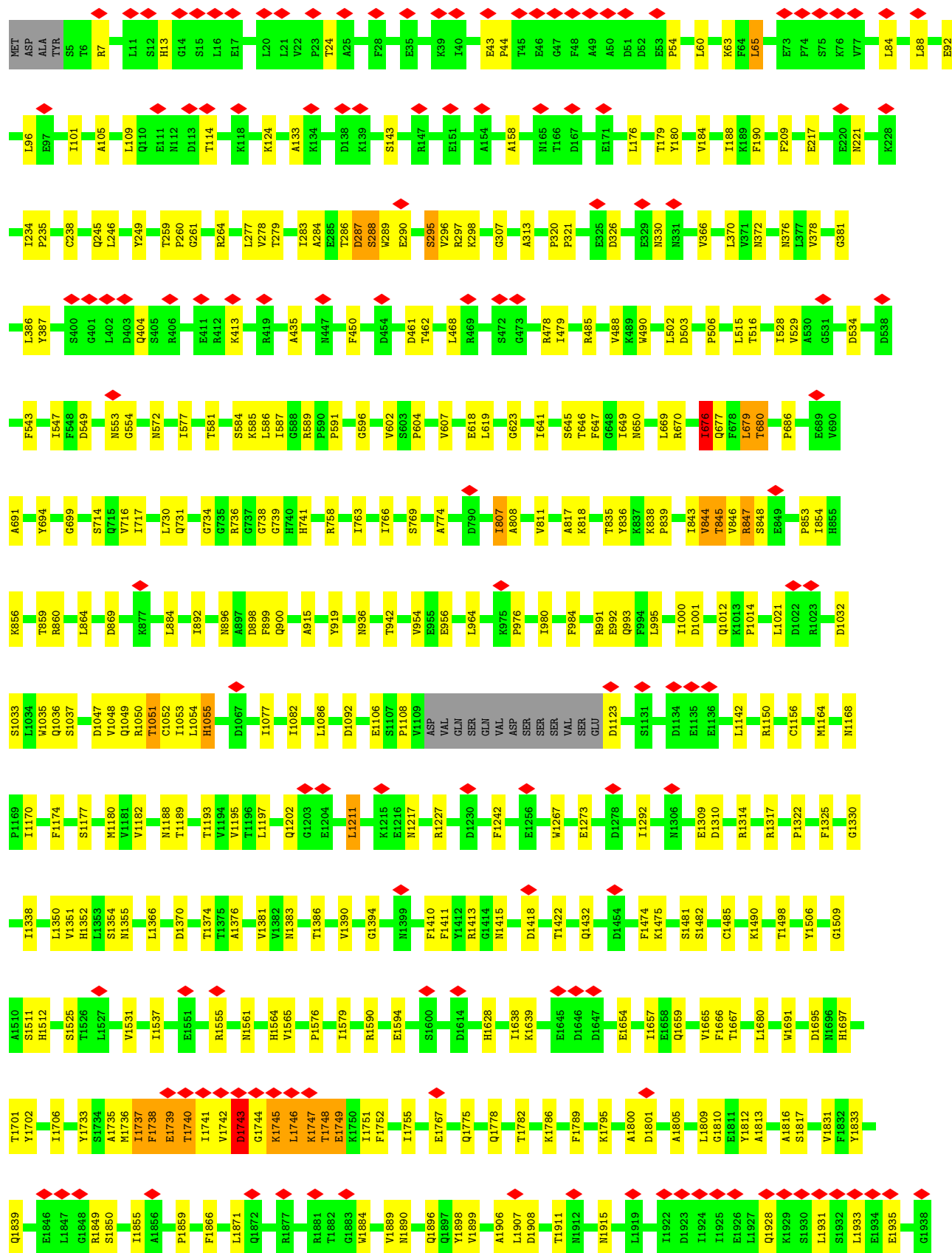
• Molecule 2: Fatty acid synthase subunit beta

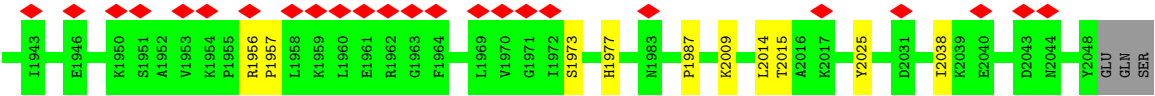




• Molecule 2: Fatty acid synthase subunit beta







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	15320	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 ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.293	Depositor
Minimum map value	-3.098	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.187	Depositor
Recommended contour level	0.6	Depositor
Map size (\AA)	399.84, 399.84, 399.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FMN, SEP

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	0.51	0/13859	0.62	7/18724 (0.0%)
1	B	0.51	0/13859	0.62	7/18724 (0.0%)
1	D	0.51	0/13859	0.62	7/18724 (0.0%)
1	F	0.51	0/13859	0.62	7/18724 (0.0%)
1	I	0.51	0/13859	0.62	7/18724 (0.0%)
1	K	0.51	0/13859	0.64	9/18724 (0.0%)
2	C	0.39	0/16342	0.58	4/22174 (0.0%)
2	E	0.39	0/16342	0.58	4/22174 (0.0%)
2	G	0.39	0/16342	0.58	4/22174 (0.0%)
2	H	0.39	0/16342	0.58	4/22174 (0.0%)
2	J	0.39	0/16342	0.58	4/22174 (0.0%)
2	L	0.39	0/16342	0.58	4/22174 (0.0%)
All	All	0.45	0/181206	0.60	68/245388 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	E	0	1
2	G	0	1
2	H	0	1
2	J	0	1
2	L	0	1
All	All	0	6

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	329	GLU	N-CA-CB	15.05	137.69	110.60
1	K	328	LEU	N-CA-C	-14.18	72.71	111.00
1	B	873	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	F	873	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	D	873	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	I	873	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	873	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	K	873	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	A	930	LEU	CA-CB-CG	5.96	129.01	115.30
1	K	930	LEU	CA-CB-CG	5.96	129.01	115.30
1	D	930	LEU	CA-CB-CG	5.96	129.00	115.30
1	I	930	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	930	LEU	CA-CB-CG	5.96	129.00	115.30
1	F	930	LEU	CA-CB-CG	5.96	129.00	115.30
2	E	65	LEU	CA-CB-CG	5.75	128.51	115.30
2	J	65	LEU	CA-CB-CG	5.75	128.51	115.30
2	G	65	LEU	CA-CB-CG	5.74	128.49	115.30
2	C	65	LEU	CA-CB-CG	5.74	128.49	115.30
2	L	65	LEU	CA-CB-CG	5.74	128.49	115.30
2	H	65	LEU	CA-CB-CG	5.74	128.49	115.30
1	D	1013	LEU	CA-CB-CG	5.71	128.42	115.30
1	I	1013	LEU	CA-CB-CG	5.71	128.42	115.30
1	B	1013	LEU	CA-CB-CG	5.70	128.42	115.30
1	F	1013	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	1013	LEU	CA-CB-CG	5.70	128.40	115.30
1	K	1013	LEU	CA-CB-CG	5.70	128.40	115.30
1	B	824	LEU	CA-CB-CG	5.46	127.85	115.30
1	F	824	LEU	CA-CB-CG	5.46	127.85	115.30
1	D	824	LEU	CA-CB-CG	5.45	127.84	115.30
1	I	824	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	824	LEU	CA-CB-CG	5.45	127.83	115.30
1	K	824	LEU	CA-CB-CG	5.45	127.83	115.30
2	C	1680	LEU	CA-CB-CG	5.41	127.75	115.30
2	H	1680	LEU	CA-CB-CG	5.41	127.75	115.30
2	E	1680	LEU	CA-CB-CG	5.39	127.71	115.30
2	J	1680	LEU	CA-CB-CG	5.39	127.71	115.30
2	G	1680	LEU	CA-CB-CG	5.39	127.70	115.30
2	L	1680	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	447	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	F	447	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	A	447	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	K	447	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	D	447	LEU	CB-CG-CD1	-5.36	101.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	447	LEU	CB-CG-CD1	-5.36	101.89	111.00
2	G	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	C	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	L	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	H	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	E	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	J	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	G	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	L	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	C	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	H	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	E	807	ILE	CG1-CB-CG2	-5.15	100.06	111.40
2	J	807	ILE	CG1-CB-CG2	-5.15	100.06	111.40
1	B	1426	LEU	CA-CB-CG	5.10	127.02	115.30
1	F	1426	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	1426	LEU	CA-CB-CG	5.09	127.01	115.30
1	K	1426	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	1426	LEU	CA-CB-CG	5.09	127.00	115.30
1	I	1426	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	1430	ARG	CA-CB-CG	5.04	124.48	113.40
1	K	1430	ARG	CA-CB-CG	5.04	124.48	113.40
1	B	1430	ARG	CA-CB-CG	5.02	124.44	113.40
1	D	1430	ARG	CA-CB-CG	5.02	124.44	113.40
1	F	1430	ARG	CA-CB-CG	5.02	124.44	113.40
1	I	1430	ARG	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1014	PRO	Peptide
2	E	1014	PRO	Peptide
2	G	1014	PRO	Peptide
2	H	1014	PRO	Peptide
2	J	1014	PRO	Peptide
2	L	1014	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13619	0	13602	244	0
1	B	13619	0	13602	241	0
1	D	13619	0	13602	242	0
1	F	13619	0	13602	242	0
1	I	13619	0	13602	243	0
1	K	13619	0	13602	240	0
2	C	15977	0	15964	290	0
2	E	15977	0	15964	289	0
2	G	15977	0	15964	294	0
2	H	15977	0	15964	287	0
2	J	15977	0	15964	293	0
2	L	15977	0	15964	288	0
3	A	48	26	26	8	0
3	B	48	26	26	7	0
3	D	48	26	26	7	0
3	F	48	26	26	7	0
3	I	48	26	26	8	0
3	K	48	26	26	7	0
4	C	31	0	19	0	0
4	E	31	0	19	0	0
4	G	31	0	19	0	0
4	H	31	0	19	0	0
4	J	31	0	19	0	0
4	L	31	0	19	0	0
All	All	178050	156	177666	2989	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 8.

