



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:53 AM UTC

PDB ID : 8KG6 / pdb_00008kg6
EMDB ID : EMD-37211
Title : Yeast replisome in state I
Authors : Dang, S.; Zhai, Y.; Feng, J.; Yu, D.; Xu, Z.
Deposited on : 2023-08-17
Resolution : 3.07 Å(reported)
Based on initial model : 6XKL

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

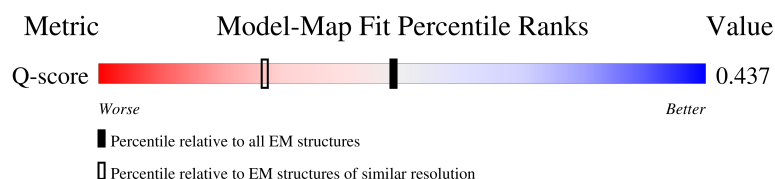
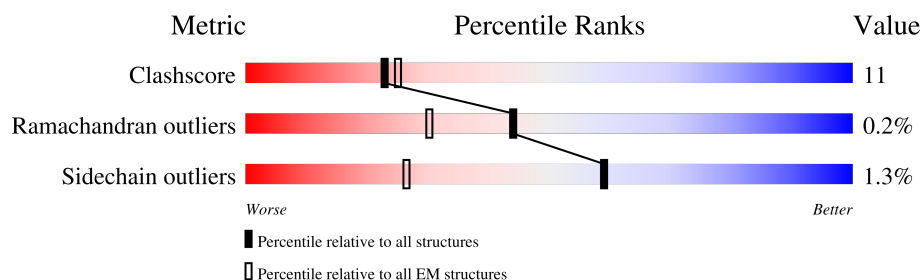
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	2	868	60% 16% • 24%
2	3	971	53% 13% • 34%
3	4	933	50% 23% • 25%
4	5	775	67% 19% • 13%

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
9	C	194	
10	D	294	
11	E	650	
12	F	927	
12	G	927	
12	H	927	
13	I	71	
14	J	61	
15	K	1238	
16	L	317	
17	M	2222	
18	N	689	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 70613 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	662	Total	C	N	O	S	0	0
			5245	3292	942	992	19		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	645	Total	C	N	O	S	0	0
			5005	3148	888	956	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	696	Total	C	N	O	S	0	0
			5494	3447	949	1067	31		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	677	Total	C	N	O	S	0	0
			5334	3345	928	1037	24		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	619	Total	C	N	O	S	0	0
			4880	3085	854	916	25		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	647	Total	C	N	O	S	0	0
			5023	3169	877	950	27		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	200	Total	C	N	O	S	0	0
			1625	1021	280	316	8		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	195	Total	C	N	O	S	0	0
			1630	1046	289	290	5		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	173	Total	C	N	O	S	0	0
			1394	907	224	256	7		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	243	Total	C	N	O	S	0	0
			2004	1276	327	389	12		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	568	Total	C	N	O	S	0	0
			4591	2930	774	873	14		

- Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	433	Total	C	N	O	S	0	0
			3467	2223	577	651	16		
12	G	421	Total	C	N	O	S	0	0
			3362	2162	555	629	16		
12	H	421	Total	C	N	O	S	0	0
			3358	2159	553	631	15		

- Molecule 13 is a DNA chain called DNA (71-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total	C	N	O	P	0	0
			722	350	112	225	35		

- Molecule 14 is a DNA chain called DNA (61-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	22	Total	C	N	O	P	0	0
			438	211	74	131	22		

- Molecule 15 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	660	Total	C	N	O	S	0	0
			5350	3466	904	961	19		

- Molecule 16 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	94	Total	C	N	O	S	0	0
			788	507	144	133	4		

- Molecule 17 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	813	Total	C	N	O	S	0	0
			6490	4202	1060	1193	35		

- Molecule 18 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	536	Total	C	N	O	S	0	0
			4254	2726	725	786	17		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

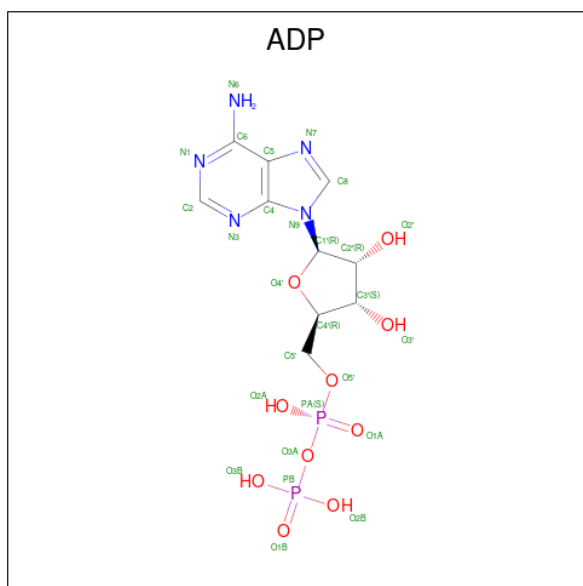
Mol	Chain	Residues	Atoms		AltConf
19	2	1	Total	Zn	0
			1	1	
19	4	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
19	5	1	Total	Zn	0
			1	1	
19	6	1	Total	Zn	0
			1	1	
19	7	1	Total	Zn	0
			1	1	
19	M	2	Total	Zn	0
			2	2	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

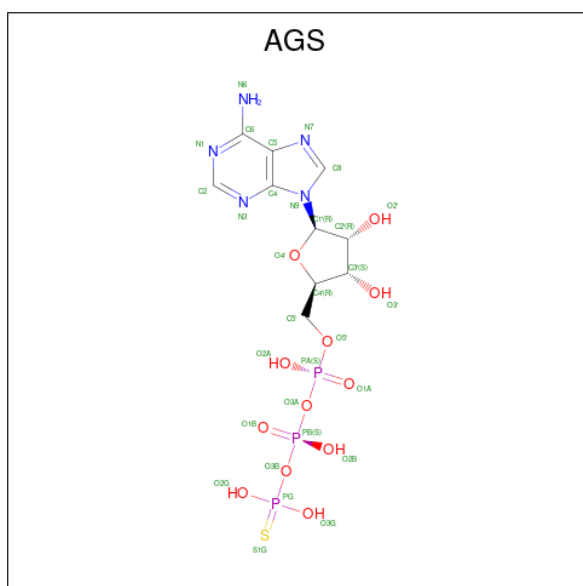
Mol	Chain	Residues	Atoms		AltConf
21	2	1	Total	Mg	0
			1	1	
21	3	1	Total	Mg	0
			1	1	

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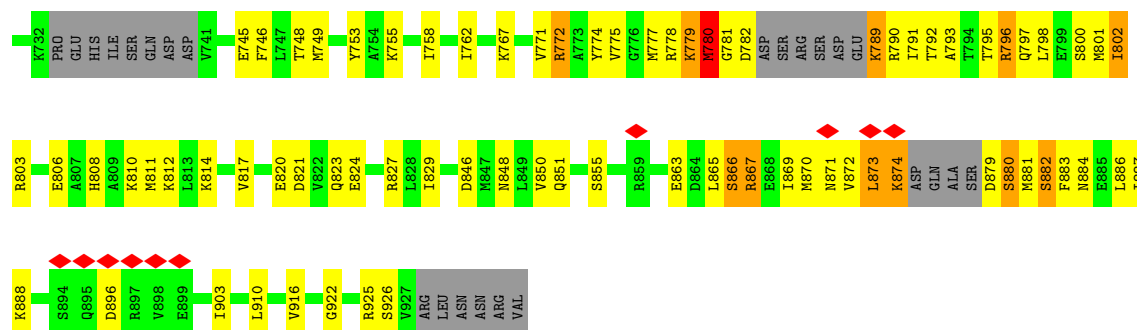
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Mol	Chain	Residues	Atoms		AltConf
21	5	1	Total	Mg	0
			1	1	
21	6	1	Total	Mg	0
			1	1	
21	7	1	Total	Mg	0
			1	1	

- Molecule 22 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).

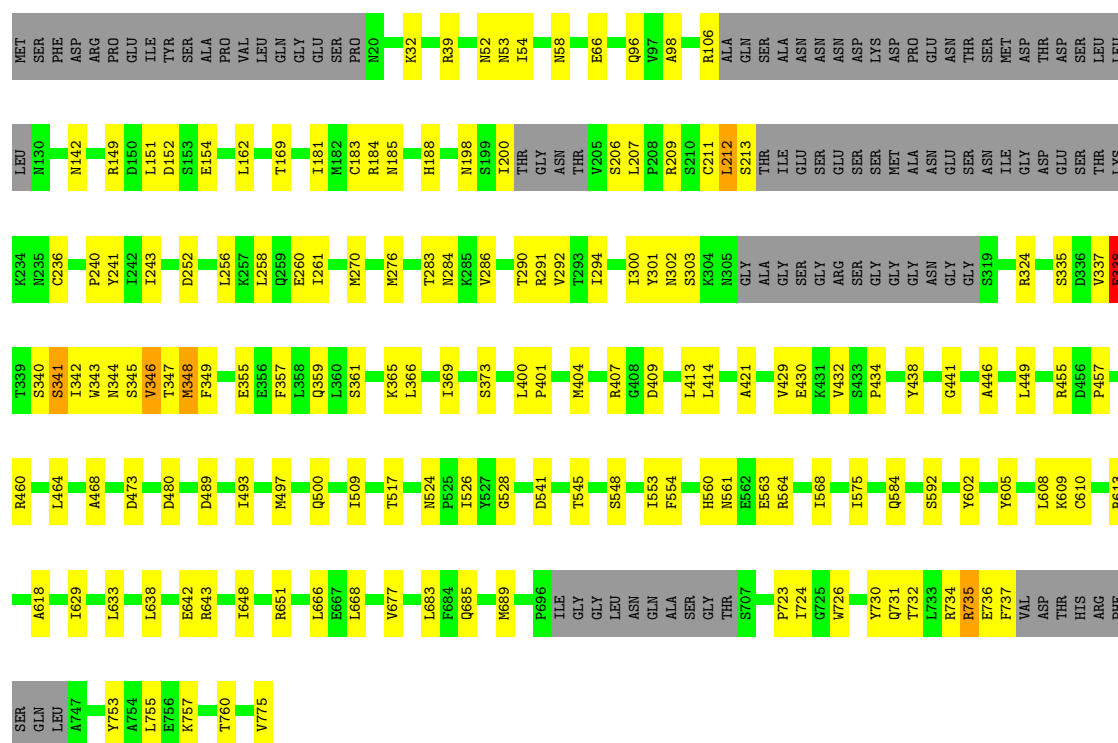


Mol	Chain	Residues	Atoms						AltConf
22	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
22	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
22	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	



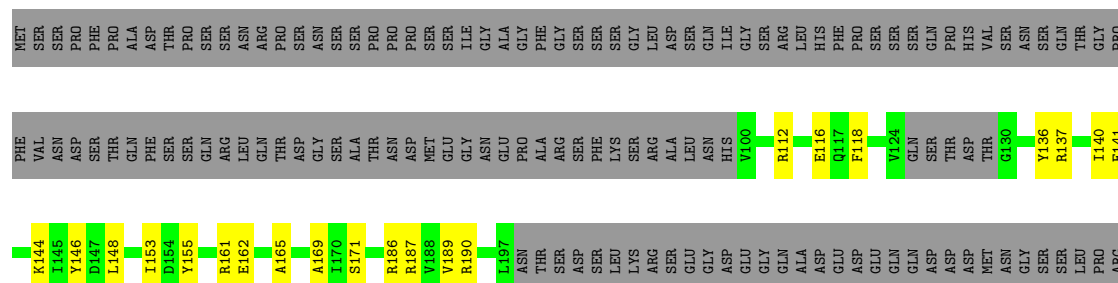
• Molecule 4: Minichromosome maintenance protein 5

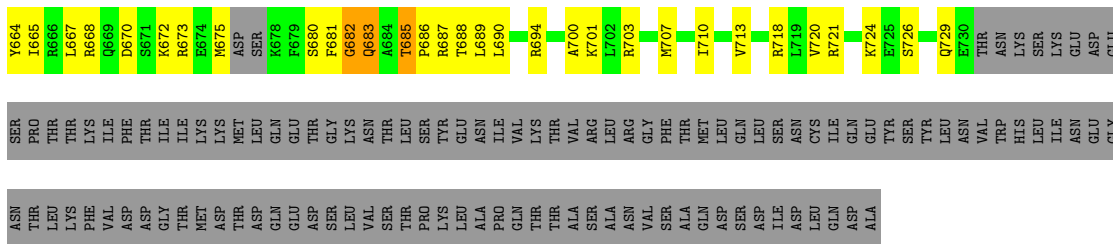
Chain 5: 67% 19% 13%



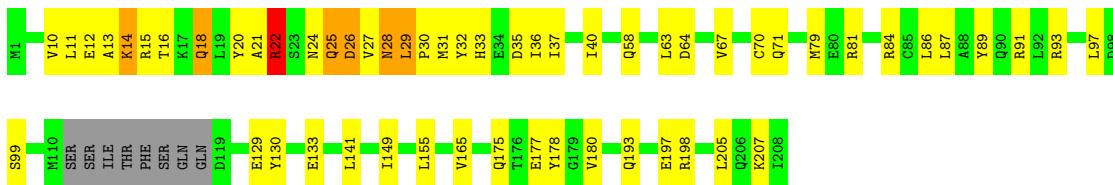
• Molecule 5: DNA replication licensing factor MCM6

Chain 6: 46% 15% 39%

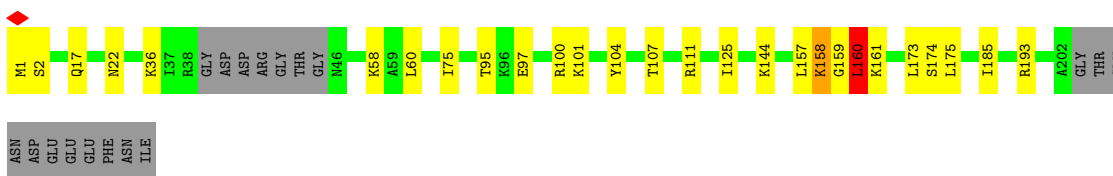
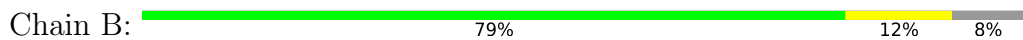




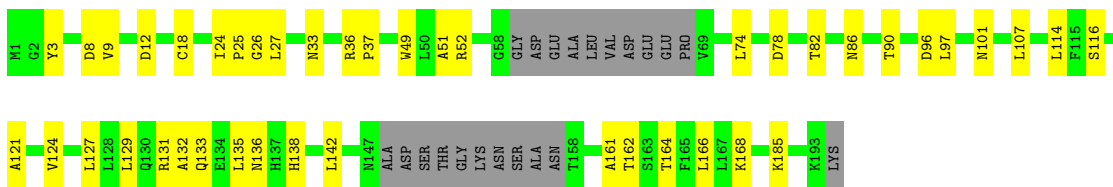
- Molecule 7: DNA replication complex GINS protein PSF1



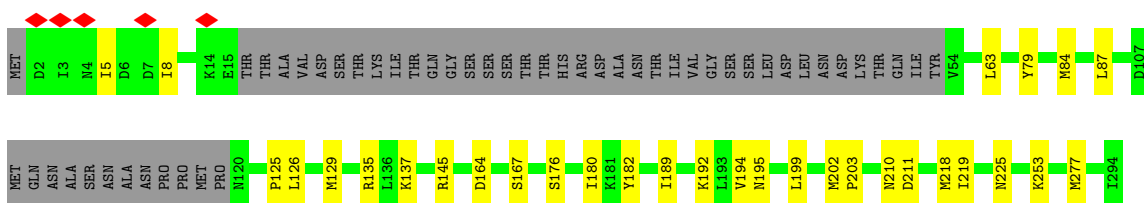
- Molecule 8: DNA replication complex GINS protein PSF2



- Molecule 9: DNA replication complex GINS protein PSF3

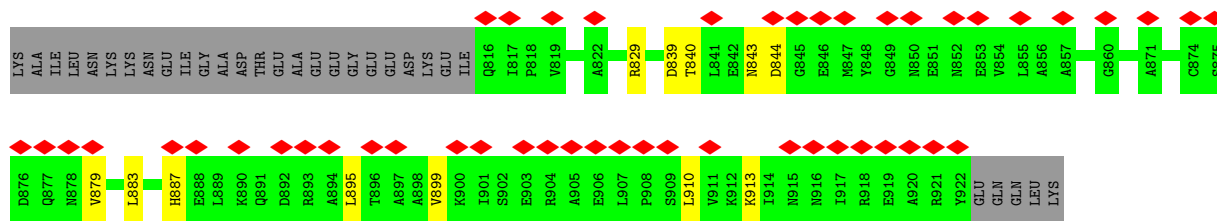


- Molecule 10: DNA replication complex GINS protein SLD5

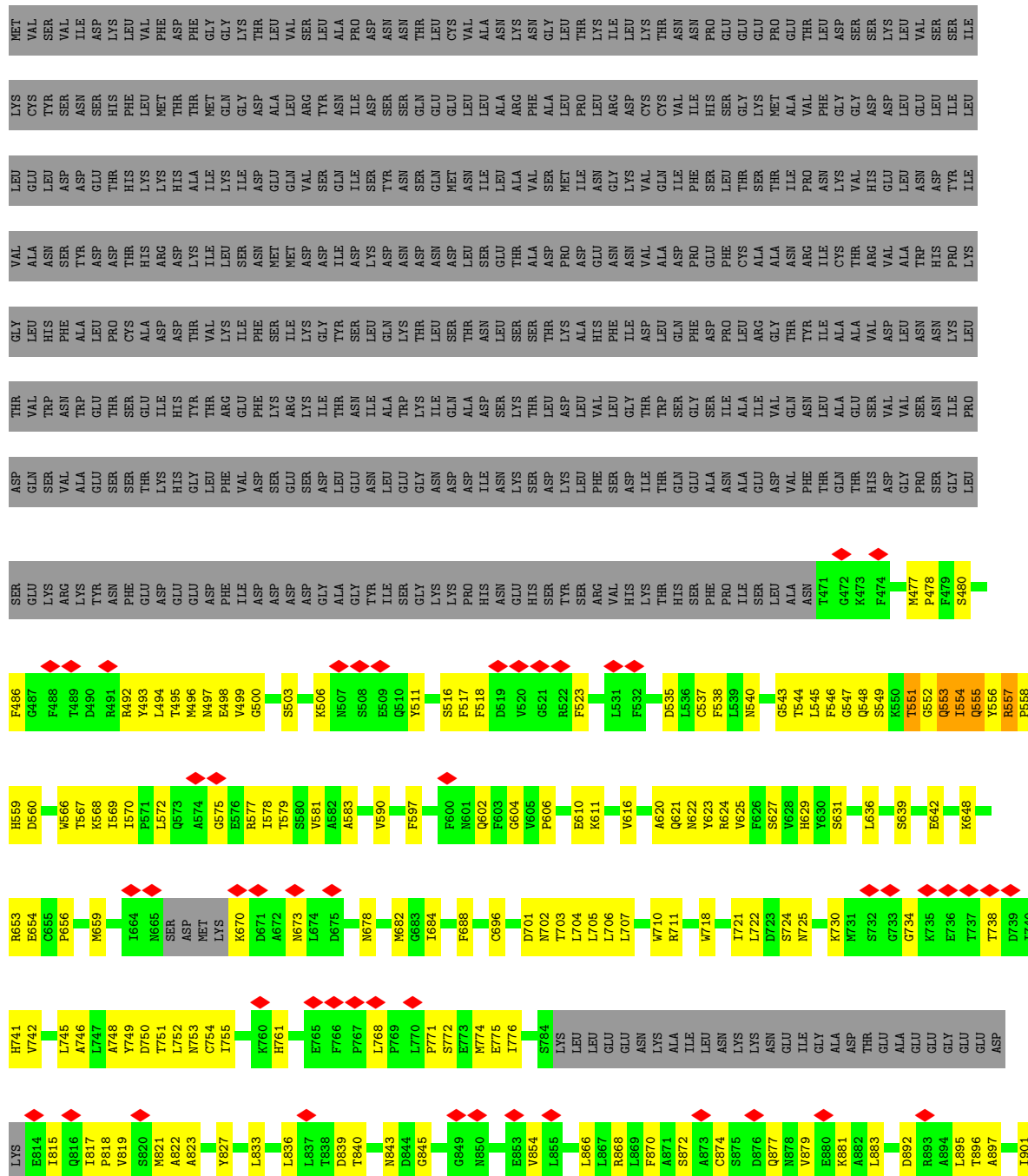
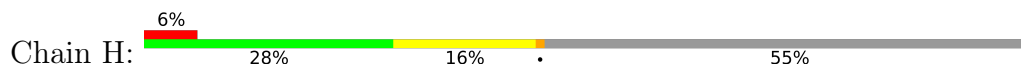


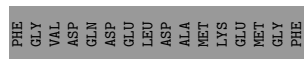
- Molecule 11: Cell division control protein 45