All (2989) 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:K:1491:ARG:CD	1:K:1750:ILE:HD11	1.37	1.55
1:D:1491:ARG:HD3	1:D:1750:ILE:CD1	1.34	1.54
1:D:1491:ARG:CD	1:D:1750:ILE:HD11	1.37	1.54
1:F:1491:ARG:CD	1:F:1750:ILE:HD11	1.37	1.54
1:A:1491:ARG:HD3	1:A:1750:ILE:CD1	1.34	1.54
1:F:1491:ARG:HD3	1:F:1750:ILE:CD1	1.34	1.54
1:B:1491:ARG:HD3	1:B:1750:ILE:CD1	1.34	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1491:ARG:CD	1:B:1750:ILE:HD11	1.37	1.53
1:A:1491:ARG:CD	1:A:1750:ILE:HD11	1.37	1.52
1:K:1491:ARG:HD3	1:K:1750:ILE:CD1	1.34	1.51
1:I:1491:ARG:HD3	1:I:1750:ILE:CD1	1.34	1.50
1:I:1491:ARG:CD	1:I:1750:ILE:HD11	1.37	1.49
2:H:847:ARG:HG3	2:H:869:ASP:OD2	1.21	1.38
1:I:1491:ARG:CD	1:I:1750:ILE:CD1	1.97	1.35
2:C:847:ARG:HG3	2:C:869:ASP:OD2	1.21	1.35
1:A:1491:ARG:CD	1:A:1750:ILE:CD1	1.97	1.34
1:K:1491:ARG:CD	1:K:1750:ILE:CD1	1.97	1.33
2:E:847:ARG:HG3	2:E:869:ASP:OD2	1.21	1.33
2:J:847:ARG:HG3	2:J:869:ASP:OD2	1.21	1.33
1:A:1491:ARG:CB	1:A:1750:ILE:HD13	1.60	1.32
1:D:1491:ARG:CB	1:D:1750:ILE:HD13	1.60	1.32
1:F:1491:ARG:CD	1:F:1750:ILE:CD1	1.97	1.32
1:I:1491:ARG:CB	1:I:1750:ILE:HD13	1.60	1.31
1:D:1491:ARG:CD	1:D:1750:ILE:CD1	1.97	1.30
1:K:1491:ARG:CB	1:K:1750:ILE:HD13	1.60	1.30
1:F:1491:ARG:CB	1:F:1750:ILE:HD13	1.60	1.30
1:B:1491:ARG:CB	1:B:1750:ILE:HD13	1.60	1.29
2:L:847:ARG:HG3	2:L:869:ASP:OD2	1.21	1.27
2:G:847:ARG:HG3	2:G:869:ASP:OD2	1.21	1.26
1:B:1491:ARG:CD	1:B:1750:ILE:CD1	1.97	1.26
1:F:1744:TYR:O	1:F:1747:ALA:CB	1.85	1.25
1:B:1744:TYR:O	1:B:1747:ALA:CB	1.85	1.25
1:K:1744:TYR:O	1:K:1747:ALA:CB	1.85	1.25
1:I:1744:TYR:O	1:I:1747:ALA:CB	1.85	1.24
1:D:1744:TYR:O	1:D:1747:ALA:CB	1.85	1.23
1:A:1744:TYR:O	1:A:1747:ALA:CB	1.85	1.23
1:A:1744:TYR:O	1:A:1747:ALA:HB2	1.03	1.21
1:F:1744:TYR:O	1:F:1747:ALA:HB2	1.03	1.20
1:K:1744:TYR:O	1:K:1747:ALA:HB2	1.03	1.19
1:I:1744:TYR:O	1:I:1747:ALA:HB2	1.03	1.19
1:D:1744:TYR:O	1:D:1747:ALA:HB2	1.03	1.19
1:A:1491:ARG:HD2	1:A:1750:ILE:HD11	1.20	1.18
1:B:1744:TYR:O	1:B:1747:ALA:HB2	1.03	1.18
2:E:1737:ILE:HB	2:E:1748:THR:HB	1.21	1.17
1:D:1491:ARG:HD3	1:D:1750:ILE:HD12	1.24	1.16
2:G:1735:ALA:O	2:G:1736:MET:HE2	1.45	1.16
2:L:1735:ALA:O	2:L:1736:MET:HE2	1.47	1.15
1:I:1491:ARG:HD2	1:I:1750:ILE:HD11	1.20	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1735:ALA:O	2:C:1736:MET:HE2	1.46	1.15
2:H:1737:ILE:HB	2:H:1748:THR:HB	1.20	1.15
2:J:1735:ALA:O	2:J:1736:MET:HE2	1.44	1.14
2:E:234:ILE:HG23	2:E:238:CYS:SG	1.87	1.14
1:F:1491:ARG:HD3	1:F:1750:ILE:HD12	1.24	1.14
2:H:234:ILE:HG23	2:H:238:CYS:SG	1.87	1.14
2:J:234:ILE:HG23	2:J:238:CYS:SG	1.87	1.14
2:C:234:ILE:HG23	2:C:238:CYS:SG	1.87	1.14
2:J:847:ARG:CG	2:J:869:ASP:OD2	1.97	1.13
2:L:1737:ILE:HB	2:L:1748:THR:HB	1.21	1.13
1:F:1491:ARG:HD2	1:F:1750:ILE:HD11	1.20	1.13
2:H:1735:ALA:O	2:H:1736:MET:HE2	1.47	1.13
1:A:848:THR:HG22	1:F:844:LEU:HD22	1.24	1.13
2:G:234:ILE:HG23	2:G:238:CYS:SG	1.87	1.13
2:G:847:ARG:CG	2:G:869:ASP:OD2	1.97	1.13
2:G:1737:ILE:HB	2:G:1748:THR:HB	1.21	1.12
2:L:234:ILE:HG23	2:L:238:CYS:SG	1.87	1.12
2:H:847:ARG:CG	2:H:869:ASP:OD2	1.97	1.12
1:D:844:LEU:HD22	1:I:848:THR:HG22	1.24	1.12
2:E:847:ARG:CG	2:E:869:ASP:OD2	1.97	1.11
2:L:847:ARG:CG	2:L:869:ASP:OD2	1.97	1.11
1:I:1491:ARG:HD3	1:I:1750:ILE:HD12	1.24	1.11
1:B:1491:ARG:HD2	1:B:1750:ILE:HD11	1.20	1.11
1:K:1491:ARG:HD3	1:K:1750:ILE:HD12	1.25	1.11
2:C:847:ARG:CG	2:C:869:ASP:OD2	1.97	1.10
2:J:1737:ILE:HB	2:J:1748:THR:HB	1.21	1.10
2:E:836:TYR:CD1	2:E:845:THR:HG21	1.87	1.10
2:E:1735:ALA:O	2:E:1736:MET:HE2	1.48	1.10
1:F:1751:GLU:HA	1:F:1754:LYS:HE3	1.32	1.10
2:H:836:TYR:CD1	2:H:845:THR:HG21	1.87	1.10
1:A:1491:ARG:HD3	1:A:1750:ILE:HD12	1.25	1.10
1:D:1491:ARG:HD2	1:D:1750:ILE:HD11	1.20	1.09
2:E:739:GLY:HA2	2:E:1054:LEU:HD23	1.10	1.09
2:L:739:GLY:HA2	2:L:1054:LEU:HD23	1.10	1.09
2:H:739:GLY:HA2	2:H:1054:LEU:HD23	1.10	1.09
2:C:1737:ILE:HB	2:C:1748:THR:HB	1.20	1.09
2:G:836:TYR:CD1	2:G:845:THR:HG21	1.87	1.09
1:B:848:THR:HG22	1:K:844:LEU:HD22	1.24	1.09
1:D:848:THR:HG22	1:I:844:LEU:HD22	1.24	1.09
2:L:836:TYR:CD1	2:L:845:THR:HG21	1.87	1.09
2:C:739:GLY:HA2	2:C:1054:LEU:HD23	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1751:GLU:HA	1:D:1754:LYS:HE3	1.32	1.08
1:I:1751:GLU:HA	1:I:1754:LYS:HE3	1.32	1.08
1:B:1491:ARG:HD3	1:B:1750:ILE:HD12	1.24	1.08
1:K:1491:ARG:HD2	1:K:1750:ILE:HD11	1.20	1.08
2:J:836:TYR:CD1	2:J:845:THR:HG21	1.87	1.08
1:B:844:LEU:HD22	1:K:848:THR:HG22	1.24	1.07
2:E:1036:GLN:HB3	2:E:1051:THR:HG23	1.36	1.07
2:J:739:GLY:HA2	2:J:1054:LEU:HD23	1.10	1.07
1:A:844:LEU:HD22	1:F:848:THR:HG22	1.24	1.07
2:G:646:THR:HB	2:G:677:GLN:HB2	1.36	1.07
2:G:1036:GLN:HB3	2:G:1051:THR:HG23	1.36	1.07
2:J:646:THR:HB	2:J:677:GLN:HB2	1.36	1.07
2:L:646:THR:HB	2:L:677:GLN:HB2	1.36	1.07
2:H:646:THR:HB	2:H:677:GLN:HB2	1.36	1.07
2:G:739:GLY:HA2	2:G:1054:LEU:HD23	1.10	1.07
2:C:646:THR:HB	2:C:677:GLN:HB2	1.36	1.07
2:C:836:TYR:CD1	2:C:845:THR:HG21	1.87	1.07
2:E:646:THR:HB	2:E:677:GLN:HB2	1.36	1.07
1:B:1751:GLU:HA	1:B:1754:LYS:HE3	1.32	1.06
2:H:1036:GLN:HB3	2:H:1051:THR:HG23	1.36	1.06
2:J:1036:GLN:HB3	2:J:1051:THR:HG23	1.36	1.06
2:L:1036:GLN:HB3	2:L:1051:THR:HG23	1.36	1.05
1:A:1751:GLU:HA	1:A:1754:LYS:HE3	1.32	1.04
2:C:1036:GLN:HB3	2:C:1051:THR:HG23	1.36	1.04
1:K:1751:GLU:HA	1:K:1754:LYS:HE3	1.32	1.04
1:A:1487:LEU:CD1	1:A:1754:LYS:HE2	1.89	1.02
1:F:1487:LEU:CD1	1:F:1754:LYS:HE2	1.89	1.02
1:I:1487:LEU:HD12	1:I:1754:LYS:HE2	1.41	1.02
1:B:1487:LEU:HD12	1:B:1754:LYS:HE2	1.41	1.02
1:F:1491:ARG:HB2	1:F:1750:ILE:HD13	1.02	1.01
1:I:1487:LEU:CD1	1:I:1754:LYS:HE2	1.90	1.01
1:D:1487:LEU:CD1	1:D:1754:LYS:HE2	1.90	1.01
1:D:1491:ARG:HB2	1:D:1750:ILE:HD13	1.02	1.01
1:K:1487:LEU:CD1	1:K:1754:LYS:HE2	1.89	1.01
2:J:1735:ALA:O	2:J:1736:MET:CE	2.09	1.01
1:B:1487:LEU:CD1	1:B:1754:LYS:HE2	1.89	1.01
2:E:1735:ALA:C	2:E:1736:MET:HE3	1.81	1.01
1:A:1491:ARG:HB2	1:A:1750:ILE:HD13	1.02	1.01
2:C:1735:ALA:O	2:C:1736:MET:CE	2.09	1.01
2:G:1735:ALA:O	2:G:1736:MET:CE	2.09	1.00
2:E:1735:ALA:O	2:E:1736:MET:CE	2.09	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1487:LEU:HD12	1:F:1754:LYS:HE2	1.41	1.00
2:H:1735:ALA:O	2:H:1736:MET:CE	2.09	1.00
1:D:1487:LEU:HD12	1:D:1754:LYS:HE2	1.41	1.00
2:L:1735:ALA:O	2:L:1736:MET:CE	2.09	1.00
1:I:1491:ARG:HB2	1:I:1750:ILE:HD13	1.02	0.99
1:K:1491:ARG:HB2	1:K:1750:ILE:HD13	1.02	0.99
1:K:1487:LEU:HD12	1:K:1754:LYS:HE2	1.41	0.99
1:A:1487:LEU:HD12	1:A:1754:LYS:HE2	1.41	0.99
2:L:1735:ALA:C	2:L:1736:MET:HE3	1.83	0.98
1:B:1491:ARG:HB2	1:B:1750:ILE:HD13	1.02	0.98
2:H:1735:ALA:C	2:H:1736:MET:HE3	1.83	0.98
2:L:1036:GLN:CB	2:L:1051:THR:HG23	1.94	0.97
2:E:1036:GLN:CB	2:E:1051:THR:HG23	1.94	0.96
2:C:1036:GLN:CB	2:C:1051:THR:HG23	1.95	0.96
2:H:1036:GLN:CB	2:H:1051:THR:HG23	1.95	0.96
2:J:1036:GLN:CB	2:J:1051:THR:HG23	1.94	0.96
2:C:1735:ALA:C	2:C:1736:MET:HE3	1.86	0.95
2:G:1036:GLN:CB	2:G:1051:THR:HG23	1.94	0.95
1:A:1751:GLU:HG3	1:A:1754:LYS:NZ	1.83	0.94
1:D:1751:GLU:HG3	1:D:1754:LYS:NZ	1.83	0.94
2:L:1735:ALA:C	2:L:1736:MET:CE	2.36	0.94
2:C:1735:ALA:C	2:C:1736:MET:CE	2.36	0.94
2:E:1735:ALA:C	2:E:1736:MET:CE	2.36	0.93
2:E:1739:GLU:HB3	2:E:1746:LEU:HD11	1.50	0.93
1:F:1751:GLU:HG3	1:F:1754:LYS:NZ	1.83	0.93
2:H:1735:ALA:C	2:H:1736:MET:CE	2.36	0.93
1:K:1751:GLU:HG3	1:K:1754:LYS:NZ	1.83	0.93
2:G:1735:ALA:C	2:G:1736:MET:CE	2.36	0.93
2:J:1735:ALA:C	2:J:1736:MET:CE	2.36	0.93
2:J:1735:ALA:C	2:J:1736:MET:HE3	1.89	0.93
2:G:1735:ALA:C	2:G:1736:MET:HE3	1.87	0.93
1:I:1751:GLU:HG3	1:I:1754:LYS:NZ	1.83	0.92
1:B:1751:GLU:HG3	1:B:1754:LYS:NZ	1.83	0.92
1:F:1491:ARG:CB	1:F:1750:ILE:CD1	2.47	0.92
2:H:1739:GLU:HB3	2:H:1746:LEU:HD11	1.51	0.92
1:D:1491:ARG:CB	1:D:1750:ILE:CD1	2.47	0.92
2:G:739:GLY:HA2	2:G:1054:LEU:CD2	2.00	0.92
2:L:1739:GLU:HB3	2:L:1746:LEU:HD11	1.50	0.92
1:A:1491:ARG:CB	1:A:1750:ILE:CD1	2.47	0.91
1:B:848:THR:CG2	1:K:844:LEU:HD22	2.01	0.91
1:D:844:LEU:HD22	1:I:848:THR:CG2	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1491:ARG:HB2	1:I:1750:ILE:CD1	1.98	0.91
1:K:1491:ARG:CB	1:K:1750:ILE:CD1	2.47	0.91
1:I:1491:ARG:CB	1:I:1750:ILE:CD1	2.47	0.91
1:F:1491:ARG:HB2	1:F:1750:ILE:CD1	1.98	0.91
2:H:739:GLY:HA2	2:H:1054:LEU:CD2	2.00	0.91
1:D:848:THR:CG2	1:I:844:LEU:HD22	2.01	0.91
1:A:848:THR:CG2	1:F:844:LEU:HD22	2.01	0.90
2:C:1739:GLU:HB3	2:C:1746:LEU:HD11	1.51	0.90
2:L:739:GLY:HA2	2:L:1054:LEU:CD2	2.00	0.90
2:J:1739:GLU:HB3	2:J:1746:LEU:HD11	1.50	0.90
1:A:844:LEU:HD22	1:F:848:THR:CG2	2.01	0.90
2:E:739:GLY:HA2	2:E:1054:LEU:CD2	2.00	0.90
1:B:844:LEU:HD22	1:K:848:THR:CG2	2.01	0.90
2:C:739:GLY:HA2	2:C:1054:LEU:CD2	2.00	0.90
1:K:1373:ARG:NE	1:K:1550:ASP:OD2	2.05	0.90
1:F:1373:ARG:NE	1:F:1550:ASP:OD2	2.05	0.90
1:D:1491:ARG:HB2	1:D:1750:ILE:CD1	1.98	0.89
2:G:1739:GLU:HB3	2:G:1746:LEU:HD11	1.50	0.89
1:B:1373:ARG:NE	1:B:1550:ASP:OD2	2.05	0.89
1:A:1373:ARG:NE	1:A:1550:ASP:OD2	2.05	0.89
1:D:1373:ARG:NE	1:D:1550:ASP:OD2	2.05	0.89
1:B:1491:ARG:CB	1:B:1750:ILE:CD1	2.47	0.89
2:C:847:ARG:HG3	2:C:869:ASP:CG	1.93	0.89
2:J:1738:PHE:CZ	2:J:1749:GLU:HG2	2.08	0.89
2:G:1738:PHE:CZ	2:G:1749:GLU:HG2	2.08	0.89
2:G:646:THR:CB	2:G:677:GLN:HB2	2.03	0.89
2:E:847:ARG:HG3	2:E:869:ASP:CG	1.93	0.89
2:H:847:ARG:HG3	2:H:869:ASP:CG	1.93	0.89
2:J:847:ARG:HG3	2:J:869:ASP:CG	1.93	0.89
2:E:1738:PHE:CZ	2:E:1749:GLU:HG2	2.08	0.89
2:L:847:ARG:HG3	2:L:869:ASP:CG	1.93	0.88
1:I:1373:ARG:NE	1:I:1550:ASP:OD2	2.05	0.88
2:C:646:THR:CB	2:C:677:GLN:HB2	2.03	0.88
2:H:646:THR:CB	2:H:677:GLN:HB2	2.03	0.88
2:H:1738:PHE:CZ	2:H:1749:GLU:HG2	2.08	0.88
2:L:1738:PHE:CZ	2:L:1749:GLU:HG2	2.08	0.88
2:L:646:THR:CB	2:L:677:GLN:HB2	2.03	0.88
2:C:1738:PHE:CZ	2:C:1749:GLU:HG2	2.08	0.88
2:J:646:THR:CB	2:J:677:GLN:HB2	2.03	0.88
2:E:234:ILE:CG2	2:E:238:CYS:SG	2.62	0.87
2:G:847:ARG:HG3	2:G:869:ASP:CG	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:234:ILE:CG2	2:H:238:CYS:SG	2.62	0.87
1:A:1491:ARG:HB2	1:A:1750:ILE:CD1	1.98	0.87
2:C:1737:ILE:HB	2:C:1748:THR:CB	2.05	0.87
2:G:234:ILE:CG2	2:G:238:CYS:SG	2.62	0.87
2:C:234:ILE:CG2	2:C:238:CYS:SG	2.62	0.87
1:K:1491:ARG:HB2	1:K:1750:ILE:CD1	1.98	0.87
2:J:234:ILE:CG2	2:J:238:CYS:SG	2.62	0.87
2:J:246:LEU:HD23	2:J:296:VAL:HG22	1.57	0.87
2:L:234:ILE:CG2	2:L:238:CYS:SG	2.62	0.86
2:E:646:THR:CB	2:E:677:GLN:HB2	2.03	0.86
2:C:246:LEU:HD23	2:C:296:VAL:HG22	1.57	0.86
2:L:1737:ILE:HB	2:L:1748:THR:CB	2.05	0.86
2:J:739:GLY:HA2	2:J:1054:LEU:CD2	2.00	0.86
2:G:1737:ILE:HB	2:G:1748:THR:CB	2.05	0.86
2:H:1737:ILE:HB	2:H:1748:THR:CB	2.05	0.86
2:G:246:LEU:HD23	2:G:296:VAL:HG22	1.57	0.86
2:L:246:LEU:HD23	2:L:296:VAL:HG22	1.57	0.86
2:J:1737:ILE:HB	2:J:1748:THR:CB	2.05	0.85
2:E:246:LEU:HD23	2:E:296:VAL:HG22	1.57	0.85
1:B:1491:ARG:HB2	1:B:1750:ILE:CD1	1.98	0.84
1:B:1491:ARG:CG	1:B:1750:ILE:CD1	2.55	0.84
2:E:1737:ILE:HB	2:E:1748:THR:CB	2.05	0.84
1:D:1491:ARG:CG	1:D:1750:ILE:CD1	2.55	0.84
1:K:1491:ARG:CG	1:K:1750:ILE:CD1	2.55	0.84
2:H:246:LEU:HD23	2:H:296:VAL:HG22	1.57	0.84
1:I:1751:GLU:HG3	1:I:1754:LYS:HZ1	1.43	0.84
1:I:1491:ARG:CG	1:I:1750:ILE:CD1	2.55	0.84
1:F:1491:ARG:CG	1:F:1750:ILE:CD1	2.55	0.84
1:K:1561:MET:HE2	1:K:1561:MET:HA	1.60	0.83
1:D:844:LEU:CD2	1:I:848:THR:HG22	2.08	0.83
1:A:1491:ARG:CG	1:A:1750:ILE:CD1	2.55	0.83
1:B:848:THR:HG22	1:K:844:LEU:CD2	2.08	0.83
1:K:1373:ARG:CD	1:K:1550:ASP:OD2	2.27	0.83
1:B:1373:ARG:CD	1:B:1550:ASP:OD2	2.27	0.83
1:I:1373:ARG:CD	1:I:1550:ASP:OD2	2.27	0.83
1:I:1561:MET:HE2	1:I:1561:MET:HA	1.60	0.83
1:A:848:THR:HG22	1:F:844:LEU:CD2	2.08	0.83
2:E:234:ILE:HG23	2:E:238:CYS:HG	1.41	0.83
1:D:1373:ARG:CD	1:D:1550:ASP:OD2	2.27	0.82
1:B:844:LEU:CD2	1:K:848:THR:HG22	2.08	0.82
1:F:1373:ARG:CD	1:F:1550:ASP:OD2	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:LEU:CD2	1:F:848:THR:HG22	2.08	0.82
1:B:1561:MET:HA	1:B:1561:MET:HE2	1.60	0.82
1:A:1373:ARG:CD	1:A:1550:ASP:OD2	2.27	0.82
1:D:848:THR:HG22	1:I:844:LEU:CD2	2.08	0.81
1:D:1541:PHE:HE1	1:D:1557:ILE:HG13	1.45	0.81
1:F:877:LEU:CD1	3:F:2001:NDP:H2D	2.10	0.81
1:D:1491:ARG:CG	1:D:1750:ILE:HD13	2.10	0.81
1:F:1541:PHE:HE1	1:F:1557:ILE:HG13	1.45	0.81
1:B:838:MET:HA	1:B:841:GLU:OE1	1.81	0.81
1:D:877:LEU:CD1	3:D:2001:NDP:H2D	2.10	0.81
1:A:1561:MET:HE2	1:A:1561:MET:HA	1.63	0.81
1:B:1541:PHE:HE1	1:B:1557:ILE:HG13	1.45	0.81
1:K:1541:PHE:HE1	1:K:1557:ILE:HG13	1.45	0.81
2:J:260:PRO:HD3	2:J:289:TRP:CZ2	2.16	0.81
1:A:1491:ARG:CG	1:A:1750:ILE:HD13	2.10	0.81
1:A:1541:PHE:HE1	1:A:1557:ILE:HG13	1.45	0.81
2:G:1737:ILE:CB	2:G:1748:THR:HB	2.09	0.81
1:K:1491:ARG:CG	1:K:1750:ILE:HD13	2.10	0.81
1:K:1751:GLU:CA	1:K:1754:LYS:HE3	2.11	0.81
1:I:1491:ARG:CG	1:I:1750:ILE:HD13	2.10	0.81
1:B:1491:ARG:CG	1:B:1750:ILE:HD13	2.10	0.81
1:K:838:MET:HA	1:K:841:GLU:OE1	1.81	0.81
1:A:838:MET:HA	1:A:841:GLU:OE1	1.81	0.81
1:A:877:LEU:CD1	3:A:2001:NDP:H2D	2.10	0.81
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.16	0.81
1:B:1751:GLU:CA	1:B:1754:LYS:HE3	2.11	0.81
2:C:260:PRO:HD3	2:C:289:TRP:CZ2	2.16	0.81
1:K:877:LEU:CD1	3:K:2001:NDP:H2D	2.10	0.81
1:F:1673:TYR:CZ	1:F:1677:VAL:HG21	2.16	0.81
1:D:1751:GLU:CA	1:D:1754:LYS:HE3	2.11	0.80
2:G:260:PRO:HD3	2:G:289:TRP:CZ2	2.16	0.80
2:L:260:PRO:HD3	2:L:289:TRP:CZ2	2.16	0.80
1:F:1491:ARG:CG	1:F:1750:ILE:HD13	2.10	0.80
1:B:877:LEU:CD1	3:B:2001:NDP:H2D	2.10	0.80
1:D:838:MET:HA	1:D:841:GLU:OE1	1.81	0.80
1:F:1751:GLU:CA	1:F:1754:LYS:HE3	2.11	0.80
2:H:260:PRO:HD3	2:H:289:TRP:CZ2	2.16	0.80
1:I:1673:TYR:CZ	1:I:1677:VAL:HG21	2.16	0.80
1:I:838:MET:HA	1:I:841:GLU:OE1	1.81	0.80
1:I:1491:ARG:HD3	1:I:1750:ILE:HD11	1.06	0.80
1:I:1751:GLU:CA	1:I:1754:LYS:HE3	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.16	0.80
1:D:1673:TYR:CZ	1:D:1677:VAL:HG21	2.16	0.80
2:E:260:PRO:HD3	2:E:289:TRP:CZ2	2.16	0.80
1:I:877:LEU:CD1	3:I:2001:NDP:H2D	2.10	0.79
1:F:838:MET:HA	1:F:841:GLU:OE1	1.81	0.79
1:A:1751:GLU:CA	1:A:1754:LYS:HE3	2.11	0.79
2:G:295:SER:O	2:G:298:LYS:HB2	1.82	0.79
1:B:1751:GLU:HG3	1:B:1754:LYS:HZ1	1.48	0.79
1:K:1673:TYR:CZ	1:K:1677:VAL:HG21	2.16	0.79
1:I:1541:PHE:HE1	1:I:1557:ILE:HG13	1.45	0.79
2:J:1737:ILE:HG12	2:J:1748:THR:HG21	1.64	0.79
2:C:1737:ILE:HG12	2:C:1748:THR:HG21	1.64	0.79
2:H:1737:ILE:CB	2:H:1748:THR:HB	2.09	0.79
2:G:1737:ILE:H	2:G:1737:ILE:HD13	1.48	0.79
2:H:295:SER:O	2:H:298:LYS:HB2	1.82	0.79
1:B:1558:ASN:OD1	1:B:1623:TYR:HB2	1.84	0.78
2:C:295:SER:O	2:C:298:LYS:HB2	1.82	0.78
2:C:1737:ILE:HD13	2:C:1737:ILE:H	1.48	0.78
2:E:1737:ILE:HD13	2:E:1737:ILE:H	1.48	0.78
2:L:295:SER:O	2:L:298:LYS:HB2	1.82	0.78
2:L:1737:ILE:H	2:L:1737:ILE:HD13	1.48	0.78
2:J:295:SER:O	2:J:298:LYS:HB2	1.82	0.78
2:G:1737:ILE:HG12	2:G:1748:THR:HG21	1.64	0.78
1:F:1558:ASN:OD1	1:F:1623:TYR:HB2	1.84	0.78
2:E:1737:ILE:HG12	2:E:1748:THR:HG21	1.64	0.78
1:K:1558:ASN:OD1	1:K:1623:TYR:HB2	1.83	0.78
2:L:836:TYR:CD1	2:L:845:THR:CG2	2.67	0.78
2:J:1737:ILE:HD13	2:J:1737:ILE:H	1.48	0.78
1:D:1558:ASN:OD1	1:D:1623:TYR:HB2	1.84	0.78
2:E:1737:ILE:CB	2:E:1748:THR:HB	2.09	0.78
2:E:836:TYR:CD1	2:E:845:THR:CG2	2.67	0.77
1:I:1558:ASN:OD1	1:I:1623:TYR:HB2	1.84	0.77
1:A:1491:ARG:HD3	1:A:1750:ILE:HD11	1.06	0.77
2:L:1737:ILE:HG12	2:L:1748:THR:HG21	1.64	0.77
2:H:1737:ILE:HG12	2:H:1748:THR:HG21	1.64	0.77
2:G:1737:ILE:HG12	2:G:1748:THR:CG2	2.14	0.77
1:A:1558:ASN:OD1	1:A:1623:TYR:HB2	1.83	0.77
1:D:848:THR:CG2	1:I:844:LEU:CD2	2.63	0.77
2:L:1737:ILE:HG12	2:L:1748:THR:CG2	2.14	0.77
2:C:836:TYR:CD1	2:C:845:THR:CG2	2.67	0.77
2:E:295:SER:O	2:E:298:LYS:HB2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1737:ILE:HG12	2:J:1748:THR:CG2	2.14	0.77
1:A:844:LEU:CD2	1:F:848:THR:CG2	2.63	0.77
2:H:1737:ILE:HD13	2:H:1737:ILE:H	1.48	0.77
2:C:1737:ILE:HG12	2:C:1748:THR:CG2	2.14	0.77
2:E:1737:ILE:HG12	2:E:1748:THR:CG2	2.14	0.77
2:G:836:TYR:CD1	2:G:845:THR:CG2	2.67	0.77
2:J:836:TYR:CD1	2:J:845:THR:CG2	2.67	0.77
2:H:1737:ILE:HG12	2:H:1748:THR:CG2	2.14	0.76
2:E:1037:SER:CB	2:E:1053:ILE:HG12	2.16	0.76
2:L:1737:ILE:CB	2:L:1748:THR:HB	2.09	0.76
1:B:848:THR:CG2	1:K:844:LEU:CD2	2.63	0.76
2:H:1037:SER:CB	2:H:1053:ILE:HG12	2.16	0.76
1:D:844:LEU:CD2	1:I:848:THR:CG2	2.63	0.76
1:B:844:LEU:CD2	1:K:848:THR:CG2	2.63	0.76
1:D:1487:LEU:CG	1:D:1754:LYS:HE2	2.16	0.76
1:K:1487:LEU:CG	1:K:1754:LYS:HE2	2.16	0.76
1:F:1487:LEU:CG	1:F:1754:LYS:HE2	2.16	0.75
2:H:836:TYR:CD1	2:H:845:THR:CG2	2.67	0.75
1:A:848:THR:CG2	1:F:844:LEU:CD2	2.63	0.75
2:L:1037:SER:CB	2:L:1053:ILE:HG12	2.16	0.75
2:J:1737:ILE:CB	2:J:1748:THR:HB	2.09	0.75
2:G:1037:SER:CB	2:G:1053:ILE:HG12	2.16	0.75
1:D:1561:MET:HA	1:D:1561:MET:CE	2.17	0.75
2:C:1737:ILE:CB	2:C:1748:THR:HB	2.09	0.75
1:B:1487:LEU:HD12	1:B:1754:LYS:CE	2.17	0.75
1:B:1487:LEU:CG	1:B:1754:LYS:HE2	2.16	0.75
1:F:1561:MET:HA	1:F:1561:MET:CE	2.17	0.75
1:I:1561:MET:HA	1:I:1561:MET:CE	2.17	0.75
1:A:1487:LEU:CG	1:A:1754:LYS:HE2	2.16	0.74
1:B:1561:MET:HA	1:B:1561:MET:CE	2.17	0.74
1:A:1561:MET:HA	1:A:1561:MET:CE	2.16	0.74
2:C:1037:SER:CB	2:C:1053:ILE:HG12	2.16	0.74
1:K:1561:MET:HA	1:K:1561:MET:CE	2.16	0.74
2:J:1739:GLU:HB3	2:J:1746:LEU:CD1	2.18	0.74
2:J:1037:SER:CB	2:J:1053:ILE:HG12	2.16	0.74
2:H:246:LEU:CD2	2:H:296:VAL:HG22	2.18	0.74
2:G:246:LEU:CD2	2:G:296:VAL:HG22	2.18	0.74
2:C:1739:GLU:HB3	2:C:1746:LEU:CD1	2.18	0.74
1:D:1487:LEU:HD12	1:D:1754:LYS:CE	2.17	0.74
1:K:1487:LEU:HD12	1:K:1754:LYS:CE	2.17	0.74
2:G:1739:GLU:HB3	2:G:1746:LEU:CD1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:LEU:CD2	2:E:296:VAL:HG22	2.18	0.73
2:L:839:PRO:HA	2:L:844:VAL:HG13	1.70	0.73
2:J:246:LEU:CD2	2:J:296:VAL:HG22	2.18	0.73
1:K:1751:GLU:HG3	1:K:1754:LYS:HZ1	1.53	0.73
1:A:1487:LEU:HD12	1:A:1754:LYS:CE	2.17	0.73
2:G:1036:GLN:CB	2:G:1051:THR:CG2	2.66	0.73
2:L:246:LEU:CD2	2:L:296:VAL:HG22	2.18	0.73
2:C:839:PRO:HA	2:C:844:VAL:HG13	1.70	0.73
1:I:1487:LEU:CG	1:I:1754:LYS:HE2	2.16	0.73
2:C:246:LEU:CD2	2:C:296:VAL:HG22	2.18	0.73
1:F:1487:LEU:HD12	1:F:1754:LYS:CE	2.17	0.73
1:F:1561:MET:HA	1:F:1561:MET:HE2	1.70	0.73
2:H:1739:GLU:HB3	2:H:1746:LEU:CD1	2.18	0.73
2:E:839:PRO:HA	2:E:844:VAL:HG13	1.70	0.73
2:E:1739:GLU:HB3	2:E:1746:LEU:CD1	2.18	0.73
2:H:1036:GLN:CB	2:H:1051:THR:CG2	2.66	0.73
2:E:1736:MET:HB3	2:E:1751:ILE:HD12	1.71	0.73
2:L:1736:MET:HB3	2:L:1751:ILE:HD12	1.71	0.73
2:J:234:ILE:HG23	2:J:238:CYS:HG	1.53	0.73
2:H:739:GLY:CA	2:H:1054:LEU:HD23	2.05	0.72
2:L:1739:GLU:HB3	2:L:1746:LEU:CD1	2.18	0.72
1:I:1487:LEU:HD12	1:I:1754:LYS:CE	2.17	0.72
2:J:1036:GLN:CB	2:J:1051:THR:CG2	2.66	0.72
2:E:1737:ILE:CG1	2:E:1748:THR:HG21	2.19	0.72
2:J:839:PRO:HA	2:J:844:VAL:HG13	1.70	0.72
2:H:1736:MET:HB3	2:H:1751:ILE:HD12	1.71	0.72
2:C:1737:ILE:CG1	2:C:1748:THR:HG21	2.19	0.72
2:E:1036:GLN:CB	2:E:1051:THR:CG2	2.66	0.72
2:L:1170:ILE:HG23	2:L:1174:PHE:HE2	1.55	0.72
1:B:1491:ARG:HD3	1:B:1750:ILE:HD11	1.06	0.72
2:L:1737:ILE:CG1	2:L:1748:THR:HG21	2.19	0.72
2:J:1736:MET:HB3	2:J:1751:ILE:HD12	1.71	0.72
2:G:1735:ALA:C	2:G:1736:MET:HE2	2.07	0.72
2:G:1736:MET:HB3	2:G:1751:ILE:HD12	1.71	0.72
2:C:1170:ILE:HG23	2:C:1174:PHE:HE2	1.55	0.72
2:G:1737:ILE:CG1	2:G:1748:THR:HG21	2.19	0.71
2:C:1738:PHE:HZ	2:C:1749:GLU:HG2	1.55	0.71
2:C:1736:MET:HB3	2:C:1751:ILE:HD12	1.71	0.71
2:G:839:PRO:HA	2:G:844:VAL:HG13	1.70	0.71
2:G:1738:PHE:HZ	2:G:1749:GLU:HG2	1.55	0.71
1:D:340:ARG:HH12	1:D:344:GLN:HE21	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:ARG:HH12	1:F:344:GLN:HE21	1.38	0.71
1:A:877:LEU:HD11	3:A:2001:NDP:H2D	1.73	0.71
1:F:1373:ARG:NH2	1:F:1550:ASP:HB2	2.06	0.71
2:H:1737:ILE:CG1	2:H:1748:THR:HG21	2.19	0.71
2:G:1170:ILE:HG23	2:G:1174:PHE:HE2	1.55	0.71
1:D:1561:MET:HA	1:D:1561:MET:HE2	1.71	0.71
2:L:1036:GLN:CB	2:L:1051:THR:CG2	2.66	0.71
2:J:1737:ILE:CG1	2:J:1748:THR:HG21	2.19	0.71
1:D:1373:ARG:NH2	1:D:1550:ASP:HB2	2.06	0.71
2:H:839:PRO:HA	2:H:844:VAL:HG13	1.70	0.71
2:H:1170:ILE:HG23	2:H:1174:PHE:HE2	1.55	0.71
2:J:836:TYR:HD1	2:J:845:THR:HG21	1.55	0.71
2:C:1036:GLN:CB	2:C:1051:THR:CG2	2.66	0.71
1:A:1373:ARG:NH2	1:A:1550:ASP:HB2	2.06	0.71
1:B:877:LEU:HD11	3:B:2001:NDP:H2D	1.73	0.70
1:D:1751:GLU:HG3	1:D:1754:LYS:HZ1	1.53	0.70
2:E:1170:ILE:HG23	2:E:1174:PHE:HE2	1.55	0.70
2:J:1170:ILE:HG23	2:J:1174:PHE:HE2	1.55	0.70
1:B:1373:ARG:NH2	1:B:1550:ASP:HB2	2.06	0.70
2:H:1738:PHE:HB2	2:H:1987:PRO:CB	2.22	0.70
2:C:836:TYR:HD1	2:C:845:THR:HG21	1.55	0.70
1:I:877:LEU:HD11	3:I:2001:NDP:H2D	1.73	0.70
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.38	0.70
2:G:1738:PHE:HB2	2:G:1987:PRO:CB	2.22	0.70
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.38	0.70
2:E:1738:PHE:HB2	2:E:1987:PRO:CB	2.22	0.70
1:K:340:ARG:HH12	1:K:344:GLN:HE21	1.38	0.70
2:L:836:TYR:HD1	2:L:845:THR:HG21	1.55	0.70
2:L:589:ARG:NH2	2:L:677:GLN:OE1	2.25	0.70
1:K:1373:ARG:NH2	1:K:1550:ASP:HB2	2.06	0.70
1:I:1373:ARG:NH2	1:I:1550:ASP:HB2	2.06	0.70
2:L:1738:PHE:HZ	2:L:1749:GLU:HG2	1.55	0.69
1:I:340:ARG:HH12	1:I:344:GLN:HE21	1.38	0.69
2:J:1738:PHE:HB2	2:J:1987:PRO:CB	2.22	0.69
2:L:838:LYS:O	2:L:844:VAL:CG1	2.41	0.69
2:G:838:LYS:O	2:G:844:VAL:CG1	2.41	0.69
2:C:1738:PHE:HB2	2:C:1987:PRO:CB	2.22	0.69
2:E:838:LYS:O	2:E:844:VAL:CG1	2.41	0.69
2:J:1736:MET:HE2	2:J:1736:MET:HA	1.73	0.69
2:G:589:ARG:NH2	2:G:677:GLN:OE1	2.25	0.69
1:D:877:LEU:HD11	3:D:2001:NDP:H2D	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:836:TYR:HD1	2:E:845:THR:HG21	1.55	0.69
1:K:877:LEU:HD11	3:K:2001:NDP:H2D	1.73	0.69
2:L:1738:PHE:HB2	2:L:1987:PRO:CB	2.22	0.69
2:J:838:LYS:O	2:J:844:VAL:CG1	2.41	0.69
2:J:1735:ALA:C	2:J:1736:MET:HE2	2.05	0.69
2:J:1738:PHE:HZ	2:J:1749:GLU:HG2	1.55	0.69
2:E:739:GLY:CA	2:E:1054:LEU:HD23	2.05	0.69
2:H:589:ARG:NH2	2:H:677:GLN:OE1	2.25	0.69
2:J:589:ARG:NH2	2:J:677:GLN:OE1	2.25	0.69
2:G:676:ILE:O	2:G:676:ILE:HG12	1.93	0.69
2:G:838:LYS:O	2:G:844:VAL:HG12	1.93	0.69
2:E:838:LYS:O	2:E:844:VAL:HG12	1.93	0.69
2:H:1738:PHE:HZ	2:H:1749:GLU:HG2	1.55	0.69
2:C:589:ARG:NH2	2:C:677:GLN:OE1	2.25	0.69
2:H:838:LYS:O	2:H:844:VAL:HG12	1.93	0.69
2:E:589:ARG:NH2	2:E:677:GLN:OE1	2.25	0.69
1:F:1751:GLU:HA	1:F:1754:LYS:CE	2.19	0.69
2:G:1736:MET:HE2	2:G:1736:MET:HA	1.76	0.68
2:J:676:ILE:O	2:J:676:ILE:HG12	1.93	0.68
2:E:1737:ILE:H	2:E:1737:ILE:CD1	2.07	0.68
2:J:838:LYS:O	2:J:844:VAL:HG12	1.93	0.68
2:G:1738:PHE:HB2	2:G:1987:PRO:HB3	1.76	0.68
2:C:838:LYS:O	2:C:844:VAL:CG1	2.41	0.68
1:K:1491:ARG:HD3	1:K:1750:ILE:HD11	1.06	0.68
2:L:1737:ILE:H	2:L:1737:ILE:CD1	2.07	0.68
1:F:877:LEU:HD11	3:F:2001:NDP:H2D	1.73	0.68
2:H:838:LYS:O	2:H:844:VAL:CG1	2.41	0.68
2:H:1170:ILE:HG23	2:H:1174:PHE:CE2	2.28	0.68
1:A:1563:HIS:ND1	1:K:1716:LEU:HD13	2.09	0.68
1:B:1716:LEU:HD13	1:I:1563:HIS:ND1	2.09	0.68
2:C:1170:ILE:HG23	2:C:1174:PHE:CE2	2.28	0.68
1:D:1716:LEU:HD13	1:F:1563:HIS:ND1	2.09	0.68
2:E:1738:PHE:HB2	2:E:1987:PRO:HB3	1.76	0.68
2:H:676:ILE:O	2:H:676:ILE:HG12	1.93	0.68
2:H:1737:ILE:H	2:H:1737:ILE:CD1	2.07	0.68
1:I:1751:GLU:HG3	1:I:1754:LYS:CE	2.24	0.68
1:A:16:GLU:HG3	2:G:2038:ILE:HD11	1.76	0.68
2:E:1170:ILE:HG23	2:E:1174:PHE:CE2	2.28	0.68
2:L:1170:ILE:HG23	2:L:1174:PHE:CE2	2.28	0.68
2:J:1170:ILE:HG23	2:J:1174:PHE:CE2	2.28	0.68
1:B:1751:GLU:HG3	1:B:1754:LYS:CE	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:817:ALA:HB1	2:E:1053:ILE:HD11	1.75	0.68
2:H:1738:PHE:HB2	2:H:1987:PRO:HB3	1.76	0.68
2:J:1738:PHE:HB2	2:J:1987:PRO:HB3	1.76	0.68
1:A:1751:GLU:HG3	1:A:1754:LYS:CE	2.24	0.68
2:C:676:ILE:O	2:C:676:ILE:HG12	1.93	0.68
2:C:1737:ILE:H	2:C:1737:ILE:CD1	2.07	0.68
1:F:16:GLU:HG3	2:H:2038:ILE:HD11	1.76	0.68
1:B:1563:HIS:ND1	1:I:1716:LEU:HD13	2.09	0.68
2:L:817:ALA:HB1	2:L:1053:ILE:HD11	1.75	0.68
1:I:1751:GLU:HA	1:I:1754:LYS:CE	2.19	0.68
3:B:2001:NDP:H51N	3:B:2001:NDP:H2N	1.77	0.67
1:D:1563:HIS:ND1	1:F:1716:LEU:HD13	2.09	0.67
1:D:1751:GLU:HA	1:D:1754:LYS:CE	2.19	0.67
2:E:676:ILE:O	2:E:676:ILE:HG12	1.93	0.67
1:F:1373:ARG:HD2	1:F:1550:ASP:OD2	1.94	0.67
2:H:817:ALA:HB1	2:H:1053:ILE:HD11	1.75	0.67
2:G:817:ALA:HB1	2:G:1053:ILE:HD11	1.75	0.67
2:C:838:LYS:O	2:C:844:VAL:HG12	1.93	0.67
2:E:1738:PHE:HZ	2:E:1749:GLU:HG2	1.55	0.67
2:L:1738:PHE:HB2	2:L:1987:PRO:HB3	1.76	0.67
3:A:2001:NDP:H2N	3:A:2001:NDP:H51N	1.77	0.67
2:C:1738:PHE:HB2	2:C:1987:PRO:HB3	1.76	0.67
1:I:16:GLU:HG3	2:J:2038:ILE:HD11	1.76	0.67
2:G:1737:ILE:H	2:G:1737:ILE:CD1	2.07	0.67
3:K:2001:NDP:H2N	3:K:2001:NDP:H51N	1.77	0.67
2:L:1742:VAL:HB	2:L:1745:LYS:HB2	1.77	0.67
1:K:1751:GLU:HG3	1:K:1754:LYS:CE	2.24	0.67
2:L:676:ILE:HG12	2:L:676:ILE:O	1.93	0.67
3:I:2001:NDP:H2N	3:I:2001:NDP:H51N	1.77	0.67
1:A:1716:LEU:HD13	1:K:1563:HIS:ND1	2.09	0.67
2:G:1170:ILE:HG23	2:G:1174:PHE:CE2	2.28	0.67
2:C:817:ALA:HB1	2:C:1053:ILE:HD11	1.75	0.67
3:D:2001:NDP:H2N	3:D:2001:NDP:H51N	1.77	0.67
1:K:16:GLU:HG3	2:L:2038:ILE:HD11	1.76	0.67
1:F:1751:GLU:HG3	1:F:1754:LYS:CE	2.24	0.67
1:I:1373:ARG:HD2	1:I:1550:ASP:OD2	1.94	0.67
2:C:1742:VAL:HB	2:C:1745:LYS:HB2	1.76	0.67
2:L:739:GLY:CA	2:L:1054:LEU:HD23	2.05	0.67
2:L:838:LYS:O	2:L:844:VAL:HG12	1.93	0.67
2:L:1036:GLN:HB2	2:L:1051:THR:CG2	2.26	0.67
3:F:2001:NDP:H2N	3:F:2001:NDP:H51N	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1742:VAL:O	2:C:1745:LYS:N	2.29	0.66
2:E:1742:VAL:O	2:E:1745:LYS:N	2.29	0.66
2:H:124:LYS:HG2	2:H:179:THR:HA	1.77	0.66
2:G:124:LYS:HG2	2:G:179:THR:HA	1.77	0.66
2:G:1036:GLN:HB2	2:G:1051:THR:CG2	2.26	0.66
2:J:1737:ILE:H	2:J:1737:ILE:CD1	2.07	0.66
1:B:1373:ARG:HD2	1:B:1550:ASP:OD2	1.94	0.66
2:J:1036:GLN:HB2	2:J:1051:THR:CG2	2.25	0.66
2:C:124:LYS:HG2	2:C:179:THR:HA	1.77	0.66
1:D:1751:GLU:HG3	1:D:1754:LYS:CE	2.24	0.66
1:K:1373:ARG:HD2	1:K:1550:ASP:OD2	1.94	0.66
2:J:817:ALA:HB1	2:J:1053:ILE:HD11	1.75	0.66
1:D:16:GLU:HG3	2:E:2038:ILE:HD11	1.76	0.66
1:D:1373:ARG:HD2	1:D:1550:ASP:OD2	1.94	0.66
2:L:234:ILE:HG23	2:L:238:CYS:HG	1.56	0.66
2:H:1742:VAL:HB	2:H:1745:LYS:HB2	1.76	0.66
1:A:1373:ARG:HD2	1:A:1550:ASP:OD2	1.94	0.66
2:L:124:LYS:HG2	2:L:179:THR:HA	1.77	0.66
2:E:1036:GLN:HB2	2:E:1051:THR:CG2	2.25	0.66
2:J:1742:VAL:O	2:J:1745:LYS:N	2.29	0.66
2:G:1742:VAL:O	2:G:1745:LYS:N	2.29	0.66
2:E:124:LYS:HG2	2:E:179:THR:HA	1.77	0.66
2:G:1742:VAL:HB	2:G:1745:LYS:HB2	1.77	0.66
2:C:1736:MET:HE2	2:C:1736:MET:HA	1.77	0.65
1:K:32:GLN:HE22	1:K:57:ALA:HA	1.61	0.65
2:E:1742:VAL:HB	2:E:1745:LYS:HB2	1.76	0.65
2:L:1742:VAL:O	2:L:1745:LYS:N	2.29	0.65
1:F:1751:GLU:HG3	1:F:1754:LYS:HZ1	1.57	0.65
2:J:1742:VAL:HB	2:J:1745:LYS:HB2	1.76	0.65
1:K:1751:GLU:HA	1:K:1754:LYS:CE	2.19	0.65
2:H:836:TYR:HD1	2:H:845:THR:HG21	1.55	0.65
2:H:1742:VAL:O	2:H:1745:LYS:N	2.29	0.65
2:J:124:LYS:HG2	2:J:179:THR:HA	1.77	0.65
1:B:16:GLU:HG3	2:C:2038:ILE:HD11	1.76	0.65
2:C:1036:GLN:HB2	2:C:1051:THR:CG2	2.25	0.65
2:E:7:ARG:NH2	2:E:24:THR:O	2.30	0.65
1:D:1491:ARG:HD3	1:D:1750:ILE:HD11	1.06	0.65
1:A:1541:PHE:CE1	1:A:1557:ILE:HG13	2.31	0.65
1:F:1541:PHE:CE1	1:F:1557:ILE:HG13	2.31	0.65
1:B:987:ASN:HD21	2:C:993:GLN:HE22	1.45	0.65
1:D:32:GLN:HE22	1:D:57:ALA:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1036:GLN:HB2	2:H:1051:THR:CG2	2.25	0.65
2:H:1736:MET:HE2	2:H:1736:MET:HA	1.79	0.65
2:J:7:ARG:NH2	2:J:24:THR:O	2.30	0.65
1:A:1542:HIS:HB3	1:A:1553:GLU:OE1	1.97	0.65
1:B:32:GLN:HE22	1:B:57:ALA:HA	1.61	0.65
1:A:1751:GLU:HA	1:A:1754:LYS:CE	2.19	0.65
1:D:1542:HIS:HB3	1:D:1553:GLU:OE1	1.97	0.65
1:F:32:GLN:HE22	1:F:57:ALA:HA	1.61	0.65
1:F:1552:ASN:O	1:F:1556:THR:HG22	1.97	0.65
1:B:1552:ASN:O	1:B:1556:THR:HG22	1.97	0.65
1:F:1542:HIS:HB3	1:F:1553:GLU:OE1	1.97	0.65
1:I:987:ASN:HD21	2:J:993:GLN:HE22	1.45	0.65
1:A:1552:ASN:O	1:A:1556:THR:HG22	1.97	0.64
2:L:7:ARG:NH2	2:L:24:THR:O	2.30	0.64
2:H:7:ARG:NH2	2:H:24:THR:O	2.30	0.64
2:C:1174:PHE:HE1	2:C:1197:LEU:HB2	1.63	0.64
2:H:1036:GLN:HB2	2:H:1051:THR:HG23	1.80	0.64
2:H:1735:ALA:C	2:H:1736:MET:HE2	2.11	0.64
1:I:1542:HIS:HB3	1:I:1553:GLU:OE1	1.97	0.64
2:J:1174:PHE:HE1	2:J:1197:LEU:HB2	1.63	0.64
2:G:7:ARG:NH2	2:G:24:THR:O	2.30	0.64
1:K:987:ASN:HD21	2:L:993:GLN:HE22	1.45	0.64
2:L:1174:PHE:HE1	2:L:1197:LEU:HB2	1.63	0.64
2:L:1736:MET:HE2	2:L:1736:MET:HA	1.79	0.64
1:I:32:GLN:HE22	1:I:57:ALA:HA	1.61	0.64
1:K:1552:ASN:O	1:K:1556:THR:HG22	1.97	0.64
2:J:1037:SER:OG	2:J:1053:ILE:HG12	1.98	0.64
2:C:7:ARG:NH2	2:C:24:THR:O	2.30	0.64
1:D:1541:PHE:CE1	1:D:1557:ILE:HG13	2.31	0.64
2:G:739:GLY:CA	2:G:1054:LEU:HD23	2.05	0.64
1:B:1542:HIS:HB3	1:B:1553:GLU:OE1	1.97	0.64
2:E:1174:PHE:HE1	2:E:1197:LEU:HB2	1.63	0.64
2:J:647:PHE:O	2:J:677:GLN:N	2.31	0.64
1:A:32:GLN:HE22	1:A:57:ALA:HA	1.61	0.64
2:G:647:PHE:O	2:G:677:GLN:N	2.31	0.64
2:E:1036:GLN:HB2	2:E:1051:THR:HG23	1.80	0.64
2:H:647:PHE:O	2:H:677:GLN:N	2.31	0.64
2:H:848:SER:HB3	2:H:854:ILE:CD1	2.28	0.64
2:H:1747:LYS:HG3	2:H:1747:LYS:O	1.98	0.64
2:J:739:GLY:CA	2:J:1054:LEU:HD23	2.05	0.64
1:A:987:ASN:HD21	2:G:993:GLN:HE22	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:848:SER:HB3	2:E:854:ILE:CD1	2.28	0.64
1:I:1541:PHE:CE1	1:I:1557:ILE:HG13	2.31	0.64
1:D:1552:ASN:O	1:D:1556:THR:HG22	1.97	0.64
2:E:647:PHE:O	2:E:677:GLN:N	2.31	0.64
1:F:1491:ARG:HD3	1:F:1750:ILE:HD11	1.06	0.64
1:A:844:LEU:HG	1:F:844:LEU:HG	1.80	0.63
2:G:848:SER:HB3	2:G:854:ILE:CD1	2.28	0.63
2:C:1037:SER:OG	2:C:1053:ILE:HG12	1.98	0.63
2:E:1747:LYS:HG3	2:E:1747:LYS:O	1.98	0.63
2:G:836:TYR:HD1	2:G:845:THR:CG2	2.10	0.63
2:G:1174:PHE:HE1	2:G:1197:LEU:HB2	1.63	0.63
2:E:1037:SER:OG	2:E:1053:ILE:HG12	1.98	0.63
2:H:1737:ILE:CG1	2:H:1748:THR:CG2	2.76	0.63
1:K:687:SER:HB2	3:K:2001:NDP:O1N	1.99	0.63
1:A:1491:ARG:CA	1:A:1750:ILE:HD13	2.29	0.63
2:G:1747:LYS:HG3	2:G:1747:LYS:O	1.98	0.63
2:C:647:PHE:O	2:C:677:GLN:N	2.31	0.63
2:E:1737:ILE:CG1	2:E:1748:THR:CG2	2.76	0.63
2:L:848:SER:HB3	2:L:854:ILE:CD1	2.28	0.63
2:C:739:GLY:CA	2:C:1054:LEU:HD23	2.05	0.63
2:C:1747:LYS:HG3	2:C:1747:LYS:O	1.98	0.63
2:E:1742:VAL:O	2:E:1744:GLY:N	2.32	0.63
1:K:1542:HIS:HB3	1:K:1553:GLU:OE1	1.97	0.63
1:B:1751:GLU:HA	1:B:1754:LYS:CE	2.19	0.63
2:C:848:SER:HB3	2:C:854:ILE:CD1	2.28	0.63
1:I:687:SER:HB2	3:I:2001:NDP:O1N	1.99	0.63
1:I:1552:ASN:O	1:I:1556:THR:HG22	1.97	0.63
2:J:1747:LYS:HG3	2:J:1747:LYS:O	1.98	0.63
2:G:1742:VAL:O	2:G:1744:GLY:N	2.32	0.63
1:D:1685:TYR:OH	2:E:993:GLN:NE2	2.32	0.63
2:E:1736:MET:HE2	2:E:1736:MET:HA	1.81	0.63
2:E:1739:GLU:CB	2:E:1746:LEU:HD11	2.27	0.63
2:L:1037:SER:OG	2:L:1053:ILE:HG12	1.98	0.63
2:H:1174:PHE:HE1	2:H:1197:LEU:HB2	1.63	0.63
2:J:848:SER:HB3	2:J:854:ILE:CD1	2.28	0.63
2:J:1742:VAL:O	2:J:1744:GLY:N	2.32	0.63
1:A:32:GLN:HE21	1:A:57:ALA:HB2	1.64	0.63
1:A:1751:GLU:HG3	1:A:1754:LYS:HZ1	1.59	0.63
1:K:1541:PHE:CE1	1:K:1557:ILE:HG13	2.31	0.63
2:H:1742:VAL:O	2:H:1744:GLY:N	2.32	0.63
2:G:1037:SER:HB2	2:G:1053:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1037:SER:OG	2:G:1053:ILE:HG12	1.98	0.62
1:D:844:LEU:HG	1:I:844:LEU:HG	1.80	0.62
2:L:647:PHE:O	2:L:677:GLN:N	2.31	0.62
1:F:987:ASN:HD21	2:H:993:GLN:HE22	1.45	0.62
1:A:687:SER:HB2	3:A:2001:NDP:O1N	1.99	0.62
2:H:1037:SER:OG	2:H:1053:ILE:HG12	1.98	0.62
2:H:1739:GLU:CB	2:H:1746:LEU:HD11	2.27	0.62
2:G:817:ALA:HB1	2:G:1053:ILE:CD1	2.29	0.62
2:C:1737:ILE:CG1	2:C:1748:THR:CG2	2.76	0.62
2:C:1742:VAL:O	2:C:1744:GLY:N	2.32	0.62
1:D:987:ASN:HD21	2:E:993:GLN:HE22	1.45	0.62
1:K:32:GLN:HE21	1:K:57:ALA:HB2	1.64	0.62
2:L:1737:ILE:CG1	2:L:1748:THR:CG2	2.76	0.62
2:L:1739:GLU:CB	2:L:1746:LEU:HD11	2.27	0.62
2:E:817:ALA:HB1	2:E:1053:ILE:CD1	2.30	0.62
2:E:1037:SER:HB2	2:E:1053:ILE:HG12	1.81	0.62
2:L:1747:LYS:O	2:L:1747:LYS:HG3	1.98	0.62
1:I:32:GLN:HE21	1:I:57:ALA:HB2	1.64	0.62
2:G:1737:ILE:CG1	2:G:1748:THR:CG2	2.76	0.62
1:B:32:GLN:HE21	1:B:57:ALA:HB2	1.64	0.62
2:C:836:TYR:HD1	2:C:845:THR:CG2	2.10	0.62
1:D:32:GLN:HE21	1:D:57:ALA:HB2	1.64	0.62
1:D:687:SER:HB2	3:D:2001:NDP:O1N	1.99	0.62
1:K:1751:GLU:O	1:K:1754:LYS:HG2	2.00	0.62
2:L:1742:VAL:O	2:L:1744:GLY:N	2.32	0.62
2:H:1037:SER:HB2	2:H:1053:ILE:HG12	1.81	0.62
1:B:687:SER:HB2	3:B:2001:NDP:O1N	1.99	0.62
2:C:1576:PRO:HD2	2:C:1579:ILE:HD11	1.82	0.62
1:F:28:TRP:HA	1:F:31:THR:HB	1.82	0.62
2:J:1037:SER:HB2	2:J:1053:ILE:HG12	1.81	0.62
1:A:28:TRP:HA	1:A:31:THR:HB	1.82	0.62
1:B:844:LEU:HG	1:K:844:LEU:HG	1.80	0.62
1:B:1751:GLU:O	1:B:1754:LYS:HG2	2.00	0.62
1:D:1229:THR:OG1	1:D:1687:PHE:CD1	2.53	0.62
1:K:1685:TYR:OH	2:L:993:GLN:NE2	2.32	0.62
2:L:1036:GLN:HB2	2:L:1051:THR:HG23	1.80	0.62
2:J:817:ALA:HB1	2:J:1053:ILE:CD1	2.30	0.62
1:B:1229:THR:OG1	1:B:1687:PHE:CD1	2.53	0.62
2:E:836:TYR:HD1	2:E:845:THR:CG2	2.10	0.62
1:K:1301:PRO:HG3	1:K:1314:ILE:HD12	1.82	0.62
1:F:32:GLN:HE21	1:F:57:ALA:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1685:TYR:OH	2:H:993:GLN:NE2	2.32	0.62
2:G:1156:CYS:O	2:G:1168:ASN:ND2	2.33	0.62
1:B:1301:PRO:HG3	1:B:1314:ILE:HD12	1.82	0.62
1:B:1685:TYR:OH	2:C:993:GLN:NE2	2.32	0.62
2:E:1156:CYS:O	2:E:1168:ASN:ND2	2.33	0.62
2:L:1576:PRO:HD2	2:L:1579:ILE:HD11	1.82	0.62
2:H:817:ALA:HB1	2:H:1053:ILE:CD1	2.29	0.62
2:J:1737:ILE:CG1	2:J:1748:THR:CG2	2.76	0.62
1:B:1541:PHE:CE1	1:B:1557:ILE:HG13	2.31	0.61
2:C:1739:GLU:CB	2:C:1746:LEU:HD11	2.27	0.61
2:C:1036:GLN:HB2	2:C:1051:THR:HG23	1.80	0.61
1:D:1751:GLU:O	1:D:1754:LYS:HG2	2.00	0.61
2:L:1037:SER:HB2	2:L:1053:ILE:HG12	1.81	0.61
1:I:1751:GLU:O	1:I:1754:LYS:HG2	2.00	0.61
2:L:817:ALA:HB1	2:L:1053:ILE:CD1	2.29	0.61
2:L:1735:ALA:C	2:L:1736:MET:HE2	2.11	0.61
2:H:1156:CYS:O	2:H:1168:ASN:ND2	2.33	0.61
1:I:1685:TYR:OH	2:J:993:GLN:NE2	2.32	0.61
2:C:817:ALA:HB1	2:C:1053:ILE:CD1	2.29	0.61
2:E:1889:VAL:HG13	2:E:1977:HIS:HB2	1.82	0.61
1:F:687:SER:HB2	3:F:2001:NDP:O1N	1.99	0.61
1:F:1491:ARG:CA	1:F:1750:ILE:HD13	2.29	0.61
2:H:836:TYR:HD1	2:H:845:THR:CG2	2.10	0.61
1:A:1751:GLU:O	1:A:1754:LYS:HG2	2.00	0.61
1:F:1751:GLU:O	1:F:1754:LYS:HG2	2.00	0.61
2:J:836:TYR:HD1	2:J:845:THR:CG2	2.10	0.61
2:J:1576:PRO:HD2	2:J:1579:ILE:HD11	1.82	0.61
1:A:1229:THR:OG1	1:A:1687:PHE:CD1	2.53	0.61
2:C:1156:CYS:O	2:C:1168:ASN:ND2	2.33	0.61
1:D:1301:PRO:HG3	1:D:1314:ILE:HD12	1.82	0.61
1:A:1685:TYR:OH	2:G:993:GLN:NE2	2.32	0.61
1:B:442:ARG:NH1	1:B:726:GLY:O	2.34	0.61
1:D:1682:LYS:HE2	2:E:992:GLU:O	2.01	0.61
1:K:1229:THR:OG1	1:K:1687:PHE:CD1	2.53	0.61
2:H:1576:PRO:HD2	2:H:1579:ILE:HD11	1.82	0.61
1:A:1301:PRO:HG3	1:A:1314:ILE:HD12	1.82	0.61
2:G:1889:VAL:HG13	2:G:1977:HIS:HB2	1.82	0.61
1:I:28:TRP:HA	1:I:31:THR:HB	1.82	0.61
1:D:28:TRP:HA	1:D:31:THR:HB	1.82	0.60
2:E:1735:ALA:C	2:E:1736:MET:HE2	2.14	0.60
2:L:1889:VAL:HG13	2:L:1977:HIS:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1301:PRO:HG3	1:F:1314:ILE:HD12	1.82	0.60
1:F:1682:LYS:HE2	2:H:992:GLU:O	2.01	0.60
2:G:1739:GLU:CB	2:G:1746:LEU:HD11	2.27	0.60
1:B:28:TRP:HA	1:B:31:THR:HB	1.82	0.60
1:K:1682:LYS:HE2	2:L:992:GLU:O	2.01	0.60
1:I:442:ARG:NH1	1:I:726:GLY:O	2.34	0.60
2:J:1156:CYS:O	2:J:1168:ASN:ND2	2.33	0.60
2:G:1576:PRO:HD2	2:G:1579:ILE:HD11	1.82	0.60
1:B:1491:ARG:CA	1:B:1750:ILE:HD13	2.29	0.60
2:C:1037:SER:HB2	2:C:1053:ILE:HG12	1.81	0.60
1:K:442:ARG:NH1	1:K:726:GLY:O	2.34	0.60
2:L:1156:CYS:O	2:L:1168:ASN:ND2	2.33	0.60
1:I:1301:PRO:HG3	1:I:1314:ILE:HD12	1.82	0.60
2:E:1736:MET:HE3	2:E:1736:MET:N	2.16	0.60
1:K:28:TRP:HA	1:K:31:THR:HB	1.82	0.60
1:I:1682:LYS:HE2	2:J:992:GLU:O	2.01	0.60
2:J:1036:GLN:HB2	2:J:1051:THR:HG23	1.80	0.60
1:A:442:ARG:NH1	1:A:726:GLY:O	2.34	0.60
1:B:1323:LYS:NZ	1:I:1313:ASP:OD1	2.35	0.60
1:K:1491:ARG:CA	1:K:1750:ILE:HD13	2.29	0.60
2:J:1889:VAL:HG13	2:J:1977:HIS:HB2	1.82	0.60
1:B:1749:THR:HB	1:B:1874:ASP:HB3	1.83	0.60
1:F:442:ARG:NH1	1:F:726:GLY:O	2.34	0.60
2:H:1350:LEU:HD11	2:H:1410:PHE:HB3	1.84	0.60
1:I:1749:THR:HB	1:I:1874:ASP:HB3	1.83	0.60
1:A:1313:ASP:OD1	1:K:1323:LYS:NZ	2.35	0.60
1:B:1682:LYS:HE2	2:C:992:GLU:O	2.01	0.60
1:D:442:ARG:NH1	1:D:726:GLY:O	2.34	0.60
2:E:1576:PRO:HD2	2:E:1579:ILE:HD11	1.82	0.60
2:L:584:SER:HB3	2:L:591:PRO:HG3	1.84	0.60
1:A:1487:LEU:HA	1:A:1754:LYS:HD3	1.84	0.60
2:C:1123:ASP:OD1	2:C:1188:ASN:ND2	2.35	0.60
1:I:1487:LEU:HA	1:I:1754:LYS:HD3	1.84	0.60
1:A:479:ASN:ND2	1:A:613:VAL:O	2.35	0.60
2:G:584:SER:HB3	2:G:591:PRO:HG3	1.84	0.60
1:B:1313:ASP:OD1	1:I:1323:LYS:NZ	2.35	0.60
2:C:295:SER:O	2:C:298:LYS:N	2.35	0.60
1:D:1313:ASP:OD1	1:F:1323:LYS:NZ	2.35	0.60
1:D:1487:LEU:HA	1:D:1754:LYS:HD3	1.84	0.60
1:K:479:ASN:ND2	1:K:613:VAL:O	2.35	0.60
1:F:1229:THR:OG1	1:F:1687:PHE:CD1	2.53	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1889:VAL:HG13	2:H:1977:HIS:HB2	1.82	0.60
1:A:1305:CYS:HB2	1:A:1645:GLY:HA2	1.84	0.60
1:B:1487:LEU:HA	1:B:1754:LYS:HD3	1.84	0.60
2:C:584:SER:HB3	2:C:591:PRO:HG3	1.84	0.60
1:D:1323:LYS:NZ	1:F:1313:ASP:OD1	2.35	0.60
1:D:1491:ARG:CA	1:D:1750:ILE:HD13	2.29	0.60
2:L:1741:ILE:O	2:L:1741:ILE:HG22	2.02	0.60
1:F:479:ASN:ND2	1:F:613:VAL:O	2.35	0.60
1:I:982:ILE:HG23	2:J:956:GLU:HG2	1.84	0.60
1:I:1229:THR:OG1	1:I:1687:PHE:CD1	2.53	0.60
2:J:1123:ASP:OD1	2:J:1188:ASN:ND2	2.35	0.60
1:B:479:ASN:ND2	1:B:613:VAL:O	2.35	0.59
2:C:1475:LYS:HB2	2:C:1481:SER:HB2	1.84	0.59
2:J:584:SER:HB3	2:J:591:PRO:HG3	1.84	0.59
1:A:1682:LYS:HE2	2:G:992:GLU:O	2.01	0.59
2:C:1889:VAL:HG13	2:C:1977:HIS:HB2	1.82	0.59
2:E:584:SER:HB3	2:E:591:PRO:HG3	1.84	0.59
2:J:1739:GLU:CB	2:J:1746:LEU:HD11	2.27	0.59
1:A:1323:LYS:NZ	1:K:1313:ASP:OD1	2.35	0.59
2:G:1741:ILE:O	2:G:1741:ILE:HG22	2.02	0.59
2:C:1741:ILE:O	2:C:1741:ILE:HG22	2.02	0.59
1:K:1749:THR:HB	1:K:1874:ASP:HB3	1.83	0.59
1:A:1749:THR:HB	1:A:1874:ASP:HB3	1.83	0.59
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.84	0.59
1:F:1305:CYS:HB2	1:F:1645:GLY:HA2	1.84	0.59
2:H:584:SER:HB3	2:H:591:PRO:HG3	1.84	0.59
2:H:1741:ILE:HG22	2:H:1741:ILE:O	2.02	0.59
2:J:1741:ILE:HG22	2:J:1741:ILE:O	2.02	0.59
1:B:894:ARG:NH1	1:B:895:THR:O	2.36	0.59
1:D:27:ARG:HH11	2:E:2015:THR:HA	1.68	0.59
1:D:894:ARG:NH1	1:D:895:THR:O	2.36	0.59
2:E:1350:LEU:HD11	2:E:1410:PHE:HB3	1.84	0.59
2:E:1741:ILE:HG22	2:E:1741:ILE:O	2.02	0.59
2:L:836:TYR:HD1	2:L:845:THR:CG2	2.10	0.59
1:I:479:ASN:ND2	1:I:613:VAL:O	2.35	0.59
1:I:894:ARG:NH1	1:I:895:THR:O	2.36	0.59
1:I:1305:CYS:HB2	1:I:1645:GLY:HA2	1.84	0.59
2:G:295:SER:O	2:G:298:LYS:N	2.35	0.59
1:B:1305:CYS:HB2	1:B:1645:GLY:HA2	1.84	0.59
2:J:295:SER:O	2:J:298:LYS:N	2.35	0.59
2:J:1475:LYS:HB2	2:J:1481:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG21	1:A:266:LEU:HB3	1.85	0.59
1:A:982:ILE:HG23	2:G:956:GLU:HG2	1.84	0.59
1:D:479:ASN:ND2	1:D:613:VAL:O	2.35	0.59
1:D:1749:THR:HB	1:D:1874:ASP:HB3	1.83	0.59
2:L:1475:LYS:HB2	2:L:1481:SER:HB2	1.84	0.59
1:A:894:ARG:NH1	1:A:895:THR:O	2.36	0.59
2:C:1350:LEU:HD11	2:C:1410:PHE:HB3	1.84	0.59
1:K:894:ARG:NH1	1:K:895:THR:O	2.36	0.59
2:L:1123:ASP:OD1	2:L:1188:ASN:ND2	2.35	0.59
2:H:835:THR:HG22	2:H:844:VAL:HA	1.85	0.59
2:G:670:ARG:HG2	2:G:699:GLY:H	1.68	0.59
2:C:326:ASP:O	2:C:330:ASN:ND2	2.36	0.59
2:L:1350:LEU:HD11	2:L:1410:PHE:HB3	1.84	0.59
1:D:153:VAL:HG21	1:D:266:LEU:HB3	1.85	0.59
1:D:1487:LEU:HG	1:D:1754:LYS:HE2	1.84	0.59
1:K:982:ILE:HG23	2:L:956:GLU:HG2	1.84	0.59
1:K:1487:LEU:HG	1:K:1754:LYS:HE2	1.84	0.59
2:L:670:ARG:HG2	2:L:699:GLY:H	1.68	0.59
2:H:295:SER:O	2:H:298:LYS:N	2.35	0.59
2:G:1123:ASP:OD1	2:G:1188:ASN:ND2	2.35	0.58
2:C:670:ARG:HG2	2:C:699:GLY:H	1.68	0.58
1:K:153:VAL:HG21	1:K:266:LEU:HB3	1.85	0.58
1:F:1487:LEU:HA	1:F:1754:LYS:HD3	1.84	0.58
2:H:326:ASP:O	2:H:330:ASN:ND2	2.36	0.58
2:J:835:THR:HG22	2:J:844:VAL:HA	1.85	0.58
1:B:36:LEU:O	1:B:76:ARG:NH2	2.36	0.58
2:L:326:ASP:O	2:L:330:ASN:ND2	2.36	0.58
2:C:835:THR:HG22	2:C:844:VAL:HA	1.85	0.58
1:F:894:ARG:NH1	1:F:895:THR:O	2.36	0.58
1:F:1195:ALA:HB1	1:F:1200:ILE:HD12	1.85	0.58
2:H:261:GLY:N	2:H:287:ASP:O	2.37	0.58
2:G:1786:LYS:NZ	2:G:1816:ALA:O	2.35	0.58
1:B:982:ILE:HG23	2:C:956:GLU:HG2	1.84	0.58
1:D:1413:LYS:NZ	1:F:1708:ASP:OD1	2.37	0.58
1:K:1487:LEU:HA	1:K:1754:LYS:HD3	1.84	0.58
2:L:1786:LYS:NZ	2:L:1816:ALA:O	2.35	0.58
1:F:1749:THR:HB	1:F:1874:ASP:HB3	1.83	0.58
2:H:1123:ASP:OD1	2:H:1188:ASN:ND2	2.35	0.58
2:H:1475:LYS:HB2	2:H:1481:SER:HB2	1.84	0.58
1:I:27:ARG:HH11	2:J:2015:THR:HA	1.68	0.58
1:A:27:ARG:HH11	2:G:2015:THR:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1475:LYS:HB2	2:G:1481:SER:HB2	1.84	0.58
1:B:1487:LEU:HG	1:B:1754:LYS:HE2	1.84	0.58
1:D:982:ILE:HG23	2:E:956:GLU:HG2	1.84	0.58
1:D:1708:ASP:OD1	1:F:1413:LYS:NZ	2.37	0.58
2:L:261:GLY:N	2:L:287:ASP:O	2.37	0.58
2:J:864:LEU:HD23	2:J:899:PHE:HB2	1.86	0.58
1:B:27:ARG:HH11	2:C:2015:THR:HA	1.68	0.58
2:C:836:TYR:CE1	2:C:845:THR:HG21	2.37	0.58
2:C:864:LEU:HD23	2:C:899:PHE:HB2	1.86	0.58
2:E:1123:ASP:OD1	2:E:1188:ASN:ND2	2.35	0.58
2:L:864:LEU:HD23	2:L:899:PHE:HB2	1.86	0.58
2:H:670:ARG:HG2	2:H:699:GLY:H	1.68	0.58
1:I:153:VAL:HG21	1:I:266:LEU:HB3	1.85	0.58
2:G:261:GLY:N	2:G:287:ASP:O	2.37	0.58
2:G:326:ASP:O	2:G:330:ASN:ND2	2.36	0.58
2:G:836:TYR:CE1	2:G:845:THR:HG21	2.37	0.58
2:E:835:THR:HG22	2:E:844:VAL:HA	1.85	0.58
1:K:27:ARG:HH11	2:L:2015:THR:HA	1.68	0.58
1:F:982:ILE:HG23	2:H:956:GLU:HG2	1.84	0.58
2:H:1742:VAL:O	2:H:1743:ASP:C	2.42	0.58
1:I:1491:ARG:CA	1:I:1750:ILE:HD13	2.29	0.58
1:I:1749:THR:HB	1:I:1874:ASP:CG	2.24	0.58
1:A:1413:LYS:NZ	1:K:1708:ASP:OD1	2.37	0.58
1:A:1487:LEU:HG	1:A:1754:LYS:HE2	1.84	0.58
1:A:1749:THR:HB	1:A:1874:ASP:CG	2.24	0.58
2:G:864:LEU:HD23	2:G:899:PHE:HB2	1.86	0.58
2:G:1737:ILE:HD13	2:G:1737:ILE:O	2.04	0.58
1:B:1413:LYS:NZ	1:I:1708:ASP:OD1	2.37	0.58
1:D:260:ARG:HH12	1:D:300:VAL:HG21	1.69	0.58
1:K:260:ARG:HH12	1:K:300:VAL:HG21	1.69	0.58
1:K:1305:CYS:HB2	1:K:1645:GLY:HA2	1.84	0.58
2:L:1736:MET:HE3	2:L:1736:MET:N	2.18	0.58
1:F:27:ARG:HH11	2:H:2015:THR:HA	1.68	0.58
1:F:260:ARG:HH12	1:F:300:VAL:HG21	1.69	0.58
1:F:1487:LEU:HG	1:F:1754:LYS:HE2	1.84	0.58
2:J:1350:LEU:HD11	2:J:1410:PHE:HB3	1.84	0.58
1:A:1708:ASP:OD1	1:K:1413:LYS:NZ	2.37	0.58
1:D:202:GLU:HG2	1:D:203:GLU:HG3	1.86	0.58
2:E:295:SER:O	2:E:298:LYS:N	2.35	0.58
2:E:864:LEU:HD23	2:E:899:PHE:HB2	1.86	0.58
2:L:295:SER:O	2:L:298:LYS:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1036:GLN:HB3	2:G:1051:THR:CG2	2.24	0.58
2:E:326:ASP:O	2:E:330:ASN:ND2	2.36	0.58
2:E:670:ARG:HG2	2:E:699:GLY:H	1.68	0.58
2:E:1475:LYS:HB2	2:E:1481:SER:HB2	1.84	0.58
1:K:1195:ALA:HB1	1:K:1200:ILE:HD12	1.85	0.58
1:F:153:VAL:HG21	1:F:266:LEU:HB3	1.85	0.58
1:F:202:GLU:HG2	1:F:203:GLU:HG3	1.86	0.58
1:I:838:MET:CA	1:I:841:GLU:OE1	2.52	0.58
2:C:261:GLY:N	2:C:287:ASP:O	2.37	0.57
2:E:261:GLY:N	2:E:287:ASP:O	2.37	0.57
2:E:1786:LYS:NZ	2:E:1816:ALA:O	2.35	0.57
1:F:36:LEU:O	1:F:76:ARG:NH2	2.36	0.57
2:H:864:LEU:HD23	2:H:899:PHE:HB2	1.86	0.57
1:I:1487:LEU:HG	1:I:1754:LYS:HE2	1.84	0.57
1:A:260:ARG:HH12	1:A:300:VAL:HG21	1.69	0.57
2:G:1590:ARG:NH1	2:G:1594:GLU:OE1	2.38	0.57
1:B:153:VAL:HG21	1:B:266:LEU:HB3	1.85	0.57
1:B:1195:ALA:HB1	1:B:1200:ILE:HD12	1.85	0.57
1:B:1533:ILE:O	1:B:1566:ARG:NH1	2.37	0.57
1:D:1305:CYS:HB2	1:D:1645:GLY:HA2	1.84	0.57
2:E:1742:VAL:O	2:E:1743:ASP:C	2.42	0.57
1:F:1749:THR:HB	1:F:1874:ASP:CG	2.24	0.57
2:H:1036:GLN:HB3	2:H:1051:THR:CG2	2.24	0.57
1:A:202:GLU:HG2	1:A:203:GLU:HG3	1.86	0.57
2:J:261:GLY:N	2:J:287:ASP:O	2.37	0.57
2:J:1590:ARG:NH1	2:J:1594:GLU:OE1	2.38	0.57
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	1.85	0.57
2:G:835:THR:HG22	2:G:844:VAL:HA	1.85	0.57
1:B:1708:ASP:OD1	1:I:1413:LYS:NZ	2.37	0.57
1:D:32:GLN:NE2	1:D:57:ALA:HB2	2.19	0.57
2:H:1590:ARG:NH1	2:H:1594:GLU:OE1	2.37	0.57
2:J:1737:ILE:HD13	2:J:1737:ILE:O	2.04	0.57
2:J:1786:LYS:NZ	2:J:1816:ALA:O	2.35	0.57
2:G:1742:VAL:O	2:G:1743:ASP:C	2.42	0.57
1:D:36:LEU:O	1:D:76:ARG:NH2	2.36	0.57
2:E:1737:ILE:HD13	2:E:1737:ILE:O	2.04	0.57
1:K:1533:ILE:O	1:K:1566:ARG:NH1	2.37	0.57
1:F:32:GLN:NE2	1:F:57:ALA:HB2	2.19	0.57
2:H:190:PHE:HZ	2:H:297:ARG:HD2	1.69	0.57
2:J:326:ASP:O	2:J:330:ASN:ND2	2.36	0.57
1:D:1019:ILE:HG13	1:D:1316:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1195:ALA:HB1	1:D:1200:ILE:HD12	1.85	0.57
1:D:1749:THR:HB	1:D:1874:ASP:CG	2.24	0.57
2:L:1351:VAL:HG21	2:L:1413:ARG:HH21	1.70	0.57
1:I:260:ARG:HH12	1:I:300:VAL:HG21	1.69	0.57
1:I:1195:ALA:HB1	1:I:1200:ILE:HD12	1.85	0.57
1:A:36:LEU:O	1:A:76:ARG:NH2	2.36	0.57
2:G:190:PHE:HZ	2:G:297:ARG:HD2	1.69	0.57
1:B:260:ARG:HH12	1:B:300:VAL:HG21	1.69	0.57
1:B:838:MET:CA	1:B:841:GLU:OE1	2.52	0.57
1:D:1010:GLU:O	1:D:1449:LYS:NZ	2.38	0.57
2:E:1351:VAL:HG21	2:E:1413:ARG:HH21	1.70	0.57
2:L:835:THR:HG22	2:L:844:VAL:HA	1.85	0.57
2:L:1737:ILE:HD13	2:L:1737:ILE:O	2.04	0.57
2:L:1742:VAL:O	2:L:1743:ASP:C	2.42	0.57
1:A:1533:ILE:O	1:A:1566:ARG:NH1	2.37	0.57
2:C:1351:VAL:HG21	2:C:1413:ARG:HH21	1.70	0.57
2:H:619:LEU:HB3	2:H:649:ILE:HG12	1.87	0.57
2:H:1737:ILE:HD13	2:H:1737:ILE:O	2.04	0.57
2:C:859:THR:HB	2:C:1049:GLN:HA	1.87	0.57
1:D:41:THR:O	1:D:76:ARG:NH1	2.38	0.57
1:K:838:MET:CA	1:K:841:GLU:OE1	2.52	0.57
2:H:1736:MET:HE3	2:H:1736:MET:N	2.18	0.57
2:J:670:ARG:HG2	2:J:699:GLY:H	1.68	0.57
2:J:1036:GLN:HB3	2:J:1051:THR:CG2	2.24	0.57
2:G:859:THR:HB	2:G:1049:GLN:HA	1.87	0.57
2:C:1737:ILE:HD13	2:C:1737:ILE:O	2.04	0.57
1:K:202:GLU:HG2	1:K:203:GLU:HG3	1.86	0.57
1:K:1019:ILE:HG13	1:K:1316:VAL:HG13	1.87	0.57
1:K:1749:THR:HB	1:K:1874:ASP:CG	2.24	0.57
2:H:1736:MET:CE	2:H:1736:MET:HA	2.35	0.57
1:I:41:THR:O	1:I:76:ARG:NH1	2.38	0.57
1:A:764:ASP:OD1	1:A:810:LYS:NZ	2.38	0.56
2:G:619:LEU:HB3	2:G:649:ILE:HG12	1.87	0.56
2:C:1590:ARG:NH1	2:C:1594:GLU:OE1	2.37	0.56
2:C:1742:VAL:O	2:C:1743:ASP:C	2.42	0.56
1:D:764:ASP:OD1	1:D:810:LYS:NZ	2.38	0.56
1:F:1010:GLU:O	1:F:1449:LYS:NZ	2.38	0.56
2:J:1911:THR:O	2:J:1915:ASN:ND2	2.38	0.56
2:G:1911:THR:O	2:G:1915:ASN:ND2	2.38	0.56
1:B:32:GLN:NE2	1:B:57:ALA:HB2	2.19	0.56
1:B:234:SER:OG	1:K:1123:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1749:THR:HB	1:B:1874:ASP:CG	2.24	0.56
1:D:234:SER:OG	1:I:1123:GLN:NE2	2.38	0.56
1:D:1533:ILE:O	1:D:1566:ARG:NH1	2.37	0.56
2:E:1590:ARG:NH1	2:E:1594:GLU:OE1	2.38	0.56
1:K:41:THR:O	1:K:76:ARG:NH1	2.38	0.56
1:K:764:ASP:OD1	1:K:810:LYS:NZ	2.38	0.56
2:L:96:LEU:HD11	2:L:101:ILE:HG22	1.88	0.56