• Molecule 12: DNA polymerase alpha-binding protein

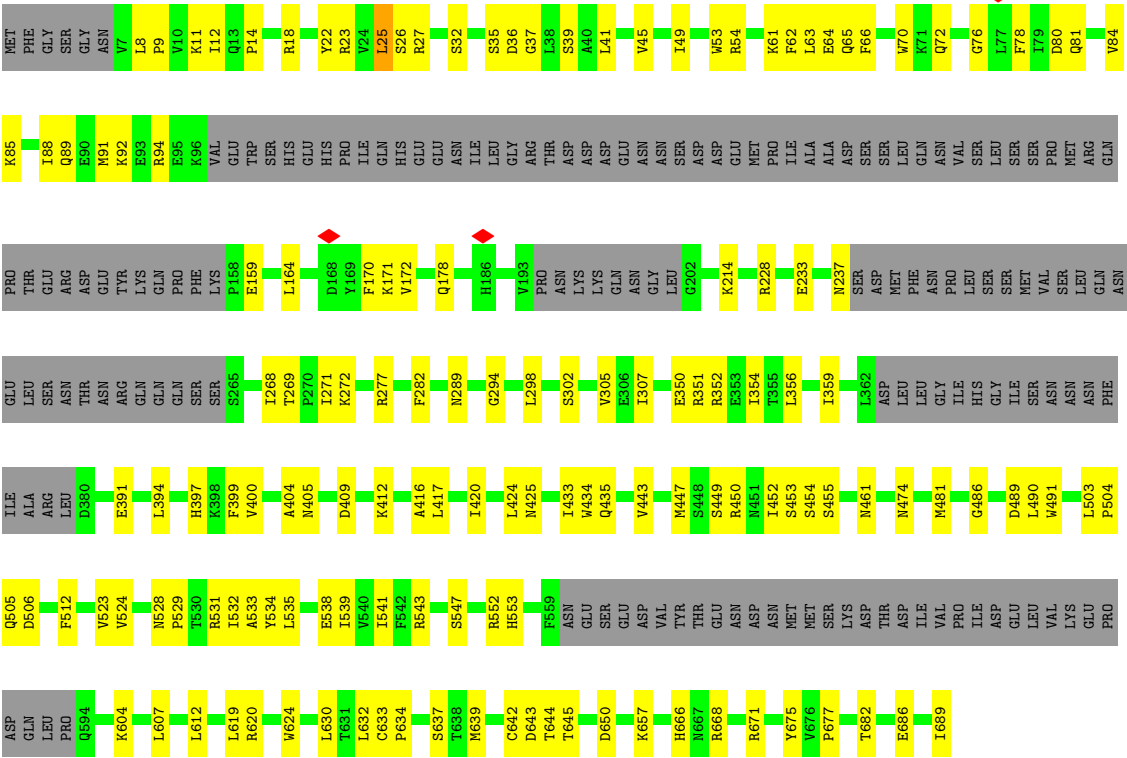




Chain M: 27% 9% 63%

R2073	Gln	A1809	M1608	Pro	E1410	T1321	Leu	Ser	Ile	Met	Ser	Glu	Arg
R2086	D1932	L1810	P1611	Ser	K1411	W1322	Ile	Lys	Asp	Val	Val	Val	Tyr
L2107	V1939	L1812	F1611	Asn	E1412	E1323	Pro	Lys	Gly	Lys	Gly	Gly	Glu
C2130	Q1940	L1813	S1616	Ala	T1415	F1324	Met	Asn	Lys	Asp	Asn	Phe	Phe
V2131	F1944	M1814	L1617	Gln	S1416	L1325	Asp	Val	Tyr	Gly	Trp	Gly	Gly
R2132	S1815	S1816	Asn	Glu	I1417	D1329	Glu	Pro	Arg	Gln	Leu	Ala	Leu
C2133	A1817	L1816	Val	Ile	F1418	G1330	Asp	Thr	Glu	Gln	Asp	Ser	Ala
Q2143	A1817	L1731	Glu	Met	M1419	G1331	Tyr	Met	Gly	Gln	Val	Gly	Ile
I2147	S1818	L1732	Leu	Met	F1423	E1332	Val	Gly	Gly	Lys	Leu	Ala	Thr
R2151	M1819	L1739	Pro	Lys	V1424	P1333	Gly	Lys	Gly	Tyr	Asp	Cys	Trp
Q2160	Q1820	L1749	Gln	Lys	G1425	G1334	Trp	Lys	Ser	Ile	Phe	Leu	Lys
R2163	Q1821	Ile	Leu	Asn	H1434	V1335	Asn	Asp	Ala	Ser	Gly	Arg	Gly
Y2174	M1822	Asn	Asn	Met	Q1435	L1336	Tyr	Ile	Gln	Ser	Leu	Ala	Thr
E2186	A1825	Asp	Trp	Gly	Q1438	E1337	Lys	Asp	Ile	Phe	Glu	Ile	Ile
A2205	K1826	Glu	Q1628	Gln	I1438	V1338	Lys	Phe	Thr	Asn	Ala	Gln	Asp
F2210	K1842	Ser	K1633	K1539	S1444	T1341	Trp	Glu	Ile	Ala	Glu	Thr	Pro
D2211	A1843	Asp	V1636	K1540	F1447	V1346	Lys	Pro	Pro	Val	Asp	Ala	Ala
L2212	L1844	Val	H1637	I1552	F1457	K1360	Ile	Thr	Ala	Val	Leu	Lys	Arg
L2213	V1848	Asn	H1638	I1556	K1457	F1361	Gln	Val	Ala	Thr	Val	Lys	Lys
C2216	V1848	Asn	V1639	N1557	K1450	K1362	Ala	Glu	Leu	Glu	Ser	Phe	His
T2221	I1858	Met	S1641	F1558	K1453	K1372	Arg	Glu	Gln	Ala	Leu	Val	Ala
Ile	R1863	Gly	S1644	E1559	A1454	L1375	Asp	Asn	Gly	Ile	Ile	Glu	Arg
	M1864	Ile	M1644	F1563	L1455	I1376	Arg	Ala	Val	Ile	Cys	Lys	Asp
	Q1865	Asp	M1657	I1566	G1456	I1377	Lys	Lys	Ser	Pro	Glu	Arg	Glu
	K1868	Lys	I1658	S1567	K1457	E1377	Arg	Ile	Ala	Val	Asn	Lys	Ala
	K1869	Asp	P1659	K1568	G1458	K1378	Asp	Val	Pro	Ala	Arg	Lys	Lys
	T1870	Ala	I1660	L1569	I1459	S1379	Gln	Ile	Pro	Ile	Ser	Met	Met
	S1882	Val	C1661	L1572	L1477	L1383	Phe	Ala	Arg	Ala	Ser	Glu	Val
	M1886	Asn	L1665	L1573	M1482	P1384	Gly	Thr	Glu	Ala	Lys	Leu	Val
	K1887	Ser	M1668	S1574	Y1486	N1385	Asn	Lys	Pro	Ile	Lys	Thr	Thr
	A1888	Pro	D1669	Q1575	L1487	Asn	Pro	Lys	Asp	Tyr	Glu	Asp	Ser
	T1891	Glu	Y1670	K1579	L1488	Ser	Ser	Val	Lys	Arg	Glu	Trp	Gln
	W1906	F1778	I1671	L1580	H1489	Asn	Glu	Val	Arg	Phe	Gln	Cys	Lys
	M1912	N1769	L1675	K1581	S1493	Pro	Arg	Lys	Lys	Leu	Lys	Leu	His
	D1913	R1792	Y1676	E1582	I1494	Ala	Ser	Arg	Ile	Arg	Phe	Pro	Lys
	K1914	G1793	A1677	R1584	G1495	Gly	Ala	Lys	Ala	Arg	Val	Lys	Val
	S1918	M1794	R1678	G1585	Y1496	Gln	Leu	Arg	Thr	Trp	Phe	Ser	Ile
	A1921	L1795	N1684	L1586	F1499	Leu	Ser	Gln	Lys	Leu	Gly	Pro	Asn
	C1922	K1796	M1689	Q1587	S1500	Phe	Met	Leu	Asp	Pro	Thr	Glu	Ser
	L1922	E1797	M1690	L1589	L1501	Lys	Ile	Thr	Lys	Pro	Ala	Thr	Phe
	D1924	W1798	E1691	Q1593	F1502	Ile	Arg	Asn	Phe	Ser	Arg	Lys	Tyr
	S2065	D1800	D1697	T1598	K1503	T1401	Lys	Glu	Lys	Leu	Arg	Ala	Ala
	T2068	Ile	H1698	K1599	T1510	L1402	Gln	Asp	Glu	Glu	Leu	Gly	Phe
	L2070	L1803	N1704	L1601	I1511	E1404	Ala	Pro	Thr	Asp	Gly	Ile	Thr
		K1804	D1707	L1604	Leu	S1405	Glu	Leu	Leu	Leu	Tyr	Pro	Glu
		N1806	N1708	I1604	Val	V1406	Ser	Val	Thr	Ile	Phe	Ser	Arg
					Leu	F1407	Y1317	Leu	Lys	Arg	Gly	Asn	Lys
						L1408	N1318	Leu	Phe	Thr	Val	Gly	Lys
							S1320	Pro		Ile			Arg

● Molecule 18: DNA polymerase epsilon subunit B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	384519	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.382	Depositor
Minimum map value	-1.647	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	572.39996, 572.39996, 572.39996	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2	0.25	0/5334	0.34	0/7203
2	3	0.26	0/5091	0.36	0/6914
3	4	0.29	1/5566 (0.0%)	0.46	1/7519 (0.0%)
4	5	0.30	0/5407	0.41	0/7302
5	6	0.20	0/4957	0.31	0/6684
6	7	0.21	0/5097	0.37	1/6896 (0.0%)
7	A	0.34	0/1645	0.48	0/2215
8	B	0.26	0/1663	0.41	1/2249 (0.0%)
9	C	0.20	0/1426	0.28	0/1929
10	D	0.19	0/2040	0.31	0/2755
11	E	0.19	0/4677	0.28	0/6335
12	F	0.13	0/3553	0.28	0/4811
12	G	0.09	0/3448	0.27	0/4675
12	H	0.21	0/3443	0.33	0/4668
13	I	0.20	0/805	0.39	0/1244
14	J	0.14	0/488	0.29	0/747
15	K	0.21	0/5449	0.36	0/7340
16	L	0.09	0/804	0.22	0/1074
17	M	0.26	0/6632	0.42	2/8976 (0.0%)
18	N	0.17	0/4345	0.32	0/5884
All	All	0.23	1/71870 (0.0%)	0.36	5/97420 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	567	CYS	N-CA	5.08	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	160	LEU	N-CA-C	-7.40	104.38	113.19
6	7	364	LYS	N-CA-C	-6.42	105.17	112.87
17	M	1810	ASP	CA-C-N	-5.69	112.86	120.54
17	M	1810	ASP	C-N-CA	-5.69	112.86	120.54
3	4	567	CYS	CB-CA-C	-5.41	109.28	117.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	790	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5245	0	5289	107	0
2	3	5005	0	5043	94	0
3	4	5494	0	5531	197	0
4	5	5334	0	5383	113	0
5	6	4880	0	4914	126	0
6	7	5023	0	5042	140	0
7	A	1625	0	1621	53	0
8	B	1630	0	1685	20	0
9	C	1394	0	1405	34	0
10	D	2004	0	2001	29	0
11	E	4591	0	4567	80	0
12	F	3467	0	3410	91	0
12	G	3362	0	3299	74	0
12	H	3358	0	3283	115	0
13	I	722	0	407	16	0
14	J	438	0	249	10	0
15	K	5350	0	5519	155	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	788	0	827	16	0
17	M	6490	0	6446	159	0
18	N	4254	0	4256	106	0
19	2	1	0	0	0	0
19	4	1	0	0	0	0
19	5	1	0	0	0	0
19	6	1	0	0	0	0
19	7	1	0	0	0	0
19	M	2	0	0	0	0
20	2	27	0	12	2	0
20	3	27	0	12	1	0
21	2	1	0	0	0	0
21	3	1	0	0	0	0
21	5	1	0	0	0	0
21	6	1	0	0	0	0
21	7	1	0	0	0	0
22	5	31	0	12	3	0
22	6	31	0	12	2	0
22	7	31	0	12	1	0
All	All	70613	0	70237	1578	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 11.