1:F:1019:ILE:HG13	1:F:1316:VAL:HG13	1.87	0.56
2:H:1911:THR:O	2:H:1915:ASN:ND2	2.38	0.56
1:A:41:THR:O	1:A:76:ARG:NH1	2.38	0.56
1:A:1106:ILE:HA	1:A:1188:GLN:HE22	1.70	0.56
1:A:1123:GLN:NE2	1:F:234:SER:OG	2.38	0.56
2:G:84:LEU:HD12	2:G:133:ALA:HB2	1.88	0.56
2:G:96:LEU:HD11	2:G:101:ILE:HG22	1.88	0.56
2:G:1736:MET:CE	2:G:1736:MET:HA	2.35	0.56
1:K:32:GLN:NE2	1:K:57:ALA:HB2	2.19	0.56
1:K:1010:GLU:O	1:K:1449:LYS:NZ	2.38	0.56
1:F:764:ASP:OD1	1:F:810:LYS:NZ	2.38	0.56
1:F:1106:ILE:HA	1:F:1188:GLN:HE22	1.70	0.56
1:F:1533:ILE:O	1:F:1566:ARG:NH1	2.37	0.56
2:H:84:LEU:HD12	2:H:133:ALA:HB2	1.88	0.56
2:H:1351:VAL:HG21	2:H:1413:ARG:HH21	1.70	0.56
1:I:202:GLU:HG2	1:I:203:GLU:HG3	1.86	0.56
1:I:1533:ILE:O	1:I:1566:ARG:NH1	2.37	0.56
2:J:619:LEU:HB3	2:J:649:ILE:HG12	1.87	0.56
2:J:1742:VAL:O	2:J:1743:ASP:C	2.42	0.56
1:B:764:ASP:OD1	1:B:810:LYS:NZ	2.38	0.56
2:E:619:LEU:HB3	2:E:649:ILE:HG12	1.87	0.56
1:I:32:GLN:HE22	1:I:57:ALA:CA	2.18	0.56
2:J:1351:VAL:HG21	2:J:1413:ARG:HH21	1.70	0.56
2:C:190:PHE:HZ	2:C:297:ARG:HD2	1.69	0.56
2:C:619:LEU:HB3	2:C:649:ILE:HG12	1.87	0.56
1:A:32:GLN:NE2	1:A:57:ALA:HB2	2.19	0.56
1:B:32:GLN:HE22	1:B:57:ALA:CA	2.19	0.56
1:B:41:THR:O	1:B:76:ARG:NH1	2.38	0.56
1:B:1019:ILE:HG13	1:B:1316:VAL:HG13	1.87	0.56
1:B:1491:ARG:HB2	1:B:1750:ILE:HG21	1.87	0.56
2:C:96:LEU:HD11	2:C:101:ILE:HG22	1.87	0.56
1:D:1123:GLN:NE2	1:I:234:SER:OG	2.38	0.56
1:K:1491:ARG:HB2	1:K:1750:ILE:HG21	1.87	0.56
2:L:1590:ARG:NH1	2:L:1594:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HG2	1:B:203:GLU:HG3	1.86	0.56
1:D:1106:ILE:HA	1:D:1188:GLN:HE22	1.70	0.56
2:E:1036:GLN:HB3	2:E:1051:THR:CG2	2.24	0.56
2:E:1736:MET:CE	2:E:1736:MET:HA	2.35	0.56
1:K:36:LEU:O	1:K:76:ARG:NH2	2.36	0.56
2:L:1736:MET:CE	2:L:1736:MET:HA	2.35	0.56
2:H:96:LEU:HD11	2:H:101:ILE:HG22	1.87	0.56
2:H:859:THR:HB	2:H:1049:GLN:HA	1.87	0.56
2:J:836:TYR:CE1	2:J:845:THR:HG21	2.37	0.56
1:A:844:LEU:O	1:F:844:LEU:HD23	2.06	0.56
1:B:1123:GLN:NE2	1:K:234:SER:OG	2.38	0.56
2:C:1911:THR:O	2:C:1915:ASN:ND2	2.38	0.56
2:E:190:PHE:HZ	2:E:297:ARG:HD2	1.69	0.56
2:E:1911:THR:O	2:E:1915:ASN:ND2	2.38	0.56
1:I:764:ASP:OD1	1:I:810:LYS:NZ	2.38	0.56
1:A:844:LEU:HD23	1:F:844:LEU:O	2.06	0.56
2:G:1736:MET:HB3	2:G:1751:ILE:CD1	2.36	0.56
2:C:1736:MET:CE	2:C:1736:MET:HA	2.35	0.56
2:C:1786:LYS:NZ	2:C:1816:ALA:O	2.35	0.56
1:I:32:GLN:NE2	1:I:57:ALA:HB2	2.19	0.56
2:J:190:PHE:HZ	2:J:297:ARG:HD2	1.69	0.56
1:B:844:LEU:HD23	1:K:844:LEU:O	2.06	0.56
1:K:836:ASP:HB3	1:K:839:TYR:HB3	1.88	0.56
1:K:1106:ILE:HA	1:K:1188:GLN:HE22	1.70	0.56
2:L:1911:THR:O	2:L:1915:ASN:ND2	2.38	0.56
1:A:1010:GLU:O	1:A:1449:LYS:NZ	2.38	0.55
1:A:1019:ILE:HG13	1:A:1316:VAL:HG13	1.87	0.55
2:G:1351:VAL:HG21	2:G:1413:ARG:HH21	1.70	0.55
1:B:1106:ILE:HA	1:B:1188:GLN:HE22	1.70	0.55
1:D:708:SER:HB3	3:D:2001:NDP:O2X	2.07	0.55
1:K:1471:LYS:HA	1:K:1761:LYS:HE2	1.89	0.55
2:L:619:LEU:HB3	2:L:649:ILE:HG12	1.87	0.55
2:L:836:TYR:CE1	2:L:845:THR:HG21	2.37	0.55
2:L:859:THR:HB	2:L:1049:GLN:HA	1.87	0.55
1:A:234:SER:OG	1:F:1123:GLN:NE2	2.38	0.55
1:A:838:MET:CA	1:A:841:GLU:OE1	2.52	0.55
2:C:461:ASP:OD2	2:C:478:ARG:NH2	2.39	0.55
2:E:84:LEU:HD12	2:E:133:ALA:HB2	1.88	0.55
1:K:32:GLN:NE2	1:K:57:ALA:HA	2.22	0.55
2:L:1737:ILE:HD13	2:L:1737:ILE:N	2.19	0.55
1:A:32:GLN:HE22	1:A:57:ALA:CA	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:GLU:O	1:B:1449:LYS:NZ	2.38	0.55
2:C:1736:MET:HB3	2:C:1751:ILE:CD1	2.36	0.55
2:L:84:LEU:HD12	2:L:133:ALA:HB2	1.88	0.55
2:J:859:THR:HB	2:J:1049:GLN:HA	1.87	0.55
1:B:836:ASP:HB3	1:B:839:TYR:HB3	1.88	0.55
2:C:84:LEU:HD12	2:C:133:ALA:HB2	1.88	0.55
2:C:1736:MET:HE3	2:C:1736:MET:N	2.21	0.55
1:D:32:GLN:HE22	1:D:57:ALA:CA	2.18	0.55
1:D:32:GLN:NE2	1:D:57:ALA:HA	2.22	0.55
1:D:1471:LYS:HA	1:D:1761:LYS:HE2	1.89	0.55
2:E:96:LEU:HD11	2:E:101:ILE:HG22	1.88	0.55
1:F:32:GLN:HE22	1:F:57:ALA:CA	2.19	0.55
1:F:838:MET:CA	1:F:841:GLU:OE1	2.52	0.55
1:I:1010:GLU:O	1:I:1449:LYS:NZ	2.38	0.55
1:I:1019:ILE:HG13	1:I:1316:VAL:HG13	1.87	0.55
2:J:84:LEU:HD12	2:J:133:ALA:HB2	1.88	0.55
1:B:708:SER:HB3	3:B:2001:NDP:O2X	2.07	0.55
1:B:844:LEU:O	1:K:844:LEU:HD23	2.06	0.55
1:D:353:ASP:OD2	1:D:359:ARG:NH2	2.40	0.55
2:E:836:TYR:CE1	2:E:845:THR:HG21	2.37	0.55
2:E:1202:GLN:HE22	2:E:1555:ARG:HH21	1.54	0.55
2:E:1928:GLN:HE22	2:E:1933:LEU:HD23	1.71	0.55
1:F:41:THR:O	1:F:76:ARG:NH1	2.38	0.55
2:H:13:HIS:HB3	2:H:60:LEU:HD11	1.89	0.55
2:H:461:ASP:OD2	2:H:478:ARG:NH2	2.39	0.55
2:G:13:HIS:HB3	2:G:60:LEU:HD11	1.89	0.55
1:D:844:LEU:HD23	1:I:844:LEU:O	2.06	0.55
1:K:32:GLN:HE22	1:K:57:ALA:CA	2.19	0.55
1:K:63:ASN:ND2	2:L:1896:GLN:OE1	2.40	0.55
2:L:461:ASP:OD2	2:L:478:ARG:NH2	2.39	0.55
2:J:1736:MET:CE	2:J:1736:MET:HA	2.35	0.55
1:D:1491:ARG:HB2	1:D:1750:ILE:HG21	1.87	0.55
2:L:13:HIS:HB3	2:L:60:LEU:HD11	1.89	0.55
2:L:190:PHE:HZ	2:L:297:ARG:HD2	1.69	0.55
1:F:708:SER:HB3	3:F:2001:NDP:O2X	2.07	0.55
1:I:1491:ARG:HB2	1:I:1750:ILE:HG21	1.87	0.55
2:J:461:ASP:OD2	2:J:478:ARG:NH2	2.39	0.55
2:J:1738:PHE:HB2	2:J:1987:PRO:HB2	1.89	0.55
1:B:1471:LYS:HA	1:B:1761:LYS:HE2	1.89	0.55
1:D:844:LEU:O	1:I:844:LEU:HD23	2.06	0.55
2:L:1482:SER:HA	2:L:1509:GLY:HA2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1736:MET:HB3	2:L:1751:ILE:CD1	2.36	0.55
2:L:1928:GLN:HE22	2:L:1933:LEU:HD23	1.71	0.55
1:F:353:ASP:OD2	1:F:359:ARG:NH2	2.40	0.55
2:H:1739:GLU:CB	2:H:1746:LEU:CD1	2.85	0.55
1:I:708:SER:HB3	3:I:2001:NDP:O2X	2.07	0.55
1:I:1106:ILE:HA	1:I:1188:GLN:HE22	1.70	0.55
1:I:1219:VAL:HG22	1:I:1384:ILE:HD13	1.89	0.55
1:A:353:ASP:OD2	1:A:359:ARG:NH2	2.40	0.55
2:G:461:ASP:OD2	2:G:478:ARG:NH2	2.39	0.55
1:B:63:ASN:ND2	2:C:1896:GLN:OE1	2.40	0.55
1:B:877:LEU:HD12	3:B:2001:NDP:H2D	1.88	0.55
1:D:838:MET:CA	1:D:841:GLU:OE1	2.52	0.55
2:E:859:THR:HB	2:E:1049:GLN:HA	1.87	0.55
1:F:836:ASP:HB3	1:F:839:TYR:HB3	1.88	0.55
2:J:96:LEU:HD11	2:J:101:ILE:HG22	1.88	0.55
1:A:257:PRO:HD2	1:A:260:ARG:HD2	1.89	0.55
1:D:836:ASP:HB3	1:D:839:TYR:HB3	1.88	0.55
1:K:877:LEU:HD12	3:K:2001:NDP:H2D	1.88	0.55
2:H:1786:LYS:NZ	2:H:1816:ALA:O	2.35	0.55
2:J:13:HIS:HB3	2:J:60:LEU:HD11	1.89	0.55
1:A:32:GLN:NE2	1:A:57:ALA:HA	2.22	0.54
1:D:257:PRO:HD2	1:D:260:ARG:HD2	1.89	0.54
2:E:1482:SER:HA	2:E:1509:GLY:HA2	1.89	0.54
2:E:1739:GLU:CB	2:E:1746:LEU:CD1	2.84	0.54
2:L:366:VAL:HG12	2:L:381:GLY:HA3	1.89	0.54
2:L:1202:GLN:HE22	2:L:1555:ARG:HH21	1.54	0.54
1:F:1471:LYS:HA	1:F:1761:LYS:HE2	1.89	0.54
1:I:36:LEU:O	1:I:76:ARG:NH2	2.36	0.54
1:A:708:SER:HB3	3:A:2001:NDP:O2X	2.07	0.54
1:A:1219:VAL:HG22	1:A:1384:ILE:HD13	1.89	0.54
1:A:1491:ARG:HB2	1:A:1750:ILE:HG21	1.87	0.54
2:C:1736:MET:CE	2:C:1736:MET:CA	2.86	0.54
1:D:63:ASN:ND2	2:E:1896:GLN:OE1	2.40	0.54
2:E:1736:MET:HB3	2:E:1751:ILE:CD1	2.36	0.54
2:L:1736:MET:CE	2:L:1736:MET:CA	2.86	0.54
1:F:1491:ARG:HB2	1:F:1750:ILE:HG21	1.87	0.54
2:H:1202:GLN:HE22	2:H:1555:ARG:HH21	1.54	0.54
1:A:836:ASP:HB3	1:A:839:TYR:HB3	1.88	0.54
2:C:1482:SER:HA	2:C:1509:GLY:HA2	1.89	0.54
2:C:1928:GLN:HE22	2:C:1933:LEU:HD23	1.71	0.54
1:I:1471:LYS:HA	1:I:1761:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:HIS:HB3	2:C:60:LEU:HD11	1.89	0.54
1:D:1219:VAL:HG22	1:D:1384:ILE:HD13	1.89	0.54
2:E:366:VAL:HG12	2:E:381:GLY:HA3	1.89	0.54
1:K:1219:VAL:HG22	1:K:1384:ILE:HD13	1.89	0.54
1:I:1561:MET:CE	1:I:1561:MET:CA	2.85	0.54
2:G:260:PRO:HD3	2:G:289:TRP:CH2	2.43	0.54
1:B:353:ASP:OD2	1:B:359:ARG:NH2	2.40	0.54
1:K:708:SER:HB3	3:K:2001:NDP:O2X	2.07	0.54
1:F:1219:VAL:HG22	1:F:1384:ILE:HD13	1.89	0.54
1:I:836:ASP:HB3	1:I:839:TYR:HB3	1.88	0.54
2:J:260:PRO:HD3	2:J:289:TRP:CH2	2.43	0.54
2:J:758:ARG:NH2	2:J:763:ILE:O	2.41	0.54
2:J:1736:MET:CE	2:J:1736:MET:CA	2.86	0.54
2:C:286:THR:HG23	2:C:286:THR:O	2.08	0.54
2:L:758:ARG:NH2	2:L:763:ILE:O	2.41	0.54
1:F:257:PRO:HD2	1:F:260:ARG:HD2	1.89	0.54
2:H:836:TYR:CE1	2:H:845:THR:HG21	2.37	0.54
1:I:32:GLN:NE2	1:I:57:ALA:HA	2.22	0.54
1:I:257:PRO:HD2	1:I:260:ARG:HD2	1.89	0.54
1:I:353:ASP:OD2	1:I:359:ARG:NH2	2.40	0.54
2:J:1202:GLN:HE22	2:J:1555:ARG:HH21	1.54	0.54
2:J:1736:MET:HB3	2:J:1751:ILE:CD1	2.36	0.54
1:A:1471:LYS:HA	1:A:1761:LYS:HE2	1.89	0.54
2:C:1738:PHE:HB2	2:C:1987:PRO:HB2	1.89	0.54
1:K:1561:MET:CE	1:K:1561:MET:CA	2.85	0.54
1:F:32:GLN:NE2	1:F:57:ALA:HA	2.22	0.54
1:I:63:ASN:ND2	2:J:1896:GLN:OE1	2.40	0.54
2:J:1383:ASN:ND2	2:J:1418:ASP:O	2.41	0.54
2:G:1383:ASN:ND2	2:G:1418:ASP:O	2.41	0.54
2:C:366:VAL:HG12	2:C:381:GLY:HA3	1.89	0.54
2:C:1383:ASN:ND2	2:C:1418:ASP:O	2.41	0.54
2:E:758:ARG:NH2	2:E:763:ILE:O	2.41	0.54
2:L:1739:GLU:CB	2:L:1746:LEU:CD1	2.84	0.54
2:H:1736:MET:CE	2:H:1736:MET:CA	2.86	0.54
2:J:1928:GLN:HE22	2:J:1933:LEU:HD23	1.71	0.54
2:G:1738:PHE:HB2	2:G:1987:PRO:HB2	1.89	0.54
2:G:1739:GLU:CB	2:G:1746:LEU:CD1	2.84	0.54
2:C:758:ARG:NH2	2:C:763:ILE:O	2.41	0.54
1:K:353:ASP:OD2	1:K:359:ARG:NH2	2.40	0.54
2:L:286:THR:HG23	2:L:286:THR:O	2.08	0.54
2:H:1383:ASN:ND2	2:H:1418:ASP:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1482:SER:HA	2:G:1509:GLY:HA2	1.89	0.54
1:B:257:PRO:HD2	1:B:260:ARG:HD2	1.89	0.54
2:E:461:ASP:OD2	2:E:478:ARG:NH2	2.39	0.54
1:F:63:ASN:ND2	2:H:1896:GLN:OE1	2.40	0.54
2:J:1032:ASP:OD2	2:J:1035:TRP:NE1	2.41	0.54
2:G:1202:GLN:HE22	2:G:1555:ARG:HH21	1.54	0.53
2:E:13:HIS:HB3	2:E:60:LEU:HD11	1.89	0.53
2:H:758:ARG:NH2	2:H:763:ILE:O	2.41	0.53
1:A:63:ASN:ND2	2:G:1896:GLN:OE1	2.40	0.53
1:A:1751:GLU:HG3	1:A:1754:LYS:HZ2	1.71	0.53
1:B:1219:VAL:HG22	1:B:1384:ILE:HD13	1.89	0.53
2:C:734:GLY:H	2:C:769:SER:HB3	1.74	0.53
2:C:1177:SER:OG	2:C:1180:MET:SD	2.63	0.53
1:D:1561:MET:CE	1:D:1561:MET:CA	2.85	0.53
2:H:1736:MET:HB3	2:H:1751:ILE:CD1	2.36	0.53
2:G:1928:GLN:HE22	2:G:1933:LEU:HD23	1.71	0.53
1:B:739:GLN:O	1:B:798:ASN:ND2	2.42	0.53
2:E:1736:MET:CE	2:E:1736:MET:CA	2.86	0.53
2:H:734:GLY:H	2:H:769:SER:HB3	1.74	0.53
2:J:366:VAL:HG12	2:J:381:GLY:HA3	1.89	0.53
2:G:758:ARG:NH2	2:G:763:ILE:O	2.41	0.53
2:G:1736:MET:CE	2:G:1736:MET:CA	2.86	0.53
1:F:1561:MET:CE	1:F:1561:MET:CA	2.86	0.53
1:I:236:LYS:HG2	1:I:273:PRO:HD2	1.90	0.53
1:I:877:LEU:HD12	3:I:2001:NDP:H2D	1.88	0.53
2:J:286:THR:HG23	2:J:286:THR:O	2.08	0.53
2:J:734:GLY:H	2:J:769:SER:HB3	1.74	0.53
2:G:602:VAL:HG21	2:G:623:GLY:HA3	1.91	0.53
2:G:734:GLY:H	2:G:769:SER:HB3	1.74	0.53
2:C:1202:GLN:HE22	2:C:1555:ARG:HH21	1.54	0.53
1:D:1019:ILE:HG21	1:D:1316:VAL:HG22	1.90	0.53
1:K:257:PRO:HD2	1:K:260:ARG:HD2	1.89	0.53
1:K:739:GLN:O	1:K:798:ASN:ND2	2.42	0.53
2:H:1928:GLN:HE22	2:H:1933:LEU:HD23	1.71	0.53
2:G:286:THR:HG23	2:G:286:THR:O	2.08	0.53
2:G:650:ASN:OD1	2:G:680:THR:HG22	2.09	0.53
2:L:1383:ASN:ND2	2:L:1418:ASP:O	2.41	0.53
2:H:366:VAL:HG12	2:H:381:GLY:HA3	1.89	0.53
2:H:1695:ASP:OD1	2:H:1706:ILE:N	2.42	0.53
2:J:1482:SER:HA	2:J:1509:GLY:HA2	1.89	0.53
1:A:1544:THR:HG21	1:A:1546:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:PRO:HD3	2:C:289:TRP:CH2	2.43	0.53
1:D:877:LEU:HD12	3:D:2001:NDP:H2D	1.88	0.53
2:E:260:PRO:HD3	2:E:289:TRP:CH2	2.43	0.53
2:E:650:ASN:OD1	2:E:680:THR:HG22	2.09	0.53
2:E:1383:ASN:ND2	2:E:1418:ASP:O	2.41	0.53
1:K:1544:THR:HG21	1:K:1546:THR:OG1	2.09	0.53
2:H:602:VAL:HG21	2:H:623:GLY:HA3	1.91	0.53
2:H:650:ASN:OD1	2:H:680:THR:HG22	2.09	0.53
2:G:366:VAL:HG12	2:G:381:GLY:HA3	1.89	0.53
2:G:774:ALA:HB2	2:G:1077:ILE:HA	1.91	0.53
2:E:1738:PHE:HB2	2:E:1987:PRO:HB2	1.89	0.53
2:L:602:VAL:HG21	2:L:623:GLY:HA3	1.91	0.53
1:F:1019:ILE:HG21	1:F:1316:VAL:HG22	1.90	0.53
2:H:286:THR:HG23	2:H:286:THR:O	2.08	0.53
1:I:1544:THR:HG21	1:I:1546:THR:OG1	2.09	0.53
1:A:774:ILE:HG22	3:A:2001:NDP:N7A	2.24	0.53
1:A:1544:THR:CG2	1:A:1546:THR:OG1	2.57	0.53
1:F:1544:THR:CG2	1:F:1546:THR:OG1	2.57	0.53
2:H:260:PRO:HD3	2:H:289:TRP:CH2	2.43	0.53
2:H:774:ALA:HB2	2:H:1077:ILE:HA	1.91	0.53
1:I:1544:THR:CG2	1:I:1546:THR:OG1	2.57	0.53
2:J:1739:GLU:CB	2:J:1746:LEU:CD1	2.84	0.53
1:A:236:LYS:HG2	1:A:273:PRO:HD2	1.90	0.53
1:A:1545:SER:O	1:A:1545:SER:OG	2.27	0.53
1:B:32:GLN:NE2	1:B:57:ALA:HA	2.22	0.53
2:C:1032:ASP:OD2	2:C:1035:TRP:NE1	2.41	0.53
1:K:236:LYS:HG2	1:K:273:PRO:HD2	1.90	0.53
2:L:260:PRO:HD3	2:L:289:TRP:CH2	2.43	0.53
1:F:1545:SER:O	1:F:1545:SER:OG	2.27	0.53
2:J:602:VAL:HG21	2:J:623:GLY:HA3	1.91	0.53
2:J:1695:ASP:OD1	2:J:1706:ILE:N	2.42	0.53
1:A:413:LEU:HD12	1:A:439:ILE:HG21	1.91	0.52
1:A:697:LEU:HD21	1:A:732:LEU:HD23	1.91	0.52
1:A:1561:MET:CE	1:A:1561:MET:CA	2.85	0.52
2:G:1736:MET:HE3	2:G:1736:MET:N	2.23	0.52
1:B:1544:THR:HG21	1:B:1546:THR:OG1	2.09	0.52
2:C:1739:GLU:CB	2:C:1746:LEU:CD1	2.85	0.52
1:D:774:ILE:HG22	3:D:2001:NDP:N7A	2.24	0.52
2:E:286:THR:HG23	2:E:286:THR:O	2.08	0.52
2:E:734:GLY:H	2:E:769:SER:HB3	1.74	0.52
1:F:413:LEU:HD12	1:F:439:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:650:ASN:OD1	2:J:680:THR:HG22	2.09	0.52
2:G:297:ARG:HG2	2:G:297:ARG:HH11	1.74	0.52
2:L:649:ILE:O	2:L:679:LEU:HD22	2.09	0.52
2:L:650:ASN:OD1	2:L:680:THR:HG22	2.09	0.52
1:F:774:ILE:HG22	3:F:2001:NDP:N7A	2.24	0.52
2:H:1309:GLU:O	2:H:1317:ARG:NH1	2.42	0.52
2:H:1482:SER:HA	2:H:1509:GLY:HA2	1.89	0.52
1:I:739:GLN:O	1:I:798:ASN:ND2	2.42	0.52
2:J:297:ARG:HG2	2:J:297:ARG:HH11	1.74	0.52
2:G:1695:ASP:OD1	2:G:1706:ILE:N	2.42	0.52
1:B:774:ILE:HG22	3:B:2001:NDP:N7A	2.24	0.52
1:B:1019:ILE:HG21	1:B:1316:VAL:HG22	1.90	0.52
1:B:1561:MET:CE	1:B:1561:MET:CA	2.86	0.52
2:C:1309:GLU:O	2:C:1317:ARG:NH1	2.42	0.52
1:D:1749:THR:HB	1:D:1874:ASP:CB	2.39	0.52
2:E:1695:ASP:OD1	2:E:1706:ILE:N	2.42	0.52
1:K:1749:THR:HB	1:K:1874:ASP:CB	2.39	0.52
2:L:1738:PHE:HB2	2:L:1987:PRO:HB2	1.89	0.52
2:G:1490:LYS:HB3	2:G:1498:THR:HB	1.92	0.52
1:B:236:LYS:HG2	1:B:273:PRO:HD2	1.90	0.52
2:C:602:VAL:HG21	2:C:623:GLY:HA3	1.91	0.52
1:D:236:LYS:HG2	1:D:273:PRO:HD2	1.90	0.52
1:K:1544:THR:CG2	1:K:1546:THR:OG1	2.57	0.52
2:L:734:GLY:H	2:L:769:SER:HB3	1.74	0.52
1:F:1749:THR:HB	1:F:1874:ASP:CB	2.39	0.52
2:H:1490:LYS:HB3	2:H:1498:THR:HB	1.92	0.52
2:E:649:ILE:O	2:E:679:LEU:HD22	2.09	0.52
2:L:847:ARG:HG2	2:L:869:ASP:OD2	2.03	0.52
2:L:1736:MET:CE	2:L:1736:MET:N	2.73	0.52
1:F:1544:THR:HG21	1:F:1546:THR:OG1	2.09	0.52
2:H:1738:PHE:HB2	2:H:1987:PRO:HB2	1.89	0.52
1:I:206:LEU:HD23	1:I:209:LEU:HD12	1.92	0.52
1:A:1749:THR:HB	1:A:1874:ASP:CB	2.39	0.52
2:E:1177:SER:OG	2:E:1180:MET:SD	2.63	0.52
2:E:1490:LYS:HB3	2:E:1498:THR:HB	1.92	0.52
2:E:1736:MET:CE	2:E:1736:MET:N	2.73	0.52
1:K:1019:ILE:HG21	1:K:1316:VAL:HG22	1.90	0.52
1:A:1491:ARG:NH1	1:A:1744:TYR:O	2.43	0.52
2:G:649:ILE:O	2:G:679:LEU:HD22	2.09	0.52
2:G:1736:MET:CE	2:G:1736:MET:N	2.73	0.52
1:D:1544:THR:CG2	1:D:1546:THR:OG1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1544:THR:HG21	1:D:1546:THR:OG1	2.09	0.52
2:E:847:ARG:HG2	2:E:869:ASP:OD2	2.03	0.52
2:E:1032:ASP:OD2	2:E:1035:TRP:NE1	2.41	0.52
1:F:236:LYS:HG2	1:F:273:PRO:HD2	1.90	0.52
1:F:471:THR:HG22	1:F:610:THR:HG21	1.92	0.52
1:I:1491:ARG:NH1	1:I:1744:TYR:O	2.43	0.52
2:J:217:GLU:OE2	2:J:221:ASN:ND2	2.37	0.52
1:A:206:LEU:HD23	1:A:209:LEU:HD12	1.92	0.52
1:B:1544:THR:CG2	1:B:1546:THR:OG1	2.57	0.52
2:C:649:ILE:O	2:C:679:LEU:HD22	2.09	0.52
2:C:1737:ILE:CD1	2:C:1737:ILE:N	2.73	0.52
1:K:1744:TYR:C	1:K:1747:ALA:CB	2.75	0.52
2:L:774:ALA:HB2	2:L:1077:ILE:HA	1.91	0.52
1:I:774:ILE:HG22	3:I:2001:NDP:N7A	2.24	0.52
2:J:1490:LYS:HB3	2:J:1498:THR:HB	1.92	0.52
1:B:1749:THR:HB	1:B:1874:ASP:CB	2.39	0.52
2:C:1695:ASP:OD1	2:C:1706:ILE:N	2.42	0.52
2:C:1736:MET:CE	2:C:1736:MET:N	2.73	0.52
1:D:90:TYR:OH	2:E:1659:GLN:NE2	2.43	0.52
1:D:697:LEU:HD21	1:D:732:LEU:HD23	1.91	0.52
1:D:844:LEU:HD23	1:I:848:THR:HG23	1.92	0.52
1:D:881:ASN:HB3	1:D:944:ARG:HH22	1.75	0.52
1:K:774:ILE:HG22	3:K:2001:NDP:N7A	2.24	0.52
2:L:1695:ASP:OD1	2:L:1706:ILE:N	2.42	0.52
1:F:881:ASN:HB3	1:F:944:ARG:HH22	1.75	0.52
2:H:1032:ASP:OD2	2:H:1035:TRP:NE1	2.41	0.52
2:H:1189:THR:O	2:H:1193:THR:OG1	2.28	0.52
2:H:1736:MET:CE	2:H:1736:MET:N	2.73	0.52
1:A:29:ILE:HD11	2:G:1898:TYR:HE1	1.75	0.52
1:A:877:LEU:HD12	3:A:2001:NDP:H2D	1.88	0.52
1:A:1019:ILE:HG21	1:A:1316:VAL:HG22	1.90	0.52
2:G:1737:ILE:HD13	2:G:1737:ILE:N	2.19	0.52
1:B:206:LEU:HD23	1:B:209:LEU:HD12	1.92	0.52
2:C:650:ASN:OD1	2:C:680:THR:HG22	2.09	0.52
1:D:29:ILE:HD11	2:E:1898:TYR:HE1	1.75	0.52
1:D:1064:ASN:ND2	1:D:1073:THR:OG1	2.43	0.52
2:E:1738:PHE:HB3	2:E:1833:TYR:OH	2.10	0.52
1:K:29:ILE:HD11	2:L:1898:TYR:HE1	1.75	0.52
1:K:271:ASN:HB2	1:K:290:MET:HE1	1.92	0.52
1:F:206:LEU:HD23	1:F:209:LEU:HD12	1.92	0.52
1:F:739:GLN:O	1:F:798:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1064:ASN:ND2	1:F:1073:THR:OG1	2.43	0.52
2:J:1736:MET:CE	2:J:1736:MET:N	2.73	0.52
1:A:739:GLN:O	1:A:798:ASN:ND2	2.42	0.51
1:B:413:LEU:HD12	1:B:439:ILE:HG21	1.91	0.51
1:B:505:LYS:HA	1:B:954:ARG:HD3	1.92	0.51
2:C:297:ARG:HG2	2:C:297:ARG:HH11	1.74	0.51
1:D:471:THR:HG22	1:D:610:THR:HG21	1.92	0.51
1:K:90:TYR:OH	2:L:1659:GLN:NE2	2.43	0.51
1:K:505:LYS:HA	1:K:954:ARG:HD3	1.92	0.51
1:K:697:LEU:HD21	1:K:732:LEU:HD23	1.91	0.51
2:L:1032:ASP:OD2	2:L:1035:TRP:NE1	2.41	0.51
1:F:877:LEU:HD12	3:F:2001:NDP:H2D	1.88	0.51
1:I:505:LYS:HA	1:I:954:ARG:HD3	1.92	0.51
2:J:649:ILE:O	2:J:679:LEU:HD22	2.09	0.51
1:A:801:ARG:NH2	1:F:789:GLU:OE1	2.43	0.51
1:B:789:GLU:OE1	1:K:801:ARG:NH2	2.43	0.51
1:B:848:THR:HG23	1:K:844:LEU:HD23	1.92	0.51
1:B:1491:ARG:NH1	1:B:1744:TYR:O	2.43	0.51
2:C:774:ALA:HB2	2:C:1077:ILE:HA	1.91	0.51
2:C:1037:SER:OG	2:C:1053:ILE:CD1	2.59	0.51
2:C:1037:SER:HB2	2:C:1053:ILE:CG1	2.40	0.51
1:F:90:TYR:OH	2:H:1659:GLN:NE2	2.43	0.51
2:H:297:ARG:HG2	2:H:297:ARG:HH11	1.74	0.51
1:I:1019:ILE:HG21	1:I:1316:VAL:HG22	1.90	0.51
1:I:1749:THR:HB	1:I:1874:ASP:CB	2.39	0.51
1:A:789:GLU:OE1	1:F:801:ARG:NH2	2.43	0.51
1:A:848:THR:HG23	1:F:844:LEU:HD23	1.92	0.51
2:C:209:PHE:HE1	2:C:235:PRO:HB2	1.75	0.51
2:E:1931:LEU:HD22	2:E:1935:GLU:HG2	1.92	0.51
2:L:1037:SER:HB2	2:L:1053:ILE:CG1	2.41	0.51
2:L:1738:PHE:HB3	2:L:1833:TYR:OH	2.11	0.51
1:F:1491:ARG:NH1	1:F:1744:TYR:O	2.43	0.51
1:I:14:LEU:HD13	1:I:14:LEU:C	2.31	0.51
1:I:1545:SER:O	1:I:1545:SER:OG	2.27	0.51
2:J:1037:SER:HB2	2:J:1053:ILE:CG1	2.41	0.51
2:J:1738:PHE:HB3	2:J:1833:TYR:OH	2.10	0.51
2:J:1931:LEU:HD22	2:J:1935:GLU:HG2	1.92	0.51
1:A:881:ASN:HB3	1:A:944:ARG:HH22	1.75	0.51
1:A:1064:ASN:ND2	1:A:1073:THR:OG1	2.43	0.51
1:B:29:ILE:HD11	2:C:1898:TYR:HE1	1.75	0.51
1:D:206:LEU:HD23	1:D:209:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:602:VAL:HG21	2:E:623:GLY:HA3	1.91	0.51
2:E:774:ALA:HB2	2:E:1077:ILE:HA	1.91	0.51
1:K:206:LEU:HD23	1:K:209:LEU:HD12	1.92	0.51
1:K:413:LEU:HD12	1:K:439:ILE:HG21	1.91	0.51
2:L:1931:LEU:HD22	2:L:1935:GLU:HG2	1.92	0.51
1:F:29:ILE:HD11	2:H:1898:TYR:HE1	1.75	0.51
1:F:271:ASN:HB2	1:F:290:MET:HE1	1.93	0.51
1:F:697:LEU:HD21	1:F:732:LEU:HD23	1.91	0.51
2:H:209:PHE:HE1	2:H:235:PRO:HB2	1.75	0.51
1:I:90:TYR:OH	2:J:1659:GLN:NE2	2.43	0.51
2:J:1189:THR:O	2:J:1193:THR:OG1	2.28	0.51
2:G:143:SER:OG	2:G:547:ILE:O	2.29	0.51
2:G:217:GLU:OE2	2:G:221:ASN:ND2	2.37	0.51
1:B:697:LEU:HD21	1:B:732:LEU:HD23	1.91	0.51
1:D:801:ARG:NH2	1:I:789:GLU:OE1	2.43	0.51
2:L:297:ARG:HG2	2:L:297:ARG:HH11	1.74	0.51
2:L:1037:SER:OG	2:L:1053:ILE:CD1	2.59	0.51
2:H:848:SER:HB3	2:H:854:ILE:HD11	1.93	0.51
2:H:1738:PHE:HB3	2:H:1833:TYR:OH	2.10	0.51
1:I:1505:GLN:O	1:I:1509:GLY:N	2.43	0.51
2:J:297:ARG:HG2	2:J:297:ARG:NH1	2.26	0.51
1:A:271:ASN:HB2	1:A:290:MET:HE1	1.93	0.51
2:G:1738:PHE:HB3	2:G:1833:TYR:OH	2.11	0.51
1:B:271:ASN:HB2	1:B:290:MET:HE1	1.92	0.51
2:C:1752:PHE:HB3	2:C:1755:ILE:HD13	1.92	0.51
2:E:297:ARG:NH1	2:E:297:ARG:HG2	2.26	0.51
2:L:1177:SER:OG	2:L:1180:MET:SD	2.63	0.51
2:H:649:ILE:O	2:H:679:LEU:HD22	2.09	0.51
1:A:14:LEU:HD13	1:A:14:LEU:C	2.31	0.51
1:A:471:THR:HG22	1:A:610:THR:HG21	1.92	0.51
1:B:801:ARG:NH2	1:K:789:GLU:OE1	2.43	0.51
1:B:1505:GLN:O	1:B:1509:GLY:N	2.43	0.51
1:D:789:GLU:OE1	1:I:801:ARG:NH2	2.43	0.51
1:K:1064:ASN:ND2	1:K:1073:THR:OG1	2.43	0.51
1:F:14:LEU:C	1:F:14:LEU:HD13	2.31	0.51
1:I:413:LEU:HD12	1:I:439:ILE:HG21	1.91	0.51
1:A:505:LYS:HA	1:A:954:ARG:HD3	1.92	0.51
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.93	0.51
1:B:14:LEU:HD13	1:B:14:LEU:C	2.31	0.51
1:B:1064:ASN:ND2	1:B:1073:THR:OG1	2.43	0.51
2:E:848:SER:HB3	2:E:854:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1309:GLU:O	2:E:1317:ARG:NH1	2.42	0.51
2:L:217:GLU:OE2	2:L:221:ASN:ND2	2.37	0.51
2:L:1490:LYS:HB3	2:L:1498:THR:HB	1.92	0.51
2:L:1775:GLN:OE1	2:L:1839:GLN:NE2	2.44	0.51
2:H:297:ARG:HG2	2:H:297:ARG:NH1	2.26	0.51
1:I:1064:ASN:ND2	1:I:1073:THR:OG1	2.43	0.51
2:J:774:ALA:HB2	2:J:1077:ILE:HA	1.91	0.51
2:J:1037:SER:OG	2:J:1053:ILE:CD1	2.59	0.51
1:A:950:THR:HA	1:A:953:VAL:HG12	1.93	0.51
1:A:995:LEU:HD13	1:A:1674:VAL:HG22	1.93	0.51
1:D:271:ASN:HB2	1:D:290:MET:HE1	1.93	0.51
1:D:739:GLN:O	1:D:798:ASN:ND2	2.42	0.51
2:E:1037:SER:OG	2:E:1053:ILE:CD1	2.59	0.51
2:E:1037:SER:HB2	2:E:1053:ILE:CG1	2.41	0.51
2:E:1322:PRO:HG2	2:E:1325:PHE:HB2	1.93	0.51
2:L:297:ARG:HG2	2:L:297:ARG:NH1	2.26	0.51
2:H:1037:SER:OG	2:H:1053:ILE:CD1	2.59	0.51
2:H:1037:SER:HB2	2:H:1053:ILE:CG1	2.40	0.51
1:I:471:THR:HG22	1:I:610:THR:HG21	1.92	0.51
1:I:697:LEU:HD21	1:I:732:LEU:HD23	1.91	0.51
1:I:1039:MET:HG3	1:I:1580:LEU:HD11	1.93	0.51
2:J:1752:PHE:HB3	2:J:1755:ILE:HD13	1.92	0.51
1:A:90:TYR:OH	2:G:1659:GLN:NE2	2.43	0.51
2:G:209:PHE:HE1	2:G:235:PRO:HB2	1.75	0.51
2:G:297:ARG:HG2	2:G:297:ARG:NH1	2.26	0.51
2:G:1037:SER:OG	2:G:1053:ILE:CD1	2.59	0.51
1:B:90:TYR:OH	2:C:1659:GLN:NE2	2.43	0.51
1:B:471:THR:HG22	1:B:610:THR:HG21	1.92	0.51
2:C:297:ARG:HG2	2:C:297:ARG:NH1	2.26	0.51
2:C:1189:THR:O	2:C:1193:THR:OG1	2.28	0.51
2:C:1738:PHE:HB3	2:C:1833:TYR:OH	2.10	0.51
1:D:413:LEU:HD12	1:D:439:ILE:HG21	1.91	0.51
2:E:209:PHE:HE1	2:E:235:PRO:HB2	1.75	0.51
2:E:1752:PHE:HB3	2:E:1755:ILE:HD13	1.92	0.51
1:K:881:ASN:HB3	1:K:944:ARG:HH22	1.75	0.51
1:K:1491:ARG:NH1	1:K:1744:TYR:O	2.43	0.51
2:L:209:PHE:HE1	2:L:235:PRO:HB2	1.75	0.51
2:L:1036:GLN:HB3	2:L:1051:THR:CG2	2.24	0.51
2:L:1189:THR:O	2:L:1193:THR:OG1	2.28	0.51
2:L:1267:TRP:NE1	2:L:1273:GLU:O	2.39	0.51
2:J:209:PHE:HE1	2:J:235:PRO:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1322:PRO:HG2	2:J:1325:PHE:HB2	1.93	0.51
2:J:1775:GLN:OE1	2:J:1839:GLN:NE2	2.44	0.51
1:A:364:GLU:OE1	1:F:364:GLU:OE1	2.29	0.50
1:B:1406:MET:HB3	1:B:1654:ILE:HG22	1.93	0.50
2:C:1490:LYS:HB3	2:C:1498:THR:HB	1.92	0.50
1:D:1491:ARG:NH1	1:D:1744:TYR:O	2.43	0.50
2:L:848:SER:HB3	2:L:854:ILE:HD11	1.93	0.50
1:A:844:LEU:HD23	1:F:848:THR:HG23	1.92	0.50
2:G:1931:LEU:HD22	2:G:1935:GLU:HG2	1.92	0.50
1:B:844:LEU:HD23	1:K:848:THR:HG23	1.92	0.50
1:B:1039:MET:HG3	1:B:1580:LEU:HD11	1.93	0.50
1:D:505:LYS:HA	1:D:954:ARG:HD3	1.92	0.50
1:D:995:LEU:HD13	1:D:1674:VAL:HG22	1.93	0.50
2:E:1189:THR:O	2:E:1193:THR:OG1	2.28	0.50
2:L:1752:PHE:HB3	2:L:1755:ILE:HD13	1.92	0.50
1:F:950:THR:HA	1:F:953:VAL:HG12	1.93	0.50
2:H:1931:LEU:HD22	2:H:1935:GLU:HG2	1.92	0.50
1:I:881:ASN:HB3	1:I:944:ARG:HH22	1.75	0.50
1:I:1406:MET:HB3	1:I:1654:ILE:HG22	1.93	0.50
2:J:143:SER:OG	2:J:547:ILE:O	2.29	0.50
2:J:1177:SER:OG	2:J:1180:MET:SD	2.63	0.50
2:G:1032:ASP:OD2	2:G:1035:TRP:NE1	2.41	0.50
2:G:1189:THR:O	2:G:1193:THR:OG1	2.28	0.50
2:G:1752:PHE:HB3	2:G:1755:ILE:HD13	1.92	0.50
1:B:32:GLN:HA	1:B:35:PHE:CE1	2.47	0.50
1:B:881:ASN:HB3	1:B:944:ARG:HH22	1.75	0.50
1:B:1545:SER:O	1:B:1545:SER:OG	2.27	0.50
2:L:1322:PRO:HG2	2:L:1325:PHE:HB2	1.93	0.50
2:H:686:PRO:HB2	2:H:691:ALA:HB2	1.93	0.50
2:H:1752:PHE:HB3	2:H:1755:ILE:HD13	1.92	0.50
1:I:641:ARG:NH2	1:I:925:ASP:OD2	2.45	0.50
1:I:995:LEU:HD13	1:I:1674:VAL:HG22	1.93	0.50
2:J:892:ILE:O	2:J:896:ASN:ND2	2.45	0.50
2:G:1037:SER:HB2	2:G:1053:ILE:CG1	2.41	0.50
2:C:1931:LEU:HD22	2:C:1935:GLU:HG2	1.92	0.50
2:E:297:ARG:HG2	2:E:297:ARG:HH11	1.74	0.50
2:E:954:VAL:HG11	2:E:984:PHE:HE1	1.77	0.50
1:K:1773:VAL:HG22	1:K:1879:VAL:HG22	1.94	0.50
2:L:1142:LEU:O	2:L:1150:ARG:NH2	2.45	0.50
1:F:995:LEU:HD13	1:F:1674:VAL:HG22	1.93	0.50
1:I:29:ILE:HD11	2:J:1898:TYR:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:254:TRP:NE1	1:I:288:ASP:OD1	2.42	0.50
2:J:1309:GLU:O	2:J:1317:ARG:NH1	2.42	0.50
1:A:1017:ARG:NH1	1:A:1511:ASP:OD2	2.42	0.50
1:A:1406:MET:HB3	1:A:1654:ILE:HG22	1.93	0.50
1:A:1505:GLN:O	1:A:1509:GLY:N	2.43	0.50
2:G:1322:PRO:HG2	2:G:1325:PHE:HB2	1.93	0.50
1:B:400:ARG:NH1	1:B:1358:HIS:O	2.40	0.50
1:D:14:LEU:HD13	1:D:14:LEU:C	2.31	0.50
1:D:1773:VAL:HG22	1:D:1879:VAL:HG22	1.94	0.50
2:E:846:VAL:HG21	2:E:856:LYS:HD2	1.94	0.50
1:K:32:GLN:HA	1:K:35:PHE:CE1	2.47	0.50
1:K:641:ARG:NH2	1:K:925:ASP:OD2	2.45	0.50
2:L:954:VAL:HG11	2:L:984:PHE:HE1	1.77	0.50
2:J:1639:LYS:NZ	2:J:1654:GLU:OE1	2.44	0.50
1:B:364:GLU:OE1	1:K:364:GLU:OE1	2.29	0.50
1:B:995:LEU:HD13	1:B:1674:VAL:HG22	1.93	0.50
1:B:1773:VAL:HG22	1:B:1879:VAL:HG22	1.94	0.50
2:C:1775:GLN:OE1	2:C:1839:GLN:NE2	2.44	0.50
1:D:848:THR:HG23	1:I:844:LEU:HD23	1.92	0.50
1:D:1542:HIS:CB	1:D:1553:GLU:OE1	2.59	0.50
1:D:1673:TYR:CE1	1:D:1677:VAL:HG21	2.47	0.50
1:K:14:LEU:C	1:K:14:LEU:HD13	2.31	0.50
1:K:1673:TYR:CE1	1:K:1677:VAL:CG2	2.95	0.50
2:L:846:VAL:HG21	2:L:856:LYS:HD2	1.94	0.50
1:F:32:GLN:HA	1:F:35:PHE:CE1	2.47	0.50
1:F:1744:TYR:C	1:F:1747:ALA:CB	2.75	0.50
1:I:1542:HIS:CB	1:I:1553:GLU:OE1	2.59	0.50
1:A:1039:MET:HG3	1:A:1580:LEU:HD11	1.93	0.50
1:A:1744:TYR:C	1:A:1747:ALA:CB	2.75	0.50
2:G:686:PRO:HB2	2:G:691:ALA:HB2	1.93	0.50
2:E:65:LEU:HD11	2:E:88:LEU:HD23	1.94	0.50
2:E:686:PRO:HB2	2:E:691:ALA:HB2	1.93	0.50
1:K:995:LEU:HD13	1:K:1674:VAL:HG22	1.93	0.50
2:L:65:LEU:HD11	2:L:88:LEU:HD23	1.94	0.50
1:I:1673:TYR:CE1	1:I:1677:VAL:HG21	2.47	0.50
2:J:65:LEU:HD11	2:J:88:LEU:HD23	1.94	0.50
2:J:92:GLU:HA	2:J:96:LEU:HB2	1.94	0.50
1:A:32:GLN:HA	1:A:35:PHE:CE1	2.47	0.50
1:A:1542:HIS:CB	1:A:1553:GLU:OE1	2.59	0.50
2:G:92:GLU:HA	2:G:96:LEU:HB2	1.94	0.50
2:C:65:LEU:HD11	2:C:88:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:LEU:O	2:C:1150:ARG:NH2	2.45	0.50
1:D:1017:ARG:NH1	1:D:1511:ASP:OD2	2.42	0.50
2:E:1142:LEU:O	2:E:1150:ARG:NH2	2.45	0.50
1:K:1542:HIS:CB	1:K:1553:GLU:OE1	2.59	0.50
1:K:1673:TYR:CE1	1:K:1677:VAL:HG21	2.47	0.50
1:I:1751:GLU:HG3	1:I:1754:LYS:HE3	1.94	0.50
2:J:847:ARG:HG2	2:J:869:ASP:OD2	2.03	0.50
2:J:848:SER:HB3	2:J:854:ILE:HD11	1.93	0.50
1:B:1751:GLU:HG3	1:B:1754:LYS:HE3	1.94	0.50
2:C:217:GLU:OE2	2:C:221:ASN:ND2	2.37	0.50
2:C:892:ILE:O	2:C:896:ASN:ND2	2.45	0.50
1:D:1673:TYR:CE1	1:D:1677:VAL:CG2	2.95	0.50
1:K:471:THR:HG22	1:K:610:THR:HG21	1.92	0.50
1:F:505:LYS:HA	1:F:954:ARG:HD3	1.92	0.50
1:F:1542:HIS:CB	1:F:1553:GLU:OE1	2.59	0.50
1:I:950:THR:HA	1:I:953:VAL:HG12	1.93	0.50
1:I:1744:TYR:C	1:I:1747:ALA:CB	2.75	0.50
2:J:1314:ARG:HB2	2:J:1317:ARG:HD3	1.94	0.50
1:A:1578:LYS:HD2	1:A:1583:HIS:HA	1.94	0.49
1:A:1673:TYR:CE1	1:A:1677:VAL:HG21	2.47	0.49
1:A:1687:PHE:C	1:A:1687:PHE:CD2	2.86	0.49
1:B:641:ARG:NH2	1:B:925:ASP:OD2	2.45	0.49
1:B:1486:LEU:HD21	1:B:1761:LYS:HZ2	1.76	0.49
1:B:1542:HIS:CB	1:B:1553:GLU:OE1	2.59	0.49
1:K:1039:MET:HG3	1:K:1580:LEU:HD11	1.93	0.49
1:K:1406:MET:HB3	1:K:1654:ILE:HG22	1.93	0.49
2:L:1314:ARG:HB2	2:L:1317:ARG:HD3	1.94	0.49
1:F:641:ARG:NH2	1:F:925:ASP:OD2	2.45	0.49
1:F:1773:VAL:HG22	1:F:1879:VAL:HG22	1.94	0.49
2:H:846:VAL:HG21	2:H:856:LYS:HD2	1.94	0.49
2:H:1775:GLN:OE1	2:H:1839:GLN:NE2	2.44	0.49
2:J:1736:MET:HE3	2:J:1736:MET:N	2.26	0.49
1:A:1751:GLU:HG3	1:A:1754:LYS:HE3	1.94	0.49
1:B:1673:TYR:CE1	1:B:1677:VAL:CG2	2.95	0.49
1:B:1687:PHE:C	1:B:1687:PHE:CD2	2.86	0.49
2:C:92:GLU:HA	2:C:96:LEU:HB2	1.94	0.49
1:D:364:GLU:OE1	1:I:364:GLU:OE1	2.29	0.49
1:D:1687:PHE:C	1:D:1687:PHE:CD2	2.86	0.49
2:G:892:ILE:O	2:G:896:ASN:ND2	2.45	0.49
2:G:1314:ARG:HB2	2:G:1317:ARG:HD3	1.94	0.49
2:E:1639:LYS:NZ	2:E:1654:GLU:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:503:ASP:HB3	2:L:529:VAL:HA	1.94	0.49
2:H:92:GLU:HA	2:H:96:LEU:HB2	1.94	0.49
2:H:1177:SER:OG	2:H:1180:MET:SD	2.63	0.49
1:I:32:GLN:HA	1:I:35:PHE:CE1	2.47	0.49
2:J:1142:LEU:O	2:J:1150:ARG:NH2	2.45	0.49
1:A:641:ARG:NH2	1:A:925:ASP:OD2	2.45	0.49
1:A:1373:ARG:CZ	1:A:1550:ASP:HB2	2.43	0.49
2:G:954:VAL:HG11	2:G:984:PHE:HE1	1.77	0.49
2:G:1142:LEU:O	2:G:1150:ARG:NH2	2.45	0.49
2:C:1322:PRO:HG2	2:C:1325:PHE:HB2	1.93	0.49
1:D:1039:MET:HG3	1:D:1580:LEU:HD11	1.93	0.49
2:E:1314:ARG:HB2	2:E:1317:ARG:HD3	1.94	0.49
2:E:1537:ILE:HD12	2:E:1628:HIS:HD2	1.78	0.49
1:K:1505:GLN:O	1:K:1509:GLY:N	2.43	0.49
1:K:1687:PHE:C	1:K:1687:PHE:CD2	2.86	0.49
1:K:1751:GLU:HG3	1:K:1754:LYS:HE3	1.94	0.49
2:H:954:VAL:HG11	2:H:984:PHE:HE1	1.77	0.49
1:I:1578:LYS:HD2	1:I:1583:HIS:HA	1.94	0.49
1:A:1773:VAL:HG22	1:A:1879:VAL:HG22	1.94	0.49
2:G:65:LEU:HD11	2:G:88:LEU:HD23	1.94	0.49
2:G:1775:GLN:OE1	2:G:1839:GLN:NE2	2.44	0.49
1:B:1578:LYS:HD2	1:B:1583:HIS:HA	1.95	0.49
2:C:807:ILE:HG23	2:C:818:LYS:HB3	1.95	0.49
2:E:892:ILE:O	2:E:896:ASN:ND2	2.45	0.49
1:K:32:GLN:NE2	1:K:57:ALA:CA	2.76	0.49
1:F:1373:ARG:CZ	1:F:1550:ASP:HB2	2.43	0.49
1:F:1406:MET:HB3	1:F:1654:ILE:HG22	1.93	0.49
2:H:65:LEU:HD11	2:H:88:LEU:HD23	1.94	0.49
2:H:1142:LEU:O	2:H:1150:ARG:NH2	2.45	0.49
1:I:1373:ARG:CZ	1:I:1550:ASP:HB2	2.43	0.49
1:I:1673:TYR:CE1	1:I:1677:VAL:CG2	2.95	0.49
2:J:1267:TRP:NE1	2:J:1273:GLU:O	2.39	0.49
1:B:32:GLN:NE2	1:B:57:ALA:CA	2.76	0.49
2:C:846:VAL:HG21	2:C:856:LYS:HD2	1.94	0.49
2:C:1037:SER:OG	2:C:1053:ILE:CG1	2.61	0.49
1:D:1373:ARG:CZ	1:D:1550:ASP:HB2	2.43	0.49
2:E:1775:GLN:OE1	2:E:1839:GLN:NE2	2.44	0.49
1:K:413:LEU:HD12	1:K:439:ILE:HD13	1.95	0.49
1:K:950:THR:HA	1:K:953:VAL:HG12	1.93	0.49
1:F:1578:LYS:HD2	1:F:1583:HIS:HA	1.95	0.49
1:F:1751:GLU:HG3	1:F:1754:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1322:PRO:HG2	2:H:1325:PHE:HB2	1.93	0.49
1:I:413:LEU:HD12	1:I:439:ILE:HD13	1.95	0.49
2:J:686:PRO:HB2	2:J:691:ALA:HB2	1.93	0.49
2:J:807:ILE:HG23	2:J:818:LYS:HB3	1.95	0.49
2:J:1736:MET:O	2:J:1751:ILE:HG13	2.13	0.49
1:A:32:GLN:NE2	1:A:57:ALA:CA	2.76	0.49
1:B:950:THR:HA	1:B:953:VAL:HG12	1.93	0.49
1:B:1673:TYR:CE1	1:B:1677:VAL:HG21	2.47	0.49
2:C:847:ARG:HG2	2:C:869:ASP:OD2	2.03	0.49
2:C:954:VAL:HG11	2:C:984:PHE:HE1	1.77	0.49
1:D:32:GLN:HA	1:D:35:PHE:CE1	2.47	0.49
1:D:950:THR:HA	1:D:953:VAL:HG12	1.93	0.49
1:D:1406:MET:HB3	1:D:1654:ILE:HG22	1.93	0.49
1:D:1751:GLU:HG3	1:D:1754:LYS:HE3	1.94	0.49
1:D:1775:LEU:HD23	1:D:1877:GLN:HB3	1.95	0.49
2:E:92:GLU:HA	2:E:96:LEU:HB2	1.94	0.49
1:K:688:ILE:HG13	1:K:875:THR:HG21	1.95	0.49
2:L:295:SER:O	2:L:298:LYS:CB	2.59	0.49
2:L:1309:GLU:O	2:L:1317:ARG:NH1	2.42	0.49
2:L:1639:LYS:NZ	2:L:1654:GLU:OE1	2.44	0.49
1:F:1017:ARG:NH1	1:F:1511:ASP:OD2	2.42	0.49
1:I:32:GLN:NE2	1:I:57:ALA:CA	2.76	0.49
2:J:503:ASP:HB3	2:J:529:VAL:HA	1.94	0.49
1:A:1673:TYR:CE1	1:A:1677:VAL:CG2	2.95	0.49
2:G:295:SER:O	2:G:298:LYS:CB	2.59	0.49
2:G:503:ASP:HB3	2:G:529:VAL:HA	1.94	0.49
2:C:848:SER:HB3	2:C:854:ILE:HD11	1.93	0.49
1:D:413:LEU:HD12	1:D:439:ILE:HD13	1.95	0.49
1:D:520:ARG:NH2	1:D:606:ASP:OD2	2.46	0.49
2:E:217:GLU:OE2	2:E:221:ASN:ND2	2.37	0.49
1:K:1775:LEU:HD23	1:K:1877:GLN:HB3	1.95	0.49
2:L:1048:VAL:O	2:L:1048:VAL:HG12	2.13	0.49
2:L:1537:ILE:HD12	2:L:1628:HIS:HD2	1.77	0.49
1:F:1673:TYR:CE1	1:F:1677:VAL:CG2	2.95	0.49
2:H:646:THR:OG1	2:H:677:GLN:OE1	2.28	0.49
2:H:892:ILE:O	2:H:896:ASN:ND2	2.45	0.49
2:H:1537:ILE:HD12	2:H:1628:HIS:HD2	1.77	0.49
2:H:1639:LYS:NZ	2:H:1654:GLU:OE1	2.44	0.49
1:I:1026:GLU:OE1	1:I:1594:ASN:ND2	2.40	0.49
1:I:1687:PHE:C	1:I:1687:PHE:CD2	2.86	0.49
1:I:1773:VAL:HG22	1:I:1879:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:846:VAL:HG21	2:G:856:LYS:HD2	1.94	0.49
2:G:1537:ILE:HD12	2:G:1628:HIS:HD2	1.77	0.49
1:B:413:LEU:HD12	1:B:439:ILE:HD13	1.95	0.49
1:D:32:GLN:NE2	1:D:57:ALA:CA	2.76	0.49
1:D:641:ARG:NH2	1:D:925:ASP:OD2	2.45	0.49
1:K:893:VAL:HG11	1:K:930:LEU:HD23	1.95	0.49
2:L:892:ILE:O	2:L:896:ASN:ND2	2.45	0.49
1:F:413:LEU:HD12	1:F:439:ILE:HD13	1.95	0.49
1:A:413:LEU:HD12	1:A:439:ILE:HD13	1.95	0.49
2:G:1736:MET:O	2:G:1751:ILE:HG13	2.13	0.49
2:C:503:ASP:HB3	2:C:529:VAL:HA	1.94	0.49
2:C:1314:ARG:HB2	2:C:1317:ARG:HD3	1.94	0.49
1:D:688:ILE:HG13	1:D:875:THR:HG21	1.95	0.49
2:L:1037:SER:OG	2:L:1053:ILE:CG1	2.61	0.49
2:J:372:ASN:HB3	2:J:515:LEU:HD21	1.95	0.49
2:J:846:VAL:HG21	2:J:856:LYS:HD2	1.94	0.49
1:A:520:ARG:NH2	1:A:606:ASP:OD2	2.46	0.48
2:G:807:ILE:HG23	2:G:818:LYS:HB3	1.95	0.48
1:B:1470:LEU:HD13	1:B:1489:ARG:HG2	1.95	0.48
1:D:781:LEU:HD12	1:D:784:ILE:HD12	1.95	0.48
1:K:520:ARG:NH2	1:K:606:ASP:OD2	2.46	0.48
1:K:1119:LYS:NZ	1:K:1337:GLU:OE2	2.46	0.48
1:F:1039:MET:HG3	1:F:1580:LEU:HD11	1.93	0.48
1:F:1673:TYR:CE1	1:F:1677:VAL:HG21	2.47	0.48
1:F:1687:PHE:C	1:F:1687:PHE:CD2	2.86	0.48
2:H:1037:SER:OG	2:H:1053:ILE:CG1	2.61	0.48
1:I:688:ILE:HG13	1:I:875:THR:HG21	1.95	0.48
1:A:893:VAL:HG11	1:A:930:LEU:HD23	1.95	0.48
2:C:1048:VAL:O	2:C:1048:VAL:HG12	2.13	0.48
2:C:1537:ILE:HD12	2:C:1628:HIS:HD2	1.77	0.48
2:E:372:ASN:HB3	2:E:515:LEU:HD21	1.95	0.48
1:K:1470:LEU:HD13	1:K:1489:ARG:HG2	1.95	0.48
1:K:1578:LYS:HD2	1:K:1583:HIS:HA	1.94	0.48
2:L:92:GLU:HA	2:L:96:LEU:HB2	1.94	0.48
2:L:686:PRO:HB2	2:L:691:ALA:HB2	1.93	0.48
1:F:32:GLN:NE2	1:F:57:ALA:CA	2.76	0.48
2:H:847:ARG:HG2	2:H:869:ASP:OD2	2.03	0.48
1:I:271:ASN:HB2	1:I:290:MET:HE1	1.94	0.48
2:J:1537:ILE:HD12	2:J:1628:HIS:HD2	1.78	0.48
1:A:1830:GLY:HA2	1:A:1831:GLY:HA2	1.62	0.48
2:C:143:SER:OG	2:C:547:ILE:O	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1119:LYS:NZ	1:D:1337:GLU:OE2	2.46	0.48
2:E:503:ASP:HB3	2:E:529:VAL:HA	1.94	0.48
2:L:1182:VAL:HG22	2:L:1197:LEU:HD23	1.95	0.48
2:L:1697:HIS:O	2:L:1701:THR:OG1	2.28	0.48
1:F:1505:GLN:O	1:F:1509:GLY:N	2.43	0.48
2:G:1737:ILE:CD1	2:G:1737:ILE:N	2.73	0.48
1:B:520:ARG:NH2	1:B:606:ASP:OD2	2.46	0.48
1:B:844:LEU:CD2	1:K:848:THR:HG23	2.43	0.48
1:B:1373:ARG:CZ	1:B:1550:ASP:HB2	2.43	0.48
2:C:1182:VAL:HG22	2:C:1197:LEU:HD23	1.95	0.48
1:D:848:THR:HG23	1:I:844:LEU:CD2	2.43	0.48
1:D:1026:GLU:OE1	1:D:1594:ASN:ND2	2.40	0.48
1:D:1470:LEU:HD13	1:D:1489:ARG:HG2	1.95	0.48
2:E:1736:MET:O	2:E:1751:ILE:HG13	2.13	0.48
2:L:807:ILE:HG23	2:L:818:LYS:HB3	1.95	0.48
2:L:1740:THR:O	2:L:1740:THR:OG1	2.31	0.48
1:F:781:LEU:HD12	1:F:784:ILE:HD12	1.95	0.48
1:F:1467:LEU:HD22	1:F:1757:GLU:OE2	2.14	0.48
2:H:1736:MET:O	2:H:1751:ILE:HG13	2.13	0.48
2:J:1037:SER:OG	2:J:1053:ILE:CG1	2.61	0.48
2:G:372:ASN:HB3	2:G:515:LEU:HD21	1.95	0.48
1:B:688:ILE:HG13	1:B:875:THR:HG21	1.94	0.48
2:C:1639:LYS:NZ	2:C:1654:GLU:OE1	2.44	0.48
1:D:18:LEU:HD13	2:E:1812:TYR:HE1	1.79	0.48
1:D:893:VAL:HG11	1:D:930:LEU:HD23	1.95	0.48
1:D:1030:TRP:O	1:D:1035:THR:OG1	2.31	0.48
1:K:18:LEU:HD13	2:L:1812:TYR:HE1	1.79	0.48
1:K:1373:ARG:CZ	1:K:1550:ASP:HB2	2.43	0.48
1:F:520:ARG:NH2	1:F:606:ASP:OD2	2.46	0.48
1:F:1470:LEU:HD13	1:F:1489:ARG:HG2	1.95	0.48
1:F:1775:LEU:HD23	1:F:1877:GLN:HB3	1.95	0.48
2:H:1767:GLU:OE2	2:H:1849:ARG:NE	2.36	0.48
2:J:596:GLY:N	2:J:618:GLU:OE1	2.46	0.48
2:J:1182:VAL:HG22	2:J:1197:LEU:HD23	1.96	0.48
1:A:688:ILE:HG13	1:A:875:THR:HG21	1.95	0.48
2:G:607:VAL:HG11	2:G:619:LEU:HD13	1.96	0.48
2:G:1048:VAL:O	2:G:1048:VAL:HG12	2.13	0.48
2:G:1182:VAL:HG22	2:G:1197:LEU:HD23	1.95	0.48
2:G:1309:GLU:O	2:G:1317:ARG:NH1	2.42	0.48
2:G:1639:LYS:NZ	2:G:1654:GLU:OE1	2.44	0.48
1:B:254:TRP:NE1	1:B:288:ASP:OD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1775:LEU:HD23	1:B:1877:GLN:HB3	1.95	0.48
2:C:686:PRO:HB2	2:C:691:ALA:HB2	1.93	0.48
2:C:1736:MET:O	2:C:1751:ILE:HG13	2.13	0.48
1:D:868:ILE:HB	1:D:925:ASP:HA	1.95	0.48
1:D:1173:LEU:HD13	1:F:1173:LEU:HD13	1.96	0.48
2:E:1048:VAL:O	2:E:1048:VAL:HG12	2.13	0.48
1:F:46:GLU:OE2	2:H:1667:THR:OG1	2.32	0.48
1:F:893:VAL:HG11	1:F:930:LEU:HD23	1.95	0.48
2:H:372:ASN:HB3	2:H:515:LEU:HD21	1.95	0.48
1:I:1470:LEU:HD13	1:I:1489:ARG:HG2	1.95	0.48
1:I:1486:LEU:HD21	1:I:1761:LYS:HZ2	1.78	0.48
2:J:1697:HIS:O	2:J:1701:THR:OG1	2.28	0.48
1:A:781:LEU:HD12	1:A:784:ILE:HD12	1.95	0.48
2:G:836:TYR:HD1	2:G:845:THR:HG21	1.55	0.48
1:B:1119:LYS:NZ	1:B:1337:GLU:OE2	2.46	0.48
1:B:1173:LEU:HD13	1:I:1173:LEU:HD13	1.96	0.48
2:C:277:LEU:HD21	2:C:468:LEU:HD11	1.96	0.48
2:C:372:ASN:HB3	2:C:515:LEU:HD21	1.95	0.48
2:C:1737:ILE:HG12	2:C:1748:THR:HG22	1.95	0.48
1:D:1578:LYS:HD2	1:D:1583:HIS:HA	1.94	0.48
1:K:868:ILE:HB	1:K:925:ASP:HA	1.95	0.48
1:K:1751:GLU:HG3	1:K:1754:LYS:HZ2	1.77	0.48
1:F:254:TRP:NE1	1:F:288:ASP:OD1	2.42	0.48
2:J:607:VAL:HG11	2:J:619:LEU:HD13	1.96	0.48
1:A:848:THR:HG23	1:F:844:LEU:CD2	2.43	0.48
1:A:1173:LEU:HD13	1:K:1173:LEU:HD13	1.96	0.48
1:A:1467:LEU:HD22	1:A:1757:GLU:OE2	2.14	0.48
1:A:1470:LEU:HD13	1:A:1489:ARG:HG2	1.95	0.48
1:B:1467:LEU:HD22	1:B:1757:GLU:OE2	2.14	0.48
1:D:1467:LEU:HD22	1:D:1757:GLU:OE2	2.14	0.48
2:L:1736:MET:O	2:L:1751:ILE:HG13	2.13	0.48
1:F:1751:GLU:HG3	1:F:1754:LYS:HZ2	1.73	0.48
2:H:1737:ILE:CD1	2:H:1737:ILE:N	2.73	0.48
1:I:18:LEU:HD13	2:J:1812:TYR:HE1	1.79	0.48
1:A:1486:LEU:HD21	1:A:1761:LYS:HZ2	1.78	0.48
1:B:893:VAL:HG11	1:B:930:LEU:HD23	1.95	0.48
1:D:848:THR:CG2	1:I:844:LEU:HD23	2.44	0.48
2:E:143:SER:OG	2:E:547:ILE:O	2.29	0.48
2:E:1037:SER:OG	2:E:1053:ILE:CG1	2.61	0.48
1:K:1484:GLU:OE2	1:K:1741:LYS:NZ	2.47	0.48
2:L:646:THR:OG1	2:L:677:GLN:OE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1314:ARG:HB2	2:H:1317:ARG:HD3	1.94	0.48
2:J:954:VAL:HG11	2:J:984:PHE:HE1	1.77	0.48
1:A:18:LEU:HD13	2:G:1812:TYR:HE1	1.79	0.48
1:A:868:ILE:HB	1:A:925:ASP:HA	1.95	0.48
2:E:807:ILE:HG23	2:E:818:LYS:HB3	1.95	0.48
1:K:781:LEU:HD12	1:K:784:ILE:HD12	1.95	0.48
2:H:249:TYR:HE2	2:H:260:PRO:HB3	1.79	0.48
2:H:807:ILE:HG23	2:H:818:LYS:HB3	1.95	0.48
1:I:1030:TRP:O	1:I:1035:THR:OG1	2.31	0.48
2:J:277:LEU:HD21	2:J:468:LEU:HD11	1.96	0.48
1:B:781:LEU:HD12	1:B:784:ILE:HD12	1.95	0.47
1:D:400:ARG:NH1	1:D:1358:HIS:O	2.40	0.47
1:K:1467:LEU:HD22	1:K:1757:GLU:OE2	2.14	0.47
2:H:490:TRP:HE1	2:H:516:THR:HG22	1.79	0.47
1:I:520:ARG:NH2	1:I:606:ASP:OD2	2.46	0.47
2:J:1048:VAL:O	2:J:1048:VAL:HG12	2.13	0.47
1:A:844:LEU:HD23	1:F:848:THR:CG2	2.44	0.47
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.79	0.47
1:B:1030:TRP:O	1:B:1035:THR:OG1	2.31	0.47
1:A:1775:LEU:HD23	1:A:1877:GLN:HB3	1.95	0.47
2:G:847:ARG:HG2	2:G:869:ASP:OD2	2.03	0.47
1:B:18:LEU:HD13	2:C:1812:TYR:HE1	1.79	0.47
1:B:1484:GLU:OE2	1:B:1741:LYS:NZ	2.47	0.47
1:D:1505:GLN:O	1:D:1509:GLY:N	2.43	0.47
1:D:1744:TYR:C	1:D:1747:ALA:CB	2.75	0.47
2:E:249:TYR:HE2	2:E:260:PRO:HB3	1.79	0.47
2:L:277:LEU:HD21	2:L:468:LEU:HD11	1.96	0.47
1:F:1119:LYS:NZ	1:F:1337:GLU:OE2	2.46	0.47
2:H:217:GLU:OE2	2:H:221:ASN:ND2	2.37	0.47
2:H:503:ASP:HB3	2:H:529:VAL:HA	1.94	0.47
2:H:607:VAL:HG11	2:H:619:LEU:HD13	1.96	0.47
2:H:1048:VAL:HG12	2:H:1048:VAL:O	2.13	0.47
1:I:1119:LYS:NZ	1:I:1337:GLU:OE2	2.46	0.47
1:I:1775:LEU:HD23	1:I:1877:GLN:HB3	1.95	0.47
2:J:1737:ILE:HG12	2:J:1748:THR:HG22	1.95	0.47
2:J:1737:ILE:CD1	2:J:1737:ILE:N	2.73	0.47
1:A:844:LEU:CD2	1:F:848:THR:HG23	2.43	0.47
1:B:1744:TYR:C	1:B:1747:ALA:CB	2.75	0.47
2:E:234:ILE:HG22	2:E:307:GLY:HA2	1.96	0.47
1:K:539:SER:HB2	1:K:633:GLU:HA	1.97	0.47
1:K:1030:TRP:O	1:K:1035:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:143:SER:OG	2:L:547:ILE:O	2.29	0.47
2:L:372:ASN:HB3	2:L:515:LEU:HD21	1.95	0.47
1:F:868:ILE:HB	1:F:925:ASP:HA	1.95	0.47
2:H:1737:ILE:HG12	2:H:1748:THR:HG22	1.95	0.47
1:I:781:LEU:HD12	1:I:784:ILE:HD12	1.95	0.47
1:I:1484:GLU:OE2	1:I:1741:LYS:NZ	2.47	0.47
2:J:646:THR:HB	2:J:677:GLN:CB	2.26	0.47
1:A:848:THR:CG2	1:F:844:LEU:HD23	2.44	0.47
1:B:868:ILE:HB	1:B:925:ASP:HA	1.95	0.47
2:E:553:ASN:O	2:E:556:LYS:NZ	2.39	0.47
2:L:607:VAL:HG11	2:L:619:LEU:HD13	1.96	0.47
1:F:688:ILE:HG13	1:F:875:THR:HG21	1.94	0.47
1:I:1467:LEU:HD22	1:I:1757:GLU:OE2	2.14	0.47
2:J:313:ALA:HB2	2:J:435:ALA:HB2	1.97	0.47
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.96	0.47
2:C:313:ALA:HB2	2:C:435:ALA:HB2	1.97	0.47
2:C:691:ALA:HA	2:C:694:TYR:HD2	1.80	0.47
2:E:736:ARG:NE	2:E:769:SER:O	2.48	0.47
2:L:490:TRP:HE1	2:L:516:THR:HG22	1.79	0.47
1:F:1030:TRP:O	1:F:1035:THR:OG1	2.31	0.47
1:F:1484:GLU:OE2	1:F:1741:LYS:NZ	2.47	0.47
1:A:1119:LYS:NZ	1:A:1337:GLU:OE2	2.46	0.47
1:A:1484:GLU:OE2	1:A:1741:LYS:NZ	2.47	0.47
2:G:249:TYR:HE2	2:G:260:PRO:HB3	1.79	0.47
2:G:736:ARG:NE	2:G:769:SER:O	2.48	0.47
2:C:596:GLY:N	2:C:618:GLU:OE1	2.46	0.47
2:C:607:VAL:HG11	2:C:619:LEU:HD13	1.96	0.47
2:C:1267:TRP:NE1	2:C:1273:GLU:O	2.39	0.47
1:D:1486:LEU:HD21	1:D:1761:LYS:HZ2	1.79	0.47
2:E:1737:ILE:CD1	2:E:1737:ILE:N	2.73	0.47
2:E:1908:ASP:HA	2:E:1911:THR:HG22	1.97	0.47
2:L:596:GLY:N	2:L:618:GLU:OE1	2.46	0.47
1:F:1010:GLU:HA	1:F:1664:ALA:HA	1.96	0.47
1:I:539:SER:HB2	1:I:633:GLU:HA	1.97	0.47
2:J:490:TRP:HE1	2:J:516:THR:HG22	1.79	0.47
2:J:587:ILE:HG13	2:J:589:ARG:H	1.80	0.47
2:G:313:ALA:HB2	2:G:435:ALA:HB2	1.97	0.47
2:G:587:ILE:HG13	2:G:589:ARG:H	1.80	0.47
1:B:18:LEU:HD13	2:C:1812:TYR:CE1	2.50	0.47
2:C:234:ILE:HG22	2:C:307:GLY:HA2	1.96	0.47
1:D:1271:GLN:HB2	1:D:1274:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1428:THR:OG1	1:D:1652:GLN:NE2	2.48	0.47
2:E:277:LEU:HD21	2:E:468:LEU:HD11	1.96	0.47
2:E:1697:HIS:O	2:E:1701:THR:OG1	2.28	0.47
2:E:1855:ILE:HD12	2:E:1907:LEU:HG	1.97	0.47
1:K:1010:GLU:HA	1:K:1664:ALA:HA	1.96	0.47
1:K:1428:THR:OG1	1:K:1652:GLN:NE2	2.48	0.47
2:L:1908:ASP:HA	2:L:1911:THR:HG22	1.97	0.47
2:H:234:ILE:HG22	2:H:307:GLY:HA2	1.96	0.47
2:H:587:ILE:HG13	2:H:589:ARG:H	1.80	0.47
2:H:1182:VAL:HG22	2:H:1197:LEU:HD23	1.95	0.47
2:H:1267:TRP:NE1	2:H:1273:GLU:O	2.39	0.47
2:H:1908:ASP:HA	2:H:1911:THR:HG22	1.97	0.47
1:I:893:VAL:HG11	1:I:930:LEU:HD23	1.95	0.47
2:J:249:TYR:HE2	2:J:260:PRO:HB3	1.79	0.47
1:A:1030:TRP:O	1:A:1035:THR:OG1	2.31	0.47
2:G:1037:SER:OG	2:G:1053:ILE:CG1	2.61	0.47
2:C:54:PRO:HG3	2:C:63:LYS:HG3	1.97	0.47
2:C:1691:TRP:O	2:C:1695:ASP:N	2.40	0.47
2:C:1908:ASP:HA	2:C:1911:THR:HG22	1.97	0.47
2:E:691:ALA:HA	2:E:694:TYR:HD2	1.80	0.47
2:E:1381:VAL:O	2:E:1422:THR:OG1	2.28	0.47
2:L:587:ILE:HG13	2:L:589:ARG:H	1.80	0.47
2:L:691:ALA:HA	2:L:694:TYR:HD2	1.80	0.47
2:L:736:ARG:NE	2:L:769:SER:O	2.48	0.47
2:L:1855:ILE:HD12	2:L:1907:LEU:HG	1.97	0.47
1:F:18:LEU:HD13	2:H:1812:TYR:HE1	1.79	0.47
1:F:1271:GLN:HB2	1:F:1274:ILE:HG23	1.97	0.47
2:H:691:ALA:HA	2:H:694:TYR:HD2	1.80	0.47
2:H:1855:ILE:HD12	2:H:1907:LEU:HG	1.97	0.47
2:J:1691:TRP:O	2:J:1695:ASP:N	2.40	0.47
2:G:1908:ASP:HA	2:G:1911:THR:HG22	1.97	0.47
1:B:401:THR:HG22	1:B:733:ILE:HG12	1.97	0.47
1:B:1792:THR:HG21	1:B:1838:GLU:HG2	1.97	0.47
2:C:490:TRP:HE1	2:C:516:THR:HG22	1.79	0.47
1:D:539:SER:HB2	1:D:633:GLU:HA	1.97	0.47
2:E:490:TRP:HE1	2:E:516:THR:HG22	1.79	0.47
2:E:596:GLY:HA3	2:E:650:ASN:HD22	1.80	0.47
1:K:18:LEU:HD13	2:L:1812:TYR:CE1	2.50	0.47
2:L:313:ALA:HB2	2:L:435:ALA:HB2	1.97	0.47
1:F:1226:SER:O	1:F:1226:SER:OG	2.32	0.47
2:G:277:LEU:HD21	2:G:468:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1740:THR:O	2:G:1740:THR:OG1	2.31	0.46
2:G:1767:GLU:OE2	2:G:1849:ARG:NE	2.36	0.46
2:G:1855:ILE:HD12	2:G:1907:LEU:HG	1.97	0.46
1:B:1010:GLU:HA	1:B:1664:ALA:HA	1.96	0.46
2:C:1422:THR:HG23	2:C:1474:PHE:HB2	1.97	0.46
1:D:18:LEU:HD13	2:E:1812:TYR:CE1	2.50	0.46
1:D:46:GLU:OE2	2:E:1667:THR:OG1	2.32	0.46
1:D:254:TRP:NE1	1:D:288:ASP:OD1	2.42	0.46
1:D:1484:GLU:OE2	1:D:1741:LYS:NZ	2.47	0.46
2:E:462:THR:HG21	2:E:488:VAL:HG22	1.98	0.46
1:K:1017:ARG:NH1	1:K:1511:ASP:OD2	2.42	0.46
1:K:1852:HIS:HA	1:K:1856:LYS:HE3	1.97	0.46
2:L:1037:SER:OG	2:L:1053:ILE:HD11	2.16	0.46
2:H:736:ARG:NE	2:H:769:SER:O	2.48	0.46
2:J:234:ILE:HG22	2:J:307:GLY:HA2	1.96	0.46
1:B:1852:HIS:HA	1:B:1856:LYS:HE3	1.97	0.46
1:D:1792:THR:HG21	1:D:1838:GLU:HG2	1.97	0.46
2:L:249:TYR:HE2	2:L:260:PRO:HB3	1.79	0.46
2:L:462:THR:HG21	2:L:488:VAL:HG22	1.98	0.46
2:L:596:GLY:HA3	2:L:650:ASN:HD22	1.81	0.46
2:L:1737:ILE:HG12	2:L:1748:THR:HG22	1.95	0.46
1:F:1792:THR:HG21	1:F:1838:GLU:HG2	1.97	0.46
1:I:868:ILE:HB	1:I:925:ASP:HA	1.95	0.46
1:I:1010:GLU:HA	1:I:1664:ALA:HA	1.96	0.46
2:J:691:ALA:HA	2:J:694:TYR:HD2	1.80	0.46
2:J:1037:SER:OG	2:J:1053:ILE:HD11	2.16	0.46
1:A:254:TRP:NE1	1:A:288:ASP:OD1	2.42	0.46
2:G:1037:SER:OG	2:G:1053:ILE:HD11	2.16	0.46
2:G:1691:TRP:O	2:G:1695:ASP:N	2.40	0.46
2:C:249:TYR:HE2	2:C:260:PRO:HB3	1.79	0.46
1:D:32:GLN:NE2	1:D:57:ALA:CB	2.78	0.46
2:E:864:LEU:HD22	2:E:898:ASP:HB2	1.97	0.46
1:F:18:LEU:HD13	2:H:1812:TYR:CE1	2.50	0.46
2:H:313:ALA:HB2	2:H:435:ALA:HB2	1.97	0.46
1:I:18:LEU:HD13	2:J:1812:TYR:CE1	2.50	0.46
1:I:1792:THR:HG21	1:I:1838:GLU:HG2	1.97	0.46
1:A:1428:THR:OG1	1:A:1652:GLN:NE2	2.48	0.46
2:G:462:THR:HG21	2:G:488:VAL:HG22	1.98	0.46
1:B:1226:SER:O	1:B:1226:SER:OG	2.32	0.46
2:C:587:ILE:HG13	2:C:589:ARG:H	1.80	0.46
2:C:835:THR:HG23	2:C:843:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1561:MET:N	1:D:1561:MET:HE3	2.31	0.46
2:E:1182:VAL:HG22	2:E:1197:LEU:HD23	1.96	0.46
1:K:254:TRP:NE1	1:K:288:ASP:OD1	2.42	0.46
2:L:234:ILE:HG22	2:L:307:GLY:HA2	1.96	0.46
2:L:864:LEU:HD22	2:L:898:ASP:HB2	1.98	0.46
1:F:32:GLN:NE2	1:F:57:ALA:CB	2.79	0.46
1:F:1428:THR:OG1	1:F:1652:GLN:NE2	2.48	0.46
2:H:462:THR:HG21	2:H:488:VAL:HG22	1.98	0.46
2:H:596:GLY:HA3	2:H:650:ASN:HD22	1.81	0.46
1:I:401:THR:HG22	1:I:733:ILE:HG12	1.97	0.46
2:J:736:ARG:NE	2:J:769:SER:O	2.48	0.46
1:A:1503:ALA:HA	1:A:1506:GLN:HE21	1.81	0.46
2:G:835:THR:HG23	2:G:843:ILE:O	2.16	0.46
2:G:860:ARG:NH2	2:G:1047:ASP:OD2	2.49	0.46
1:B:488:PRO:HG3	1:B:728:LYS:HG2	1.97	0.46
1:B:1428:THR:OG1	1:B:1652:GLN:NE2	2.48	0.46
2:C:462:THR:HG21	2:C:488:VAL:HG22	1.98	0.46
2:C:1638:ILE:HD13	2:C:1657:ILE:HD13	1.98	0.46
1:D:1852:HIS:HA	1:D:1856:LYS:HE3	1.97	0.46
2:E:313:ALA:HB2	2:E:435:ALA:HB2	1.97	0.46
2:L:1037:SER:CB	2:L:1053:ILE:CG1	2.92	0.46
2:L:1737:ILE:CD1	2:L:1737:ILE:N	2.73	0.46
1:F:678:VAL:HG22	1:F:767:ALA:HB3	1.98	0.46
2:J:835:THR:HG23	2:J:843:ILE:O	2.16	0.46
1:A:539:SER:HB2	1:A:633:GLU:HA	1.97	0.46
2:G:691:ALA:HA	2:G:694:TYR:HD2	1.80	0.46
2:G:1177:SER:OG	2:G:1180:MET:SD	2.63	0.46
1:D:678:VAL:HG22	1:D:767:ALA:HB3	1.98	0.46