All (1578) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:536:ALA:HA	5:6:742:ILE:CD1	1.68	1.22
5:6:535:PRO:HB2	5:6:742:ILE:HG21	1.28	1.14
3:4:775:VAL:HB	3:4:779:LYS:HZ2	1.24	1.03
3:4:762:ILE:HG23	5:6:736:MET:HG3	1.37	1.01
3:4:775:VAL:HB	3:4:779:LYS:NZ	1.81	0.94
5:6:535:PRO:HB2	5:6:742:ILE:CG2	1.97	0.94
5:6:536:ALA:HA	5:6:742:ILE:HD13	1.47	0.94
2:3:277:ILE:HG13	2:3:320:LEU:HD13	1.48	0.94
3:4:569:ASP:HB3	3:4:682:TYR:H	1.32	0.94
17:M:1668:MET:HB3	17:M:1815:SER:CB	2.03	0.88
7:A:20:TYR:HD1	7:A:27:VAL:HG12	1.41	0.86
15:K:195:THR:HB	15:K:198:ASP:HB2	1.58	0.86
5:6:536:ALA:HA	5:6:742:ILE:HD11	1.58	0.86
17:M:1957:MET:HE1	17:M:2061:VAL:HG21	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:666:HIS:HB2	18:N:671:ARG:HE	1.44	0.82
3:4:873:LEU:HA	3:4:879:ASP:HA	1.63	0.80
5:6:734:LEU:CD2	5:6:742:ILE:HG13	2.12	0.80
12:H:555:GLN:HG3	12:H:557:ARG:HD2	1.65	0.79
5:6:734:LEU:HD21	5:6:742:ILE:HG13	1.65	0.79
17:M:1848:VAL:HG13	17:M:1858:ILE:HG13	1.65	0.78
3:4:774:TYR:CZ	3:4:778:ARG:HD2	2.19	0.78
3:4:871:ASN:HA	3:4:874:LYS:HD2	1.64	0.77
4:5:449:LEU:HD13	4:5:493:ILE:HD11	1.67	0.77
12:H:704:LEU:HB2	12:H:721:ILE:HB	1.67	0.76
15:K:668:THR:HG22	15:K:670:PRO:HD2	1.66	0.76
1:2:190:LYS:HB3	1:2:197:TRP:CZ3	2.21	0.75
12:F:509:GLU:HG2	12:F:510:GLN:HG3	1.67	0.75
15:K:414:LEU:HD13	15:K:473:VAL:HG11	1.69	0.74
1:2:185:SER:HA	1:2:188:ASN:HD22	1.50	0.74
18:N:352:ARG:HH12	18:N:538:GLU:H	1.34	0.73
5:6:536:ALA:CA	5:6:742:ILE:HD13	2.19	0.73
12:H:682:MET:HG3	12:H:684:ILE:HG12	1.68	0.73
17:M:1669:ASP:OD1	17:M:1819:TRP:HB2	1.87	0.73
17:M:1731:VAL:HG12	17:M:1869:LYS:HA	1.70	0.72
9:C:26:GLY:H	9:C:37:PRO:HB3	1.53	0.72
6:7:670:ASP:HA	6:7:673:ARG:HG2	1.68	0.72
12:F:548:GLN:HB3	12:F:552:GLY:HA2	1.71	0.72
12:F:702:ASN:HB3	12:F:724:SER:HB3	1.72	0.72
5:6:535:PRO:C	5:6:742:ILE:HD13	2.14	0.72
15:K:389:LEU:HD21	16:L:96:GLN:HG2	1.72	0.72
5:6:535:PRO:O	5:6:742:ILE:HD13	1.90	0.71
5:6:773:LEU:HD21	5:6:804:ILE:HG12	1.72	0.71
4:5:430:GLU:HG3	4:5:438:TYR:HB2	1.72	0.71
5:6:535:PRO:CB	5:6:742:ILE:HG21	2.16	0.71
17:M:1668:MET:HB3	17:M:1815:SER:HB3	1.71	0.71
18:N:70:TRP:HD1	18:N:72:GLN:HE22	1.38	0.71
13:I:58:DT:H2"	13:I:59:DT:H5"	1.73	0.71
3:4:796:ARG:HH11	22:6:1103:AGS:H5'2	1.56	0.71
12:H:879:VAL:O	12:H:913:LYS:NZ	2.23	0.71
12:H:753:ASN:HB2	12:H:771:PRO:HB2	1.73	0.71
6:7:645:ALA:HB3	6:7:701:LYS:HG3	1.72	0.70
3:4:775:VAL:CB	3:4:779:LYS:HZ2	2.03	0.70
11:E:526:ARG:NH2	11:E:563:GLN:O	2.24	0.70
17:M:1584:ARG:HA	17:M:1584:ARG:HH11	1.57	0.70
2:3:306:MET:HA	4:5:206:SER:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:506:LEU:HA	3:4:509:ILE:HD12	1.73	0.70
4:5:276:MET:HE1	4:5:294:ILE:HG13	1.74	0.70
5:6:313:MET:SD	5:6:340:ASN:ND2	2.65	0.70
18:N:481:MET:HB2	18:N:523:VAL:HG22	1.73	0.70
17:M:1657:ASN:O	17:M:1678:ARG:NH2	2.25	0.70
4:5:347:THR:HG21	4:5:609:LYS:HE2	1.74	0.70
12:G:879:VAL:O	12:G:913:LYS:NZ	2.24	0.70
4:5:407:ARG:NH1	4:5:409:ASP:O	2.25	0.69
3:4:335:SER:OG	3:4:395:GLN:NE2	2.26	0.69
17:M:2216:CYS:SG	18:N:491:TRP:NE1	2.66	0.69
3:4:374:ILE:O	3:4:377:ASN:ND2	2.26	0.69
12:H:548:GLN:NE2	12:H:553:GLN:HB2	2.08	0.68
3:4:808:HIS:ND1	3:4:821:ASP:OD1	2.26	0.68
18:N:443:VAL:HG11	18:N:490:LEU:HD22	1.74	0.68
15:K:680:GLU:HA	15:K:718:LEU:HD11	1.74	0.68
3:4:573:SER:O	3:4:577:ILE:HG12	1.93	0.68
4:5:526:ILE:HD11	4:5:541:ASP:HB3	1.76	0.68
6:7:16:ASN:ND2	6:7:100:ASP:OD2	2.27	0.68
12:H:478:PRO:HG3	12:H:549:SER:HB3	1.74	0.68
15:K:368:THR:HG22	15:K:372:THR:HB	1.75	0.68
3:4:527:ALA:HB3	3:4:537:LYS:HE2	1.76	0.68
5:6:644:MET:HE2	5:6:649:GLN:HG2	1.76	0.68
6:7:682:GLY:O	6:7:683:GLN:C	2.36	0.68
1:2:621:HIS:O	1:2:676:ARG:NH1	2.27	0.68
6:7:82:LEU:HD21	6:7:106:ILE:HD11	1.75	0.68
4:5:455:ARG:NH2	13:I:52:DT:O2	2.27	0.67
10:D:202:MET:HG3	10:D:203:PRO:HD2	1.76	0.67
15:K:366:ILE:HD11	15:K:374:LEU:HB3	1.77	0.67
17:M:1668:MET:CB	17:M:1815:SER:HB3	2.25	0.67
2:3:688:ASN:ND2	6:7:605:SER:O	2.21	0.67
5:6:140:ILE:HG22	5:6:144:LYS:HE2	1.77	0.67
5:6:568:ASP:OD2	5:6:659:GLN:NE2	2.28	0.67
15:K:414:LEU:HD22	15:K:473:VAL:HG21	1.76	0.67
17:M:1533:LYS:HA	17:M:1536:PHE:HB3	1.75	0.67
1:2:596:LEU:HD21	1:2:646:ILE:HD11	1.77	0.67
1:2:468:GLU:HG2	1:2:473:VAL:HG13	1.77	0.67
3:4:712:VAL:HG23	6:7:668:ARG:HG2	1.77	0.67
5:6:628:LEU:HD21	5:6:678:ILE:HD11	1.77	0.67
11:E:434:VAL:HG23	11:E:498:LEU:HD13	1.75	0.67
15:K:184:LEU:HA	15:K:187:ILE:HG22	1.77	0.67
1:2:191:ALA:HB1	1:2:196:GLU:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:593:ARG:HA	6:7:687:ARG:HD2	1.77	0.67
11:E:248:VAL:O	11:E:290:ARG:NH2	2.28	0.67
12:F:636:LEU:HD21	12:F:661:LEU:HD13	1.76	0.66
3:4:872:VAL:HG12	3:4:879:ASP:N	2.11	0.66
12:H:636:LEU:HD21	12:H:659:MET:HE3	1.77	0.66
5:6:310:THR:HG22	5:6:317:ILE:HG12	1.77	0.66
17:M:2205:ALA:HB2	17:M:2213:LEU:HD23	1.76	0.66
4:5:52:ASN:ND2	9:C:142:LEU:O	2.28	0.66
17:M:1671:ILE:HG22	17:M:1812:LEU:HD11	1.78	0.66
3:4:368:PRO:HG2	3:4:382:MET:HG3	1.78	0.66
12:F:478:PRO:HD3	12:F:577:ARG:HD3	1.78	0.66
11:E:435:GLY:O	11:E:494:ARG:NH2	2.29	0.65
15:K:486:GLN:HG2	15:K:501:VAL:HB	1.78	0.65
5:6:340:ASN:O	5:6:341:ARG:NH1	2.29	0.65
10:D:5:ILE:HG22	12:F:904:ARG:HH22	1.60	0.65
12:F:570:ILE:HG21	12:F:578:ILE:HD11	1.77	0.65
17:M:1732:LEU:HD12	17:M:1868:ILE:HD11	1.79	0.65
3:4:513:ALA:HA	3:4:518:LEU:HD22	1.77	0.65
5:6:536:ALA:CA	5:6:742:ILE:CD1	2.60	0.65
12:H:702:ASN:HB3	12:H:724:SER:HB3	1.78	0.65
5:6:734:LEU:HD21	5:6:742:ILE:CG1	2.27	0.65
6:7:675:MET:HE2	6:7:680:SER:HA	1.79	0.65
8:B:104:TYR:OH	8:B:111:ARG:NH1	2.30	0.65
17:M:1704:ASP:OD2	18:N:552:ARG:NH1	2.29	0.65
11:E:248:VAL:HG22	11:E:290:ARG:HH22	1.62	0.65
15:K:173:GLY:O	15:K:260:ASN:ND2	2.30	0.65
15:K:164:LYS:NZ	15:K:248:ILE:O	2.30	0.65
2:3:229:ALA:HB2	6:7:370:LEU:HD23	1.77	0.64
4:5:524:ASN:ND2	22:5:802:AGS:S1G	2.70	0.64
17:M:1379:SER:O	17:M:1684:ASN:ND2	2.30	0.64
2:3:528:ASP:OD1	2:3:531:GLN:NE2	2.31	0.64
4:5:548:SER:OG	4:5:651:ARG:NH1	2.31	0.64
6:7:230:ILE:HD12	6:7:239:ILE:HD12	1.79	0.64
12:G:704:LEU:HD12	12:G:722:LEU:HB3	1.78	0.64
2:3:400:ARG:NH1	2:3:402:ASP:O	2.30	0.64
7:A:32:TYR:CE1	7:A:37:ILE:HG13	2.32	0.64
11:E:75:ASP:O	11:E:118:ARG:NH2	2.30	0.64
17:M:1486:TYR:HB3	17:M:1502:PHE:HB3	1.79	0.64
2:3:43:ARG:HB2	2:3:136:MET:HE1	1.79	0.64
2:3:480:ASP:OD1	2:3:483:ARG:NH1	2.31	0.64
3:4:880:SER:HB2	3:4:925:ARG:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:281:ASP:OD2	11:E:406:ARG:NH1	2.30	0.64
11:E:470:ARG:HH22	11:E:621:ARG:HH21	1.43	0.64
12:F:585:PRO:O	12:F:602:GLN:NE2	2.31	0.64
17:M:2130:CYS:SG	17:M:2131:VAL:N	2.70	0.64
3:4:573:SER:C	3:4:575:SER:N	2.54	0.64
4:5:736:GLU:O	4:5:737:PHE:C	2.40	0.64
6:7:351:VAL:HG22	6:7:381:VAL:HG22	1.79	0.63
17:M:1486:TYR:HE2	17:M:1639:VAL:HA	1.63	0.63
2:3:276:VAL:HG11	2:3:294:VAL:HG11	1.80	0.63
15:K:768:LEU:HD21	16:L:129:ARG:HB3	1.80	0.63
3:4:567:CYS:SG	3:4:692:ILE:HD13	2.39	0.63
5:6:338:CYS:SG	5:6:340:ASN:ND2	2.70	0.63
7:A:16:THR:HG22	7:A:30:PRO:HG2	1.81	0.63
12:G:566:TRP:NE1	12:G:602:GLN:O	2.30	0.63
12:H:543:GLY:HA2	12:H:558:PRO:HA	1.81	0.63
2:3:310:ASN:HB3	2:3:313:THR:HB	1.79	0.63
12:F:712:SER:HB3	12:F:715:GLU:HB2	1.81	0.63
12:G:743:TRP:HB3	12:G:755:ILE:HB	1.81	0.63
12:H:670:LYS:HB3	12:H:673:ASN:HB2	1.80	0.63
18:N:443:VAL:HG23	18:N:454:SER:HB3	1.81	0.63