2:E:1767:GLU:OE2	2:E:1849:ARG:NE	2.36	0.46
1:K:1503:ALA:HA	1:K:1506:GLN:HE21	1.81	0.46
2:L:245:GLN:HE21	2:L:506:PRO:HD3	1.81	0.46
2:L:1422:THR:HG23	2:L:1474:PHE:HB2	1.97	0.46
2:H:326:ASP:OD2	2:H:387:TYR:OH	2.33	0.46
2:H:900:GLN:HB3	2:H:1050:ARG:O	2.16	0.46
2:H:1697:HIS:O	2:H:1701:THR:OG1	2.28	0.46
2:J:295:SER:O	2:J:298:LYS:CB	2.59	0.46
2:J:1422:THR:HG23	2:J:1474:PHE:HB2	1.97	0.46
1:A:18:LEU:HD13	2:G:1812:TYR:CE1	2.50	0.46
1:A:1226:SER:O	1:A:1226:SER:OG	2.32	0.46
1:B:1017:ARG:NH1	1:B:1511:ASP:OD2	2.42	0.46
2:C:736:ARG:NE	2:C:769:SER:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1037:SER:OG	2:C:1053:ILE:HD11	2.16	0.46
2:C:1292:ILE:HD11	2:C:1366:LEU:HD23	1.98	0.46
2:C:1855:ILE:HD12	2:C:1907:LEU:HG	1.97	0.46
1:K:1271:GLN:HB2	1:K:1274:ILE:HG23	1.97	0.46
2:L:1292:ILE:HD11	2:L:1366:LEU:HD23	1.98	0.46
2:L:1638:ILE:HD13	2:L:1657:ILE:HD13	1.98	0.46
2:H:54:PRO:HG3	2:H:63:LYS:HG3	1.97	0.46
2:H:835:THR:HG23	2:H:843:ILE:O	2.16	0.46
2:H:1691:TRP:O	2:H:1695:ASP:N	2.40	0.46
2:J:716:VAL:HG11	2:J:730:LEU:HD13	1.98	0.46
2:J:860:ARG:NH2	2:J:1047:ASP:OD2	2.49	0.46
2:J:1638:ILE:HD13	2:J:1657:ILE:HD13	1.98	0.46
2:J:1855:ILE:HD12	2:J:1907:LEU:HG	1.97	0.46
2:J:1908:ASP:HA	2:J:1911:THR:HG22	1.97	0.46
1:A:401:THR:HG22	1:A:733:ILE:HG12	1.97	0.46
1:A:678:VAL:HG22	1:A:767:ALA:HB3	1.98	0.46
2:G:234:ILE:HG22	2:G:307:GLY:HA2	1.96	0.46
2:G:596:GLY:HA3	2:G:650:ASN:HD22	1.81	0.46
1:B:539:SER:HB2	1:B:633:GLU:HA	1.97	0.46
2:C:596:GLY:HA3	2:C:650:ASN:HD22	1.81	0.46
2:C:864:LEU:HD22	2:C:898:ASP:HB2	1.98	0.46
1:D:488:PRO:HG3	1:D:728:LYS:HG2	1.97	0.46
2:E:295:SER:O	2:E:298:LYS:CB	2.59	0.46
2:E:587:ILE:HG13	2:E:589:ARG:H	1.80	0.46
2:E:607:VAL:HG11	2:E:619:LEU:HD13	1.96	0.46
2:E:716:VAL:HG11	2:E:730:LEU:HD13	1.98	0.46
2:E:1037:SER:CB	2:E:1053:ILE:CG1	2.92	0.46
2:L:716:VAL:HG11	2:L:730:LEU:HD13	1.98	0.46
2:H:277:LEU:HD21	2:H:468:LEU:HD11	1.96	0.46
1:A:1792:THR:HG21	1:A:1838:GLU:HG2	1.97	0.46
1:A:1852:HIS:HA	1:A:1856:LYS:HE3	1.97	0.46
2:C:326:ASP:OD2	2:C:387:TYR:OH	2.33	0.46
1:D:401:THR:HG22	1:D:733:ILE:HG12	1.97	0.46
1:D:1010:GLU:HA	1:D:1664:ALA:HA	1.96	0.46
1:D:1545:SER:O	1:D:1545:SER:OG	2.27	0.46
2:E:646:THR:HB	2:E:677:GLN:CB	2.26	0.46
1:K:400:ARG:NH1	1:K:1358:HIS:O	2.40	0.46
2:H:143:SER:OG	2:H:547:ILE:O	2.29	0.46
2:H:259:THR:OG1	2:H:288:SER:HA	2.16	0.46
1:I:1428:THR:OG1	1:I:1652:GLN:NE2	2.48	0.46
2:J:245:GLN:HE21	2:J:506:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:462:THR:HG21	2:J:488:VAL:HG22	1.98	0.46
1:A:32:GLN:NE2	1:A:57:ALA:CB	2.79	0.46
2:G:1736:MET:HE2	2:G:1736:MET:CA	2.45	0.46
1:B:430:ARG:HG2	1:B:605:LEU:HD22	1.98	0.46
2:E:1037:SER:OG	2:E:1053:ILE:HD11	2.16	0.46
1:F:488:PRO:HG3	1:F:728:LYS:HG2	1.97	0.46
1:F:1303:GLY:HA2	1:F:1649:LYS:HZ1	1.81	0.46
2:J:1338:ILE:HG22	2:J:1390:VAL:HG11	1.98	0.46
1:A:430:ARG:HG2	1:A:605:LEU:HD22	1.98	0.45
1:A:1271:GLN:HB2	1:A:1274:ILE:HG23	1.97	0.45
2:G:54:PRO:HG3	2:G:63:LYS:HG3	1.97	0.45
1:B:937:LYS:HD2	1:K:855:SER:HB2	1.98	0.45
1:B:1503:ALA:HA	1:B:1506:GLN:HE21	1.81	0.45
2:C:646:THR:HB	2:C:677:GLN:CB	2.26	0.45
2:C:1740:THR:O	2:C:1740:THR:OG1	2.31	0.45
1:D:937:LYS:HD2	1:I:855:SER:HB2	1.98	0.45
2:E:54:PRO:HG3	2:E:63:LYS:HG3	1.97	0.45
2:E:860:ARG:NH2	2:E:1047:ASP:OD2	2.49	0.45
2:E:900:GLN:HB3	2:E:1050:ARG:O	2.16	0.45
2:L:835:THR:HG23	2:L:843:ILE:O	2.16	0.45
2:L:860:ARG:NH2	2:L:1047:ASP:OD2	2.49	0.45
2:L:1811:GLU:OE2	2:L:2010:TYR:OH	2.29	0.45
1:F:1852:HIS:HA	1:F:1856:LYS:HE3	1.97	0.45
1:I:678:VAL:HG22	1:I:767:ALA:HB3	1.98	0.45
1:I:1503:ALA:HA	1:I:1506:GLN:HE21	1.81	0.45
2:J:596:GLY:HA3	2:J:650:ASN:HD22	1.80	0.45
2:J:646:THR:OG1	2:J:677:GLN:OE1	2.28	0.45
2:G:646:THR:HB	2:G:677:GLN:CB	2.26	0.45
2:G:716:VAL:HG11	2:G:730:LEU:HD13	1.98	0.45
2:G:900:GLN:HB3	2:G:1050:ARG:O	2.16	0.45
1:B:32:GLN:NE2	1:B:57:ALA:CB	2.79	0.45
2:C:716:VAL:HG11	2:C:730:LEU:HD13	1.98	0.45
2:C:900:GLN:HB3	2:C:1050:ARG:O	2.16	0.45
1:D:431:GLU:O	1:D:435:GLU:N	2.49	0.45
1:D:844:LEU:HD23	1:I:848:THR:CG2	2.44	0.45
1:D:1503:ALA:HA	1:D:1506:GLN:HE21	1.81	0.45
2:E:259:THR:OG1	2:E:288:SER:HA	2.16	0.45
2:E:1338:ILE:HG22	2:E:1390:VAL:HG11	1.98	0.45
1:K:32:GLN:NE2	1:K:57:ALA:CB	2.79	0.45
1:K:401:THR:HG22	1:K:733:ILE:HG12	1.97	0.45
1:K:719:GLN:HG3	1:K:1612:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:54:PRO:HG3	2:L:63:LYS:HG3	1.97	0.45
2:L:259:THR:OG1	2:L:288:SER:HA	2.16	0.45
2:L:278:VAL:HB	2:L:479:ILE:HD13	1.99	0.45
2:H:1338:ILE:HG22	2:H:1390:VAL:HG11	1.98	0.45
1:I:402:PHE:HE1	1:I:1612:ASP:HB2	1.81	0.45
2:J:1292:ILE:HD11	2:J:1366:LEU:HD23	1.98	0.45
2:G:1195:VAL:HG13	2:G:1211:LEU:HB3	1.98	0.45
1:B:855:SER:HB2	1:K:937:LYS:HD2	1.98	0.45
2:E:1638:ILE:HD13	2:E:1657:ILE:HD13	1.98	0.45
1:F:719:GLN:HG3	1:F:1612:ASP:HA	1.99	0.45
2:H:808:ALA:HB3	2:H:811:VAL:HG13	1.98	0.45
2:H:864:LEU:HD22	2:H:898:ASP:HB2	1.98	0.45
2:H:1195:VAL:HG13	2:H:1211:LEU:HB3	1.99	0.45
2:H:1370:ASP:OD1	2:H:1370:ASP:N	2.50	0.45
1:I:488:PRO:HG3	1:I:728:LYS:HG2	1.97	0.45
2:J:54:PRO:HG3	2:J:63:LYS:HG3	1.97	0.45
1:A:855:SER:HB2	1:F:937:LYS:HD2	1.98	0.45
2:G:259:THR:OG1	2:G:288:SER:HA	2.16	0.45
2:G:1638:ILE:HD13	2:G:1657:ILE:HD13	1.98	0.45
1:B:402:PHE:HE1	1:B:1612:ASP:HB2	1.81	0.45
2:C:860:ARG:NH2	2:C:1047:ASP:OD2	2.49	0.45
2:C:1036:GLN:HB3	2:C:1051:THR:CG2	2.24	0.45
2:C:1850:SER:HB3	2:C:1973:SER:HB2	1.99	0.45
1:D:1226:SER:O	1:D:1226:SER:OG	2.32	0.45
1:D:1233:GLU:OE2	1:D:1680:ARG:NH1	2.50	0.45
2:E:326:ASP:OD2	2:E:387:TYR:OH	2.33	0.45
2:E:1292:ILE:HD11	2:E:1366:LEU:HD23	1.98	0.45
1:K:448:ILE:HD13	1:K:481:LYS:HG2	1.99	0.45
1:K:1792:THR:HG21	1:K:1838:GLU:HG2	1.97	0.45
2:L:1330:GLY:HA2	2:L:1374:THR:HG21	1.99	0.45
1:F:1486:LEU:HD21	1:F:1761:LYS:HZ2	1.81	0.45
2:H:245:GLN:HE21	2:H:506:PRO:HD3	1.81	0.45
1:I:400:ARG:NH1	1:I:1358:HIS:O	2.40	0.45
1:I:1107:GLU:OE1	1:I:1191:THR:OG1	2.29	0.45
2:G:245:GLN:HE21	2:G:506:PRO:HD3	1.81	0.45
2:C:259:THR:OG1	2:C:288:SER:HA	2.16	0.45
2:C:320:PRO:HA	2:C:321:PRO:HD3	1.89	0.45
2:C:1338:ILE:HG22	2:C:1390:VAL:HG11	1.98	0.45
2:E:1422:THR:HG23	2:E:1474:PHE:HB2	1.97	0.45
1:K:678:VAL:HG22	1:K:767:ALA:HB3	1.98	0.45
2:H:716:VAL:HG11	2:H:730:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1037:SER:OG	2:H:1053:ILE:HD11	2.16	0.45
2:H:1638:ILE:HD13	2:H:1657:ILE:HD13	1.98	0.45
2:J:278:VAL:HB	2:J:479:ILE:HD13	1.99	0.45
2:J:1850:SER:HB3	2:J:1973:SER:HB2	1.99	0.45
1:A:402:PHE:HE1	1:A:1612:ASP:HB2	1.81	0.45
1:A:1303:GLY:HA2	1:A:1649:LYS:HZ2	1.81	0.45
2:G:1338:ILE:HG22	2:G:1390:VAL:HG11	1.98	0.45
1:B:678:VAL:HG22	1:B:767:ALA:HB3	1.98	0.45
1:B:1107:GLU:OE1	1:B:1191:THR:OG1	2.29	0.45
2:C:245:GLN:HE21	2:C:506:PRO:HD3	1.81	0.45
2:E:808:ALA:HB3	2:E:811:VAL:HG13	1.98	0.45
2:E:835:THR:HG23	2:E:843:ILE:O	2.16	0.45
2:E:1330:GLY:HA2	2:E:1374:THR:HG21	1.99	0.45
1:K:1107:GLU:OE1	1:K:1191:THR:OG1	2.29	0.45
1:K:1233:GLU:OE2	1:K:1680:ARG:NH1	2.50	0.45
1:F:1830:GLY:HA2	1:F:1831:GLY:HA2	1.62	0.45
1:I:1226:SER:O	1:I:1226:SER:OG	2.32	0.45
2:J:259:THR:OG1	2:J:288:SER:HA	2.16	0.45
2:J:1800:ALA:O	2:J:2009:LYS:NZ	2.47	0.45
2:G:847:ARG:HG2	2:G:847:ARG:H	1.41	0.45
1:B:1830:GLY:HA2	1:B:1831:GLY:HA2	1.62	0.45
2:C:1195:VAL:HG13	2:C:1211:LEU:HB3	1.99	0.45
1:K:46:GLU:OE2	2:L:1667:THR:OG1	2.32	0.45
2:L:1850:SER:HB3	2:L:1973:SER:HB2	1.99	0.45
1:F:401:THR:HG22	1:F:733:ILE:HG12	1.97	0.45
1:F:539:SER:HB2	1:F:633:GLU:HA	1.97	0.45
1:A:488:PRO:HG3	1:A:728:LYS:HG2	1.97	0.45
2:G:176:LEU:HG	2:G:180:TYR:HD2	1.82	0.45
2:G:326:ASP:OD2	2:G:387:TYR:OH	2.33	0.45
2:G:1037:SER:CB	2:G:1053:ILE:CG1	2.92	0.45
1:D:1830:GLY:HA2	1:D:1831:GLY:HA2	1.62	0.45
2:E:731:GLN:HA	2:E:766:ILE:HB	1.99	0.45
2:L:731:GLN:HA	2:L:766:ILE:HB	1.99	0.45
2:L:1195:VAL:HG13	2:L:1211:LEU:HB3	1.98	0.45
1:F:1503:ALA:HA	1:F:1506:GLN:HE21	1.81	0.45
1:I:1271:GLN:HB2	1:I:1274:ILE:HG23	1.97	0.45
1:I:1852:HIS:HA	1:I:1856:LYS:HE3	1.97	0.45
2:J:176:LEU:HG	2:J:180:TYR:HD2	1.82	0.45
1:A:719:GLN:HG3	1:A:1612:ASP:HA	1.99	0.45
2:G:278:VAL:HB	2:G:479:ILE:HD13	1.99	0.45
2:G:1422:THR:HG23	2:G:1474:PHE:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2041:ILE:HD12	2:G:2041:ILE:HA	1.87	0.45
1:B:719:GLN:HG3	1:B:1612:ASP:HA	1.99	0.45
1:B:1271:GLN:HB2	1:B:1274:ILE:HG23	1.97	0.45
1:F:1026:GLU:OE1	1:F:1594:ASN:ND2	2.40	0.45
1:F:1107:GLU:OE1	1:F:1191:THR:OG1	2.29	0.45
2:H:176:LEU:HG	2:H:180:TYR:HD2	1.82	0.45
2:H:1422:THR:HG23	2:H:1474:PHE:HB2	1.97	0.45
2:H:1800:ALA:O	2:H:2009:LYS:NZ	2.48	0.45
1:I:1233:GLU:OE2	1:I:1680:ARG:NH1	2.50	0.45
2:G:808:ALA:HB3	2:G:811:VAL:HG13	1.98	0.45
2:G:1292:ILE:HD11	2:G:1366:LEU:HD23	1.98	0.45
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.99	0.45
2:G:1789:PHE:CD2	2:G:1817:SER:HB3	2.52	0.45
1:B:1041:ALA:O	1:B:1630:THR:OG1	2.29	0.45
2:E:646:THR:OG1	2:E:677:GLN:OE1	2.28	0.45
2:E:1195:VAL:HG13	2:E:1211:LEU:HB3	1.99	0.45
2:E:1740:THR:O	2:E:1740:THR:OG1	2.31	0.45
1:K:488:PRO:HG3	1:K:728:LYS:HG2	1.97	0.45
1:F:717:TYR:CZ	1:F:721:ILE:HD11	2.52	0.45
2:H:860:ARG:NH2	2:H:1047:ASP:OD2	2.49	0.45
2:H:1086:LEU:HG	2:H:1092:ASP:HA	1.99	0.45
2:H:1292:ILE:HD11	2:H:1366:LEU:HD23	1.98	0.45
1:I:430:ARG:HG2	1:I:605:LEU:HD22	1.98	0.45
1:A:717:TYR:CZ	1:A:721:ILE:HD11	2.52	0.44
2:G:1086:LEU:HG	2:G:1092:ASP:HA	1.99	0.44
2:C:176:LEU:HG	2:C:180:TYR:HD2	1.82	0.44
1:D:448:ILE:HD13	1:D:481:LYS:HG2	1.99	0.44
1:F:1233:GLU:OE2	1:F:1680:ARG:NH1	2.50	0.44
1:F:1561:MET:N	1:F:1561:MET:HE3	2.32	0.44
2:H:553:ASN:O	2:H:556:LYS:NZ	2.39	0.44
2:H:1740:THR:O	2:H:1740:THR:OG1	2.31	0.44
1:I:32:GLN:NE2	1:I:57:ALA:CB	2.78	0.44
2:J:326:ASP:OD2	2:J:387:TYR:OH	2.33	0.44
2:J:864:LEU:HD22	2:J:898:ASP:HB2	1.97	0.44
1:B:16:GLU:CG	2:C:2038:ILE:HD11	2.46	0.44
2:C:604:PRO:HA	2:C:607:VAL:HG12	2.00	0.44
2:C:731:GLN:HA	2:C:766:ILE:HB	1.99	0.44
1:D:1020:VAL:HG11	1:D:1400:ILE:HG12	1.99	0.44
2:E:596:GLY:N	2:E:618:GLU:OE1	2.46	0.44
2:E:1782:THR:HG21	2:E:1831:VAL:HG21	2.00	0.44
2:L:176:LEU:HG	2:L:180:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:900:GLN:HB3	2:L:1050:ARG:O	2.16	0.44
2:L:1338:ILE:HG22	2:L:1390:VAL:HG11	1.98	0.44
1:F:430:ARG:HG2	1:F:605:LEU:HD22	1.98	0.44
1:F:1097:ILE:O	1:F:1101:SER:OG	2.33	0.44
2:H:596:GLY:N	2:H:618:GLU:OE1	2.46	0.44
2:H:731:GLN:HA	2:H:766:ILE:HB	1.99	0.44
2:H:1789:PHE:CD2	2:H:1817:SER:HB3	2.52	0.44
1:B:431:GLU:O	1:B:435:GLU:N	2.49	0.44
2:C:1037:SER:CB	2:C:1053:ILE:CG1	2.92	0.44
1:D:47:ILE:HD12	2:E:1666:PHE:HE1	1.83	0.44
2:E:176:LEU:HG	2:E:180:TYR:HD2	1.82	0.44
2:E:278:VAL:HB	2:E:479:ILE:HD13	1.99	0.44
1:K:16:GLU:CG	2:L:2038:ILE:HD11	2.46	0.44
1:K:1486:LEU:HD21	1:K:1761:LYS:HZ2	1.81	0.44
1:K:1694:TYR:OH	2:L:1001:ASP:OD2	2.35	0.44
2:L:326:ASP:OD2	2:L:387:TYR:OH	2.33	0.44
2:L:1789:PHE:CD2	2:L:1817:SER:HB3	2.52	0.44
1:F:431:GLU:O	1:F:435:GLU:N	2.49	0.44
2:J:320:PRO:HA	2:J:321:PRO:HD3	1.89	0.44
2:J:604:PRO:HA	2:J:607:VAL:HG12	2.00	0.44
2:J:1789:PHE:CD2	2:J:1817:SER:HB3	2.52	0.44
2:G:1782:THR:HG21	2:G:1831:VAL:HG21	2.00	0.44
1:B:774:ILE:HD11	1:B:791:ALA:HB2	1.99	0.44
1:F:1303:GLY:H	1:F:1307:THR:HG22	1.83	0.44
1:I:448:ILE:HD13	1:I:481:LYS:HG2	1.99	0.44
1:I:1491:ARG:HA	1:I:1750:ILE:CD1	2.48	0.44
2:J:1370:ASP:N	2:J:1370:ASP:OD1	2.50	0.44
2:J:1739:GLU:H	2:J:1739:GLU:HG2	1.66	0.44
1:A:1373:ARG:HH21	1:A:1550:ASP:HB2	1.83	0.44
2:G:604:PRO:HA	2:G:607:VAL:HG12	2.00	0.44
2:G:864:LEU:HD22	2:G:898:ASP:HB2	1.98	0.44
2:G:1850:SER:HB3	2:G:1973:SER:HB2	1.99	0.44
1:D:1491:ARG:HA	1:D:1750:ILE:CD1	2.48	0.44
2:E:1810:GLY:HA2	2:E:1813:ALA:HB3	2.00	0.44
2:E:1850:SER:HB3	2:E:1973:SER:HB2	1.99	0.44
1:K:1020:VAL:HG11	1:K:1400:ILE:HG12	1.99	0.44
2:L:1800:ALA:O	2:L:2009:LYS:NZ	2.47	0.44
2:L:1866:PHE:HE2	2:L:1871:LEU:HD12	1.83	0.44
1:F:47:ILE:HD12	2:H:1666:PHE:HE1	1.83	0.44
2:H:919:TYR:HE1	2:H:995:LEU:HA	1.83	0.44
1:I:1020:VAL:HG11	1:I:1400:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1810:GLY:HA2	2:J:1813:ALA:HB3	2.00	0.44
2:G:919:TYR:HE1	2:G:995:LEU:HA	1.83	0.44
1:B:448:ILE:HD13	1:B:481:LYS:HG2	1.99	0.44
2:C:278:VAL:HB	2:C:479:ILE:HD13	1.99	0.44
2:C:1086:LEU:HG	2:C:1092:ASP:HA	1.99	0.44
2:C:1628:HIS:HA	2:C:1638:ILE:HG13	2.00	0.44
2:C:1849:ARG:HH11	2:C:1957:PRO:HG2	1.83	0.44
1:D:430:ARG:HG2	1:D:605:LEU:HD22	1.98	0.44
1:D:717:TYR:CZ	1:D:721:ILE:HD11	2.52	0.44
1:D:774:ILE:HD11	1:D:791:ALA:HB2	1.99	0.44
1:D:1303:GLY:H	1:D:1307:THR:HG22	1.83	0.44
2:E:245:GLN:HE21	2:E:506:PRO:HD3	1.81	0.44
2:E:287:ASP:HB3	2:E:288:SER:H	1.59	0.44
2:E:1737:ILE:HG12	2:E:1748:THR:HG22	1.95	0.44
2:E:1800:ALA:O	2:E:2009:LYS:NZ	2.47	0.44
2:E:1866:PHE:HE2	2:E:1871:LEU:HD12	1.83	0.44
1:K:47:ILE:HD12	2:L:1666:PHE:HE1	1.83	0.44
1:K:430:ARG:HG2	1:K:605:LEU:HD22	1.98	0.44
2:L:919:TYR:HE1	2:L:995:LEU:HA	1.83	0.44
1:F:774:ILE:HD11	1:F:791:ALA:HB2	1.99	0.44
1:F:1020:VAL:HG11	1:F:1400:ILE:HG12	1.99	0.44
1:F:1373:ARG:HH21	1:F:1550:ASP:HB2	1.83	0.44
1:F:1491:ARG:HA	1:F:1750:ILE:CD1	2.48	0.44
2:H:101:ILE:O	2:H:105:ALA:N	2.51	0.44
2:H:1782:THR:HG21	2:H:1831:VAL:HG21	2.00	0.44
1:I:774:ILE:HD11	1:I:791:ALA:HB2	1.99	0.44
1:I:1373:ARG:HH21	1:I:1550:ASP:HB2	1.83	0.44
1:I:1851:LEU:HD22	1:I:1855:ALA:HB1	2.00	0.44
1:A:1303:GLY:H	1:A:1307:THR:HG22	1.82	0.44
1:A:1491:ARG:HA	1:A:1750:ILE:CD1	2.48	0.44
2:G:1381:VAL:O	2:G:1422:THR:OG1	2.28	0.44
2:G:1810:GLY:HA2	2:G:1813:ALA:HB3	2.00	0.44
2:C:1697:HIS:O	2:C:1701:THR:OG1	2.28	0.44
1:D:402:PHE:HE1	1:D:1612:ASP:HB2	1.81	0.44
1:D:719:GLN:HG3	1:D:1612:ASP:HA	1.99	0.44
2:E:919:TYR:HE1	2:E:995:LEU:HA	1.83	0.44
2:E:1730:ARG:NH1	2:E:1759:SER:O	2.43	0.44
1:K:1106:ILE:HA	1:K:1188:GLN:NE2	2.33	0.44
2:L:1086:LEU:HG	2:L:1092:ASP:HA	1.99	0.44
2:L:1691:TRP:O	2:L:1695:ASP:N	2.40	0.44
2:H:1850:SER:HB3	2:H:1973:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:719:GLN:HG3	1:I:1612:ASP:HA	1.99	0.44
1:I:1009:LEU:HG	1:I:1664:ALA:HB2	2.00	0.44
1:I:1303:GLY:H	1:I:1307:THR:HG22	1.83	0.44
2:J:1330:GLY:HA2	2:J:1374:THR:HG21	1.99	0.44
2:J:1628:HIS:HA	2:J:1638:ILE:HG13	2.00	0.44
1:A:448:ILE:HD13	1:A:481:LYS:HG2	1.99	0.44
1:A:1233:GLU:OE2	1:A:1680:ARG:NH1	2.50	0.44
2:G:731:GLN:HA	2:G:766:ILE:HB	1.99	0.44
1:B:717:TYR:CZ	1:B:721:ILE:HD11	2.52	0.44
1:B:1106:ILE:HA	1:B:1188:GLN:NE2	2.33	0.44
2:C:1789:PHE:CD2	2:C:1817:SER:HB3	2.52	0.44
2:E:641:ILE:HG12	2:E:645:SER:HB2	2.00	0.44
2:E:844:VAL:HB	2:E:845:THR:H	1.70	0.44
1:K:402:PHE:HE1	1:K:1612:ASP:HB2	1.81	0.44
2:L:264:ARG:NH1	2:L:284:ALA:O	2.51	0.44
2:L:808:ALA:HB3	2:L:811:VAL:HG13	1.98	0.44
2:L:1782:THR:HG21	2:L:1831:VAL:HG21	2.00	0.44
1:F:402:PHE:HE1	1:F:1612:ASP:HB2	1.81	0.44
1:F:448:ILE:HD13	1:F:481:LYS:HG2	1.99	0.44
2:J:900:GLN:HB3	2:J:1050:ARG:O	2.16	0.44
2:J:1086:LEU:HG	2:J:1092:ASP:HA	2.00	0.44
1:A:937:LYS:HD2	1:F:855:SER:HB2	1.98	0.44
1:A:1851:LEU:HD22	1:A:1855:ALA:HB1	2.00	0.44
2:G:101:ILE:O	2:G:105:ALA:N	2.51	0.44
2:G:596:GLY:N	2:G:618:GLU:OE1	2.46	0.44
2:C:264:ARG:NH1	2:C:284:ALA:O	2.51	0.44
2:C:844:VAL:HB	2:C:845:THR:H	1.70	0.44
2:C:1330:GLY:HA2	2:C:1374:THR:HG21	1.99	0.44
1:D:687:SER:HA	1:D:875:THR:HG22	2.00	0.44
2:E:1086:LEU:HG	2:E:1092:ASP:HA	2.00	0.44
2:E:1884:TRP:HB3	2:E:1906:ALA:HB2	2.00	0.44
2:L:604:PRO:HA	2:L:607:VAL:HG12	2.00	0.44
2:L:1810:GLY:HA2	2:L:1813:ALA:HB3	2.00	0.44
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.99	0.44
2:H:1810:GLY:HA2	2:H:1813:ALA:HB3	2.00	0.44
1:I:13:LEU:HD21	2:J:2025:TYR:CE2	2.53	0.44
1:I:16:GLU:CG	2:J:2038:ILE:HD11	2.46	0.44
1:I:717:TYR:CZ	1:I:721:ILE:HD11	2.52	0.44
2:G:1800:ALA:O	2:G:2009:LYS:NZ	2.47	0.43
1:B:1020:VAL:HG11	1:B:1400:ILE:HG12	1.99	0.43
1:B:1397:GLY:O	1:B:1680:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1851:LEU:HD22	1:B:1855:ALA:HB1	2.00	0.43
2:C:1801:ASP:HA	2:C:2009:LYS:HD3	2.00	0.43
1:D:855:SER:HB2	1:I:937:LYS:HD2	1.98	0.43
1:K:1491:ARG:HA	1:K:1750:ILE:CD1	2.48	0.43
1:I:1830:GLY:HA2	1:I:1831:GLY:HA2	1.62	0.43
2:G:984:PHE:O	2:G:991:ARG:NH1	2.52	0.43
1:K:717:TYR:CZ	1:K:721:ILE:HD11	2.52	0.43
2:L:370:LEU:HD12	2:L:378:VAL:HG21	2.01	0.43
2:L:1665:VAL:HG12	2:L:1805:ALA:HB3	2.00	0.43
2:H:1665:VAL:HG12	2:H:1805:ALA:HB3	2.00	0.43
2:H:1884:TRP:HB3	2:H:1906:ALA:HB2	2.00	0.43
2:J:641:ILE:HG12	2:J:645:SER:HB2	2.00	0.43
2:G:534:ASP:HB2	2:G:543:PHE:CE1	2.53	0.43
1:B:1026:GLU:OE1	1:B:1594:ASN:ND2	2.40	0.43
1:B:1233:GLU:OE2	1:B:1680:ARG:NH1	2.50	0.43
2:C:919:TYR:HE1	2:C:995:LEU:HA	1.83	0.43
2:C:1665:VAL:HG12	2:C:1805:ALA:HB3	2.00	0.43
2:C:1810:GLY:HA2	2:C:1813:ALA:HB3	2.00	0.43
1:D:1851:LEU:HD22	1:D:1855:ALA:HB1	2.00	0.43
2:E:370:LEU:HD12	2:E:378:VAL:HG21	2.01	0.43
2:E:1370:ASP:N	2:E:1370:ASP:OD1	2.50	0.43
2:E:1665:VAL:HG12	2:E:1805:ALA:HB3	2.00	0.43
2:E:1789:PHE:CD2	2:E:1817:SER:HB3	2.52	0.43
2:L:641:ILE:HG12	2:L:645:SER:HB2	2.00	0.43
2:L:1849:ARG:HH11	2:L:1957:PRO:HG2	1.83	0.43
2:H:264:ARG:NH1	2:H:284:ALA:O	2.51	0.43
2:H:534:ASP:HB2	2:H:543:PHE:CE1	2.53	0.43
2:J:101:ILE:O	2:J:105:ALA:N	2.51	0.43
2:J:731:GLN:HA	2:J:766:ILE:HB	1.99	0.43
2:J:1782:THR:HG21	2:J:1831:VAL:HG21	2.00	0.43
1:A:13:LEU:HD21	2:G:2025:TYR:CE2	2.53	0.43
1:A:47:ILE:HD12	2:G:1666:PHE:HE1	1.83	0.43
1:A:1107:GLU:OE1	1:A:1191:THR:OG1	2.29	0.43
2:G:1665:VAL:HG12	2:G:1805:ALA:HB3	2.00	0.43
2:C:287:ASP:HB3	2:C:288:SER:H	1.59	0.43
2:C:808:ALA:HB3	2:C:811:VAL:HG13	1.98	0.43
1:D:1694:TYR:OH	2:E:1001:ASP:OD2	2.35	0.43
1:K:1421:PRO:HB2	1:K:1552:ASN:HD22	1.84	0.43
2:L:534:ASP:HB2	2:L:543:PHE:CE1	2.53	0.43
1:F:687:SER:HA	1:F:875:THR:HG22	2.00	0.43
2:H:1174:PHE:CD1	2:H:1197:LEU:HG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:808:ALA:HB3	2:J:811:VAL:HG13	1.98	0.43
2:J:1665:VAL:HG12	2:J:1805:ALA:HB3	2.00	0.43
1:A:1020:VAL:HG11	1:A:1400:ILE:HG12	1.99	0.43
1:A:1744:TYR:HB2	1:K:1432:HIS:CE1	2.54	0.43
2:G:1866:PHE:HE2	2:G:1871:LEU:HD12	1.83	0.43
1:B:46:GLU:OE2	2:C:1667:THR:OG1	2.32	0.43
1:B:1744:TYR:HB2	1:I:1432:HIS:CE1	2.54	0.43
2:C:534:ASP:HB2	2:C:543:PHE:CE1	2.53	0.43
2:C:1370:ASP:OD1	2:C:1370:ASP:N	2.50	0.43
2:C:1782:THR:HG21	2:C:1831:VAL:HG21	2.00	0.43
2:E:264:ARG:NH1	2:E:284:ALA:O	2.51	0.43
1:K:1009:LEU:HG	1:K:1664:ALA:HB2	2.00	0.43
1:K:1397:GLY:O	1:K:1680:ARG:HG3	2.18	0.43
2:L:1174:PHE:CD1	2:L:1197:LEU:HG	2.54	0.43
2:L:1370:ASP:N	2:L:1370:ASP:OD1	2.50	0.43
2:L:1628:HIS:HA	2:L:1638:ILE:HG13	2.00	0.43
1:F:13:LEU:HD21	2:H:2025:TYR:CE2	2.53	0.43
2:J:919:TYR:HE1	2:J:995:LEU:HA	1.83	0.43
1:A:1421:PRO:HB2	1:A:1552:ASN:HD22	1.84	0.43
1:A:1694:TYR:OH	2:G:1001:ASP:OD2	2.35	0.43
2:G:1628:HIS:HA	2:G:1638:ILE:HG13	2.00	0.43
1:B:47:ILE:HD12	2:C:1666:PHE:HE1	1.83	0.43
1:B:1432:HIS:CE1	1:I:1744:TYR:HB2	2.54	0.43
1:B:1491:ARG:HA	1:B:1750:ILE:CD1	2.48	0.43
2:C:370:LEU:HD12	2:C:378:VAL:HG21	2.01	0.43
2:E:1174:PHE:CD1	2:E:1197:LEU:HG	2.54	0.43
1:K:1303:GLY:H	1:K:1307:THR:HG22	1.82	0.43
1:F:1421:PRO:HB2	1:F:1552:ASN:HD22	1.84	0.43
2:H:295:SER:O	2:H:298:LYS:CB	2.59	0.43
2:H:604:PRO:HA	2:H:607:VAL:HG12	2.00	0.43
2:H:984:PHE:O	2:H:991:ARG:NH1	2.52	0.43
2:H:1801:ASP:HA	2:H:2009:LYS:HD3	2.00	0.43
1:I:1220:VAL:HG21	1:I:1698:PHE:HD1	1.84	0.43
1:I:1694:TYR:OH	2:J:1001:ASP:OD2	2.35	0.43
2:J:109:LEU:HD22	2:J:114:THR:HG23	2.01	0.43
2:J:1849:ARG:HH11	2:J:1957:PRO:HG2	1.83	0.43
1:A:46:GLU:OE2	2:G:1667:THR:OG1	2.32	0.43
1:A:431:GLU:O	1:A:435:GLU:N	2.49	0.43
2:G:641:ILE:HG12	2:G:645:SER:HB2	2.00	0.43
2:C:109:LEU:HD22	2:C:114:THR:HG23	2.01	0.43
1:D:1106:ILE:HA	1:D:1188:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1373:ARG:HH21	1:D:1550:ASP:HB2	1.83	0.43
2:E:604:PRO:HA	2:E:607:VAL:HG12	2.00	0.43
2:E:984:PHE:O	2:E:991:ARG:NH1	2.52	0.43
1:K:774:ILE:HD11	1:K:791:ALA:HB2	1.99	0.43
2:L:109:LEU:HD22	2:L:114:THR:HG23	2.01	0.43
2:H:278:VAL:HB	2:H:479:ILE:HD13	1.99	0.43
2:H:641:ILE:HG12	2:H:645:SER:HB2	2.00	0.43
2:H:1849:ARG:HH11	2:H:1957:PRO:HG2	1.83	0.43
1:I:171:THR:HG23	1:I:174:ASP:H	1.84	0.43
1:I:431:GLU:O	1:I:435:GLU:N	2.49	0.43
1:I:1106:ILE:HA	1:I:1188:GLN:NE2	2.33	0.43
1:I:1397:GLY:O	1:I:1680:ARG:HG3	2.18	0.43
2:J:1174:PHE:CD1	2:J:1197:LEU:HG	2.54	0.43
2:J:1195:VAL:HG13	2:J:1211:LEU:HB3	1.99	0.43
2:J:1767:GLU:OE2	2:J:1849:ARG:NE	2.36	0.43
1:A:1220:VAL:HG21	1:A:1698:PHE:HD1	1.84	0.43
2:G:109:LEU:HD22	2:G:114:THR:HG23	2.01	0.43
2:G:1174:PHE:CD1	2:G:1197:LEU:HG	2.54	0.43
2:G:1801:ASP:HA	2:G:2009:LYS:HD3	2.01	0.43
2:C:295:SER:O	2:C:298:LYS:CB	2.59	0.43
2:C:1866:PHE:HE2	2:C:1871:LEU:HD12	1.83	0.43
2:C:1890:ASN:HB2	2:C:1899:VAL:HB	2.01	0.43
1:D:1421:PRO:HB2	1:D:1552:ASN:HD22	1.84	0.43
2:E:1801:ASP:HA	2:E:2009:LYS:HD3	2.00	0.43
2:L:984:PHE:O	2:L:991:ARG:NH1	2.52	0.43
2:L:2041:ILE:HD12	2:L:2041:ILE:HA	1.87	0.43
2:H:370:LEU:HD12	2:H:378:VAL:HG21	2.01	0.43
1:I:1549:ASN:ND2	1:I:1549:ASN:C	2.73	0.43
2:J:534:ASP:HB2	2:J:543:PHE:CE1	2.54	0.43
1:A:774:ILE:HD11	1:A:791:ALA:HB2	1.99	0.43
1:A:1009:LEU:HG	1:A:1664:ALA:HB2	2.00	0.43
1:A:1432:HIS:CE1	1:K:1744:TYR:HB2	2.54	0.43
1:B:1303:GLY:H	1:B:1307:THR:HG22	1.83	0.43
1:D:1432:HIS:CE1	1:F:1744:TYR:HB2	2.54	0.43
2:E:1068:GLU:HA	2:E:1069:PRO:HD3	1.92	0.43
2:E:1890:ASN:HB2	2:E:1899:VAL:HB	2.01	0.43
2:L:1381:VAL:O	2:L:1422:THR:OG1	2.28	0.43
1:F:409:ALA:HB2	1:F:442:ARG:HE	1.84	0.43
1:F:1851:LEU:HD22	1:F:1855:ALA:HB1	2.00	0.43
2:H:1628:HIS:HA	2:H:1638:ILE:HG13	2.00	0.43
2:H:1866:PHE:HE2	2:H:1871:LEU:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:264:ARG:NH1	2:J:284:ALA:O	2.51	0.43
2:J:976:PRO:O	2:J:980:ILE:N	2.48	0.43
2:J:1884:TRP:HB3	2:J:1906:ALA:HB2	2.00	0.43
1:A:16:GLU:CG	2:G:2038:ILE:HD11	2.46	0.43
2:G:370:LEU:HD12	2:G:378:VAL:HG21	2.01	0.43
2:G:1370:ASP:N	2:G:1370:ASP:OD1	2.50	0.43
1:B:848:THR:CG2	1:K:844:LEU:HD23	2.44	0.43
1:B:1421:PRO:HB2	1:B:1552:ASN:HD22	1.84	0.43
1:D:13:LEU:HD21	2:E:2025:TYR:CE2	2.53	0.43
1:D:16:GLU:CG	2:E:2038:ILE:HD11	2.46	0.43
2:E:109:LEU:HD22	2:E:114:THR:HG23	2.01	0.43
2:E:283:ILE:O	2:E:286:THR:HG22	2.19	0.43
2:E:1628:HIS:HA	2:E:1638:ILE:HG13	2.00	0.43
1:K:770:PRO:HB2	1:K:799:ILE:HG12	2.01	0.43
2:L:158:ALA:HA	2:L:502:LEU:HB2	2.01	0.43
2:L:1801:ASP:HA	2:L:2009:LYS:HD3	2.01	0.43
2:L:1884:TRP:HB3	2:L:1906:ALA:HB2	2.00	0.43
1:F:17:LEU:HD23	2:H:2014:LEU:HD23	2.01	0.43
2:H:581:THR:H	2:H:584:SER:HG	1.64	0.43
1:I:687:SER:HA	1:I:875:THR:HG22	2.00	0.43
1:I:877:LEU:HD11	3:I:2001:NDP:C2D	2.47	0.43
1:I:1421:PRO:HB2	1:I:1552:ASN:HD22	1.84	0.43
1:A:877:LEU:HD11	3:A:2001:NDP:C2D	2.47	0.42
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	2.01	0.42
2:G:264:ARG:NH1	2:G:284:ALA:O	2.51	0.42
2:G:290:GLU:N	2:G:290:GLU:CD	2.73	0.42
1:B:171:THR:HG23	1:B:174:ASP:H	1.84	0.42
2:C:158:ALA:HA	2:C:502:LEU:HB2	2.01	0.42
1:D:1009:LEU:HG	1:D:1664:ALA:HB2	2.00	0.42
1:D:1303:GLY:HA2	1:D:1649:LYS:HZ1	1.84	0.42
1:D:1744:TYR:HB2	1:F:1432:HIS:CE1	2.54	0.42
2:E:919:TYR:CE1	2:E:995:LEU:HA	2.54	0.42
1:K:13:LEU:HD21	2:L:2025:TYR:CE2	2.53	0.42
1:K:1851:LEU:HD22	1:K:1855:ALA:HB1	2.00	0.42
2:L:844:VAL:HB	2:L:845:THR:H	1.70	0.42
1:F:1009:LEU:HG	1:F:1664:ALA:HB2	2.00	0.42
1:F:1279:PHE:HB2	1:F:1282:THR:HG23	2.01	0.42
2:H:577:ILE:HB	2:H:1082:ILE:HD11	2.01	0.42
2:H:884:LEU:HD22	2:H:1021:LEU:HD12	2.01	0.42
2:H:1890:ASN:HB2	2:H:1899:VAL:HB	2.01	0.42
1:I:1017:ARG:NH1	1:I:1511:ASP:OD2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:370:LEU:HD12	2:J:378:VAL:HG21	2.01	0.42
2:J:1801:ASP:HA	2:J:2009:LYS:HD3	2.00	0.42
2:J:1890:ASN:HB2	2:J:1899:VAL:HB	2.01	0.42
1:A:33:ASP:OD2	1:A:64:LYS:NZ	2.41	0.42
1:A:1549:ASN:ND2	1:A:1549:ASN:C	2.73	0.42
2:G:158:ALA:HA	2:G:502:LEU:HB2	2.01	0.42
2:G:646:THR:OG1	2:G:677:GLN:OE1	2.28	0.42
1:B:13:LEU:HD21	2:C:2025:TYR:CE2	2.53	0.42
1:B:770:PRO:HB2	1:B:799:ILE:HG12	2.01	0.42
1:B:1549:ASN:C	1:B:1549:ASN:ND2	2.73	0.42
2:C:641:ILE:HG12	2:C:645:SER:HB2	2.00	0.42
2:C:1174:PHE:CD1	2:C:1197:LEU:HG	2.54	0.42
2:C:1884:TRP:HB3	2:C:1906:ALA:HB2	2.00	0.42
1:D:981:GLU:HA	2:E:964:LEU:HA	2.01	0.42
1:D:1397:GLY:O	1:D:1680:ARG:HG3	2.18	0.42
2:E:184:VAL:HG12	2:E:188:ILE:HG12	2.01	0.42
2:E:884:LEU:HD22	2:E:1021:LEU:HD12	2.01	0.42
2:E:1561:ASN:HB3	2:E:1564:HIS:HD2	1.84	0.42
2:E:1849:ARG:HH11	2:E:1957:PRO:HG2	1.83	0.42
2:H:109:LEU:HD22	2:H:114:THR:HG23	2.01	0.42
2:H:158:ALA:HA	2:H:502:LEU:HB2	2.01	0.42
2:H:184:VAL:HG12	2:H:188:ILE:HG12	2.01	0.42
2:H:919:TYR:CE1	2:H:995:LEU:HA	2.54	0.42
1:I:46:GLU:OE2	2:J:1667:THR:OG1	2.32	0.42
1:I:47:ILE:HD12	2:J:1666:PHE:HE1	1.83	0.42
1:I:1279:PHE:HB2	1:I:1282:THR:HG23	2.01	0.42
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	2.01	0.42
1:B:1009:LEU:HG	1:B:1664:ALA:HB2	2.00	0.42
1:B:1220:VAL:HG21	1:B:1698:PHE:HD1	1.84	0.42
2:C:184:VAL:HG12	2:C:188:ILE:HG12	2.01	0.42
2:C:884:LEU:HD22	2:C:1021:LEU:HD12	2.01	0.42
2:C:984:PHE:O	2:C:991:ARG:NH1	2.52	0.42
2:E:534:ASP:HB2	2:E:543:PHE:CE1	2.54	0.42
2:E:1386:THR:HG23	2:E:1411:PHE:HZ	1.84	0.42
1:K:1830:GLY:HA2	1:K:1831:GLY:HA2	1.62	0.42
2:L:1767:GLU:OE2	2:L:1849:ARG:NE	2.36	0.42
2:L:1890:ASN:HB2	2:L:1899:VAL:HB	2.01	0.42
1:F:1220:VAL:HG21	1:F:1698:PHE:HD1	1.84	0.42
2:J:884:LEU:HD22	2:J:1021:LEU:HD12	2.01	0.42
2:J:1386:THR:HG23	2:J:1411:PHE:HZ	1.84	0.42
2:J:1866:PHE:HE2	2:J:1871:LEU:HD12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	2.01	0.42
1:A:171:THR:HG23	1:A:174:ASP:H	1.84	0.42
1:A:1397:GLY:O	1:A:1680:ARG:HG3	2.18	0.42
2:G:184:VAL:HG12	2:G:188:ILE:HG12	2.01	0.42
2:G:919:TYR:CE1	2:G:995:LEU:HA	2.54	0.42
2:C:1730:ARG:NH1	2:C:1759:SER:O	2.43	0.42
2:C:2041:ILE:HD12	2:C:2041:ILE:HA	1.87	0.42
1:D:770:PRO:HB2	1:D:799:ILE:HG12	2.01	0.42
1:D:1279:PHE:HB2	1:D:1282:THR:HG23	2.01	0.42
2:L:184:VAL:HG12	2:L:188:ILE:HG12	2.01	0.42
2:L:283:ILE:O	2:L:286:THR:HG22	2.19	0.42
2:L:919:TYR:CE1	2:L:995:LEU:HA	2.54	0.42
2:L:1068:GLU:HA	2:L:1069:PRO:HD3	1.92	0.42
2:L:1730:ARG:NH1	2:L:1759:SER:O	2.43	0.42
1:F:171:THR:HG23	1:F:174:ASP:H	1.84	0.42
1:F:1001:VAL:HG11	1:F:1662:TYR:HB2	2.02	0.42
2:H:1310:ASP:OD1	2:H:1317:ARG:NH2	2.53	0.42
2:J:984:PHE:O	2:J:991:ARG:NH1	2.52	0.42
1:A:409:ALA:HB2	1:A:442:ARG:HE	1.84	0.42
1:A:687:SER:HA	1:A:875:THR:HG22	2.00	0.42
2:G:1737:ILE:HG12	2:G:1748:THR:HG22	1.95	0.42
2:G:1778:GLN:HA	2:G:1809:LEU:HD21	2.01	0.42
2:E:1485:CYS:HB3	2:E:1506:TYR:HB3	2.02	0.42
2:H:1068:GLU:HA	2:H:1069:PRO:HD3	1.92	0.42
1:I:35:PHE:HA	1:I:39:PHE:HD2	1.85	0.42
1:I:770:PRO:HB2	1:I:799:ILE:HG12	2.01	0.42
2:J:184:VAL:HG12	2:J:188:ILE:HG12	2.01	0.42
2:G:283:ILE:O	2:G:286:THR:HG22	2.19	0.42
2:G:577:ILE:HB	2:G:1082:ILE:HD11	2.01	0.42
2:G:1386:THR:HG23	2:G:1411:PHE:HZ	1.84	0.42
2:G:1849:ARG:HH11	2:G:1957:PRO:HG2	1.83	0.42
1:B:687:SER:HA	1:B:875:THR:HG22	2.00	0.42
1:B:1001:VAL:HG11	1:B:1662:TYR:HB2	2.02	0.42
1:D:171:THR:HG23	1:D:174:ASP:H	1.84	0.42
1:D:411:GLN:HE21	1:D:1629:LYS:HE2	1.85	0.42
2:E:528:ILE:HG21	2:E:547:ILE:HG13	2.02	0.42
1:K:17:LEU:HD23	2:L:2014:LEU:HD23	2.01	0.42
2:L:848:SER:HB3	2:L:854:ILE:HD12	2.00	0.42
1:F:35:PHE:HA	1:F:39:PHE:HD2	1.85	0.42
2:H:1037:SER:CB	2:H:1053:ILE:CG1	2.92	0.42
1:I:409:ALA:HB2	1:I:442:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:283:ILE:O	2:J:286:THR:HG22	2.19	0.42
2:G:585:LYS:HG3	2:G:1106:GLU:HB2	2.02	0.42
2:G:1884:TRP:HB3	2:G:1906:ALA:HB2	2.00	0.42
2:C:528:ILE:HG21	2:C:547:ILE:HG13	2.02	0.42
2:C:848:SER:HB3	2:C:854:ILE:HD12	2.00	0.42
2:E:290:GLU:N	2:E:290:GLU:CD	2.73	0.42
2:E:1037:SER:N	2:E:1051:THR:HG21	2.35	0.42
2:E:1267:TRP:NE1	2:E:1273:GLU:O	2.39	0.42
2:L:1265:MET:HE2	2:L:1562:PRO:HG2	2.02	0.42
2:L:1485:CYS:HB3	2:L:1506:TYR:HB3	2.02	0.42
2:H:283:ILE:O	2:H:286:THR:HG22	2.19	0.42
2:H:290:GLU:N	2:H:290:GLU:CD	2.73	0.42
2:H:549:ASP:HB3	2:H:554:GLY:HA3	2.02	0.42
2:J:158:ALA:HA	2:J:502:LEU:HB2	2.01	0.42
2:J:1310:ASP:OD1	2:J:1317:ARG:NH2	2.53	0.42
2:J:1432:GLN:N	2:J:1525:SER:O	2.52	0.42
2:G:1739:GLU:H	2:G:1739:GLU:HG2	1.66	0.42
2:C:283:ILE:O	2:C:286:THR:HG22	2.19	0.42
2:C:1485:CYS:HB3	2:C:1506:TYR:HB3	2.02	0.42
1:K:768:ILE:HG12	1:K:770:PRO:HD3	2.02	0.42
1:K:1279:PHE:HB2	1:K:1282:THR:HG23	2.01	0.42
2:L:528:ILE:HG21	2:L:547:ILE:HG13	2.02	0.42
2:L:646:THR:HB	2:L:677:GLN:CB	2.26	0.42
2:L:1037:SER:N	2:L:1051:THR:HG21	2.35	0.42
2:H:528:ILE:HG21	2:H:547:ILE:HG13	2.02	0.42
2:H:646:THR:HB	2:H:677:GLN:CB	2.26	0.42
2:H:976:PRO:O	2:H:980:ILE:N	2.48	0.42
1:I:411:GLN:HE21	1:I:1629:LYS:HE2	1.85	0.42
1:I:745:VAL:HG23	1:I:802:MET:HG2	2.02	0.42
2:J:528:ILE:HG21	2:J:547:ILE:HG13	2.02	0.42
2:J:900:GLN:HE22	2:J:1033:SER:HB2	1.85	0.42
1:A:400:ARG:NH1	1:A:1358:HIS:O	2.40	0.42
2:G:1037:SER:N	2:G:1051:THR:HG21	2.35	0.42
1:B:409:ALA:HB2	1:B:442:ARG:HE	1.84	0.42
1:B:411:GLN:HE21	1:B:1629:LYS:HE2	1.85	0.42
2:C:1310:ASP:OD1	2:C:1317:ARG:NH2	2.53	0.42
1:D:409:ALA:HB2	1:D:442:ARG:HE	1.84	0.42
1:D:633:GLU:H	1:D:653:ARG:HH22	1.68	0.42
2:E:577:ILE:HB	2:E:1082:ILE:HD11	2.01	0.42
2:E:848:SER:HB3	2:E:854:ILE:HD12	2.00	0.42
2:E:1310:ASP:OD1	2:E:1317:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:THR:HG23	1:K:174:ASP:H	1.84	0.42
1:K:1001:VAL:HG11	1:K:1662:TYR:HB2	2.02	0.42
2:L:1310:ASP:OD1	2:L:1317:ARG:NH2	2.53	0.42
1:F:1397:GLY:O	1:F:1680:ARG:HG3	2.18	0.42
1:F:1411:THR:HG22	1:F:1648:GLN:HG3	2.02	0.42
2:H:1376:ALA:HA	2:H:1394:GLY:HA2	2.02	0.42
2:H:1739:GLU:H	2:H:1739:GLU:HG2	1.66	0.42
2:J:714:SER:HA	2:J:717:ILE:HD12	2.02	0.42
2:J:1740:THR:O	2:J:1740:THR:OG1	2.31	0.42
2:J:1778:GLN:HA	2:J:1809:LEU:HD21	2.01	0.42
1:A:411:GLN:HE21	1:A:1629:LYS:HE2	1.85	0.42
1:A:1411:THR:HG22	1:A:1648:GLN:HG3	2.02	0.42
2:G:1217:ASN:HB3	2:G:1242:PHE:HB3	2.02	0.42
2:G:1859:PRO:HG3	2:G:1871:LEU:HD13	2.02	0.42
1:B:35:PHE:HA	1:B:39:PHE:HD2	1.85	0.42
1:B:1279:PHE:HB2	1:B:1282:THR:HG23	2.01	0.42
2:C:290:GLU:CD	2:C:290:GLU:N	2.73	0.42
2:C:1783:LEU:HD23	2:C:1783:LEU:HA	1.92	0.42
1:D:768:ILE:HG12	1:D:770:PRO:HD3	2.02	0.42
2:E:158:ALA:HA	2:E:502:LEU:HB2	2.01	0.42
2:E:1778:GLN:HA	2:E:1809:LEU:HD21	2.01	0.42
1:K:981:GLU:HA	2:L:964:LEU:HA	2.01	0.42
1:K:1549:ASN:ND2	1:K:1549:ASN:C	2.73	0.42
2:L:714:SER:HA	2:L:717:ILE:HD12	2.02	0.42
2:L:1386:THR:HG23	2:L:1411:PHE:HZ	1.84	0.42
2:L:1690:VAL:HG21	2:L:1787:ALA:HA	2.02	0.42
1:F:1649:LYS:HE3	1:F:1649:LYS:HB2	1.90	0.42
2:H:1386:THR:HG23	2:H:1411:PHE:HZ	1.84	0.42
2:H:1485:CYS:HB3	2:H:1506:TYR:HB3	2.02	0.42
1:I:1303:GLY:HA2	1:I:1649:LYS:HZ1	1.84	0.42
2:J:290:GLU:N	2:J:290:GLU:CD	2.73	0.42
2:J:1859:PRO:HG3	2:J:1871:LEU:HD13	2.02	0.42
1:A:1106:ILE:HA	1:A:1188:GLN:NE2	2.33	0.41
2:G:1376:ALA:HA	2:G:1394:GLY:HA2	2.02	0.41
1:B:17:LEU:HD23	2:C:2014:LEU:HD23	2.01	0.41
1:B:768:ILE:HG12	1:B:770:PRO:HD3	2.02	0.41
2:C:101:ILE:O	2:C:105:ALA:N	2.51	0.41
2:C:1386:THR:HG23	2:C:1411:PHE:HZ	1.84	0.41
2:C:1561:ASN:HB3	2:C:1564:HIS:HD2	1.85	0.41
1:D:35:PHE:HA	1:D:39:PHE:HD2	1.85	0.41
2:E:549:ASP:HB3	2:E:554:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:714:SER:HA	2:E:717:ILE:HD12	2.02	0.41
2:E:741:HIS:HB3	2:E:853:PRO:HB2	2.02	0.41
2:E:900:GLN:HE22	2:E:1033:SER:HB2	1.85	0.41
1:K:35:PHE:HA	1:K:39:PHE:HD2	1.85	0.41
1:K:411:GLN:HE21	1:K:1629:LYS:HE2	1.85	0.41
1:K:687:SER:HA	1:K:875:THR:HG22	2.00	0.41
2:L:260:PRO:CD	2:L:289:TRP:CH2	3.03	0.41
2:L:298:LYS:HB3	2:L:450:PHE:HE1	1.85	0.41
2:L:884:LEU:HD22	2:L:1021:LEU:HD12	2.01	0.41
1:F:770:PRO:HB2	1:F:799:ILE:HG12	2.01	0.41
1:F:981:GLU:HA	2:H:964:LEU:HA	2.01	0.41
1:F:1106:ILE:HA	1:F:1188:GLN:NE2	2.33	0.41
1:F:1549:ASN:ND2	1:F:1549:ASN:C	2.73	0.41
2:H:585:LYS:HG3	2:H:1106:GLU:HB2	2.02	0.41
2:H:900:GLN:HE22	2:H:1033:SER:HB2	1.85	0.41
2:H:1037:SER:N	2:H:1051:THR:HG21	2.35	0.41
2:H:1432:GLN:N	2:H:1525:SER:O	2.52	0.41
2:J:43:GLU:HA	2:J:44:PRO:HD3	1.93	0.41
2:J:1561:ASN:HB3	2:J:1564:HIS:HD2	1.84	0.41
1:A:770:PRO:HB2	1:A:799:ILE:HG12	2.01	0.41
1:A:1112:ASN:HD22	1:A:1258:ARG:HH22	1.68	0.41
2:G:714:SER:HA	2:G:717:ILE:HD12	2.02	0.41
2:G:738:GLY:CA	2:G:1055:HIS:O	2.68	0.41
2:G:884:LEU:HD22	2:G:1021:LEU:HD12	2.01	0.41
2:G:976:PRO:O	2:G:980:ILE:N	2.48	0.41
2:G:1310:ASP:OD1	2:G:1317:ARG:NH2	2.53	0.41
2:G:1697:HIS:O	2:G:1701:THR:OG1	2.28	0.41
1:B:981:GLU:HA	2:C:964:LEU:HA	2.01	0.41
1:B:1107:GLU:HA	1:B:1108:PRO:HD3	1.92	0.41
2:C:549:ASP:HB3	2:C:554:GLY:HA3	2.02	0.41
2:C:919:TYR:CE1	2:C:995:LEU:HA	2.54	0.41
2:C:1265:MET:HE2	2:C:1562:PRO:HG2	2.02	0.41
2:C:1376:ALA:HA	2:C:1394:GLY:HA2	2.02	0.41
2:C:1690:VAL:HG21	2:C:1787:ALA:HA	2.02	0.41
2:C:1859:PRO:HG3	2:C:1871:LEU:HD13	2.03	0.41
1:D:1041:ALA:O	1:D:1630:THR:OG1	2.29	0.41
1:D:1112:ASN:HD22	1:D:1258:ARG:HH22	1.69	0.41
2:E:586:LEU:HD12	2:E:1108:PRO:HD3	2.03	0.41
1:K:633:GLU:H	1:K:653:ARG:HH22	1.68	0.41
2:G:1267:TRP:NE1	2:G:1273:GLU:O	2.39	0.41
1:B:1694:TYR:OH	2:C:1001:ASP:OD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:VAL:HG23	1:D:802:MET:HG2	2.02	0.41
1:D:1549:ASN:ND2	1:D:1549:ASN:C	2.73	0.41
2:L:1561:ASN:HB3	2:L:1564:HIS:HD2	1.85	0.41
1:F:411:GLN:HE21	1:F:1629:LYS:HE2	1.85	0.41
1:F:1112:ASN:HD22	1:F:1258:ARG:HH22	1.69	0.41
2:H:738:GLY:CA	2:H:1055:HIS:O	2.68	0.41
2:H:848:SER:HB3	2:H:854:ILE:HD12	2.00	0.41
2:H:1778:GLN:HA	2:H:1809:LEU:HD21	2.01	0.41
2:J:549:ASP:HB3	2:J:554:GLY:HA3	2.02	0.41
2:J:1037:SER:N	2:J:1051:THR:HG21	2.35	0.41
1:A:745:VAL:HG23	1:A:802:MET:HG2	2.02	0.41
1:A:981:GLU:HA	2:G:964:LEU:HA	2.01	0.41
1:B:885:ALA:HA	1:B:888:ILE:HG22	2.03	0.41
2:C:260:PRO:CD	2:C:289:TRP:CH2	3.03	0.41
2:C:298:LYS:HB3	2:C:450:PHE:HE1	1.85	0.41
2:E:260:PRO:CD	2:E:289:TRP:CH2	3.03	0.41
1:K:1238:VAL:HG22	1:K:1392:LEU:HD11	2.02	0.41
1:F:768:ILE:HG12	1:F:770:PRO:HD3	2.02	0.41
1:I:885:ALA:HA	1:I:888:ILE:HG22	2.03	0.41
2:J:585:LYS:HG3	2:J:1106:GLU:HB2	2.02	0.41
2:J:919:TYR:CE1	2:J:995:LEU:HA	2.54	0.41
2:J:1736:MET:HE2	2:J:1736:MET:CA	2.42	0.41
1:A:885:ALA:HA	1:A:888:ILE:HG22	2.03	0.41
1:B:633:GLU:H	1:B:653:ARG:HH22	1.68	0.41
1:B:745:VAL:HG23	1:B:802:MET:HG2	2.02	0.41
2:C:577:ILE:HB	2:C:1082:ILE:HD11	2.01	0.41
2:C:900:GLN:HE22	2:C:1033:SER:HB2	1.85	0.41
2:C:1735:ALA:C	2:C:1736:MET:HE2	2.09	0.41
2:C:1778:GLN:HA	2:C:1809:LEU:HD21	2.01	0.41
2:C:1811:GLU:OE2	2:C:2010:TYR:OH	2.29	0.41
1:D:17:LEU:HD23	2:E:2014:LEU:HD23	2.01	0.41
1:D:1001:VAL:HG11	1:D:1662:TYR:HB2	2.02	0.41
2:E:658:MET:HG3	2:E:661:TRP:CZ2	2.56	0.41
1:K:409:ALA:HB2	1:K:442:ARG:HE	1.84	0.41
1:K:745:VAL:HG23	1:K:802:MET:HG2	2.02	0.41
1:K:1112:ASN:HD22	1:K:1258:ARG:HH22	1.68	0.41
1:K:1223:PHE:HA	1:K:1226:SER:HB3	2.03	0.41
2:L:1778:GLN:HA	2:L:1809:LEU:HD21	2.01	0.41
1:F:400:ARG:NH1	1:F:1358:HIS:O	2.40	0.41
2:H:1052:CYS:O	2:H:1052:CYS:SG	2.79	0.41
1:I:768:ILE:HG12	1:I:770:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:738:GLY:CA	2:J:1055:HIS:O	2.68	0.41
2:J:1217:ASN:HB3	2:J:1242:PHE:HB3	2.02	0.41
1:A:1001:VAL:HG11	1:A:1662:TYR:HB2	2.02	0.41
1:A:1238:VAL:HG22	1:A:1392:LEU:HD11	2.02	0.41
2:G:528:ILE:HG21	2:G:547:ILE:HG13	2.02	0.41
1:B:16:GLU:OE1	1:B:16:GLU:HA	2.21	0.41
1:B:18:LEU:O	1:B:21:GLN:HG3	2.21	0.41
2:C:915:ALA:HA	2:C:1000:ILE:HD11	2.03	0.41
2:C:1800:ALA:O	2:C:2009:LYS:NZ	2.48	0.41
1:D:1220:VAL:HG21	1:D:1698:PHE:HD1	1.84	0.41
1:D:1238:VAL:HG22	1:D:1392:LEU:HD11	2.02	0.41
2:E:585:LYS:HG3	2:E:1106:GLU:HB2	2.02	0.41
1:K:856:GLU:OE1	1:K:858:TRP:NE1	2.45	0.41
1:K:885:ALA:HA	1:K:888:ILE:HG22	2.03	0.41
2:L:327:SER:OG	2:L:333:GLY:O	2.32	0.41
2:L:577:ILE:HB	2:L:1082:ILE:HD11	2.01	0.41
2:L:1511:SER:OG	2:L:1512:HIS:N	2.54	0.41
2:L:1859:PRO:HG3	2:L:1871:LEU:HD13	2.02	0.41
2:H:658:MET:HG3	2:H:661:TRP:CZ2	2.56	0.41
2:H:741:HIS:HB3	2:H:853:PRO:HB2	2.02	0.41
1:I:981:GLU:HA	2:J:964:LEU:HA	2.01	0.41
1:I:1112:ASN:HD22	1:I:1258:ARG:HH22	1.69	0.41
2:J:577:ILE:HB	2:J:1082:ILE:HD11	2.01	0.41
2:J:1227:ARG:HD2	2:J:1565:VAL:HG11	2.02	0.41
2:J:1352:HIS:NE2	2:J:1354:SER:O	2.54	0.41
1:A:768:ILE:HG12	1:A:770:PRO:HD3	2.02	0.41
1:B:1223:PHE:HA	1:B:1226:SER:HB3	2.03	0.41
2:C:586:LEU:HD12	2:C:1108:PRO:HD3	2.03	0.41
2:C:738:GLY:CA	2:C:1055:HIS:O	2.68	0.41
1:D:1223:PHE:HA	1:D:1226:SER:HB3	2.03	0.41
1:D:1411:THR:HG22	1:D:1648:GLN:HG3	2.02	0.41
2:E:73:GLU:HA	2:E:74:PRO:HD3	1.89	0.41
2:E:581:THR:H	2:E:584:SER:HG	1.65	0.41
2:E:674:TYR:HA	2:E:675:PRO:HD3	1.90	0.41
2:E:807:ILE:HD13	2:E:807:ILE:HG21	1.88	0.41
2:E:1859:PRO:HG3	2:E:1871:LEU:HD13	2.02	0.41
1:K:1545:SER:O	1:K:1545:SER:OG	2.27	0.41
2:L:586:LEU:HD12	2:L:1108:PRO:HD3	2.03	0.41
2:L:915:ALA:HA	2:L:1000:ILE:HD11	2.03	0.41
1:F:18:LEU:O	1:F:21:GLN:HG3	2.21	0.41
2:H:726:PHE:HA	2:H:727:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1561:ASN:HB3	2:H:1564:HIS:HD2	1.85	0.41
1:I:17:LEU:HD23	2:J:2014:LEU:HD23	2.01	0.41
1:I:18:LEU:O	1:I:21:GLN:HG3	2.21	0.41
1:I:1238:VAL:HG22	1:I:1392:LEU:HD11	2.02	0.41
2:J:1170:ILE:O	2:J:1174:PHE:HD2	2.04	0.41
1:A:1082:GLU:HA	1:A:1083:PRO:HD3	1.94	0.41
1:A:1223:PHE:HA	1:A:1226:SER:HB3	2.03	0.41
1:B:1112:ASN:HD22	1:B:1258:ARG:HH22	1.69	0.41
2:C:714:SER:HA	2:C:717:ILE:HD12	2.02	0.41
2:C:1352:HIS:NE2	2:C:1354:SER:O	2.54	0.41
2:C:1737:ILE:HD13	2:C:1737:ILE:N	2.19	0.41
2:E:1052:CYS:O	2:E:1052:CYS:SG	2.79	0.41
2:E:1265:MET:HE2	2:E:1562:PRO:HG2	2.03	0.41
1:K:18:LEU:O	1:K:21:GLN:HG3	2.21	0.41
2:L:1217:ASN:HB3	2:L:1242:PHE:HB3	2.02	0.41
2:L:1376:ALA:HA	2:L:1394:GLY:HA2	2.02	0.41
2:H:586:LEU:HD12	2:H:1108:PRO:HD3	2.03	0.41
2:H:1227:ARG:HD2	2:H:1565:VAL:HG11	2.02	0.41
2:H:1783:LEU:HD23	2:H:1783:LEU:HA	1.92	0.41
1:I:16:GLU:HA	1:I:16:GLU:OE1	2.21	0.41
1:I:1411:THR:HG22	1:I:1648:GLN:HG3	2.02	0.41
1:A:35:PHE:HA	1:A:39:PHE:HD2	1.85	0.41
1:A:1423:LYS:NZ	1:K:1712:GLU:OE2	2.49	0.41
2:G:320:PRO:HA	2:G:321:PRO:HD3	1.89	0.41
2:G:586:LEU:HD12	2:G:1108:PRO:HD3	2.03	0.41
2:G:741:HIS:HB3	2:G:853:PRO:HB2	2.02	0.41
2:G:942:THR:HB	2:G:1012:GLN:HG3	2.03	0.41
2:G:1052:CYS:SG	2:G:1052:CYS:O	2.79	0.41
2:G:1170:ILE:O	2:G:1174:PHE:HD2	2.04	0.41
2:G:1511:SER:OG	2:G:1512:HIS:N	2.54	0.41
2:G:1561:ASN:HB3	2:G:1564:HIS:HD2	1.85	0.41
2:G:1690:VAL:HG21	2:G:1787:ALA:HA	2.02	0.41
1:B:14:LEU:HD13	1:B:14:LEU:O	2.21	0.41
1:B:1712:GLU:OE2	1:I:1423:LYS:NZ	2.49	0.41
1:B:1751:GLU:CB	1:B:1754:LYS:HE3	2.51	0.41
2:C:741:HIS:HE1	2:C:836:TYR:HE1	1.68	0.41
2:C:1037:SER:N	2:C:1051:THR:HG21	2.35	0.41
2:C:1511:SER:OG	2:C:1512:HIS:N	2.54	0.41
2:E:298:LYS:HB3	2:E:450:PHE:HE1	1.85	0.41
2:E:738:GLY:CA	2:E:1055:HIS:O	2.68	0.41
2:E:915:ALA:HA	2:E:1000:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1690:VAL:HG21	2:E:1787:ALA:HA	2.02	0.41
2:E:1916:PHE:O	2:E:1920:GLN:N	2.48	0.41
1:K:1220:VAL:HG21	1:K:1698:PHE:HD1	1.84	0.41
1:K:1649:LYS:HB2	1:K:1649:LYS:HE3	1.90	0.41
2:L:290:GLU:N	2:L:290:GLU:CD	2.73	0.41
2:L:900:GLN:HE22	2:L:1033:SER:HB2	1.85	0.41
2:L:942:THR:HB	2:L:1012:GLN:HG3	2.03	0.41
2:L:1739:GLU:H	2:L:1739:GLU:HG2	1.66	0.41
1:F:633:GLU:H	1:F:653:ARG:HH22	1.68	0.41
1:F:1223:PHE:HA	1:F:1226:SER:HB3	2.03	0.41
2:H:260:PRO:CD	2:H:289:TRP:CH2	3.03	0.41
2:H:942:THR:HB	2:H:1012:GLN:HG3	2.03	0.41
2:H:1170:ILE:O	2:H:1174:PHE:HD2	2.04	0.41
2:H:1217:ASN:HB3	2:H:1242:PHE:HB3	2.02	0.41
2:H:1690:VAL:HG21	2:H:1787:ALA:HA	2.02	0.41
2:H:1859:PRO:HG3	2:H:1871:LEU:HD13	2.03	0.41
1:I:1001:VAL:HG11	1:I:1662:TYR:HB2	2.02	0.41
1:I:1223:PHE:HA	1:I:1226:SER:HB3	2.03	0.41
2:J:260:PRO:HG2	2:J:289:TRP:CZ3	2.56	0.41
2:J:260:PRO:CD	2:J:289:TRP:CH2	3.03	0.41
2:J:741:HIS:HE1	2:J:836:TYR:HE1	1.68	0.41
2:J:848:SER:HB3	2:J:854:ILE:HD12	2.00	0.41
2:J:1485:CYS:HB3	2:J:1506:TYR:HB3	2.02	0.41
2:J:1702:TYR:O	2:J:1733:TYR:OH	2.30	0.41
1:A:14:LEU:HD13	1:A:14:LEU:O	2.21	0.41
2:G:260:PRO:HG2	2:G:289:TRP:CZ3	2.56	0.41
2:G:658:MET:HG3	2:G:661:TRP:CZ2	2.56	0.41
2:G:747:HIS:O	2:G:751:LEU:N	2.54	0.41
2:G:1068:GLU:HA	2:G:1069:PRO:HD3	1.92	0.41
2:C:43:GLU:HA	2:C:44:PRO:HD3	1.93	0.41
2:C:585:LYS:HG3	2:C:1106:GLU:HB2	2.02	0.41
2:C:942:THR:HB	2:C:1012:GLN:HG3	2.03	0.41
2:E:942:THR:HB	2:E:1012:GLN:HG3	2.03	0.41
1:K:14:LEU:HD13	1:K:14:LEU:O	2.21	0.41
1:K:371:LEU:HD23	1:K:371:LEU:HA	1.93	0.41
2:L:585:LYS:HG3	2:L:1106:GLU:HB2	2.02	0.41
2:L:741:HIS:HB3	2:L:853:PRO:HB2	2.02	0.41
2:J:581:THR:H	2:J:584:SER:HG	1.65	0.41
2:J:586:LEU:HD12	2:J:1108:PRO:HD3	2.03	0.41
2:J:691:ALA:HA	2:J:694:TYR:CD2	2.56	0.41
2:J:1511:SER:OG	2:J:1512:HIS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1227:ARG:HD2	2:G:1565:VAL:HG11	2.02	0.40
2:G:1485:CYS:HB3	2:G:1506:TYR:HB3	2.02	0.40
1:B:1264:ARG:NH2	1:B:1271:GLN:O	2.54	0.40
2:C:646:THR:OG1	2:C:677:GLN:OE1	2.28	0.40
2:C:1170:ILE:O	2:C:1174:PHE:HD2	2.04	0.40
2:C:1217:ASN:HB3	2:C:1242:PHE:HB3	2.02	0.40
2:E:1737:ILE:HD13	2:E:1737:ILE:N	2.19	0.40
2:L:549:ASP:HB3	2:L:554:GLY:HA3	2.02	0.40
2:L:658:MET:HG3	2:L:661:TRP:CZ2	2.56	0.40
2:L:1227:ARG:HD2	2:L:1565:VAL:HG11	2.02	0.40
1:F:745:VAL:HG23	1:F:802:MET:HG2	2.02	0.40
1:F:1238:VAL:HG22	1:F:1392:LEU:HD11	2.02	0.40
2:J:915:ALA:HA	2:J:1000:ILE:HD11	2.03	0.40
2:J:1082:ILE:HD13	2:J:1082:ILE:HG21	1.91	0.40
2:J:1376:ALA:HA	2:J:1394:GLY:HA2	2.02	0.40
2:G:190:PHE:CZ	2:G:297:ARG:HD2	2.54	0.40
2:G:549:ASP:HB3	2:G:554:GLY:HA3	2.02	0.40
2:G:848:SER:HB3	2:G:854:ILE:HD12	2.00	0.40
2:G:900:GLN:HE22	2:G:1033:SER:HB2	1.85	0.40
2:G:1352:HIS:NE2	2:G:1354:SER:O	2.54	0.40
1:B:856:GLU:OE1	1:B:858:TRP:NE1	2.45	0.40
1:B:1553:GLU:HA	1:B:1556:THR:HG22	2.04	0.40
2:C:260:PRO:HG2	2:C:289:TRP:CZ3	2.56	0.40
2:C:741:HIS:HB3	2:C:853:PRO:HB2	2.02	0.40
2:C:1767:GLU:OE2	2:C:1849:ARG:NE	2.36	0.40
1:D:14:LEU:HD13	1:D:14:LEU:O	2.21	0.40
2:E:327:SER:OG	2:E:333:GLY:O	2.32	0.40
2:E:1227:ARG:HD2	2:E:1565:VAL:HG11	2.02	0.40
1:K:403:ASP:OD1	1:K:731:THR:OG1	2.30	0.40
1:K:1264:ARG:NH2	1:K:1271:GLN:O	2.54	0.40
2:L:381:GLY:H	2:L:386:LEU:HD11	1.87	0.40
2:L:1432:GLN:N	2:L:1525:SER:O	2.52	0.40
1:F:13:LEU:HG	2:H:2019:PHE:HE1	1.87	0.40
1:F:14:LEU:HD13	1:F:14:LEU:O	2.21	0.40
2:H:381:GLY:H	2:H:386:LEU:HD11	1.86	0.40
2:H:1730:ARG:NH1	2:H:1759:SER:O	2.43	0.40
2:J:404:GLN:HE22	2:J:413:LYS:HB2	1.87	0.40
2:J:741:HIS:HB3	2:J:853:PRO:HB2	2.02	0.40
1:A:18:LEU:O	1:A:21:GLN:HG3	2.21	0.40
1:A:498:GLY:HA2	1:A:873:ARG:HH22	1.86	0.40
1:A:1264:ARG:NH2	1:A:1271:GLN:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:73:GLU:HA	2:G:74:PRO:HD3	1.89	0.40
2:G:1265:MET:HE2	2:G:1562:PRO:HG2	2.02	0.40
1:B:1238:VAL:HG22	1:B:1392:LEU:HD11	2.02	0.40
1:B:1411:THR:HG22	1:B:1648:GLN:HG3	2.02	0.40
2:C:381:GLY:H	2:C:386:LEU:HD11	1.86	0.40
2:C:533:LEU:HB3	2:C:544:LYS:HB3	2.04	0.40
2:C:1052:CYS:SG	2:C:1052:CYS:O	2.79	0.40
2:C:1227:ARG:HD2	2:C:1565:VAL:HG11	2.02	0.40
1:D:2:LYS:HA	1:D:3:PRO:HD3	1.96	0.40
1:D:13:LEU:HG	2:E:2019:PHE:HE1	1.87	0.40
1:D:1521:PRO:O	1:D:1525:ALA:N	2.46	0.40
1:K:1411:THR:HG22	1:K:1648:GLN:HG3	2.02	0.40
1:F:885:ALA:HA	1:F:888:ILE:HG22	2.03	0.40
2:H:714:SER:HA	2:H:717:ILE:HD12	2.02	0.40
2:H:807:ILE:HG21	2:H:807:ILE:HD13	1.88	0.40
2:H:915:ALA:HA	2:H:1000:ILE:HD11	2.03	0.40
2:H:1849:ARG:HD3	2:H:1957:PRO:HB3	2.03	0.40
1:I:498:GLY:HA2	1:I:873:ARG:HH22	1.87	0.40
1:I:521:LYS:HB3	1:I:523:SER:H	1.87	0.40
1:I:1560:MET:HG3	1:I:1561:MET:HE3	2.04	0.40
1:I:1751:GLU:CB	1:I:1754:LYS:HE3	2.51	0.40
2:J:190:PHE:CZ	2:J:297:ARG:HD2	2.54	0.40
2:J:298:LYS:HB3	2:J:450:PHE:HE1	1.85	0.40
2:J:942:THR:HB	2:J:1012:GLN:HG3	2.03	0.40
1:A:1385:GLN:NE2	1:A:1594:ASN:OD1	2.52	0.40
1:A:1521:PRO:O	1:A:1525:ALA:N	2.46	0.40
2:G:298:LYS:HB3	2:G:450:PHE:HE1	1.85	0.40
2:G:1849:ARG:HD3	2:G:1957:PRO:HB3	2.03	0.40
1:B:1291:LEU:HB3	1:B:1292:ILE:H	1.68	0.40
1:D:521:LYS:HB3	1:D:523:SER:H	1.87	0.40
1:D:885:ALA:HA	1:D:888:ILE:HG22	2.03	0.40
1:D:1559:GLU:OE2	1:F:1716:LEU:HD11	2.22	0.40
1:D:1751:GLU:O	1:D:1754:LYS:CG	2.69	0.40
2:E:533:LEU:HB3	2:E:544:LYS:HB3	2.04	0.40
2:E:846:VAL:CG2	2:E:856:LYS:HD2	2.52	0.40
1:K:16:GLU:OE1	1:K:16:GLU:HA	2.21	0.40
1:K:1303:GLY:HA2	1:K:1649:LYS:NZ	2.37	0.40
1:K:1553:GLU:HA	1:K:1556:THR:HG22	2.04	0.40
1:K:1783:ASN:HB3	1:K:1786:PHE:HD2	1.86	0.40
2:L:1170:ILE:O	2:L:1174:PHE:HD2	2.04	0.40
2:L:1352:HIS:NE2	2:L:1354:SER:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:GLU:CG	2:H:2038:ILE:HD11	2.46	0.40
2:H:298:LYS:HB3	2:H:450:PHE:HE1	1.85	0.40
1:I:633:GLU:H	1:I:653:ARG:HH22	1.68	0.40
1:I:1264:ARG:NH2	1:I:1271:GLN:O	2.54	0.40
2:J:381:GLY:H	2:J:386:LEU:HD11	1.87	0.40
2:J:1381:VAL:O	2:J:1422:THR:OG1	2.28	0.40
2:J:1531:VAL:HG11	2:J:1795:LYS:HA	2.04	0.40
2:J:1737:ILE:HD13	2:J:1737:ILE:N	2.19	0.40
1:A:1157:ILE:HA	1:A:1158:PRO:HD3	1.93	0.40
1:A:1559:GLU:OE2	1:K:1716:LEU:HD11	2.22	0.40
2:G:260:PRO:CD	2:G:289:TRP:CH2	3.03	0.40
2:G:582:LYS:HD3	2:G:1108:PRO:HB3	2.04	0.40
2:G:691:ALA:HA	2:G:694:TYR:CD2	2.56	0.40
2:G:846:VAL:CG2	2:G:856:LYS:HD2	2.52	0.40
2:G:915:ALA:HA	2:G:1000:ILE:HD11	2.03	0.40
2:G:1201:VAL:HG11	2:G:1226:ASN:HB2	2.03	0.40
1:B:521:LYS:HB3	1:B:523:SER:H	1.87	0.40
2:C:404:GLN:HE22	2:C:413:LYS:HB2	1.87	0.40
1:D:18:LEU:O	1:D:21:GLN:HG3	2.21	0.40
1:D:1716:LEU:HD11	1:F:1559:GLU:OE2	2.22	0.40
2:E:1304:VAL:HA	2:E:1584:PHE:HE1	1.87	0.40
2:E:1739:GLU:H	2:E:1739:GLU:HG2	1.66	0.40
2:L:738:GLY:CA	2:L:1055:HIS:O	2.68	0.40
2:L:1052:CYS:O	2:L:1052:CYS:SG	2.79	0.40
1:F:16:GLU:OE1	1:F:16:GLU:HA	2.21	0.40
2:H:1352:HIS:NE2	2:H:1354:SER:O	2.54	0.40
1:I:1119:LYS:HE2	1:I:1341:PHE:CG	2.57	0.40
1:I:1491:ARG:CA	1:I:1750:ILE:CD1	2.96	0.40
2:J:846:VAL:CG2	2:J:856:LYS:HD2	2.52	0.40
2:J:1052:CYS:O	2:J:1052:CYS:SG	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	48	79
1	B	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	48	79
1	D	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	48	79
1	F	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	48	79
1	I	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	48	79
1	K	1737/1887 (92%)	1649 (95%)	85 (5%)	3 (0%)	44	74
2	C	2027/2051 (99%)	1899 (94%)	125 (6%)	3 (0%)	48	79
2	E	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	48	79
2	G	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	48	79
2	H	2027/2051 (99%)	1899 (94%)	125 (6%)	3 (0%)	48	79
2	J	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	48	79
2	L	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	48	79
All	All	22584/23628 (96%)	21289 (94%)	1264 (6%)	31 (0%)	50	79

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	1743	ASP
2	C	1743	ASP
2	E	1743	ASP
2	L	1743	ASP
2	H	1743	ASP
2	J	1743	ASP
1	K	329	GLU
2	G	287	ASP
2	C	287	ASP
2	E	287	ASP
2	L	287	ASP
2	H	287	ASP
2	J	287	ASP
1	A	1291	LEU
1	B	1291	LEU
1	D	1291	LEU
1	K	1291	LEU
1	F	1291	LEU
1	I	1291	LEU

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Mol	Chain	Res	Type
2	C	676	ILE
2	E	676	ILE
2	H	676	ILE
2	J	676	ILE
2	G	676	ILE
2	L	676	ILE
1	B	1292	ILE
1	D	1292	ILE
1	F	1292	ILE
1	I	1292	ILE
1	A	1292	ILE
1	K	1292	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1475/1565 (94%)	1455 (99%)	20 (1%)	62	81
1	B	1475/1565 (94%)	1455 (99%)	20 (1%)	62	81
1	D	1475/1565 (94%)	1455 (99%)	20 (1%)	62	81
1	F	1475/1565 (94%)	1455 (99%)	20 (1%)	62	81
1	I	1475/1565 (94%)	1455 (99%)	20 (1%)	62	81
1	K	1475/1565 (94%)	1455 (99%)	20 (1%)	62	81
2	C	1770/1789 (99%)	1739 (98%)	31 (2%)	54	76
2	E	1770/1789 (99%)	1739 (98%)	31 (2%)	54	76
2	G	1770/1789 (99%)	1739 (98%)	31 (2%)	54	76
2	H	1770/1789 (99%)	1739 (98%)	31 (2%)	54	76
2	J	1770/1789 (99%)	1739 (98%)	31 (2%)	54	76
2	L	1770/1789 (99%)	1739 (98%)	31 (2%)	54	76
All	All	19470/20124 (97%)	19164 (98%)	306 (2%)	58	79