1:2:191:ALA:HB2	1:2:200:GLN:HE21	1.63	0.63
7:A:20:TYR:CD1	7:A:27:VAL:HG12	2.30	0.63
12:G:776:ILE:O	12:G:829:ARG:NH1	2.32	0.63
6:7:569:PRO:HA	6:7:584:ILE:HG13	1.81	0.63
17:M:2130:CYS:HB3	17:M:2133:CYS:SG	2.38	0.63
6:7:462:PRO:HD3	6:7:569:PRO:HD2	1.79	0.62
12:H:874:CYS:O	12:H:877:GLN:NE2	2.32	0.62
1:2:624:MET:HE2	1:2:646:ILE:HG13	1.81	0.62
17:M:1486:TYR:OH	17:M:1638:HIS:ND1	2.27	0.62
2:3:52:ASN:ND2	2:3:90:ASN:O	2.32	0.62
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.33	0.62
3:4:779:LYS:O	3:4:781:GLY:N	2.32	0.62
15:K:97:ASN:OD1	15:K:98:LYS:N	2.32	0.62
4:5:346:VAL:HG22	4:5:347:THR:H	1.63	0.62
5:6:596:VAL:HG22	5:6:631:ALA:HB2	1.81	0.62
6:7:89:GLN:OE1	6:7:102:LEU:N	2.33	0.62
18:N:490:LEU:HB3	18:N:491:TRP:HE3	1.64	0.62
1:2:194:TYR:CZ	1:2:259:PHE:HE1	2.18	0.62
5:6:112:ARG:NH2	15:K:246:ASP:OD1	2.32	0.62
5:6:773:LEU:HD12	5:6:803:MET:HE2	1.80	0.62
2:3:483:ARG:HD3	2:3:539:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:583:TYR:HB3	15:K:587:PHE:HD2	1.65	0.62
17:M:1509:ILE:HD13	17:M:1556:ILE:HG23	1.82	0.62
4:5:212:LEU:HB3	4:5:241:TYR:OH	2.00	0.61
2:3:253:HIS:NE2	2:3:451:GLU:OE2	2.29	0.61
12:H:566:TRP:NE1	12:H:602:GLN:O	2.31	0.61
18:N:643:ASP:OD1	18:N:644:THR:N	2.33	0.61
11:E:285:ALA:O	11:E:289:ASN:ND2	2.32	0.61
15:K:368:THR:HG21	16:L:101:GLU:OE2	2.00	0.61
2:3:402:ASP:HB3	2:3:511:SER:HB3	1.83	0.61
7:A:12:GLU:HG3	7:A:33:HIS:CE1	2.34	0.61
13:I:34:DT:H3	14:J:28:DA:H61	1.49	0.61
2:3:365:GLN:NE2	2:3:375:ASP:OD1	2.30	0.61
15:K:386:LYS:NZ	16:L:86:ASP:OD1	2.33	0.61
18:N:532:ILE:HB	18:N:539:ILE:HB	1.82	0.61
9:C:101:ASN:HD21	9:C:107:LEU:HD12	1.65	0.61
18:N:449:SER:OG	18:N:450:ARG:NH1	2.34	0.61
3:4:440:ARG:NH1	15:K:359:ARG:O	2.33	0.61
7:A:177:GLU:OE1	18:N:27:ARG:NH2	2.34	0.61
15:K:682:PHE:HB3	15:K:722:MET:HE1	1.82	0.61
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.81	0.61
12:F:614:PRO:HD2	12:F:631:SER:HB3	1.83	0.61
15:K:70:LYS:O	15:K:149:GLN:NE2	2.33	0.61
1:2:190:LYS:HG3	15:K:81:TYR:CB	2.31	0.60
4:5:149:ARG:NH2	4:5:270:MET:O	2.35	0.60
4:5:184:ARG:N	4:5:240:PRO:O	2.30	0.60
11:E:24:SER:O	11:E:55:GLN:NE2	2.34	0.60
15:K:414:LEU:HB3	15:K:470:LEU:HD13	1.83	0.60
18:N:172:VAL:HG11	18:N:524:VAL:HG11	1.84	0.60
3:4:425:ASP:OD1	5:6:375:ARG:NH2	2.34	0.60
6:7:508:LEU:HD11	6:7:557:LEU:HD11	1.83	0.60
12:H:548:GLN:HE22	12:H:553:GLN:HB2	1.65	0.60
18:N:171:LYS:HG2	18:N:533:ALA:HB3	1.82	0.60
12:H:480:SER:HG	12:H:495:THR:HG1	1.50	0.60
13:I:36:DG:N2	14:J:26:DC:N3	2.43	0.60
3:4:315:ARG:NH2	3:4:411:THR:O	2.33	0.60
3:4:775:VAL:CB	3:4:779:LYS:NZ	2.62	0.60
6:7:289:CYS:SG	6:7:294:THR:OG1	2.59	0.60
1:2:190:LYS:HE2	15:K:28:ALA:HB3	1.84	0.60
3:4:865:LEU:HD11	3:4:903:ILE:HG23	1.83	0.60
6:7:273:VAL:HG21	6:7:278:PHE:HB3	1.84	0.60
17:M:2163:ARG:NH1	17:M:2186:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:431:LYS:NZ	1:2:452:GLU:OE1	2.25	0.60
3:4:725:THR:HA	3:4:728:TYR:HD2	1.66	0.60
4:5:337:VAL:O	4:5:338:GLU:HB2	2.01	0.60
12:F:605:VAL:HG13	12:H:881:LYS:HE2	1.81	0.60
1:2:613:ASN:ND2	1:2:616:ASP:OD2	2.27	0.60
3:4:746:PHE:HA	3:4:749:MET:HE3	1.84	0.60
3:4:771:VAL:HG13	5:6:728:ALA:HB3	1.83	0.60
5:6:190:ARG:HH22	15:K:252:THR:HG22	1.66	0.60
6:7:700:ALA:HA	6:7:707:MET:HE3	1.82	0.60
12:G:557:ARG:HD2	12:G:565:ASN:HD22	1.65	0.60
12:G:662:PRO:HB3	12:G:665:ASN:HB2	1.84	0.60
12:H:597:PHE:HB3	12:H:610:GLU:HB3	1.84	0.60
18:N:425:ASN:O	18:N:474:ASN:ND2	2.34	0.60
3:4:628:VAL:HA	3:4:670:SER:HB2	1.83	0.59
3:4:916:VAL:HA	3:4:926:SER:HA	1.84	0.59
4:5:32:LYS:NZ	4:5:96:GLN:OE1	2.30	0.59
5:6:334:PRO:O	15:K:221:THR:OG1	2.20	0.59
7:A:58:GLN:HG2	7:A:63:LEU:HB2	1.84	0.59
17:M:1444:SER:HB2	17:M:1477:LEU:HD11	1.84	0.59
17:M:1690:ASN:HB2	17:M:1697:ASP:HB2	1.84	0.59
1:2:782:ASP:HB3	17:M:2086:ARG:HG2	1.82	0.59
4:5:211:CYS:HB2	4:5:236:CYS:HB2	1.84	0.59
12:F:485:PRO:HB3	12:F:679:PHE:HB2	1.84	0.59
12:F:610:GLU:OE2	12:F:653:ARG:NH2	2.35	0.59
11:E:642:GLU:O	11:E:645:THR:OG1	2.20	0.59
12:H:570:ILE:HG21	12:H:578:ILE:HD11	1.85	0.59
12:H:722:LEU:HD12	12:H:776:ILE:HA	1.84	0.59
12:H:910:LEU:HD12	12:H:913:LYS:HE2	1.84	0.59
2:3:303:ALA:HA	4:5:243:ILE:HD12	1.83	0.59
12:F:721:ILE:HG22	12:F:776:ILE:HB	1.84	0.59
8:B:160:LEU:HD11	8:B:185:ILE:HD11	1.84	0.59
12:H:480:SER:OG	12:H:495:THR:OG1	2.20	0.59
5:6:727:LEU:O	5:6:731:ILE:HD12	2.03	0.59
6:7:453:ASP:O	6:7:694:ARG:NH1	2.36	0.59
11:E:41:ALA:HB1	11:E:255:ILE:HD12	1.84	0.59
12:F:707:LEU:HB3	12:F:710:TRP:HB3	1.85	0.59
2:3:363:LEU:HD22	2:3:656:LEU:HD13	1.84	0.59
5:6:300:VAL:HG13	5:6:386:VAL:HG11	1.85	0.59
17:M:1322:TRP:CD1	17:M:1325:LEU:HD13	2.38	0.59
7:A:141:LEU:HD21	10:D:182:TYR:HB2	1.85	0.59
12:F:866:LEU:HD13	12:F:889:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:885:LEU:HD21	12:G:605:VAL:HG21	1.85	0.59
15:K:288:GLU:HA	15:K:291:PHE:HB3	1.84	0.59
17:M:1819:TRP:O	17:M:1822:ASN:N	2.29	0.59
18:N:612:LEU:HD12	18:N:630:LEU:HA	1.83	0.58
6:7:658:ASP:O	6:7:661:VAL:HG12	2.02	0.58
12:G:705:LEU:HD11	12:H:611:LYS:HD3	1.84	0.58
3:4:181:TRP:HD1	15:K:365:SER:HB3	1.67	0.58
3:4:824:GLU:OE2	3:4:827:ARG:NH2	2.36	0.58
9:C:18:CYS:HB3	9:C:74:LEU:HD23	1.85	0.58
15:K:79:ALA:HB1	15:K:159:HIS:HD2	1.68	0.58
9:C:82:THR:O	9:C:86:ASN:ND2	2.37	0.58
12:F:533:GLY:O	12:F:548:GLN:NE2	2.36	0.58
12:H:545:LEU:HD11	12:H:554:ILE:HG23	1.84	0.58
15:K:772:GLU:HB3	16:L:134:ARG:HH22	1.69	0.58
3:4:269:ILE:HD11	3:4:305:PRO:HG3	1.84	0.58
7:A:21:ALA:O	7:A:22:ARG:C	2.46	0.58
12:H:895:LEU:HD21	12:H:918:ARG:HA	1.85	0.58
5:6:260:GLU:OE1	5:6:352:ARG:NH1	2.36	0.58
10:D:8:ILE:HD13	12:F:901:ILE:HG12	1.85	0.58
12:F:478:PRO:HG3	12:F:549:SER:HB3	1.86	0.58
2:3:312:ASN:HD22	4:5:200:ILE:C	2.12	0.58
15:K:251:ASN:OD1	15:K:433:ASN:ND2	2.36	0.58
5:6:406:ASP:OD1	5:6:408:THR:OG1	2.22	0.57
6:7:367:LYS:HG3	13:I:47:DT:N3	2.19	0.57
11:E:127:ARG:NH1	11:E:147:THR:OG1	2.36	0.57
15:K:746:LEU:HD12	16:L:84:SER:HB2	1.85	0.57
17:M:1882:SER:O	17:M:1886:MET:HG2	2.04	0.57
15:K:191:ARG:NH1	15:K:272:SER:O	2.37	0.57
4:5:493:ILE:HG22	4:5:497:MET:HG3	1.86	0.57
11:E:244:GLY:HA3	11:E:602:LEU:HB3	1.86	0.57
12:G:730:LYS:HA	12:G:734:GLY:HA2	1.87	0.57
3:4:203:TYR:HB3	3:4:221:ASP:HA	1.87	0.57
1:2:186:LEU:HD11	1:2:206:THR:HG22	1.86	0.57
5:6:581:LYS:NZ	5:6:683:ASN:OD1	2.38	0.57
6:7:718:ARG:HG2	6:7:721:ARG:HH22	1.69	0.57
3:4:772:ARG:HB3	3:4:772:ARG:CZ	2.34	0.57
11:E:466:LEU:O	11:E:470:ARG:HG2	2.04	0.57
17:M:1888:ALA:O	17:M:1891:THR:OG1	2.22	0.57
4:5:409:ASP:OD2	4:5:500:GLN:NE2	2.37	0.57
6:7:656:VAL:HG13	6:7:713:VAL:HG11	1.86	0.57
17:M:1528:LEU:HD21	17:M:1633:LYS:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:341:MET:SD	2:3:341:MET:N	2.77	0.57
11:E:148:VAL:HA	11:E:152:LEU:HD13	1.86	0.57
18:N:675:TYR:HD1	18:N:682:THR:HG22	1.70	0.57
1:2:738:LEU:N	1:2:742:GLN:HE21	2.03	0.57
4:5:730:TYR:CE2	4:5:734:ARG:HD3	2.40	0.57
7:A:198:ARG:NH1	18:N:32:SER:OG	2.38	0.57
5:6:169:ALA:HB2	15:K:339:LEU:HD21	1.86	0.57
8:B:97:GLU:OE1	8:B:100:ARG:NH1	2.38	0.57
12:H:827:TYR:HE1	12:H:866:LEU:HG	1.69	0.57
17:M:1322:TRP:HE1	17:M:1659:PRO:HG3	1.70	0.57
17:M:2107:LEU:HD13	18:N:447:MET:HG3	1.87	0.57
2:3:402:ASP:OD2	2:3:493:GLN:NE2	2.36	0.56
11:E:620:VAL:HG22	11:E:632:ILE:HD13	1.87	0.56
1:2:527:VAL:HG21	4:5:575:ILE:HG23	1.86	0.56
5:6:640:GLU:OE1	5:6:683:ASN:ND2	2.36	0.56
7:A:175:GLN:HE21	18:N:35:SER:HA	1.70	0.56
10:D:8:ILE:HG21	12:F:901:ILE:HD11	1.87	0.56
11:E:350:LEU:HA	11:E:355:GLY:HA3	1.87	0.56
17:M:1593:GLN:NE2	17:M:1617:LEU:O	2.38	0.56
2:3:519:VAL:HG22	2:3:534:ALA:HB2	1.88	0.56
3:4:567:CYS:SG	3:4:568:GLY:N	2.73	0.56
14:J:27:DA:H5'	16:L:47:LYS:HE3	1.87	0.56
15:K:62:PHE:HE1	15:K:75:ALA:HB2	1.69	0.56
15:K:577:PRO:HG3	15:K:591:CYS:HB2	1.87	0.56
15:K:766:PRO:O	16:L:129:ARG:NH1	2.38	0.56
17:M:1333:PRO:HG2	17:M:1407:PHE:O	2.05	0.56
18:N:8:LEU:HD12	18:N:9:PRO:HD2	1.86	0.56
1:2:774:ILE:HG22	1:2:776:PRO:HD3	1.86	0.56
1:2:473:VAL:O	1:2:765:LYS:NZ	2.38	0.56
2:3:434:GLY:HA2	2:3:478:MET:HG2	1.87	0.56
3:4:573:SER:O	3:4:575:SER:N	2.39	0.56
12:H:730:LYS:HE2	12:H:815:ILE:HB	1.86	0.56
1:2:625:GLU:HG2	1:2:808:ARG:HH21	1.71	0.56
7:A:79:MET:HE1	10:D:203:PRO:HG3	1.86	0.56
8:B:95:THR:HG23	8:B:144:LYS:HE3	1.86	0.56
12:F:624:ARG:NH2	12:F:642:GLU:OE2	2.39	0.56
1:2:423:GLU:H	1:2:460:GLU:HB2	1.70	0.56
3:4:570:PRO:HD3	3:4:677:PRO:HD2	1.87	0.56
6:7:479:ARG:NH2	6:7:515:LEU:O	2.39	0.56
12:G:722:LEU:HD12	12:G:776:ILE:HA	1.86	0.56
1:2:185:SER:HA	1:2:188:ASN:ND2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:190:LYS:HG2	1:2:191:ALA:N	2.20	0.56
5:6:514:ASN:O	5:6:518:GLU:HG2	2.06	0.56
3:4:386:HIS:HB3	5:6:450:TYR:HE2	1.70	0.56
15:K:191:ARG:HD2	15:K:194:ARG:NH2	2.21	0.56
1:2:340:ASN:ND2	1:2:346:SER:O	2.39	0.56
3:4:573:SER:HA	3:4:576:GLN:HB2	1.88	0.56
6:7:335:VAL:HG12	6:7:378:ALA:HB3	1.88	0.56
15:K:342:GLU:HA	15:K:345:MET:HG2	1.88	0.56
8:B:17:GLN:HG3	8:B:125:ILE:HD11	1.88	0.55
11:E:519:ILE:HG22	11:E:528:CYS:HB2	1.87	0.55
12:H:705:LEU:HB3	12:H:718:TRP:HE3	1.71	0.55
4:5:400:LEU:HD12	4:5:404:MET:HG3	1.87	0.55
7:A:84:ARG:NH2	9:C:8:ASP:OD2	2.31	0.55
12:F:692:TYR:HB3	12:F:840:THR:HG21	1.87	0.55
1:2:307:ARG:NH2	1:2:402:LEU:O	2.37	0.55
3:4:304:ARG:HB3	3:4:465:HIS:HB2	1.87	0.55
9:C:142:LEU:HD21	9:C:185:LYS:HA	1.87	0.55
12:H:555:GLN:HG3	12:H:557:ARG:CD	2.35	0.55
1:2:794:ARG:NH1	1:2:805:ILE:O	2.39	0.55
12:H:552:GLY:HA3	12:H:570:ILE:HB	1.89	0.55
13:I:36:DG:H4'	15:K:401:ARG:HH21	1.71	0.55
17:M:1812:LEU:HA	17:M:1815:SER:OG	2.06	0.55
3:4:568:GLY:HA2	3:4:707:LEU:HD23	1.89	0.55
3:4:871:ASN:O	3:4:874:LYS:HB2	2.07	0.55
12:F:566:TRP:NE1	12:F:602:GLN:O	2.30	0.55
12:G:910:LEU:HD12	12:G:913:LYS:HE2	1.89	0.55
12:H:581:VAL:HG12	12:H:590:VAL:HG23	1.88	0.55
3:4:397:ILE:HB	3:4:417:LEU:HB2	1.88	0.55
5:6:730:HIS:O	5:6:734:LEU:HG	2.06	0.55
5:6:795:ILE:HD12	5:6:799:GLN:HG2	1.88	0.55
17:M:1341:THR:HA	17:M:1346:VAL:HG12	1.89	0.55
1:2:543:GLY:HA3	1:2:683:VAL:HB	1.89	0.55
2:3:500:ALA:HB2	13:I:52:DT:H5''	1.88	0.55
15:K:416:ASN:HB2	15:K:420:ASN:HD21	1.72	0.55
17:M:1416:SER:C	17:M:1424:LEU:HD12	2.31	0.55
7:A:129:GLU:OE2	10:D:192:LYS:NZ	2.37	0.55
12:G:490:ASP:HA	12:G:506:LYS:HE2	1.89	0.55
17:M:1739:LEU:HD23	17:M:1863:ARG:HG2	1.89	0.55
20:2:902:ADP:C8	5:6:797:VAL:HG11	2.42	0.55
2:3:312:ASN:HA	4:5:198:ASN:ND2	2.21	0.55
6:7:414:LEU:HB3	6:7:433:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:547:LYS:HE3	15:K:605:TYR:HE1	1.71	0.54
3:4:202:LYS:HD2	3:4:222:GLU:HA	1.89	0.54
8:B:174:SER:OG	8:B:175:LEU:N	2.38	0.54
12:F:477:MET:HG2	12:F:478:PRO:HD2	1.89	0.54
17:M:1604:ILE:HG22	17:M:1608:ASN:ND2	2.22	0.54
18:N:271:ILE:HD13	18:N:305:VAL:HG12	1.88	0.54
2:3:301:LEU:HG	2:3:318:LYS:O	2.08	0.54
6:7:82:LEU:HD12	6:7:206:PRO:HA	1.89	0.54
7:A:99:SER:OG	8:B:1:MET:N	2.41	0.54
15:K:192:LEU:H	15:K:192:LEU:HD22	1.73	0.54
18:N:417:LEU:HD21	18:N:434:TRP:HZ3	1.72	0.54
1:2:181:LEU:HD23	1:2:185:SER:OG	2.08	0.54
1:2:502:ALA:HB3	1:2:512:LYS:HE2	1.90	0.54
3:4:774:TYR:CD2	3:4:798:LEU:HD12	2.43	0.54
5:6:319:ASP:OD1	5:6:320:ASN:N	2.39	0.54
12:F:706:LEU:HD22	12:F:721:ILE:HG13	1.89	0.54
17:M:1482:MET:HB3	17:M:1589:LEU:HD13	1.89	0.54
1:2:684:ARG:NH2	1:2:847:ASP:O	2.40	0.54
3:4:573:SER:C	3:4:575:SER:H	2.14	0.54
18:N:233:GLU:O	18:N:237:ASN:N	2.37	0.54
5:6:335:ASN:ND2	5:6:337:SER:OG	2.41	0.54
12:G:624:ARG:HA	12:G:642:GLU:HA	1.89	0.54
12:G:840:THR:HG23	12:G:844:ASP:HB2	1.89	0.54
12:H:540:ASN:ND2	12:H:583:ALA:O	2.34	0.54
15:K:99:CYS:SG	15:K:181:ARG:NH1	2.81	0.54
15:K:131:LEU:O	15:K:135:MET:HG2	2.08	0.54
15:K:195:THR:HG22	15:K:197:ARG:H	1.72	0.54
15:K:723:LEU:HD23	16:L:85:TYR:HB2	1.88	0.54
18:N:272:LYS:HB2	18:N:302:SER:HB2	1.88	0.54
3:4:873:LEU:CA	3:4:879:ASP:HA	2.35	0.54
6:7:140:ASP:OD1	6:7:199:ARG:NH2	2.41	0.54
10:D:210:ASN:HB2	10:D:219:ILE:HD11	1.90	0.54
12:H:535:ASP:N	12:H:547:GLY:O	2.39	0.54
3:4:440:ARG:NH2	3:4:462:ASP:OD2	2.40	0.54
17:M:1819:TRP:O	17:M:1820:VAL:C	2.51	0.54
4:5:149:ARG:NH2	4:5:260:GLU:OE2	2.33	0.54
10:D:195:ASN:HA	10:D:199:LEU:HB2	1.89	0.54
18:N:170:PHE:HD1	18:N:534:TYR:HA	1.72	0.54
4:5:290:THR:HG22	4:5:337:VAL:HG11	1.90	0.54
4:5:413:LEU:HD23	4:5:553:ILE:HG23	1.90	0.54
5:6:578:SER:OG	5:6:717:ASP:OD2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:158:LYS:HA	8:B:161:LYS:HD3	1.89	0.54
12:F:582:ALA:HB2	12:F:618:LEU:HB3	1.90	0.54
12:G:548:GLN:HB2	12:G:552:GLY:HA2	1.89	0.54
3:4:682:TYR:OH	3:4:707:LEU:HD11	2.08	0.53
4:5:441:GLY:N	4:5:480:ASP:O	2.41	0.53
7:A:193:GLN:NE2	7:A:197:GLU:OE1	2.41	0.53
12:H:498:GLU:HA	12:H:745:LEU:HD21	1.89	0.53
13:I:47:DT:H2''	13:I:48:DT:H5'	1.90	0.53
15:K:460:PHE:O	15:K:464:GLN:NE2	2.36	0.53
6:7:459:MET:SD	6:7:597:LEU:HD21	2.49	0.53
7:A:84:ARG:NH1	9:C:12:ASP:OD2	2.38	0.53
12:G:516:SER:HA	12:G:525:GLU:HG3	1.90	0.53
12:G:711:ARG:HH22	12:G:843:ASN:HB2	1.74	0.53
15:K:463:GLU:HB3	15:K:466:ARG:HB2	1.91	0.53
18:N:298:LEU:HD13	18:N:307:ILE:HG21	1.88	0.53
18:N:391:GLU:HG2	18:N:535:LEU:HD13	1.90	0.53
1:2:190:LYS:HB3	1:2:197:TRP:HZ3	1.67	0.53
3:4:568:GLY:CA	3:4:707:LEU:HD23	2.38	0.53
13:I:44:DT:H2''	13:I:45:DG:H5'	1.90	0.53
2:3:683:TYR:OH	2:3:687:ARG:NH1	2.40	0.53
3:4:387:ASN:HD21	5:6:325:PHE:HZ	1.56	0.53
4:5:39:ARG:NH2	11:E:314:ASP:OD2	2.42	0.53
7:A:10:VAL:HG11	9:C:9:VAL:HG11	1.90	0.53
12:H:492:ARG:HH12	12:H:494:LEU:HD23	1.73	0.53
17:M:1321:THR:HG21	17:M:1477:LEU:HD21	1.90	0.53
3:4:634:PHE:HB3	3:4:675:ALA:HB2	1.90	0.53
6:7:264:GLN:HA	15:K:374:LEU:HD11	1.90	0.53
15:K:530:HIS:HA	15:K:533:MET:HE2	1.91	0.53
5:6:623:ILE:HG21	5:6:672:LEU:HD21	1.91	0.53
6:7:682:GLY:HA2	6:7:724:LYS:NZ	2.24	0.53
15:K:669:GLU:HG2	15:K:709:LEU:HD23	1.90	0.53
15:K:750:LYS:HD2	16:L:78:ILE:HG12	1.89	0.53
2:3:391:LYS:HB2	2:3:399:LEU:HB2	1.91	0.53
8:B:159:GLY:C	8:B:161:LYS:H	2.16	0.53
12:G:883:LEU:HD13	12:G:913:LYS:HD2	1.91	0.53
17:M:1589:LEU:HG	17:M:1611:PRO:HB2	1.91	0.53
18:N:14:PRO:HG3	18:N:39:SER:HA	1.91	0.53
18:N:506:ASP:N	18:N:506:ASP:OD1	2.42	0.53
3:4:340:PRO:HG3	5:6:452:ILE:HG13	1.91	0.53
3:4:772:ARG:O	3:4:775:VAL:HG22	2.08	0.53
11:E:121:TYR:HB3	11:E:143:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:432:THR:HG21	2:3:442:LEU:HD21	1.91	0.53
10:D:211:ASP:H	10:D:218:MET:HE2	1.74	0.53
11:E:526:ARG:HH12	11:E:562:LYS:HB3	1.74	0.53
1:2:790:TYR:CZ	1:2:794:ARG:HD2	2.44	0.53
5:6:283:LYS:O	5:6:286:SER:OG	2.21	0.53
3:4:570:PRO:HB3	3:4:676:ASN:ND2	2.24	0.52
6:7:410:VAL:HG23	6:7:414:LEU:HD23	1.92	0.52
12:G:502:VAL:HG22	12:G:515:VAL:HG22	1.91	0.52
3:4:568:GLY:HA3	3:4:708:VAL:O	2.10	0.52
5:6:641:PHE:HB3	5:6:682:ALA:HB2	1.90	0.52
6:7:195:ASN:ND2	6:7:256:GLU:OE1	2.42	0.52
17:M:1572:ARG:O	17:M:1575:GLN:HG3	2.09	0.52