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	407	ASN
1	A	427	ASN
1	A	457	ASN
1	A	536	THR
1	A	738	ASN
1	A	761	LEU
1	A	873	ARG
1	A	894	ARG
1	A	1064	ASN
1	A	1208	VAL
1	A	1283	MET
1	A	1288	ASN
1	A	1367	ARG
1	A	1411	THR
1	A	1430	ARG
1	A	1442	ASN
1	A	1546	THR
1	A	1549	ASN
1	A	1585	LYS
2	G	279	THR
2	G	288	SER
2	G	295	SER
2	G	376	ASN
2	G	485	ARG
2	G	553	ASN
2	G	572	ASN
2	G	669	LEU
2	G	676	ILE
2	G	679	LEU
2	G	680	THR
2	G	844	VAL
2	G	845	THR
2	G	847	ARG
2	G	936	ASN
2	G	1051	THR
2	G	1055	HIS
2	G	1164	MET
2	G	1355	ASN
2	G	1415	ASN
2	G	1737	ILE
2	G	1738	PHE
2	G	1739	GLU

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Mol	Chain	Res	Type
2	G	1740	THR
2	G	1743	ASP
2	G	1745	LYS
2	G	1746	LEU
2	G	1747	LYS
2	G	1748	THR
2	G	1749	GLU
2	G	1956	ARG
1	B	356	ASN
1	B	407	ASN
1	B	427	ASN
1	B	457	ASN
1	B	536	THR
1	B	738	ASN
1	B	761	LEU
1	B	873	ARG
1	B	894	ARG
1	B	1064	ASN
1	B	1208	VAL
1	B	1283	MET
1	B	1288	ASN
1	B	1367	ARG
1	B	1411	THR
1	B	1430	ARG
1	B	1442	ASN
1	B	1546	THR
1	B	1549	ASN
1	B	1585	LYS
2	C	279	THR
2	C	288	SER
2	C	295	SER
2	C	376	ASN
2	C	485	ARG
2	C	553	ASN
2	C	572	ASN
2	C	669	LEU
2	C	676	ILE
2	C	679	LEU
2	C	680	THR
2	C	844	VAL
2	C	845	THR
2	C	847	ARG

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Mol	Chain	Res	Type
2	C	936	ASN
2	C	1051	THR
2	C	1055	HIS
2	C	1164	MET
2	C	1355	ASN
2	C	1415	ASN
2	C	1737	ILE
2	C	1738	PHE
2	C	1739	GLU
2	C	1740	THR
2	C	1743	ASP
2	C	1745	LYS
2	C	1746	LEU
2	C	1747	LYS
2	C	1748	THR
2	C	1749	GLU
2	C	1956	ARG
1	D	356	ASN
1	D	407	ASN
1	D	427	ASN
1	D	457	ASN
1	D	536	THR
1	D	738	ASN
1	D	761	LEU
1	D	873	ARG
1	D	894	ARG
1	D	1064	ASN
1	D	1208	VAL
1	D	1283	MET
1	D	1288	ASN
1	D	1367	ARG
1	D	1411	THR
1	D	1430	ARG
1	D	1442	ASN
1	D	1546	THR
1	D	1549	ASN
1	D	1585	LYS
2	E	279	THR
2	E	288	SER
2	E	295	SER
2	E	376	ASN
2	E	485	ARG

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Mol	Chain	Res	Type
2	E	553	ASN
2	E	572	ASN
2	E	669	LEU
2	E	676	ILE
2	E	679	LEU
2	E	680	THR
2	E	844	VAL
2	E	845	THR
2	E	847	ARG
2	E	936	ASN
2	E	1051	THR
2	E	1055	HIS
2	E	1164	MET
2	E	1355	ASN
2	E	1415	ASN
2	E	1737	ILE
2	E	1738	PHE
2	E	1739	GLU
2	E	1740	THR
2	E	1743	ASP
2	E	1745	LYS
2	E	1746	LEU
2	E	1747	LYS
2	E	1748	THR
2	E	1749	GLU
2	E	1956	ARG
1	K	356	ASN
1	K	407	ASN
1	K	427	ASN
1	K	457	ASN
1	K	536	THR
1	K	738	ASN
1	K	761	LEU
1	K	873	ARG
1	K	894	ARG
1	K	1064	ASN
1	K	1208	VAL
1	K	1283	MET
1	K	1288	ASN
1	K	1367	ARG
1	K	1411	THR
1	K	1430	ARG

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Mol	Chain	Res	Type
1	K	1442	ASN
1	K	1546	THR
1	K	1549	ASN
1	K	1585	LYS
2	L	279	THR
2	L	288	SER
2	L	295	SER
2	L	376	ASN
2	L	485	ARG
2	L	553	ASN
2	L	572	ASN
2	L	669	LEU
2	L	676	ILE
2	L	679	LEU
2	L	680	THR
2	L	844	VAL
2	L	845	THR
2	L	847	ARG
2	L	936	ASN
2	L	1051	THR
2	L	1055	HIS
2	L	1164	MET
2	L	1355	ASN
2	L	1415	ASN
2	L	1737	ILE
2	L	1738	PHE
2	L	1739	GLU
2	L	1740	THR
2	L	1743	ASP
2	L	1745	LYS
2	L	1746	LEU
2	L	1747	LYS
2	L	1748	THR
2	L	1749	GLU
2	L	1956	ARG
1	F	356	ASN
1	F	407	ASN
1	F	427	ASN
1	F	457	ASN
1	F	536	THR
1	F	738	ASN
1	F	761	LEU

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Mol	Chain	Res	Type
1	F	873	ARG
1	F	894	ARG
1	F	1064	ASN
1	F	1208	VAL
1	F	1283	MET
1	F	1288	ASN
1	F	1367	ARG
1	F	1411	THR
1	F	1430	ARG
1	F	1442	ASN
1	F	1546	THR
1	F	1549	ASN
1	F	1585	LYS
2	H	279	THR
2	H	288	SER
2	H	295	SER
2	H	376	ASN
2	H	485	ARG
2	H	553	ASN
2	H	572	ASN
2	H	669	LEU
2	H	676	ILE
2	H	679	LEU
2	H	680	THR
2	H	844	VAL
2	H	845	THR
2	H	847	ARG
2	H	936	ASN
2	H	1051	THR
2	H	1055	HIS
2	H	1164	MET
2	H	1355	ASN
2	H	1415	ASN
2	H	1737	ILE
2	H	1738	PHE
2	H	1739	GLU
2	H	1740	THR
2	H	1743	ASP
2	H	1745	LYS
2	H	1746	LEU
2	H	1747	LYS
2	H	1748	THR

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Mol	Chain	Res	Type
2	H	1749	GLU
2	H	1956	ARG
1	I	356	ASN
1	I	407	ASN
1	I	427	ASN
1	I	457	ASN
1	I	536	THR
1	I	738	ASN
1	I	761	LEU
1	I	873	ARG
1	I	894	ARG
1	I	1064	ASN
1	I	1208	VAL
1	I	1283	MET
1	I	1288	ASN
1	I	1367	ARG
1	I	1411	THR
1	I	1430	ARG
1	I	1442	ASN
1	I	1546	THR
1	I	1549	ASN
1	I	1585	LYS
2	J	279	THR
2	J	288	SER
2	J	295	SER
2	J	376	ASN
2	J	485	ARG
2	J	553	ASN
2	J	572	ASN
2	J	669	LEU
2	J	676	ILE
2	J	679	LEU
2	J	680	THR
2	J	844	VAL
2	J	845	THR
2	J	847	ARG
2	J	936	ASN
2	J	1051	THR
2	J	1055	HIS
2	J	1164	MET
2	J	1355	ASN
2	J	1415	ASN

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Mol	Chain	Res	Type
2	J	1737	ILE
2	J	1738	PHE
2	J	1739	GLU
2	J	1740	THR
2	J	1743	ASP
2	J	1745	LYS
2	J	1746	LEU
2	J	1747	LYS
2	J	1748	THR
2	J	1749	GLU
2	J	1956	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (293) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	214	GLN
1	A	271	ASN
1	A	335	HIS
1	A	344	GLN
1	A	407	ASN
1	A	427	ASN
1	A	457	ASN
1	A	738	ASN
1	A	792	HIS
1	A	1064	ASN
1	A	1112	ASN
1	A	1123	GLN
1	A	1188	GLN
1	A	1239	HIS
1	A	1442	ASN
1	A	1506	GLN
1	A	1510	ASN
1	A	1549	ASN
1	A	1610	ASN
1	A	1652	GLN
1	A	1845	ASN
2	G	13	HIS
2	G	354	ASN
2	G	376	ASN
2	G	404	GLN
2	G	428	HIS

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Mol	Chain	Res	Type
2	G	440	ASN
2	G	553	ASN
2	G	572	ASN
2	G	612	ASN
2	G	747	HIS
2	G	936	ASN
2	G	993	GLN
2	G	1036	GLN
2	G	1049	GLN
2	G	1151	HIS
2	G	1202	GLN
2	G	1355	ASN
2	G	1415	ASN
2	G	1476	ASN
2	G	1564	HIS
2	G	1581	HIS
2	G	1628	HIS
2	G	1659	GLN
2	G	1928	GLN
2	G	1977	HIS
2	G	2000	ASN
1	B	32	GLN
1	B	214	GLN
1	B	271	ASN
1	B	335	HIS
1	B	344	GLN
1	B	356	ASN
1	B	407	ASN
1	B	427	ASN
1	B	457	ASN
1	B	738	ASN
1	B	792	HIS
1	B	1064	ASN
1	B	1112	ASN
1	B	1123	GLN
1	B	1188	GLN
1	B	1239	HIS
1	B	1442	ASN
1	B	1506	GLN
1	B	1510	ASN
1	B	1549	ASN
1	B	1610	ASN

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Mol	Chain	Res	Type
1	B	1652	GLN
1	B	1845	ASN
2	C	13	HIS
2	C	354	ASN
2	C	376	ASN
2	C	404	GLN
2	C	428	HIS
2	C	440	ASN
2	C	553	ASN
2	C	572	ASN
2	C	612	ASN
2	C	747	HIS
2	C	936	ASN
2	C	993	GLN
2	C	1036	GLN
2	C	1049	GLN
2	C	1151	HIS
2	C	1202	GLN
2	C	1355	ASN
2	C	1415	ASN
2	C	1476	ASN
2	C	1564	HIS
2	C	1581	HIS
2	C	1628	HIS
2	C	1659	GLN
2	C	1928	GLN
2	C	1977	HIS
2	C	2000	ASN
1	D	32	GLN
1	D	214	GLN
1	D	271	ASN
1	D	335	HIS
1	D	344	GLN
1	D	407	ASN
1	D	427	ASN
1	D	457	ASN
1	D	719	GLN
1	D	738	ASN
1	D	792	HIS
1	D	1064	ASN
1	D	1112	ASN
1	D	1123	GLN

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Mol	Chain	Res	Type
1	D	1188	GLN
1	D	1239	HIS
1	D	1442	ASN
1	D	1506	GLN
1	D	1510	ASN
1	D	1549	ASN
1	D	1552	ASN
1	D	1610	ASN
1	D	1652	GLN
1	D	1845	ASN
2	E	13	HIS
2	E	354	ASN
2	E	376	ASN
2	E	404	GLN
2	E	428	HIS
2	E	440	ASN
2	E	553	ASN
2	E	572	ASN
2	E	612	ASN
2	E	747	HIS
2	E	936	ASN
2	E	993	GLN
2	E	1036	GLN
2	E	1049	GLN
2	E	1151	HIS
2	E	1202	GLN
2	E	1355	ASN
2	E	1415	ASN
2	E	1476	ASN
2	E	1564	HIS
2	E	1581	HIS
2	E	1628	HIS
2	E	1659	GLN
2	E	1928	GLN
2	E	1977	HIS
2	E	2000	ASN
1	K	32	GLN
1	K	214	GLN
1	K	271	ASN
1	K	335	HIS
1	K	344	GLN
1	K	407	ASN

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Mol	Chain	Res	Type
1	K	427	ASN
1	K	457	ASN
1	K	719	GLN
1	K	738	ASN
1	K	792	HIS
1	K	1064	ASN
1	K	1112	ASN
1	K	1123	GLN
1	K	1188	GLN
1	K	1239	HIS
1	K	1442	ASN
1	K	1506	GLN
1	K	1510	ASN
1	K	1549	ASN
1	K	1610	ASN
1	K	1652	GLN
1	K	1845	ASN
2	L	13	HIS
2	L	354	ASN
2	L	376	ASN
2	L	428	HIS
2	L	440	ASN
2	L	553	ASN
2	L	572	ASN
2	L	612	ASN
2	L	747	HIS
2	L	936	ASN
2	L	993	GLN
2	L	1036	GLN
2	L	1049	GLN
2	L	1151	HIS
2	L	1202	GLN
2	L	1355	ASN
2	L	1415	ASN
2	L	1476	ASN
2	L	1564	HIS
2	L	1581	HIS
2	L	1628	HIS
2	L	1659	GLN
2	L	1928	GLN
2	L	1977	HIS
2	L	2000	ASN

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Mol	Chain	Res	Type
1	F	32	GLN
1	F	214	GLN
1	F	271	ASN
1	F	335	HIS
1	F	344	GLN
1	F	407	ASN
1	F	427	ASN
1	F	457	ASN
1	F	738	ASN
1	F	792	HIS
1	F	1064	ASN
1	F	1112	ASN
1	F	1123	GLN
1	F	1188	GLN
1	F	1239	HIS
1	F	1442	ASN
1	F	1506	GLN
1	F	1510	ASN
1	F	1549	ASN
1	F	1552	ASN
1	F	1610	ASN
1	F	1652	GLN
1	F	1845	ASN
2	H	13	HIS
2	H	354	ASN
2	H	376	ASN
2	H	404	GLN
2	H	428	HIS
2	H	440	ASN
2	H	553	ASN
2	H	572	ASN
2	H	612	ASN
2	H	747	HIS
2	H	936	ASN
2	H	993	GLN
2	H	1036	GLN
2	H	1049	GLN
2	H	1151	HIS
2	H	1202	GLN
2	H	1355	ASN
2	H	1415	ASN
2	H	1476	ASN

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Mol	Chain	Res	Type
2	H	1564	HIS
2	H	1581	HIS
2	H	1628	HIS
2	H	1659	GLN
2	H	1928	GLN
2	H	1977	HIS
2	H	2000	ASN
1	I	32	GLN
1	I	214	GLN
1	I	271	ASN
1	I	335	HIS
1	I	344	GLN
1	I	356	ASN
1	I	407	ASN
1	I	427	ASN
1	I	457	ASN
1	I	719	GLN
1	I	738	ASN
1	I	792	HIS
1	I	1064	ASN
1	I	1112	ASN
1	I	1123	GLN
1	I	1188	GLN
1	I	1239	HIS
1	I	1442	ASN
1	I	1506	GLN
1	I	1510	ASN
1	I	1549	ASN
1	I	1610	ASN
1	I	1652	GLN
2	J	13	HIS
2	J	354	ASN
2	J	376	ASN
2	J	404	GLN
2	J	428	HIS
2	J	440	ASN
2	J	553	ASN
2	J	572	ASN
2	J	612	ASN
2	J	747	HIS
2	J	936	ASN
2	J	993	GLN

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Mol	Chain	Res	Type
2	J	1036	GLN
2	J	1049	GLN
2	J	1151	HIS
2	J	1202	GLN
2	J	1355	ASN
2	J	1415	ASN
2	J	1476	ASN
2	J	1564	HIS
2	J	1581	HIS
2	J	1628	HIS
2	J	1659	GLN
2	J	1928	GLN
2	J	1977	HIS
2	J	2000	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	SEP	I	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.79	2 (25%)
1	SEP	B	1440	1	8,9,10	1.46	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	D	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	F	1440	1	8,9,10	1.46	1 (12%)	8,12,14	1.79	2 (25%)
1	SEP	A	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	K	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.79	2 (25%)

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
1	SEP	I	1440	1	-	0/5/8/10	-
1	SEP	B	1440	1	-	2/5/8/10	-
1	SEP	D	1440	1	-	2/5/8/10	-
1	SEP	F	1440	1	-	0/5/8/10	-
1	SEP	A	1440	1	-	2/5/8/10	-
1	SEP	K	1440	1	-	0/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1440	SEP	P-O1P	3.19	1.60	1.50
1	A	1440	SEP	P-O1P	3.18	1.60	1.50
1	I	1440	SEP	P-O1P	3.18	1.60	1.50
1	B	1440	SEP	P-O1P	3.18	1.60	1.50
1	K	1440	SEP	P-O1P	3.18	1.60	1.50
1	D	1440	SEP	P-O1P	3.17	1.60	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	K	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	B	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	F	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	D	1440	SEP	P-OG-CB	-3.52	108.60	118.30
1	I	1440	SEP	P-OG-CB	-3.52	108.60	118.30
1	D	1440	SEP	OG-CB-CA	2.53	110.61	108.14
1	I	1440	SEP	OG-CB-CA	2.53	110.61	108.14
1	B	1440	SEP	OG-CB-CA	2.52	110.60	108.14
1	F	1440	SEP	OG-CB-CA	2.52	110.60	108.14
1	A	1440	SEP	OG-CB-CA	2.51	110.59	108.14
1	K	1440	SEP	OG-CB-CA	2.51	110.59	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1440	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
1	B	1440	SEP	CB-OG-P-O1P
1	D	1440	SEP	CB-OG-P-O1P
1	A	1440	SEP	CB-OG-P-O3P
1	B	1440	SEP	CB-OG-P-O3P
1	D	1440	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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	FMN	E	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	9 (18%)
3	NDP	I	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.69	12 (22%)
3	NDP	K	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)
4	FMN	J	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	9 (18%)
4	FMN	H	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.30	9 (18%)
3	NDP	A	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)
4	FMN	G	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	8 (16%)
4	FMN	C	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.30	9 (18%)
3	NDP	D	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.69	12 (22%)
4	FMN	L	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	8 (16%)
3	NDP	B	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)
3	NDP	F	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)

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	FMN	E	2101	-	-	5/18/18/18	0/3/3/3
3	NDP	I	2001	-	-	12/30/77/77	0/5/5/5
3	NDP	K	2001	-	-	12/30/77/77	0/5/5/5
4	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	H	2101	-	-	5/18/18/18	0/3/3/3
3	NDP	A	2001	-	-	12/30/77/77	0/5/5/5
4	FMN	G	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	C	2101	-	-	5/18/18/18	0/3/3/3
3	NDP	D	2001	-	-	12/30/77/77	0/5/5/5
4	FMN	L	2101	-	-	5/18/18/18	0/3/3/3
3	NDP	B	2001	-	-	12/30/77/77	0/5/5/5
3	NDP	F	2001	-	-	12/30/77/77	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2101	FMN	C4A-N5	3.31	1.37	1.30
4	J	2101	FMN	C4A-N5	3.31	1.37	1.30
4	C	2101	FMN	C4A-N5	3.29	1.37	1.30
4	H	2101	FMN	C4A-N5	3.29	1.37	1.30
4	G	2101	FMN	C4A-N5	3.28	1.37	1.30
4	L	2101	FMN	C4A-N5	3.28	1.37	1.30
3	A	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	K	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	D	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	I	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	B	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	F	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	A	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	K	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	B	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	F	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	D	2001	NDP	C3B-C4B	-2.51	1.46	1.53
3	I	2001	NDP	C3B-C4B	-2.51	1.46	1.53
3	A	2001	NDP	O4D-C4D	-2.47	1.39	1.45
3	K	2001	NDP	O4D-C4D	-2.47	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	NDP	O4D-C4D	-2.46	1.39	1.45
3	F	2001	NDP	O4D-C4D	-2.46	1.39	1.45
3	D	2001	NDP	O4D-C4D	-2.44	1.39	1.45
3	I	2001	NDP	O4D-C4D	-2.44	1.39	1.45
3	B	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	F	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	A	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	K	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	D	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	I	2001	NDP	C5A-N7A	-2.23	1.31	1.39
4	E	2101	FMN	C10-N1	2.21	1.37	1.33
4	J	2101	FMN	C10-N1	2.21	1.37	1.33
4	G	2101	FMN	C10-N1	2.18	1.37	1.33
4	L	2101	FMN	C10-N1	2.18	1.37	1.33
4	C	2101	FMN	C10-N1	2.18	1.37	1.33
4	H	2101	FMN	C10-N1	2.18	1.37	1.33
3	D	2001	NDP	C6N-N1N	-2.18	1.31	1.37
3	I	2001	NDP	C6N-N1N	-2.18	1.31	1.37
3	A	2001	NDP	C6N-N1N	-2.16	1.31	1.37
3	K	2001	NDP	C6N-N1N	-2.16	1.31	1.37
3	B	2001	NDP	C6N-N1N	-2.16	1.31	1.37
3	F	2001	NDP	C6N-N1N	-2.16	1.31	1.37
4	C	2101	FMN	C4A-C10	-2.16	1.37	1.44
4	H	2101	FMN	C4A-C10	-2.16	1.37	1.44
4	E	2101	FMN	C4A-C10	-2.14	1.37	1.44
4	J	2101	FMN	C4A-C10	-2.14	1.37	1.44
4	G	2101	FMN	C4A-C10	-2.13	1.37	1.44
4	L	2101	FMN	C4A-C10	-2.13	1.37	1.44