3:4:569:ASP:HA	3:4:677:PRO:HG3	1.91	0.52
3:4:851:GLN:O	3:4:855:SER:N	2.39	0.52
6:7:366:LEU:HD11	14:J:16:DA:O4'	2.10	0.52
6:7:558:ASN:HD22	6:7:560:ARG:HH12	1.57	0.52
12:F:914:ILE:HA	12:F:917:ILE:HD12	1.91	0.52
17:M:1616:SER:O	18:N:450:ARG:NE	2.38	0.52
1:2:528:ASN:ND2	4:5:584:GLN:OE1	2.43	0.52
3:4:372:GLU:HB3	15:K:683:ARG:HH12	1.74	0.52
11:E:127:ARG:O	11:E:129:TRP:N	2.43	0.52
12:G:731:MET:SD	12:G:732:SER:N	2.82	0.52
3:4:796:ARG:NH1	22:6:1103:AGS:H5'2	2.23	0.52
4:5:261:ILE:HG23	4:5:291:ARG:HH21	1.74	0.52
12:H:497:ASN:C	12:H:745:LEU:HD11	2.34	0.52
4:5:169:THR:HG22	4:5:256:LEU:HD22	1.91	0.52
4:5:258:LEU:HB2	4:5:276:MET:SD	2.49	0.52
5:6:734:LEU:HD21	5:6:742:ILE:CD1	2.40	0.52
6:7:685:THR:O	6:7:688:THR:N	2.42	0.52
7:A:13:ALA:HB2	7:A:89:TYR:HD1	1.74	0.52
11:E:529:VAL:HG22	11:E:570:ALA:HB3	1.91	0.52
15:K:84:LEU:HA	15:K:88:LEU:HB2	1.92	0.52
3:4:645:LEU:HA	3:4:648:VAL:HG12	1.91	0.52
5:6:312:ASP:HA	5:6:315:ARG:HH22	1.75	0.52
6:7:141:VAL:HA	6:7:144:ASN:HD21	1.75	0.52
6:7:500:ASP:HB2	6:7:501:PRO:HD3	1.91	0.52
6:7:618:TYR:HB3	6:7:626:PRO:HG3	1.91	0.52
12:G:482:ALA:HB1	12:G:496:MET:HG2	1.90	0.52
12:G:728:ILE:HD12	12:G:740:ILE:HB	1.92	0.52
15:K:453:LEU:O	15:K:457:THR:HG23	2.10	0.52
15:K:718:LEU:O	15:K:722:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:2147:ILE:O	17:M:2151:ARG:HG2	2.09	0.52
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.91	0.52
2:3:716:ARG:NH2	2:3:722:ASN:OD1	2.43	0.52
3:4:762:ILE:HA	3:4:817:VAL:HB	1.91	0.52
3:4:812:LYS:HB2	3:4:814:LYS:HZ2	1.75	0.52
11:E:594:THR:H	11:E:597:THR:HB	1.74	0.52
18:N:178:GLN:HE22	18:N:531:ARG:HD2	1.74	0.52
18:N:352:ARG:HH11	18:N:637:SER:H	1.56	0.52
18:N:409:ASP:OD1	18:N:461:ASN:ND2	2.39	0.52
1:2:211:LEU:HD13	1:2:271:PHE:HD1	1.74	0.52
3:4:802:ILE:HD11	5:6:732:VAL:HG22	1.92	0.52
6:7:366:LEU:HD22	14:J:15:DC:H2"	1.91	0.52
6:7:513:LEU:HD13	6:7:540:VAL:HG21	1.91	0.52
11:E:525:TYR:HE2	11:E:527:LEU:HD12	1.75	0.52
12:F:491:ARG:HD2	12:F:766:PHE:CD1	2.44	0.52
12:H:597:PHE:N	12:H:610:GLU:O	2.39	0.52
12:H:755:ILE:HG12	12:H:768:LEU:HD11	1.92	0.52
17:M:1641:SER:O	17:M:1644:SER:OG	2.26	0.52
18:N:66:PHE:HE1	18:N:80:ASP:HB3	1.75	0.52
4:5:734:ARG:NH2	4:5:735:ARG:HH22	2.08	0.51
7:A:175:GLN:HA	7:A:180:VAL:HG23	1.92	0.51
12:G:672:ALA:HB2	12:G:760:LYS:HE3	1.92	0.51
15:K:256:SER:HA	15:K:259:LYS:HG2	1.92	0.51
1:2:577:THR:HG22	1:2:596:LEU:HD12	1.91	0.51
3:4:408:ASP:HB2	6:7:517:ASP:HB3	1.92	0.51
6:7:311:GLN:HB3	6:7:335:VAL:HG23	1.92	0.51
17:M:1360:LYS:HG3	17:M:1362:LYS:HG3	1.91	0.51
17:M:1671:ILE:CG2	17:M:1812:LEU:HD11	2.40	0.51
18:N:36:ASP:HB2	18:N:78:PHE:CZ	2.45	0.51
1:2:472:ASP:HB3	1:2:475:SER:HB3	1.93	0.51
3:4:274:GLN:HG3	15:K:383:VAL:HG22	1.92	0.51
3:4:333:LEU:HG	3:4:400:GLN:HB2	1.92	0.51
7:A:22:ARG:HB3	7:A:25:GLN:NE2	2.25	0.51
11:E:527:LEU:HD11	11:E:641:LEU:HD13	1.91	0.51
17:M:1486:TYR:HH	17:M:1638:HIS:HD1	1.56	0.51
3:4:261:LEU:HB2	3:4:268:VAL:HG11	1.92	0.51
3:4:569:ASP:H	3:4:709:LEU:CD2	2.24	0.51
3:4:866:SER:HB3	3:4:867:ARG:NH1	2.25	0.51
5:6:112:ARG:NH1	5:6:116:GLU:OE2	2.43	0.51
6:7:521:CYS:HB2	6:7:561:THR:HG21	1.90	0.51
7:A:20:TYR:O	7:A:21:ALA:C	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:13:ASN:HD21	12:F:524:ARG:HH22	1.59	0.51
12:G:883:LEU:HG	12:G:887:HIS:CE1	2.44	0.51
15:K:770:ASN:HB3	15:K:773:VAL:HG22	1.92	0.51
3:4:375:ASP:H	15:K:681:ARG:HH22	1.57	0.51
11:E:256:TYR:OH	11:E:298:GLU:OE1	2.25	0.51
12:G:534:TYR:HA	12:G:548:GLN:HG3	1.91	0.51
12:H:543:GLY:HA3	12:H:556:TYR:CE1	2.45	0.51
8:B:22:ASN:OD1	10:D:135:ARG:NH2	2.42	0.51
12:F:910:LEU:O	12:F:914:ILE:HG12	2.10	0.51
12:G:688:PHE:HE2	12:G:744:PRO:HB2	1.76	0.51
12:G:697:ILE:HB	12:G:705:LEU:HB2	1.91	0.51
17:M:1810:ASP:O	17:M:1813:VAL:HG22	2.10	0.51
17:M:1948:ILE:HB	17:M:2034:ASP:HB3	1.91	0.51
6:7:664:TYR:HB2	6:7:689:LEU:HD21	1.92	0.51
6:7:685:THR:O	6:7:686:PRO:C	2.53	0.51
12:F:918:ARG:NE	12:F:922:TYR:OH	2.44	0.51
15:K:141:VAL:HG11	15:K:150:ILE:HD13	1.91	0.51
15:K:489:ARG:HH12	15:K:493:ASP:HB3	1.76	0.51
17:M:1604:ILE:O	17:M:1608:ASN:ND2	2.43	0.51
1:2:376:ASN:O	1:2:380:THR:OG1	2.26	0.51
3:4:408:ASP:OD1	3:4:408:ASP:N	2.44	0.51
3:4:910:LEU:HB3	3:4:916:VAL:HG22	1.92	0.51
6:7:358:ALA:HB2	6:7:375:TYR:CD1	2.46	0.51
12:G:701:ASP:OD1	12:G:701:ASP:N	2.43	0.51
15:K:206:LEU:HB3	15:K:289:ILE:HD11	1.92	0.51
1:2:446:VAL:HA	5:6:303:GLU:HA	1.93	0.51
1:2:604:CYS:HB3	1:2:646:ILE:HD13	1.92	0.51
5:6:312:ASP:OD1	5:6:312:ASP:N	2.42	0.51
12:F:634:HIS:CD2	12:H:656:PRO:HB3	2.46	0.51
17:M:1488:LEU:HA	17:M:1593:GLN:HB3	1.92	0.51
17:M:1668:MET:HB3	17:M:1815:SER:HB2	1.92	0.51
2:3:306:MET:O	4:5:207:LEU:HG	2.11	0.51
3:4:506:LEU:O	3:4:510:ARG:HG2	2.11	0.51
3:4:568:GLY:HA2	3:4:707:LEU:CD2	2.41	0.51
12:F:636:LEU:O	12:G:634:HIS:NE2	2.44	0.51
12:H:706:LEU:HD13	12:H:721:ILE:HG13	1.92	0.51
18:N:88:ILE:O	18:N:91:MET:HG3	2.11	0.51
5:6:511:ASP:OD1	5:6:512:GLU:N	2.44	0.50
5:6:722:LYS:O	5:6:725:THR:OG1	2.20	0.50
5:6:833:GLN:O	5:6:837:ARG:NH1	2.43	0.50
9:C:131:ARG:NH2	9:C:168:LYS:O	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:357:GLN:HB2	5:6:386:VAL:HG13	1.93	0.50
5:6:696:ARG:HG2	5:6:706:MET:HE1	1.93	0.50
12:F:886:ALA:HA	12:F:889:LEU:HD23	1.93	0.50
17:M:1486:TYR:CE1	17:M:1488:LEU:HB3	2.46	0.50
18:N:650:ASP:OD1	18:N:657:LYS:NZ	2.44	0.50
2:3:411:PRO:HG3	4:5:545:THR:HG22	1.93	0.50
3:4:682:TYR:CZ	3:4:707:LEU:HD21	2.45	0.50
11:E:412:THR:HG22	11:E:418:SER:HA	1.92	0.50
15:K:562:SER:O	15:K:563:ARG:NE	2.37	0.50
18:N:11:LYS:NZ	18:N:12:ILE:O	2.44	0.50
3:4:798:LEU:HA	3:4:801:MET:HE2	1.93	0.50
4:5:342:ILE:HG21	4:5:608:LEU:HD11	1.92	0.50
6:7:152:ARG:NH1	15:K:371:LYS:O	2.44	0.50
18:N:486:GLY:N	18:N:489:ASP:OD2	2.36	0.50
15:K:296:ASP:OD1	15:K:296:ASP:N	2.45	0.50
2:3:280:ASP:O	2:3:283:VAL:HG22	2.12	0.50
3:4:590:TYR:OH	3:4:632:ASP:OD2	2.21	0.50
12:G:589:ILE:HD13	12:G:625:VAL:HG11	1.93	0.50
12:H:918:ARG:NE	12:H:922:TYR:OH	2.44	0.50
15:K:475:TYR:HD2	15:K:476:LEU:HD12	1.76	0.50
17:M:1918:SER:HB2	17:M:1939:TRP:HE1	1.76	0.50
17:M:1958:MET:HE3	17:M:1958:MET:HA	1.93	0.50
2:3:455:ARG:HH12	13:I:51:DT:H1'	1.76	0.50
5:6:162:GLU:CD	15:K:332:GLY:HA3	2.37	0.50
5:6:311:CYS:HB2	5:6:340:ASN:ND2	2.27	0.50
6:7:591:LEU:HB3	6:7:681:PHE:HZ	1.76	0.50
7:A:141:LEU:HD11	10:D:182:TYR:CD1	2.47	0.50
1:2:866:LEU:HD21	17:M:2070:LEU:HD22	1.94	0.50
2:3:312:ASN:ND2	4:5:200:ILE:O	2.45	0.50
2:3:571:TYR:CZ	4:5:401:PRO:HD3	2.46	0.50
12:F:708:SER:HA	12:F:836:LEU:HD21	1.93	0.50
12:G:777:ARG:HA	12:G:829:ARG:HD3	1.93	0.50
12:H:575:GLY:O	12:H:577:ARG:NH1	2.45	0.50
18:N:668:ARG:HE	18:N:689:ILE:HG21	1.77	0.50
11:E:578:THR:HG22	11:E:633:ARG:HD2	1.94	0.50
12:H:711:ARG:HH12	12:H:839:ASP:HB3	1.77	0.50
12:H:817:ILE:HG12	12:H:822:ALA:HB2	1.94	0.50
15:K:181:ARG:HA	15:K:184:LEU:HG	1.94	0.50
17:M:2037:ILE:HG13	17:M:2047:VAL:HB	1.93	0.50
1:2:244:VAL:HG21	1:2:271:PHE:HE2	1.77	0.49
20:2:902:ADP:O2B	5:6:798:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:573:PRO:HB2	2:3:576:TYR:HD2	1.78	0.49
3:4:800:SER:O	3:4:803:ARG:HB2	2.12	0.49
4:5:183:CYS:HB3	4:5:188:HIS:H	1.77	0.49
5:6:155:TYR:OH	5:6:171:SER:OG	2.28	0.49
5:6:536:ALA:N	5:6:742:ILE:HD13	2.26	0.49
7:A:12:GLU:O	7:A:16:THR:HG23	2.12	0.49
11:E:165:LEU:O	11:E:226:ARG:NH2	2.45	0.49