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2001	NDP	O4D-C4D-C5D	-4.20	95.54	109.37
3	I	2001	NDP	O4D-C4D-C5D	-4.20	95.54	109.37
3	A	2001	NDP	O4D-C4D-C5D	-4.20	95.56	109.37
3	K	2001	NDP	O4D-C4D-C5D	-4.20	95.56	109.37
3	B	2001	NDP	O4D-C4D-C5D	-4.19	95.58	109.37
3	F	2001	NDP	O4D-C4D-C5D	-4.19	95.58	109.37
3	D	2001	NDP	N3A-C2A-N1A	-4.07	122.31	128.68
3	I	2001	NDP	N3A-C2A-N1A	-4.07	122.31	128.68
3	A	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68
3	K	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68
3	F	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68
3	A	2001	NDP	C5B-C4B-C3B	-3.89	100.60	115.18
3	K	2001	NDP	C5B-C4B-C3B	-3.89	100.60	115.18
3	B	2001	NDP	C5B-C4B-C3B	-3.89	100.61	115.18
3	F	2001	NDP	C5B-C4B-C3B	-3.89	100.61	115.18
3	D	2001	NDP	C5B-C4B-C3B	-3.89	100.62	115.18
3	I	2001	NDP	C5B-C4B-C3B	-3.89	100.62	115.18
4	G	2101	FMN	C4-N3-C2	-3.45	119.27	125.64
4	L	2101	FMN	C4-N3-C2	-3.45	119.27	125.64
4	C	2101	FMN	C4-N3-C2	-3.45	119.27	125.64
4	E	2101	FMN	C4-N3-C2	-3.45	119.28	125.64
4	J	2101	FMN	C4-N3-C2	-3.45	119.28	125.64
4	H	2101	FMN	C4-N3-C2	-3.43	119.31	125.64
3	A	2001	NDP	C4A-C5A-N7A	-3.31	105.95	109.40
3	K	2001	NDP	C4A-C5A-N7A	-3.31	105.95	109.40
3	D	2001	NDP	C4A-C5A-N7A	-3.30	105.96	109.40
3	I	2001	NDP	C4A-C5A-N7A	-3.30	105.96	109.40
3	B	2001	NDP	C4A-C5A-N7A	-3.29	105.97	109.40
3	F	2001	NDP	C4A-C5A-N7A	-3.29	105.97	109.40
3	B	2001	NDP	O2B-C2B-C1B	3.07	121.17	110.10
3	F	2001	NDP	O2B-C2B-C1B	3.07	121.17	110.10
3	D	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
3	I	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
3	A	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
3	K	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
4	G	2101	FMN	C4A-C4-N3	2.93	120.64	113.19
4	L	2101	FMN	C4A-C4-N3	2.93	120.64	113.19
4	E	2101	FMN	C4A-C4-N3	2.93	120.62	113.19
4	J	2101	FMN	C4A-C4-N3	2.93	120.62	113.19
3	B	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
3	F	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
3	D	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
3	I	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
4	C	2101	FMN	C4A-C4-N3	2.92	120.61	113.19
3	A	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	B	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	D	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	K	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	F	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	I	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
4	H	2101	FMN	C4A-C4-N3	2.92	120.61	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	NDP	O3B-C3B-C2B	2.91	119.43	111.17
3	K	2001	NDP	O3B-C3B-C2B	2.91	119.43	111.17
4	G	2101	FMN	O4-C4-C4A	-2.73	119.36	126.60
4	L	2101	FMN	O4-C4-C4A	-2.73	119.36	126.60
3	A	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	K	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	B	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	F	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	D	2001	NDP	C1D-N1N-C2N	-2.72	116.58	121.11
3	I	2001	NDP	C1D-N1N-C2N	-2.72	116.58	121.11
4	E	2101	FMN	O4-C4-C4A	-2.72	119.40	126.60
4	J	2101	FMN	O4-C4-C4A	-2.72	119.40	126.60
4	C	2101	FMN	O4-C4-C4A	-2.71	119.41	126.60
4	H	2101	FMN	O4-C4-C4A	-2.71	119.41	126.60
4	E	2101	FMN	C4A-C10-N10	2.55	120.21	116.48
4	J	2101	FMN	C4A-C10-N10	2.55	120.21	116.48
4	C	2101	FMN	C4A-C10-N10	2.52	120.17	116.48
4	H	2101	FMN	C4A-C10-N10	2.52	120.17	116.48
4	G	2101	FMN	C4A-C10-N10	2.51	120.15	116.48
4	L	2101	FMN	C4A-C10-N10	2.51	120.15	116.48
4	E	2101	FMN	C4A-C10-N1	-2.35	119.27	124.73
4	J	2101	FMN	C4A-C10-N1	-2.35	119.27	124.73
3	D	2001	NDP	O2B-P2B-O1X	-2.34	100.34	109.39
3	I	2001	NDP	O2B-P2B-O1X	-2.34	100.34	109.39
3	A	2001	NDP	O2B-P2B-O1X	-2.34	100.35	109.39
3	K	2001	NDP	O2B-P2B-O1X	-2.34	100.35	109.39
3	B	2001	NDP	O2B-P2B-O1X	-2.34	100.36	109.39
3	F	2001	NDP	O2B-P2B-O1X	-2.34	100.36	109.39
4	G	2101	FMN	C4A-C10-N1	-2.34	119.30	124.73
4	L	2101	FMN	C4A-C10-N1	-2.34	119.30	124.73
4	C	2101	FMN	C4A-C10-N1	-2.33	119.33	124.73
4	H	2101	FMN	C4A-C10-N1	-2.33	119.33	124.73
3	A	2001	NDP	O2N-PN-O1N	2.32	123.70	112.24
3	K	2001	NDP	O2N-PN-O1N	2.32	123.70	112.24
3	B	2001	NDP	O2N-PN-O1N	2.32	123.69	112.24
3	F	2001	NDP	O2N-PN-O1N	2.32	123.69	112.24
3	D	2001	NDP	O2N-PN-O1N	2.31	123.68	112.24
3	I	2001	NDP	O2N-PN-O1N	2.31	123.68	112.24
3	A	2001	NDP	O3X-P2B-O2X	2.23	116.15	107.64
3	K	2001	NDP	O3X-P2B-O2X	2.23	116.15	107.64
4	G	2101	FMN	O4'-C4'-C5'	-2.23	104.91	109.92
4	L	2101	FMN	O4'-C4'-C5'	-2.23	104.91	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2001	NDP	O3X-P2B-O2X	2.23	116.14	107.64
3	I	2001	NDP	O3X-P2B-O2X	2.23	116.14	107.64
4	C	2101	FMN	O4'-C4'-C5'	-2.22	104.92	109.92
4	H	2101	FMN	O4'-C4'-C5'	-2.22	104.92	109.92
3	B	2001	NDP	O3X-P2B-O2X	2.22	116.14	107.64
3	F	2001	NDP	O3X-P2B-O2X	2.22	116.14	107.64
4	E	2101	FMN	O4'-C4'-C5'	-2.22	104.93	109.92
4	J	2101	FMN	O4'-C4'-C5'	-2.22	104.93	109.92
4	G	2101	FMN	C9A-C5A-N5	-2.18	120.07	122.43
4	L	2101	FMN	C9A-C5A-N5	-2.18	120.07	122.43
3	D	2001	NDP	O3B-C3B-C4B	-2.17	104.79	111.05
3	I	2001	NDP	O3B-C3B-C4B	-2.17	104.79	111.05
3	A	2001	NDP	O3B-C3B-C4B	-2.16	104.79	111.05
3	K	2001	NDP	O3B-C3B-C4B	-2.16	104.79	111.05
3	B	2001	NDP	O3B-C3B-C4B	-2.16	104.81	111.05
3	F	2001	NDP	O3B-C3B-C4B	-2.16	104.81	111.05
4	E	2101	FMN	C9A-C5A-N5	-2.15	120.09	122.43
4	J	2101	FMN	C9A-C5A-N5	-2.15	120.09	122.43
4	C	2101	FMN	C9A-C5A-N5	-2.14	120.11	122.43
4	H	2101	FMN	C9A-C5A-N5	-2.14	120.11	122.43
4	G	2101	FMN	C5A-C9A-N10	2.08	120.10	117.95
4	L	2101	FMN	C5A-C9A-N10	2.08	120.10	117.95
4	E	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	J	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	C	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	H	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	E	2101	FMN	C4-C4A-C10	2.02	120.19	116.79
4	J	2101	FMN	C4-C4A-C10	2.02	120.19	116.79
4	C	2101	FMN	C4-C4A-C10	2.00	120.16	116.79
4	H	2101	FMN	C4-C4A-C10	2.00	120.16	116.79

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	NDP	C5D-O5D-PN-O3
3	B	2001	NDP	C5D-O5D-PN-O3
3	D	2001	NDP	C5D-O5D-PN-O3
3	K	2001	NDP	C5D-O5D-PN-O3
3	F	2001	NDP	C5D-O5D-PN-O3
3	I	2001	NDP	C5D-O5D-PN-O3
4	G	2101	FMN	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
4	C	2101	FMN	O3'-C3'-C4'-C5'
4	E	2101	FMN	O3'-C3'-C4'-C5'
4	L	2101	FMN	O3'-C3'-C4'-C5'
4	H	2101	FMN	O3'-C3'-C4'-C5'
4	J	2101	FMN	O3'-C3'-C4'-C5'
3	A	2001	NDP	C1B-C2B-O2B-P2B
3	B	2001	NDP	C1B-C2B-O2B-P2B
3	D	2001	NDP	C1B-C2B-O2B-P2B
3	K	2001	NDP	C1B-C2B-O2B-P2B
3	F	2001	NDP	C1B-C2B-O2B-P2B
3	I	2001	NDP	C1B-C2B-O2B-P2B
4	G	2101	FMN	C2'-C3'-C4'-C5'
4	C	2101	FMN	C2'-C3'-C4'-C5'
4	E	2101	FMN	C2'-C3'-C4'-C5'
4	L	2101	FMN	C2'-C3'-C4'-C5'
4	H	2101	FMN	C2'-C3'-C4'-C5'
4	J	2101	FMN	C2'-C3'-C4'-C5'
4	G	2101	FMN	C2'-C3'-C4'-O4'
4	C	2101	FMN	C2'-C3'-C4'-O4'
4	E	2101	FMN	C2'-C3'-C4'-O4'
4	L	2101	FMN	C2'-C3'-C4'-O4'
4	H	2101	FMN	C2'-C3'-C4'-O4'
4	J	2101	FMN	C2'-C3'-C4'-O4'
4	G	2101	FMN	O3'-C3'-C4'-O4'
4	C	2101	FMN	O3'-C3'-C4'-O4'
4	E	2101	FMN	O3'-C3'-C4'-O4'
4	L	2101	FMN	O3'-C3'-C4'-O4'
4	H	2101	FMN	O3'-C3'-C4'-O4'
4	J	2101	FMN	O3'-C3'-C4'-O4'
3	A	2001	NDP	O4D-C4D-C5D-O5D
3	K	2001	NDP	O4D-C4D-C5D-O5D
3	A	2001	NDP	PN-O3-PA-O5B
3	B	2001	NDP	PN-O3-PA-O5B
3	D	2001	NDP	PN-O3-PA-O5B
3	K	2001	NDP	PN-O3-PA-O5B
3	F	2001	NDP	PN-O3-PA-O5B
3	I	2001	NDP	PN-O3-PA-O5B
3	B	2001	NDP	O4D-C4D-C5D-O5D
3	D	2001	NDP	O4D-C4D-C5D-O5D
3	F	2001	NDP	O4D-C4D-C5D-O5D
3	I	2001	NDP	O4D-C4D-C5D-O5D
3	A	2001	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	B	2001	NDP	C2B-O2B-P2B-O1X
3	D	2001	NDP	C2B-O2B-P2B-O1X
3	K	2001	NDP	C2B-O2B-P2B-O1X
3	F	2001	NDP	C2B-O2B-P2B-O1X
3	I	2001	NDP	C2B-O2B-P2B-O1X
4	G	2101	FMN	C4'-C5'-O5'-P
4	C	2101	FMN	C4'-C5'-O5'-P
4	E	2101	FMN	C4'-C5'-O5'-P
4	L	2101	FMN	C4'-C5'-O5'-P
4	H	2101	FMN	C4'-C5'-O5'-P
4	J	2101	FMN	C4'-C5'-O5'-P
3	A	2001	NDP	C5D-O5D-PN-O1N
3	B	2001	NDP	C5D-O5D-PN-O1N
3	D	2001	NDP	C5D-O5D-PN-O1N
3	K	2001	NDP	C5D-O5D-PN-O1N
3	F	2001	NDP	C5D-O5D-PN-O1N
3	I	2001	NDP	C5D-O5D-PN-O1N
3	A	2001	NDP	C2D-C1D-N1N-C6N
3	B	2001	NDP	C2D-C1D-N1N-C6N
3	D	2001	NDP	C2D-C1D-N1N-C6N
3	K	2001	NDP	C2D-C1D-N1N-C6N
3	F	2001	NDP	C2D-C1D-N1N-C6N
3	I	2001	NDP	C2D-C1D-N1N-C6N
3	A	2001	NDP	O4D-C1D-N1N-C6N
3	B	2001	NDP	O4D-C1D-N1N-C6N
3	D	2001	NDP	O4D-C1D-N1N-C6N
3	K	2001	NDP	O4D-C1D-N1N-C6N
3	F	2001	NDP	O4D-C1D-N1N-C6N
3	I	2001	NDP	O4D-C1D-N1N-C6N
3	A	2001	NDP	PA-O3-PN-O1N
3	B	2001	NDP	PA-O3-PN-O1N
3	D	2001	NDP	PA-O3-PN-O1N
3	K	2001	NDP	PA-O3-PN-O1N
3	F	2001	NDP	PA-O3-PN-O1N
3	I	2001	NDP	PA-O3-PN-O1N
3	A	2001	NDP	C3B-C2B-O2B-P2B
3	B	2001	NDP	C3B-C2B-O2B-P2B
3	D	2001	NDP	C3B-C2B-O2B-P2B
3	K	2001	NDP	C3B-C2B-O2B-P2B
3	F	2001	NDP	C3B-C2B-O2B-P2B
3	I	2001	NDP	C3B-C2B-O2B-P2B
3	A	2001	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
3	B	2001	NDP	C2B-O2B-P2B-O3X
3	D	2001	NDP	C2B-O2B-P2B-O3X
3	K	2001	NDP	C2B-O2B-P2B-O3X
3	F	2001	NDP	C2B-O2B-P2B-O3X
3	I	2001	NDP	C2B-O2B-P2B-O3X
3	A	2001	NDP	O4B-C4B-C5B-O5B
3	B	2001	NDP	O4B-C4B-C5B-O5B
3	D	2001	NDP	O4B-C4B-C5B-O5B
3	K	2001	NDP	O4B-C4B-C5B-O5B
3	F	2001	NDP	O4B-C4B-C5B-O5B
3	I	2001	NDP	O4B-C4B-C5B-O5B

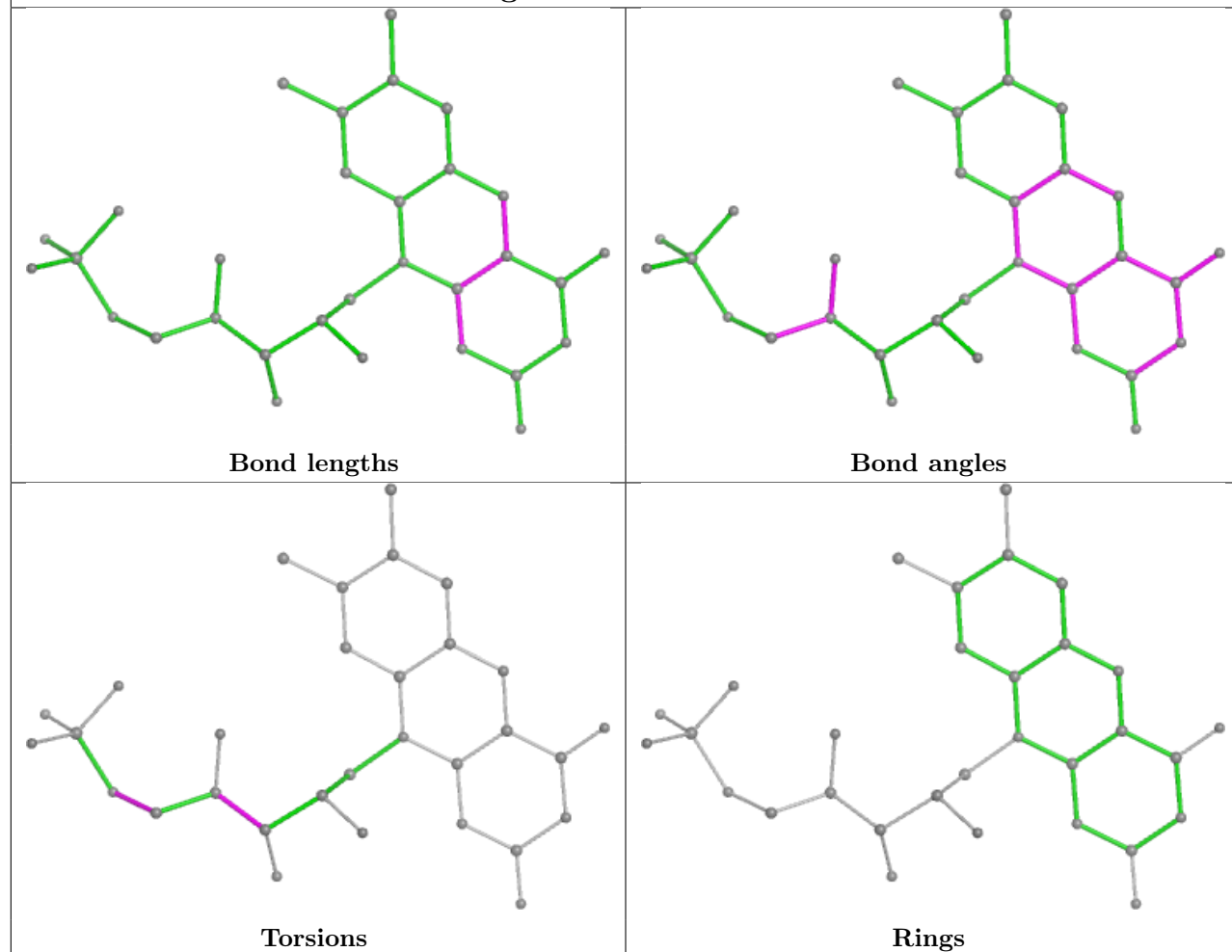
There are no ring outliers.

6 monomers are involved in 44 short contacts:

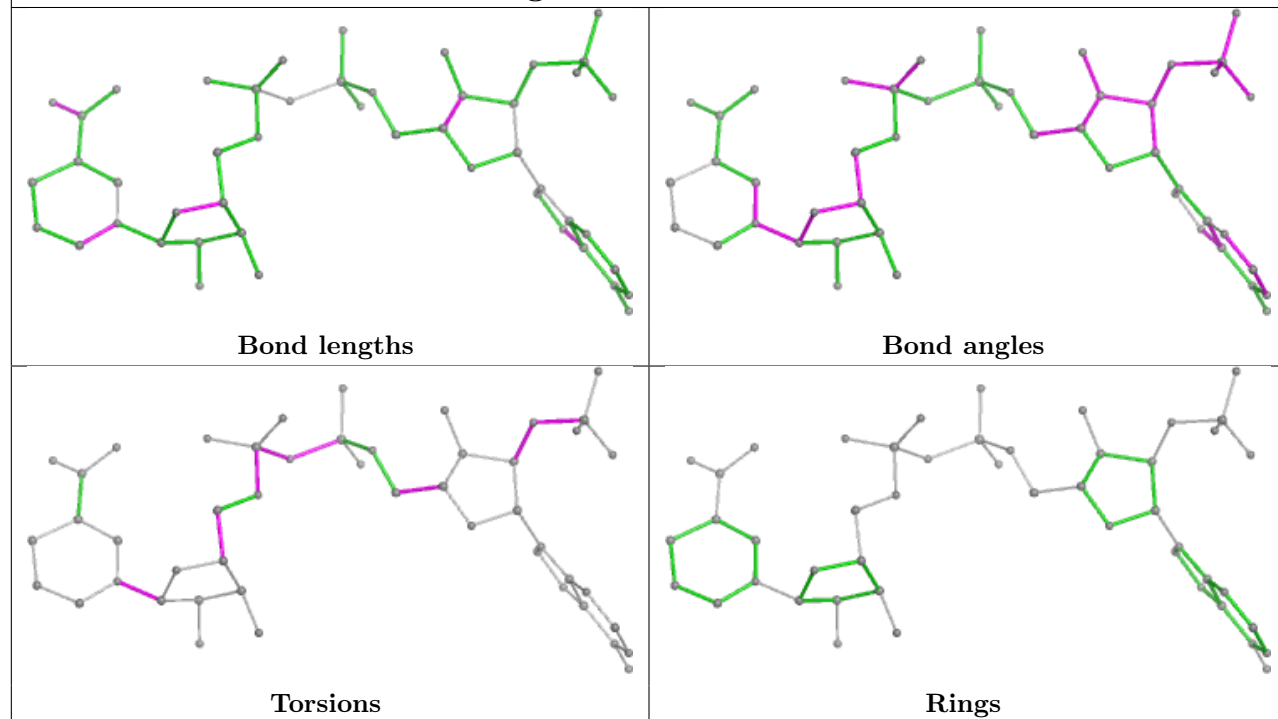
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2001	NDP	8	0
3	K	2001	NDP	7	0
3	A	2001	NDP	8	0
3	D	2001	NDP	7	0
3	B	2001	NDP	7	0
3	F	2001	NDP	7	0

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

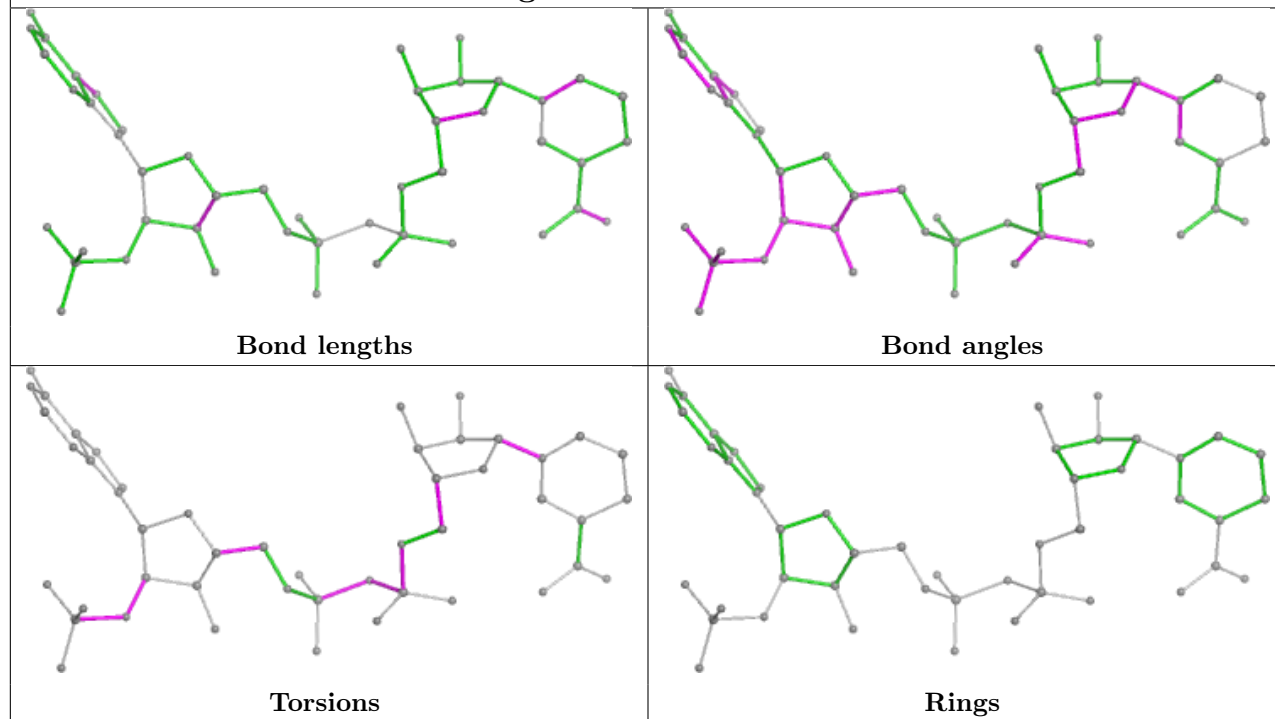
Ligand FMN E 2101



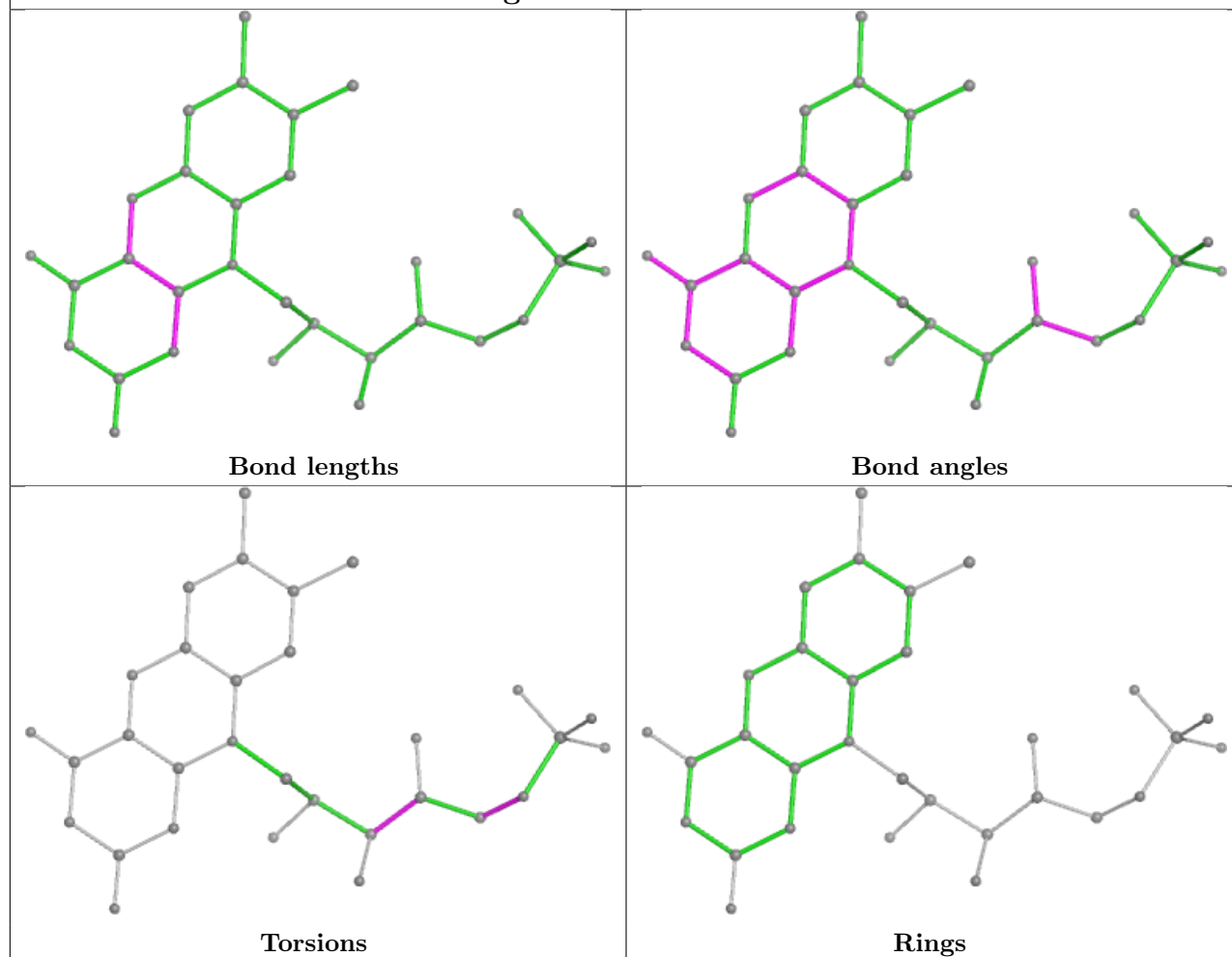
Ligand NDP I 2001



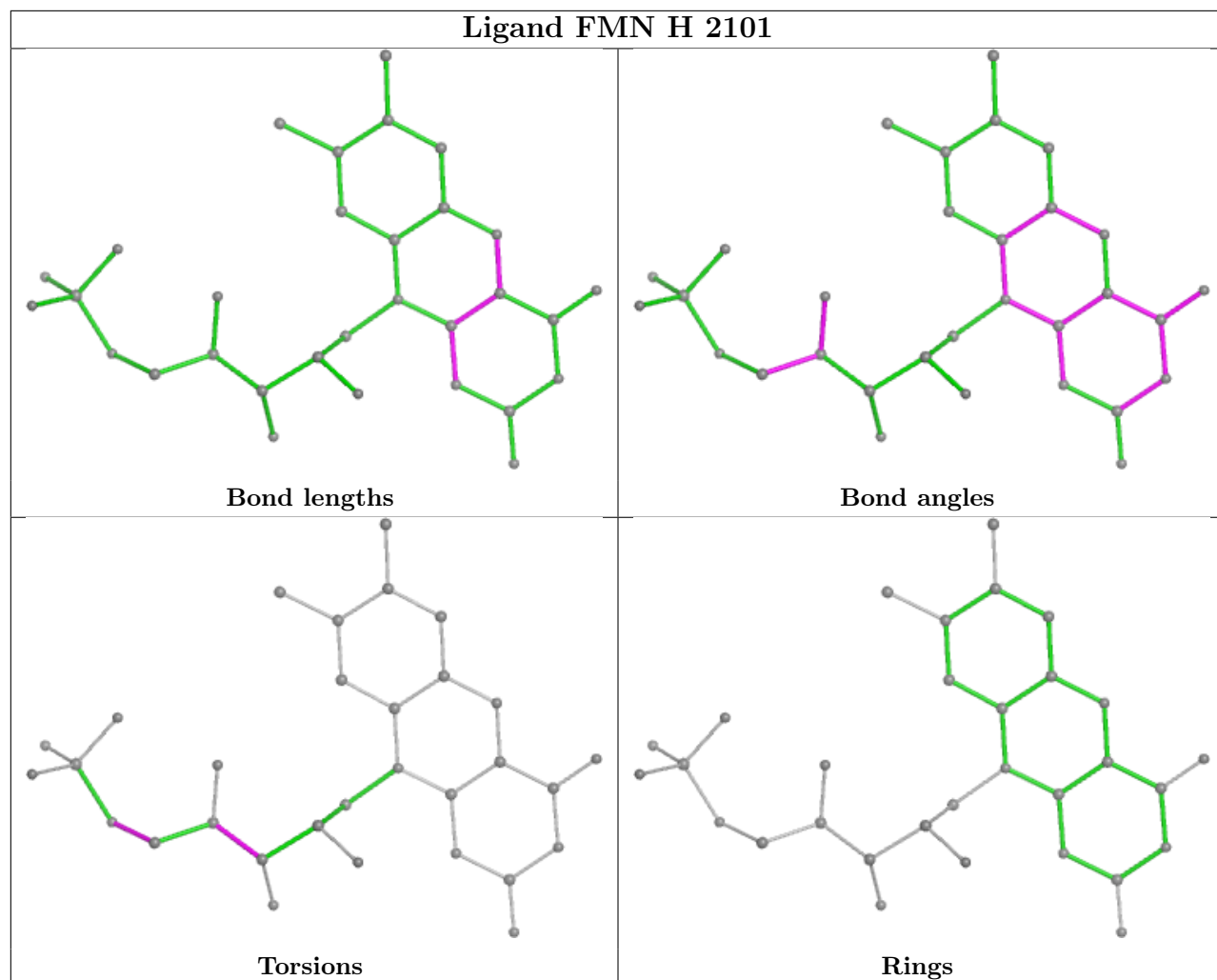
Ligand NDP K 2001



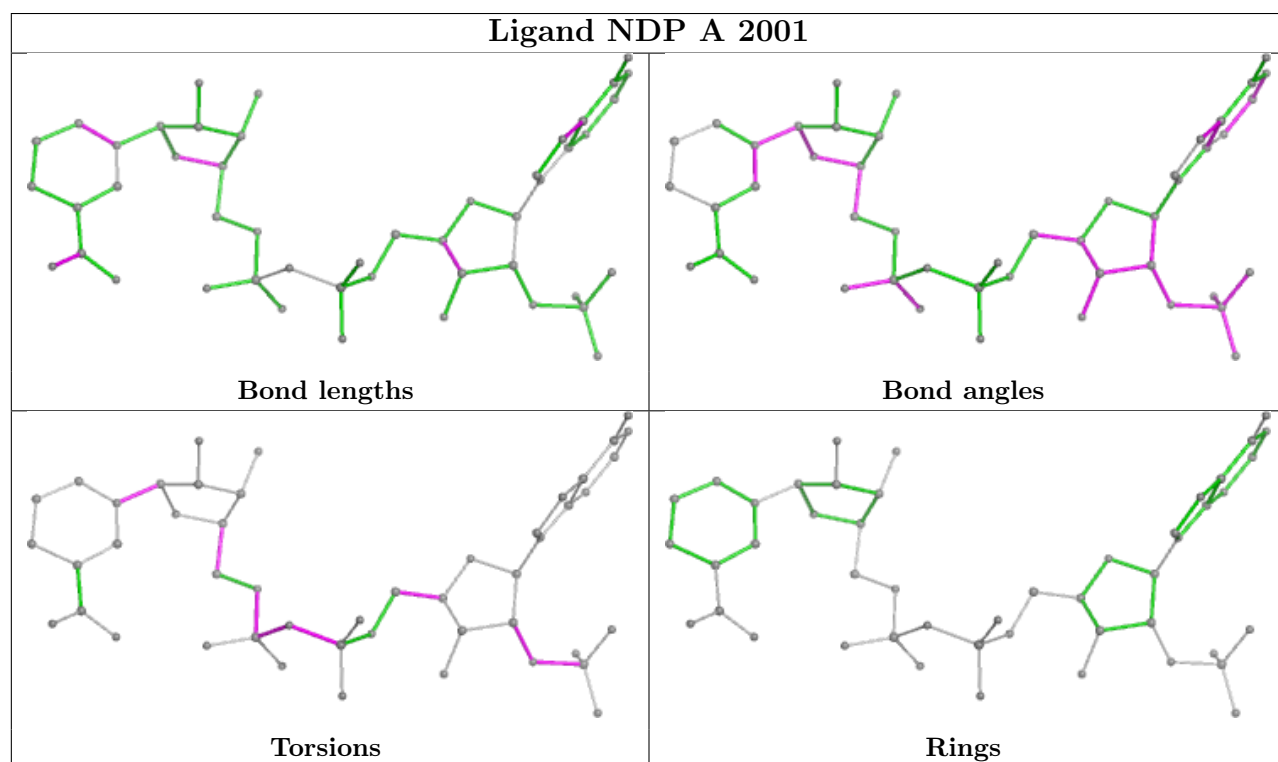
Ligand FMN J 2101

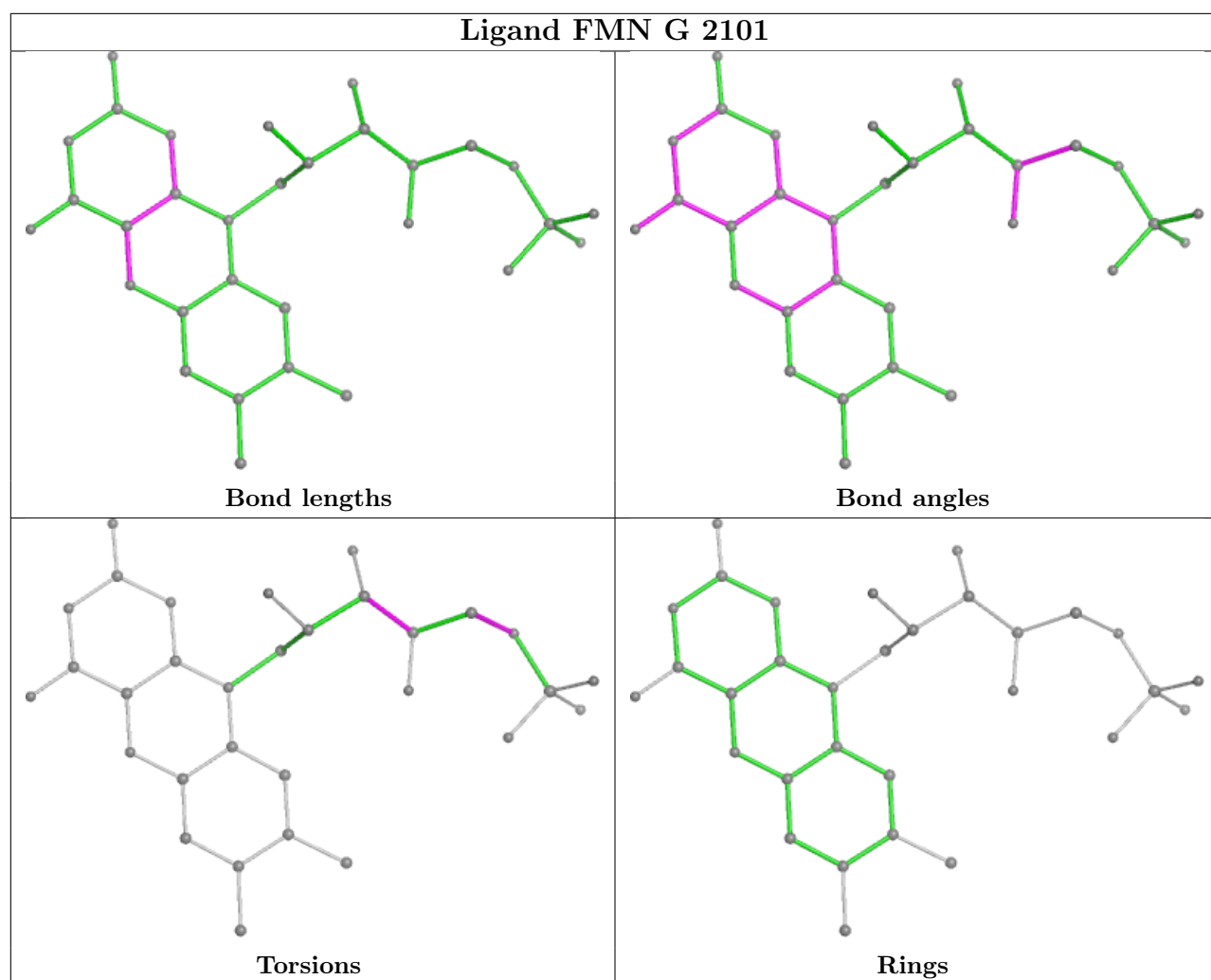


Ligand FMN H 2101

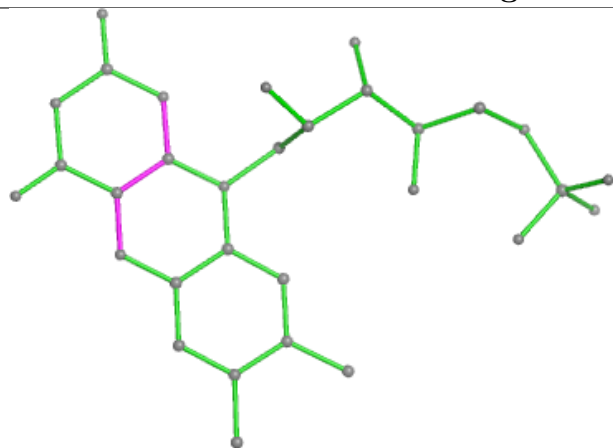


Ligand NDP A 2001

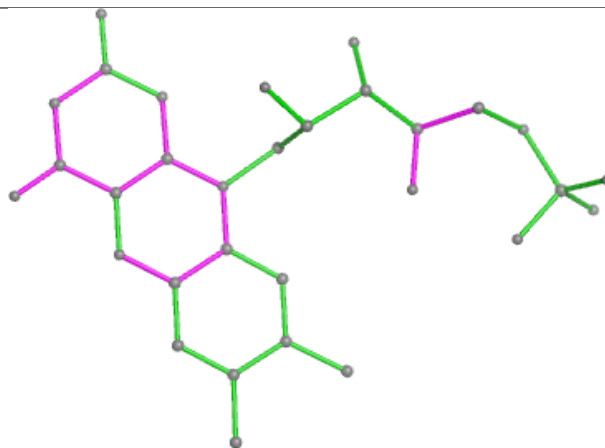




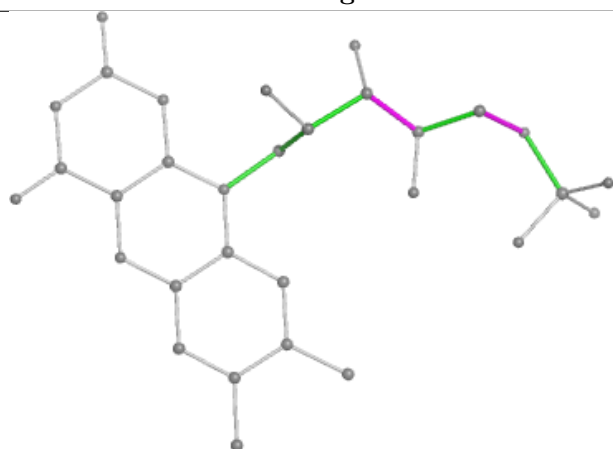
Ligand FMN C 2101



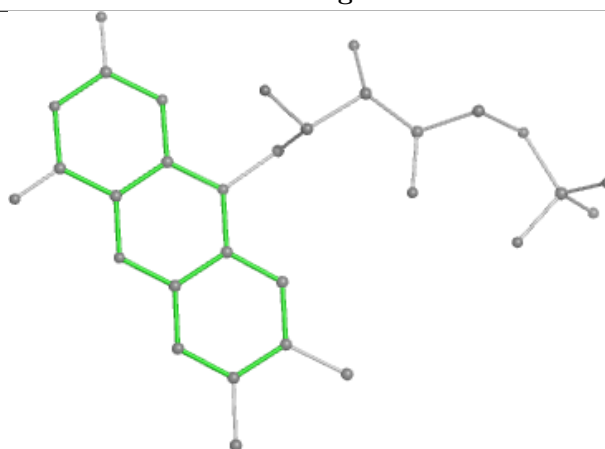
Bond lengths



Bond angles

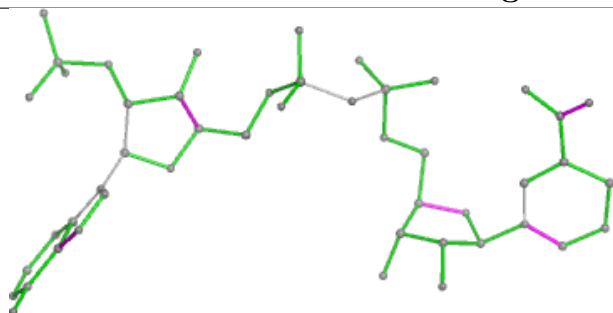


Torsions

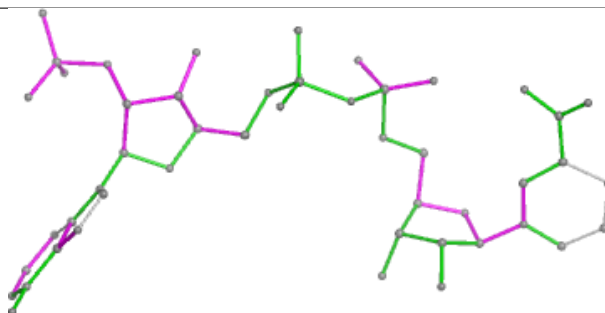


Rings

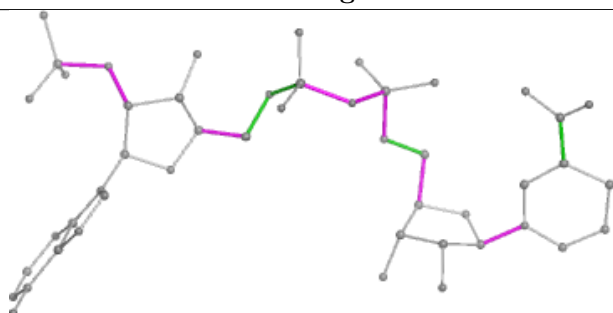
Ligand NDP D 2001



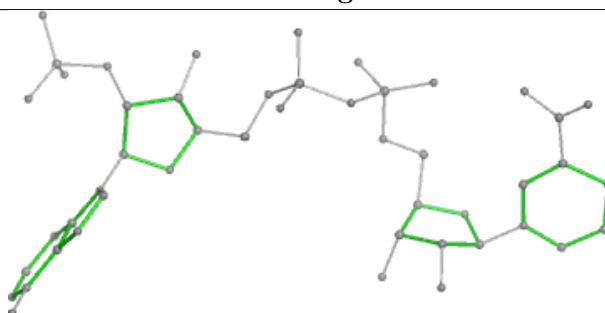
Bond lengths



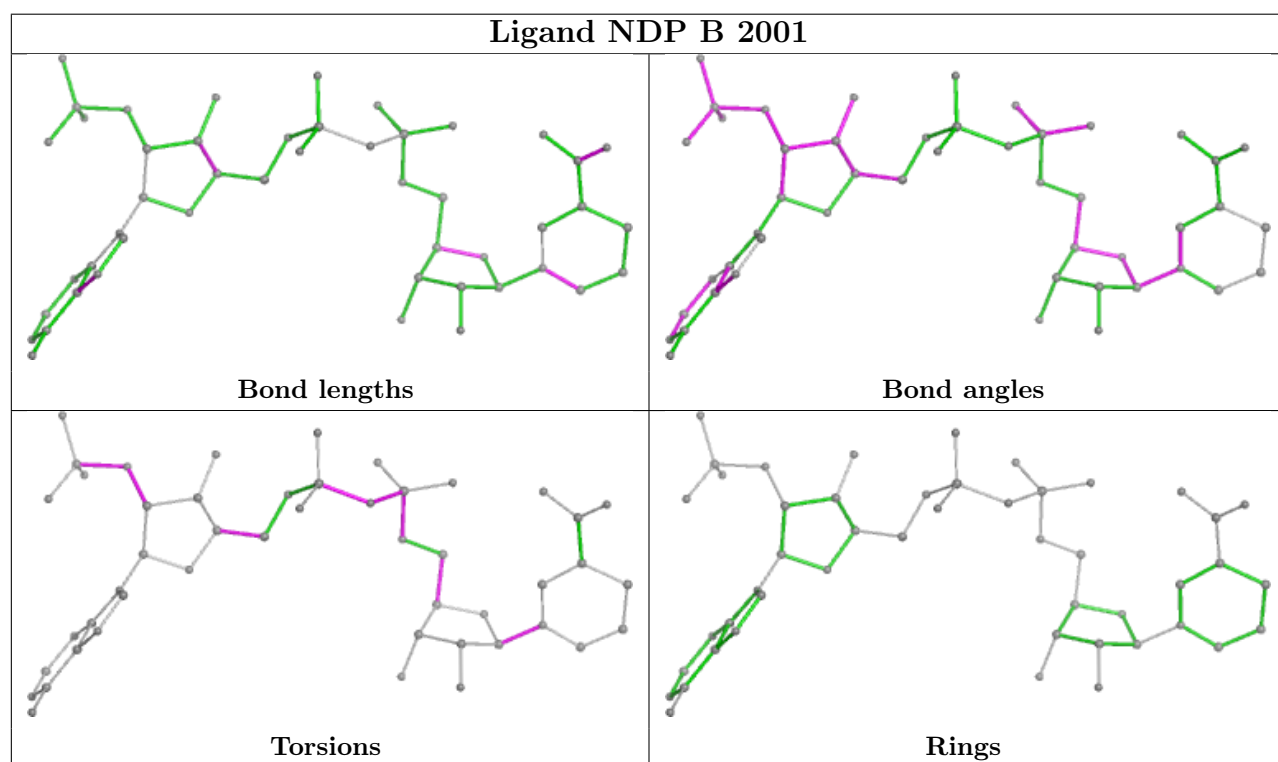
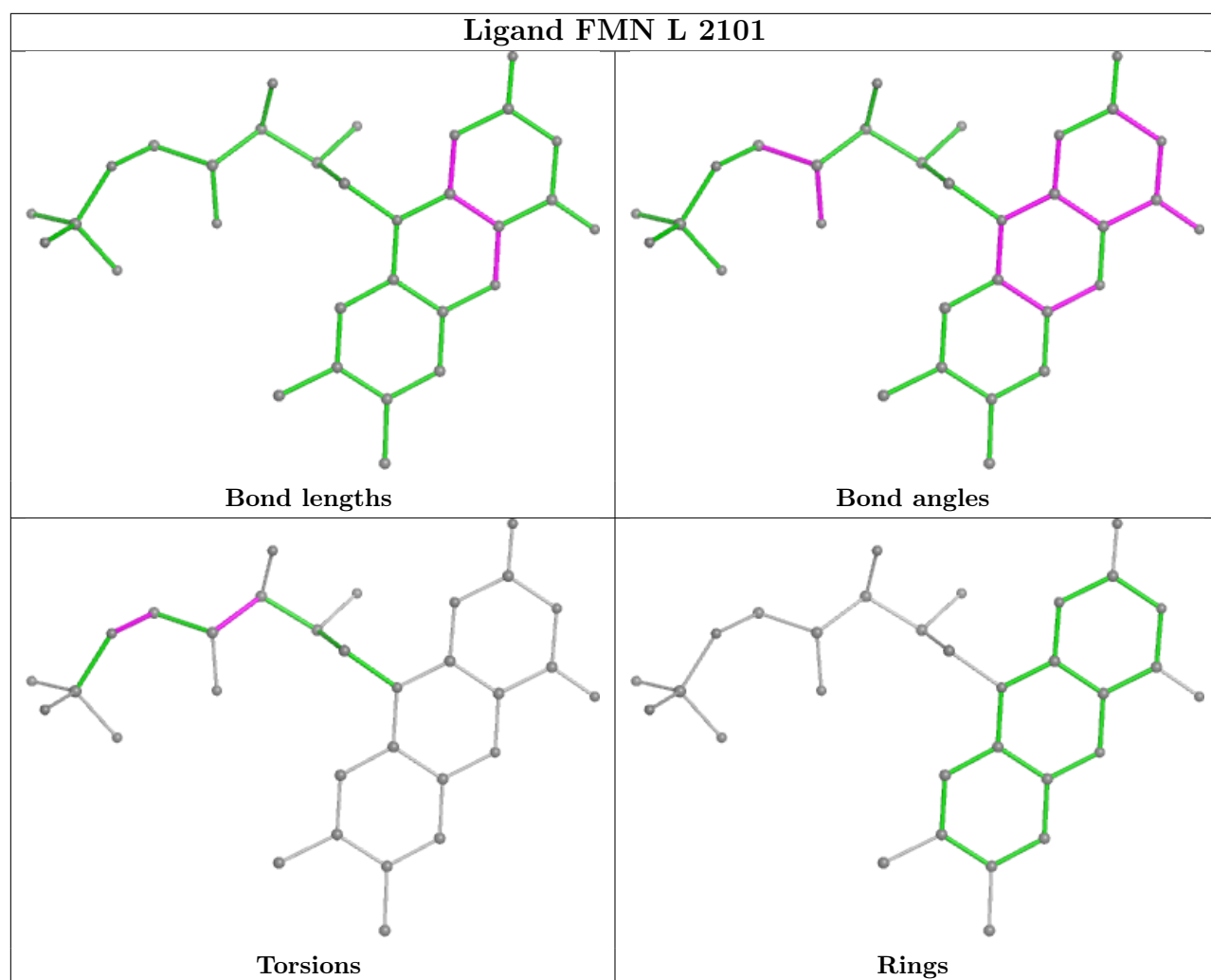
Bond angles

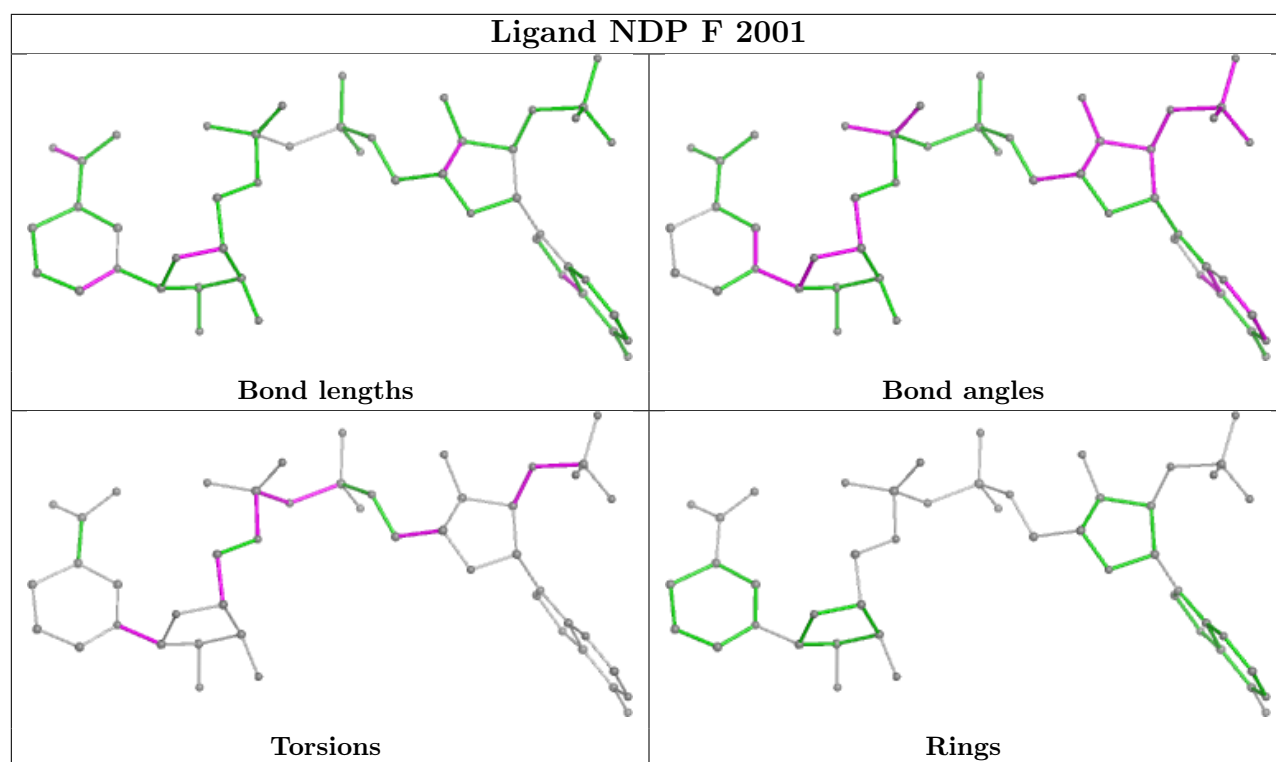


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

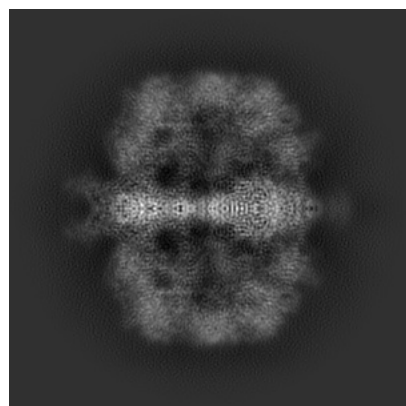
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10420. These allow visual inspection of the internal detail of the map and identification of artifacts.

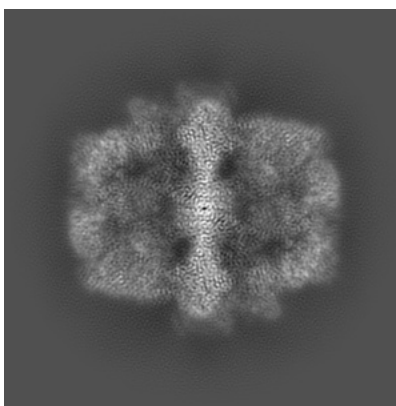
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

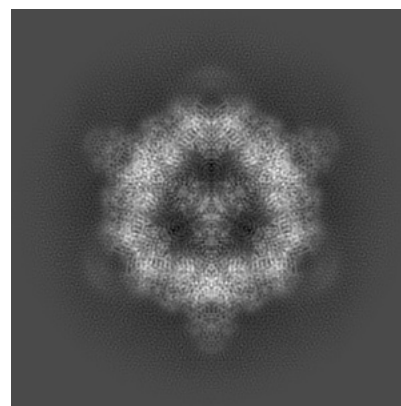
6.1.1 Primary map



X

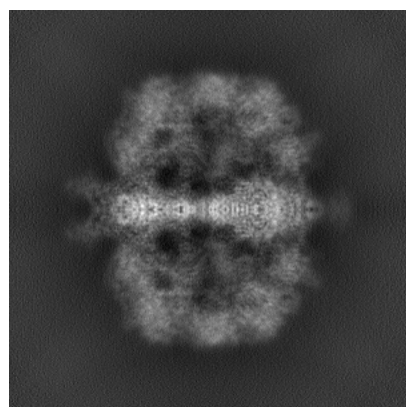


Y

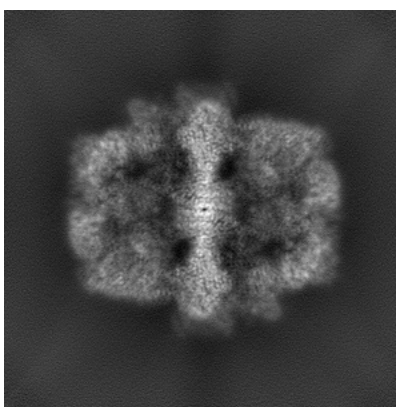


Z

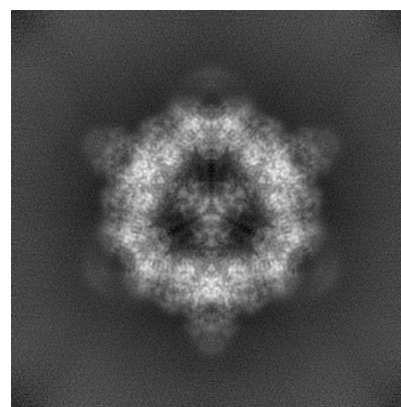
6.1.2 Raw map



X



Y

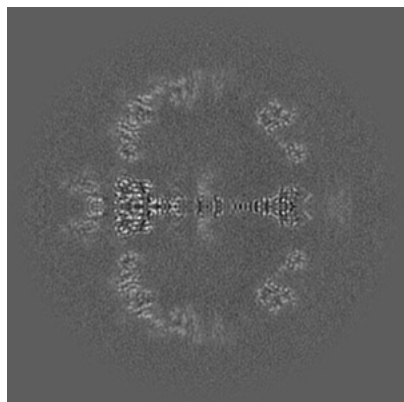


Z

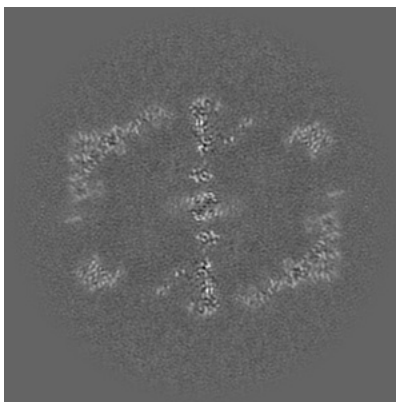
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

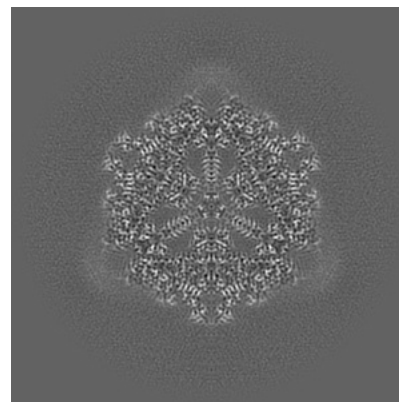
6.2.1 Primary map



X Index: 240

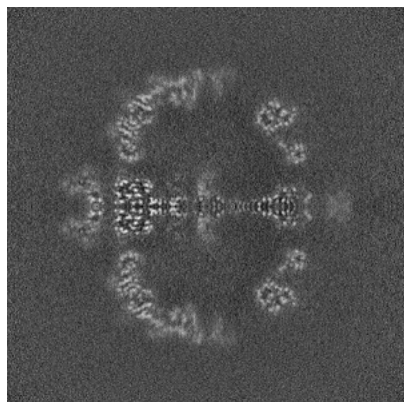


Y Index: 240

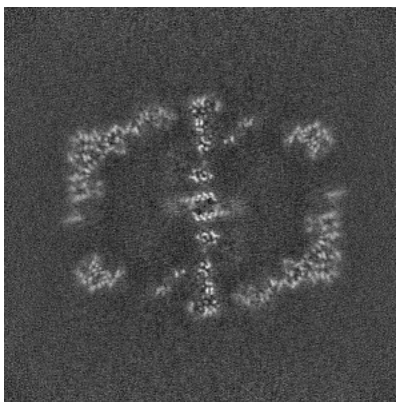


Z Index: 240

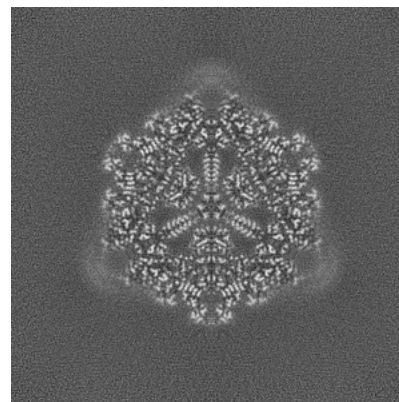
6.2.2 Raw map



X Index: 240



Y Index: 240

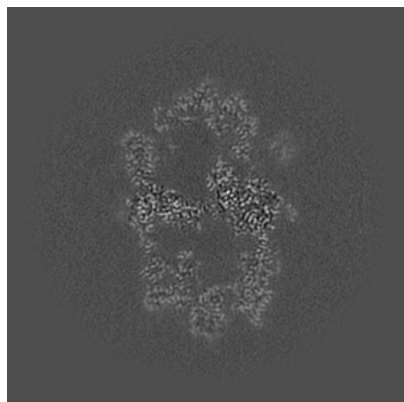


Z Index: 240

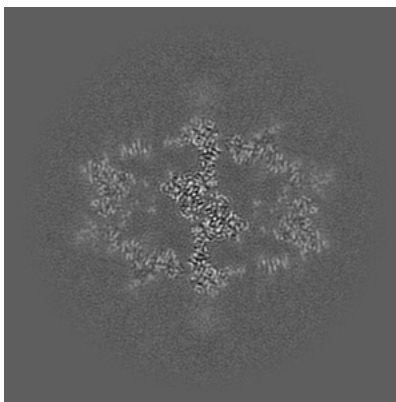
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

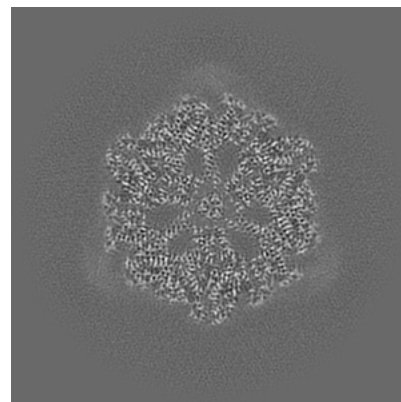
6.3.1 Primary map



X Index: 319

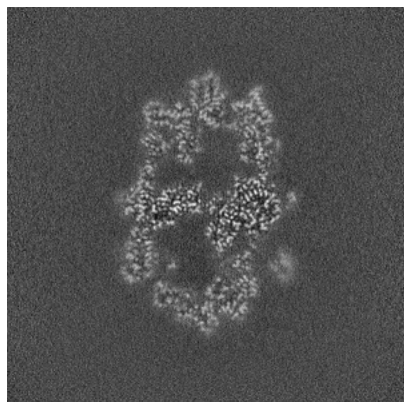


Y Index: 161

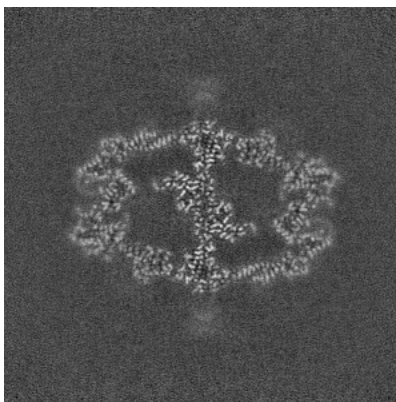


Z Index: 236

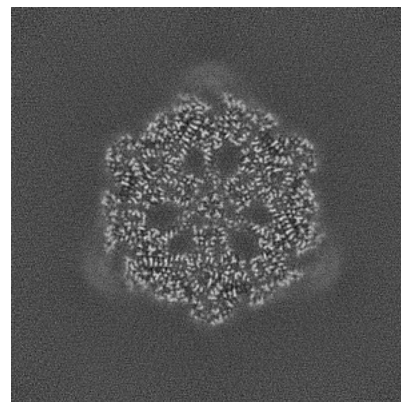
6.3.2 Raw map



X Index: 160



Y Index: 169

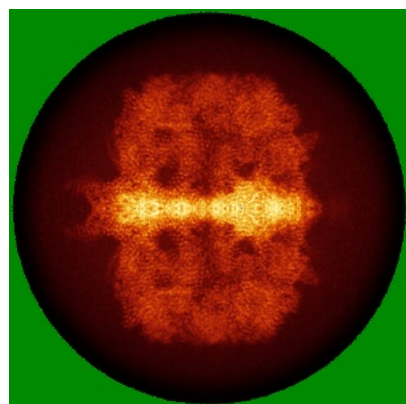


Z Index: 235

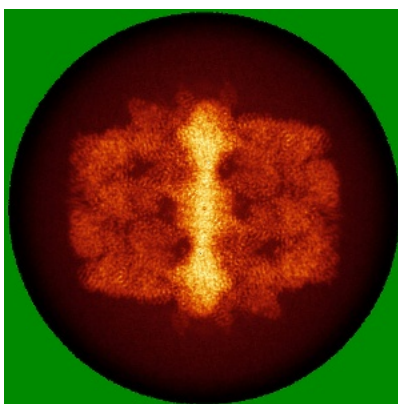
The images above show the largest variance slices of the map in three orthogonal directions.

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

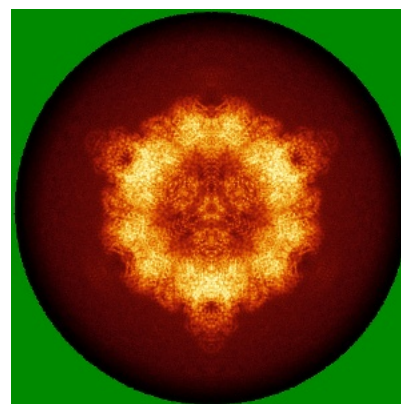
6.4.1 Primary map



X

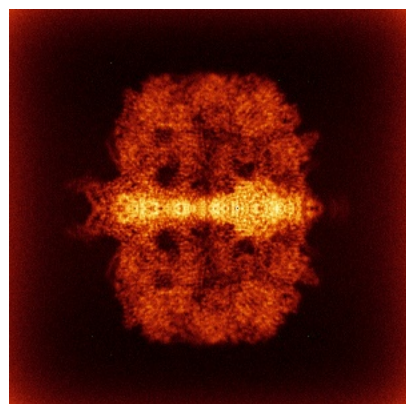


Y

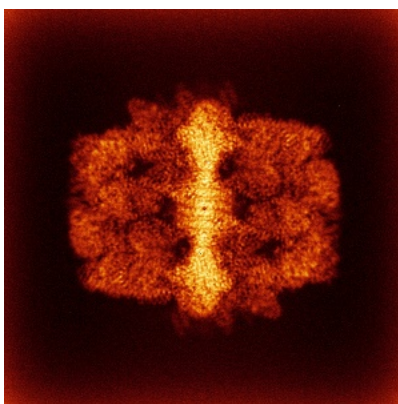


Z

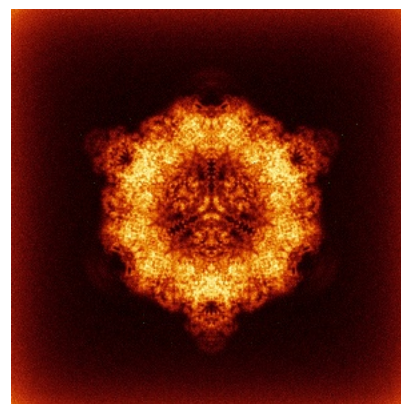
6.4.2 Raw map



X



Y

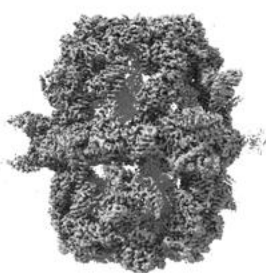


Z

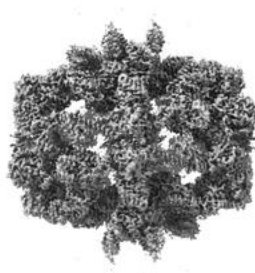
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

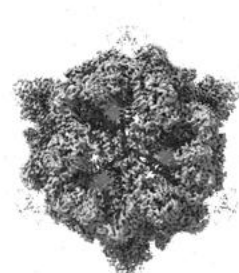
6.5.1 Primary map



X



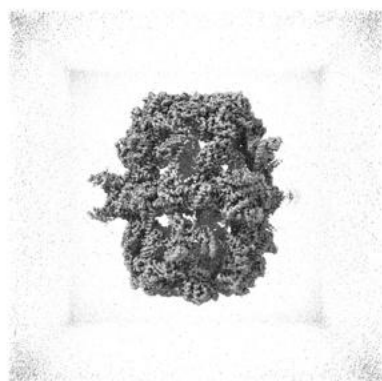
Y



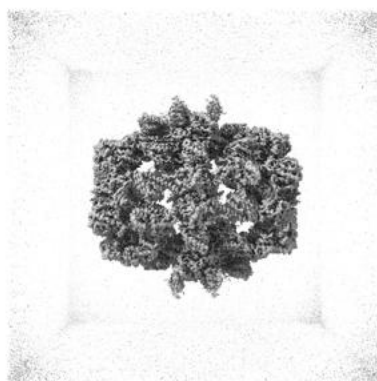
Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

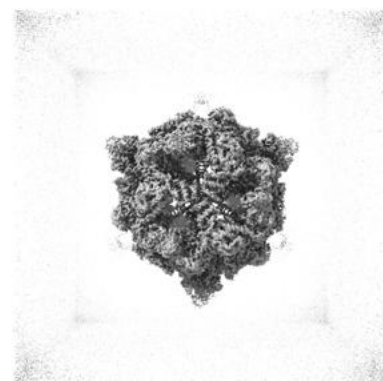
6.5.2 Raw map



X



Y



Z

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

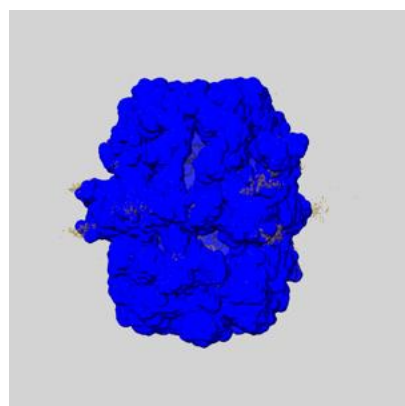
6.6 Mask visualisation [i](#)

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

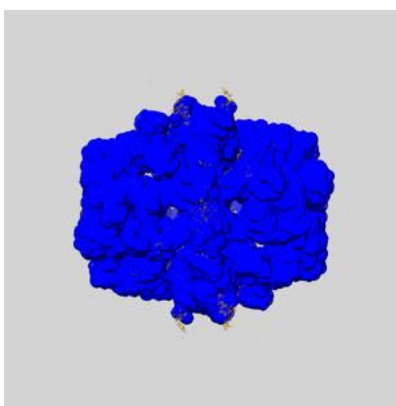
A mask typically either:

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

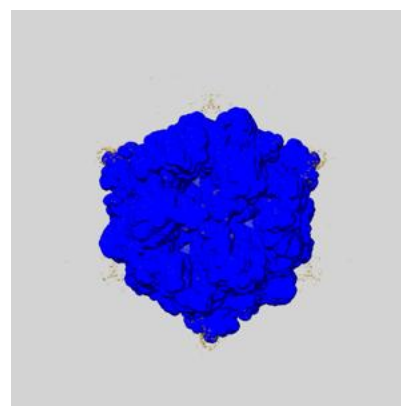
6.6.1 emd_10420_msk_1.map [i](#)



X



Y

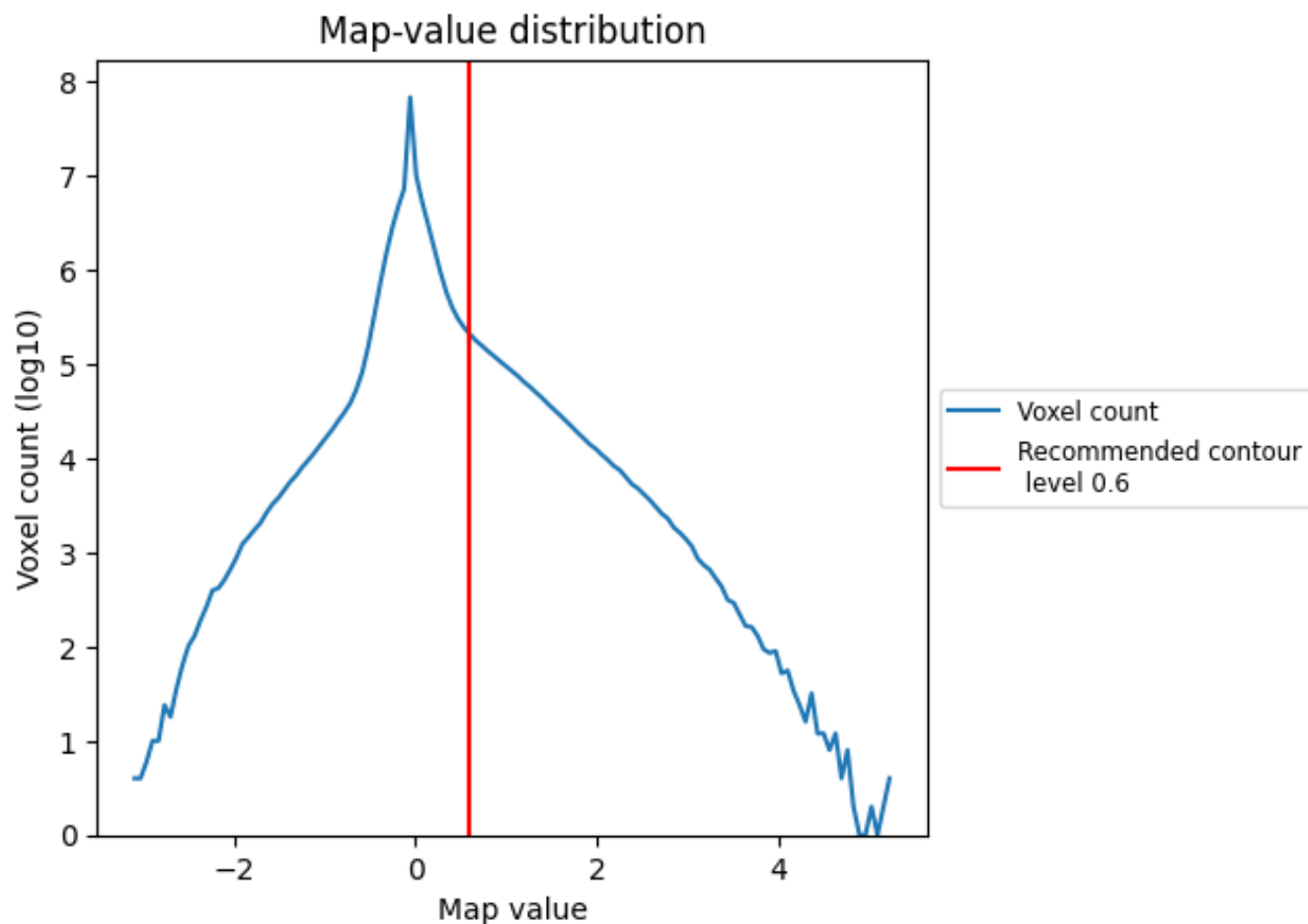


Z

7 Map analysis [i](#)

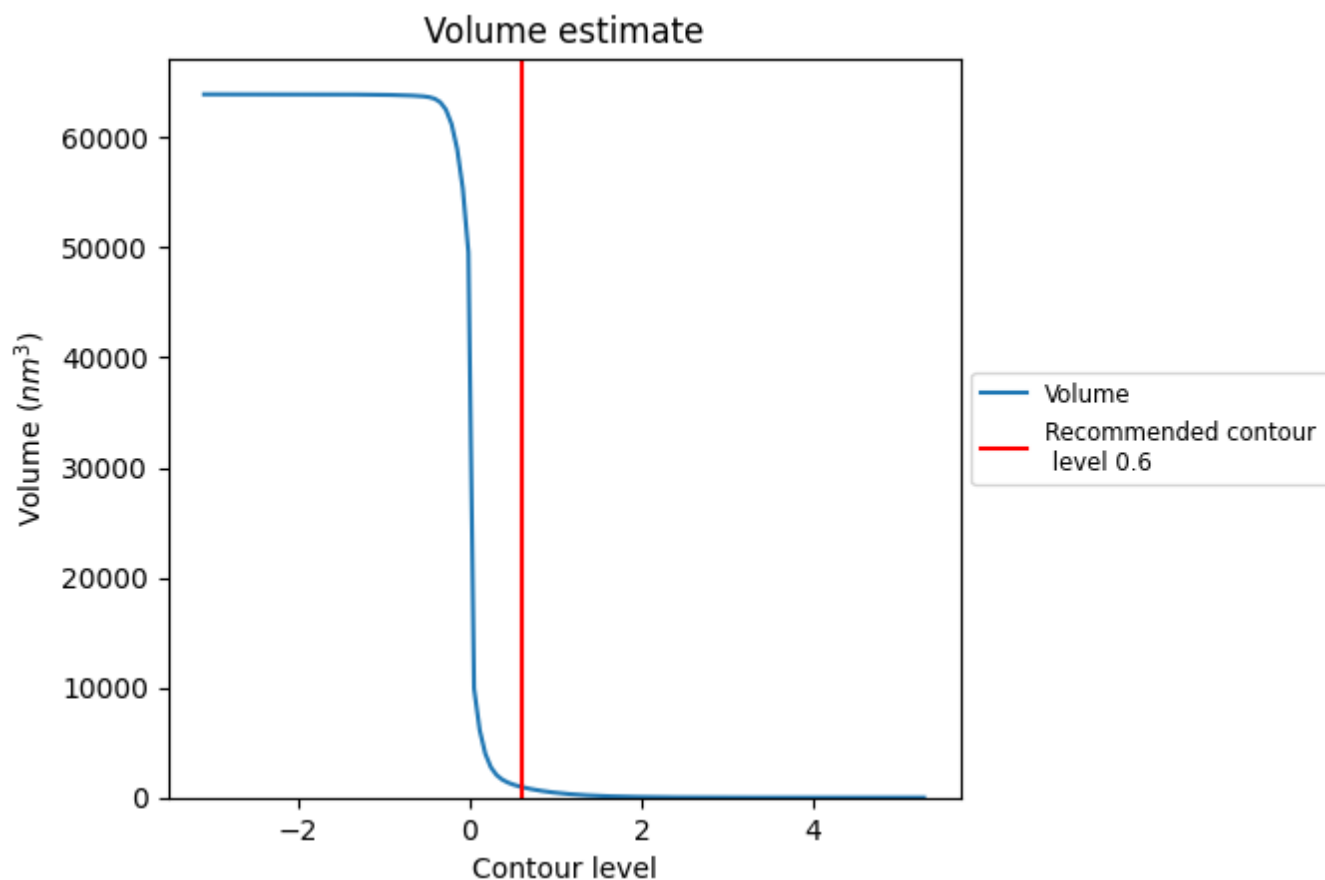
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

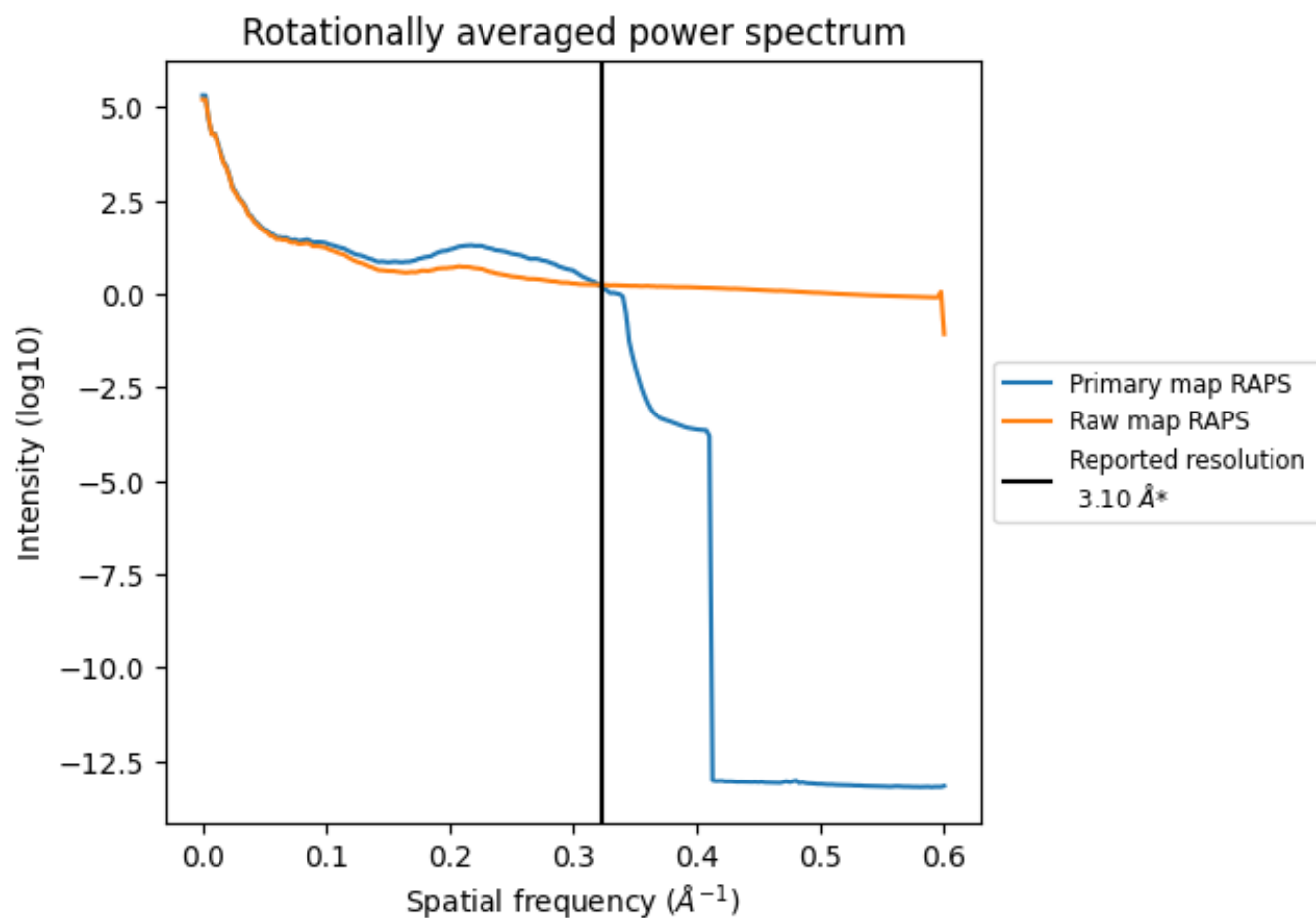
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 970 nm³; this corresponds to an approximate mass of 876 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 ⓘ

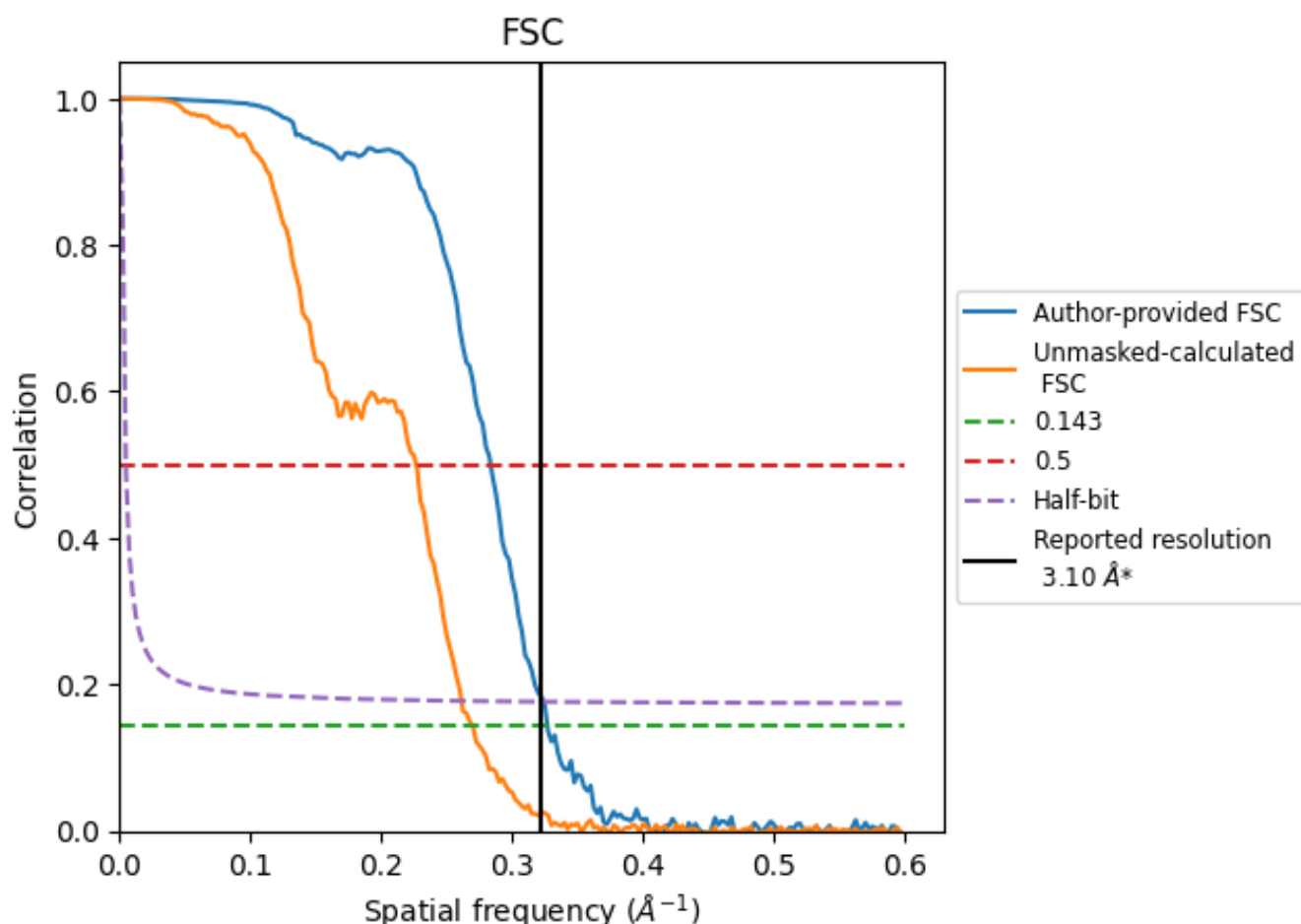


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

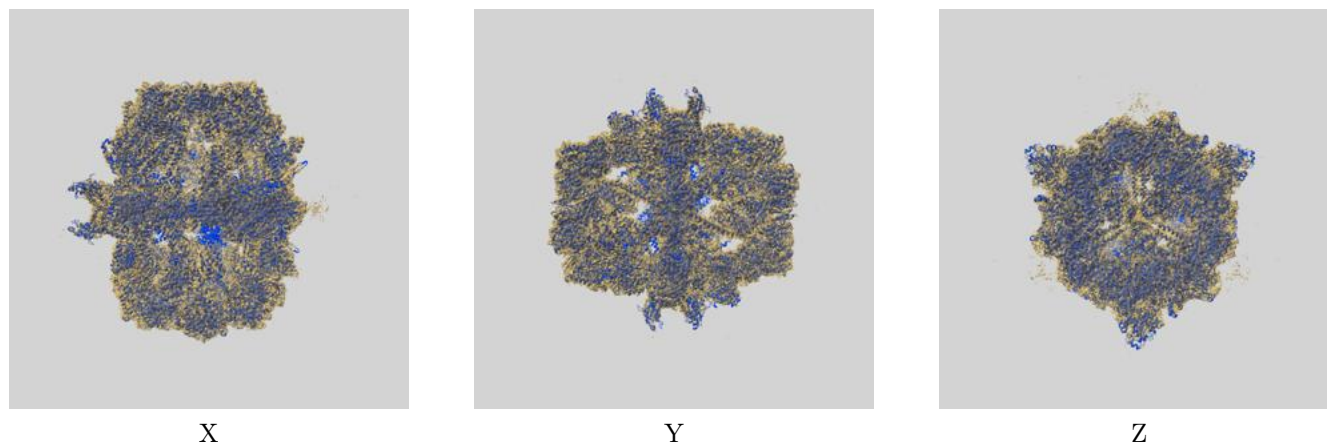
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.52	3.09
Unmasked-calculated*	3.70	4.41	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

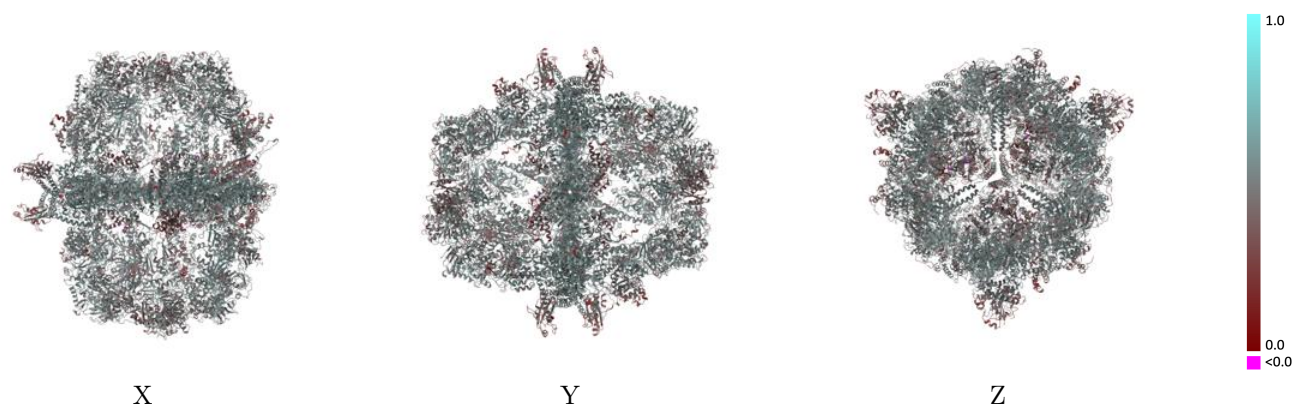
This section contains information regarding the fit between EMDB map EMD-10420 and PDB model 6TA1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



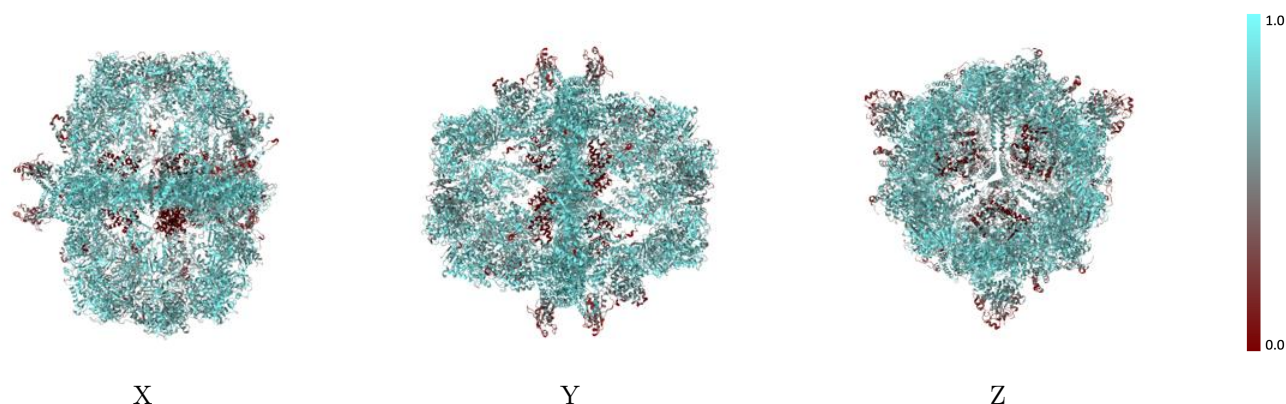
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



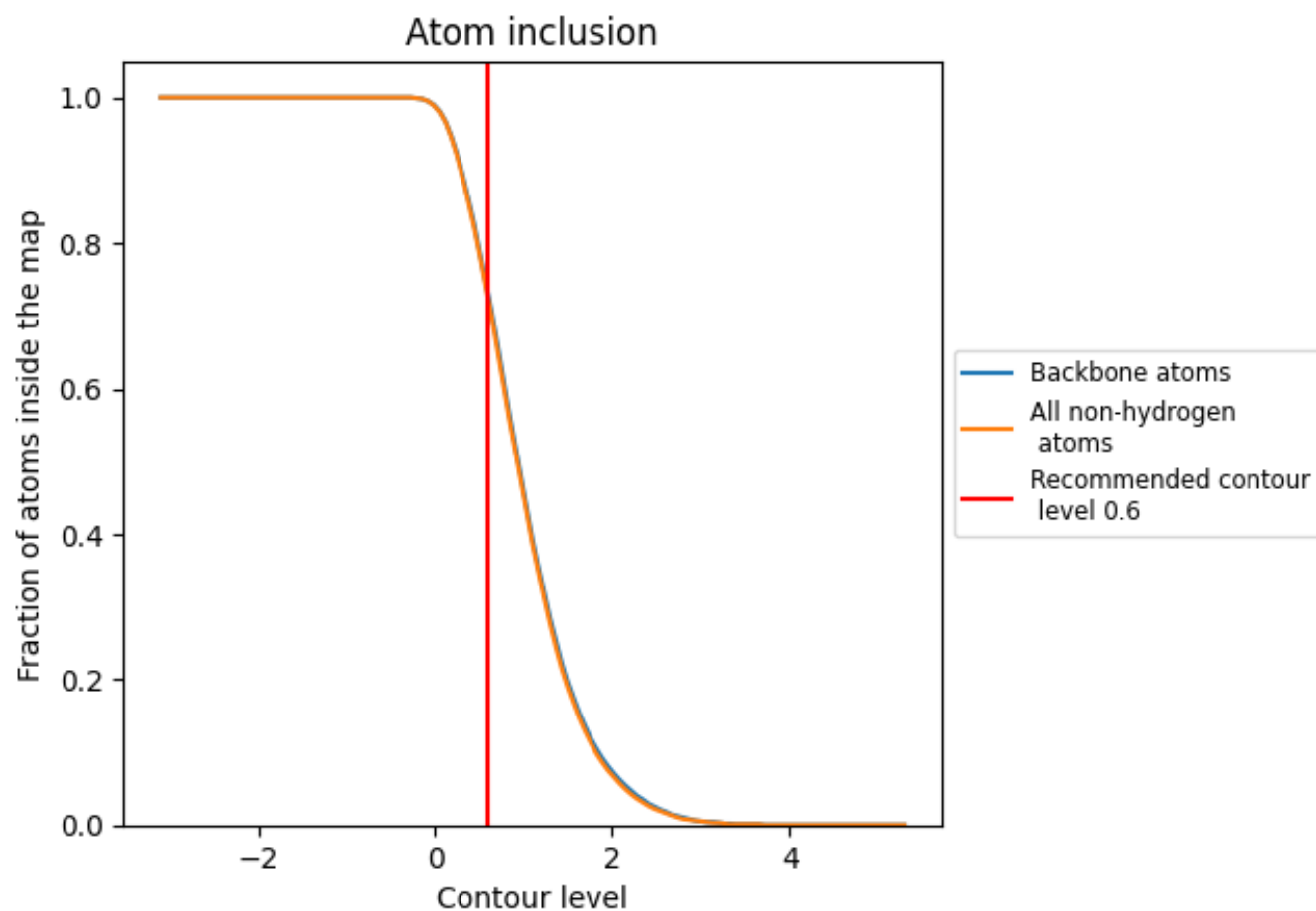
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7220	<div><div></div></div> 0.4880
A	<div><div></div></div> 0.7170	<div><div></div></div> 0.4960
B	<div><div></div></div> 0.7150	<div><div></div></div> 0.4950
C	<div><div></div></div> 0.7340	<div><div></div></div> 0.4810
D	<div><div></div></div> 0.7150	<div><div></div></div> 0.4950
E	<div><div></div></div> 0.7330	<div><div></div></div> 0.4810
F	<div><div></div></div> 0.7150	<div><div></div></div> 0.4950
G	<div><div></div></div> 0.7350	<div><div></div></div> 0.4820
H	<div><div></div></div> 0.7340	<div><div></div></div> 0.4810
I	<div><div></div></div> 0.7150	<div><div></div></div> 0.4950
J	<div><div></div></div> 0.7330	<div><div></div></div> 0.4810
K	<div><div></div></div> 0.7170	<div><div></div></div> 0.4960
L	<div><div></div></div> 0.7350	<div><div></div></div> 0.4820

1.0

0.0

<0.0