12:H:818:PRO:HG2	12:H:821:MET:HB3	1.93	0.49
15:K:746:LEU:HD11	16:L:88:LEU:HG	1.93	0.49
17:M:1455:LEU:O	17:M:1459:ILE:HG12	2.11	0.49
17:M:1494:ILE:HD12	17:M:1496:TYR:HE1	1.77	0.49
3:4:884:ASN:O	3:4:888:LYS:HG2	2.12	0.49
4:5:300:ILE:HG23	4:5:324:ARG:HB3	1.93	0.49
17:M:1418:PHE:HB2	17:M:1423:VAL:HG23	1.94	0.49
17:M:2065:SER:OG	17:M:2068:THR:OG1	2.30	0.49
1:2:188:ASN:CG	1:2:188:ASN:O	2.55	0.49
3:4:245:ALA:HB1	3:4:258:TYR:HE1	1.77	0.49
3:4:778:ARG:NH1	3:4:793:ALA:O	2.45	0.49
4:5:151:LEU:HD11	4:5:162:LEU:HD13	1.93	0.49
4:5:341:SER:HB2	4:5:345:SER:N	2.27	0.49
4:5:446:ALA:HB2	4:5:489:ASP:HA	1.92	0.49
12:F:589:ILE:HD11	12:F:643:LEU:HD11	1.94	0.49
12:H:546:PHE:HB2	12:H:555:GLN:HB3	1.93	0.49
12:H:819:VAL:HG13	12:H:868:ARG:HH21	1.76	0.49
17:M:1789:ASN:OD1	17:M:1792:ARG:NH1	2.38	0.49
18:N:351:ARG:HB2	18:N:354:ILE:HG13	1.93	0.49
3:4:863:GLU:HB2	3:4:867:ARG:HH22	1.77	0.49
5:6:771:SER:O	5:6:775:GLU:HG2	2.13	0.49
10:D:164:ASP:HB3	10:D:167:SER:HB3	1.93	0.49
12:G:624:ARG:HD3	12:G:640:LEU:HD11	1.95	0.49
12:H:544:THR:OG1	12:H:559:HIS:NE2	2.36	0.49
15:K:479:PHE:O	15:K:483:VAL:HG22	2.11	0.49
3:4:274:GLN:NE2	3:4:278:ASP:OD2	2.45	0.49
3:4:569:ASP:N	3:4:682:TYR:HB2	2.26	0.49
5:6:136:TYR:O	5:6:140:ILE:HG13	2.12	0.49
5:6:141:GLU:HA	5:6:144:LYS:HD2	1.95	0.49
5:6:276:ILE:HB	5:6:363:GLU:HG3	1.94	0.49
17:M:1450:LYS:HB3	17:M:1454:ALA:HB3	1.94	0.49
17:M:1665:LEU:HD13	18:N:450:ARG:HG2	1.94	0.49
17:M:1940:GLN:HE22	17:M:1944:PHE:HE1	1.60	0.49
18:N:81:GLN:HE21	18:N:85:LYS:HZ2	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:230:ARG:NH1	1:2:243:GLU:O	2.45	0.49
5:6:296:ARG:HH22	5:6:358:LYS:HE3	1.77	0.49
9:C:101:ASN:ND2	9:C:107:LEU:HD12	2.26	0.49
12:F:502:VAL:HG23	12:F:539:LEU:HD11	1.94	0.49
12:F:883:LEU:HB2	12:F:913:LYS:HD3	1.94	0.49
12:G:775:GLU:HG3	12:G:829:ARG:HH12	1.78	0.49
18:N:405:ASN:OD1	18:N:543:ARG:NH2	2.46	0.49
11:E:617:ASP:OD1	11:E:617:ASP:N	2.46	0.49
12:H:738:THR:O	12:H:741:HIS:NE2	2.45	0.49
12:H:823:ALA:HB3	12:H:868:ARG:HD2	1.93	0.49
17:M:2026:ILE:HG23	17:M:2027:LEU:HG	1.95	0.49
17:M:2049:ASN:HB3	17:M:2052:LEU:HB3	1.95	0.49
3:4:192:THR:O	3:4:196:ASN:ND2	2.46	0.49
3:4:625:ASP:OD1	3:4:625:ASP:N	2.44	0.49
5:6:146:TYR:HB2	5:6:148:LEU:HD22	1.93	0.49
5:6:187:ARG:HH21	15:K:428:PHE:HE2	1.60	0.49
12:F:496:MET:HB3	12:F:745:LEU:HD22	1.95	0.49
17:M:1532:TYR:HD2	17:M:1640:LEU:HD12	1.78	0.49
1:2:325:THR:HG22	1:2:326:ARG:HG2	1.93	0.49
12:F:778:MET:HE1	12:F:832:VAL:HG11	1.93	0.49
12:F:820:SER:HA	12:F:868:ARG:NH1	2.27	0.49
12:F:896:THR:OG1	12:F:918:ARG:NH1	2.45	0.49
15:K:295:LYS:HG3	15:K:417:SER:HB3	1.95	0.49
18:N:543:ARG:HA	18:N:642:CYS:HB3	1.95	0.49
2:3:305:GLY:O	2:3:306:MET:C	2.56	0.49
2:3:308:GLN:HG2	4:5:209:ARG:HH12	1.78	0.49
3:4:370:ARG:HA	3:4:379:PRO:HA	1.94	0.49
3:4:802:ILE:HG21	5:6:735:HIS:CG	2.48	0.49
4:5:685:GLN:HA	4:5:689:MET:HB2	1.94	0.49
6:7:360:TYR:O	6:7:365:ALA:HB2	2.13	0.49
6:7:402:MET:O	6:7:402:MET:HE3	2.13	0.49
11:E:328:LEU:HD13	11:E:496:ILE:HG23	1.94	0.49
12:H:627:SER:N	12:H:639:SER:O	2.45	0.49
12:F:597:PHE:N	12:F:610:GLU:O	2.39	0.48
16:L:108:PHE:O	16:L:112:MET:HG2	2.13	0.48
5:6:533:ILE:HG13	5:6:548:LEU:HB2	1.95	0.48
11:E:333:SER:OG	11:E:336:ASP:OD2	2.30	0.48
12:G:708:SER:HB2	12:G:717:LYS:HB2	1.94	0.48
12:H:705:LEU:HB3	12:H:718:TRP:CE3	2.49	0.48
2:3:235:ASP:HB2	2:3:241:LEU:HD11	1.94	0.48
2:3:585:ARG:HG2	2:3:587:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:315:ARG:O	6:7:341:ARG:NH1	2.46	0.48
3:4:767:LYS:HD2	5:6:736:MET:HE1	1.95	0.48
5:6:137:ARG:O	5:6:141:GLU:HG2	2.14	0.48
5:6:586:LYS:HA	5:6:589:VAL:HG12	1.96	0.48
7:A:133:GLU:CD	10:D:189:ILE:HG12	2.38	0.48
12:F:658:PRO:HB2	12:G:611:LYS:HG2	1.95	0.48
12:G:503:SER:OG	12:G:514:THR:OG1	2.24	0.48
12:H:749:TYR:CZ	12:H:854:VAL:HB	2.48	0.48
15:K:87:ASP:O	15:K:91:ILE:HG12	2.13	0.48
15:K:489:ARG:NH1	15:K:493:ASP:HB3	2.28	0.48
15:K:714:ASP:O	15:K:718:LEU:HD23	2.14	0.48
2:3:303:ALA:HA	4:5:243:ILE:CD1	2.43	0.48
4:5:355:GLU:OE2	4:5:359:GLN:NE2	2.40	0.48
4:5:629:ILE:HG22	4:5:648:ILE:HG21	1.96	0.48
5:6:734:LEU:CD2	5:6:742:ILE:CD1	2.91	0.48
7:A:22:ARG:HB3	7:A:25:GLN:HE21	1.77	0.48
12:F:820:SER:HA	12:F:868:ARG:HH12	1.77	0.48
12:H:653:ARG:HG3	12:H:654:GLU:HG2	1.96	0.48
15:K:74:VAL:O	15:K:78:VAL:HG23	2.13	0.48
1:2:194:TYR:O	1:2:195:SER:C	2.55	0.48
3:4:820:GLU:HA	3:4:823:GLN:NE2	2.28	0.48
4:5:449:LEU:HD23	4:5:468:ALA:HB3	1.94	0.48
7:A:25:GLN:O	7:A:26:ASP:C	2.55	0.48
12:H:556:TYR:O	12:H:558:PRO:HD3	2.14	0.48
12:H:742:VAL:HG13	12:H:754:CYS:HB2	1.94	0.48
1:2:222:THR:HG23	1:2:224:ARG:HG2	1.94	0.48
1:2:364:CYS:HB2	1:2:373:PHE:HZ	1.78	0.48
1:2:527:VAL:HB	1:2:531:HIS:HB3	1.94	0.48
1:2:688:ASP:HB2	1:2:691:ALA:HB3	1.95	0.48
2:3:347:ILE:O	2:3:351:ASN:ND2	2.35	0.48
4:5:340:SER:O	4:5:344:ASN:HA	2.14	0.48
12:F:778:MET:HE2	12:F:829:ARG:HG2	1.96	0.48
15:K:445:ILE:HA	15:K:449:PHE:HB2	1.95	0.48
1:2:271:PHE:CD2	1:2:295:VAL:HG11	2.49	0.48
3:4:251:TYR:HD2	3:4:254:THR:HG23	1.77	0.48
15:K:710:LEU:HG	15:K:715:LEU:HD13	1.96	0.48
17:M:1410:GLU:O	17:M:1411:LYS:C	2.56	0.48
2:3:486:ILE:O	2:3:490:MET:HG3	2.13	0.48
3:4:640:SER:O	3:4:643:SER:OG	2.30	0.48
4:5:457:PRO:HA	4:5:460:ARG:NH2	2.29	0.48
6:7:260:TYR:HB3	6:7:298:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:12:ASP:OD1	9:C:52:ARG:NH2	2.46	0.48
11:E:513:ILE:HD11	11:E:530:LEU:HD21	1.95	0.48
18:N:23:ARG:O	18:N:27:ARG:HB2	2.13	0.48
1:2:201:PRO:HD2	15:K:21:ARG:NH2	2.29	0.48
1:2:849:GLN:HG3	1:2:857:LEU:HD12	1.96	0.48
4:5:188:HIS:CD2	4:5:213:SER:C	2.92	0.48
4:5:365:LYS:O	4:5:369:ILE:HG12	2.14	0.48
12:G:592:THR:HG1	12:G:596:TYR:H	1.60	0.48
12:G:752:LEU:N	12:G:773:GLU:OE2	2.47	0.48
17:M:1412:GLU:HG3	17:M:1415:THR:H	1.78	0.48
1:2:782:ASP:OD1	1:2:782:ASP:N	2.45	0.48
3:4:863:GLU:HB2	3:4:867:ARG:NH2	2.29	0.48
6:7:331:LEU:HD21	6:7:376:LEU:HB2	1.94	0.48
12:G:755:ILE:HG23	12:G:769:PRO:HD2	1.96	0.48
15:K:441:ILE:O	15:K:445:ILE:HG12	2.13	0.48
17:M:1566:ILE:HA	17:M:1569:LEU:HB2	1.96	0.48
2:3:462:MET:HG3	2:3:470:VAL:HG21	1.96	0.47
3:4:181:TRP:CD1	15:K:365:SER:HB3	2.49	0.47
3:4:362:ARG:HH21	15:K:377:SER:HB2	1.79	0.47
4:5:760:THR:OG1	4:5:775:VAL:O	2.31	0.47
5:6:625:ALA:HA	5:6:629:MET:HE2	1.96	0.47
11:E:316:LEU:HD12	11:E:413:LEU:HD13	1.95	0.47
11:E:526:ARG:HG3	11:E:565:LEU:HD23	1.95	0.47
17:M:2160:GLN:O	18:N:214:LYS:NZ	2.43	0.47
18:N:214:LYS:HB2	18:N:624:TRP:CD2	2.49	0.47
1:2:324:VAL:HG12	1:2:420:PRO:HA	1.96	0.47
3:4:571:SER:O	3:4:574:LYS:HB2	2.13	0.47
5:6:529:LEU:HD11	5:6:754:TYR:CE2	2.49	0.47
6:7:584:ILE:HG22	6:7:586:LEU:HD23	1.95	0.47
11:E:381:ASP:N	11:E:381:ASP:OD1	2.44	0.47
12:F:629:HIS:NE2	12:F:639:SER:OG	2.32	0.47
15:K:412:GLU:HB2	15:K:420:ASN:ND2	2.29	0.47
1:2:444:PHE:O	1:2:446:VAL:N	2.46	0.47
4:5:344:ASN:HB2	4:5:348:MET:CE	2.44	0.47
5:6:734:LEU:CD2	5:6:742:ILE:CG1	2.87	0.47
6:7:152:ARG:HH22	15:K:372:THR:HA	1.80	0.47
12:F:522:ARG:HH21	12:F:523:PHE:HZ	1.61	0.47
12:H:754:CYS:O	12:H:772:SER:N	2.48	0.47
12:H:883:LEU:N	12:H:913:LYS:HZ1	2.12	0.47
15:K:158:LYS:O	15:K:162:VAL:HG23	2.14	0.47
1:2:353:GLN:HA	1:2:359:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:374:ILE:HD12	15:K:681:ARG:HD3	1.96	0.47
6:7:363:PHE:C	6:7:365:ALA:N	2.70	0.47
6:7:703:ARG:HB2	6:7:707:MET:HE2	1.96	0.47
11:E:148:VAL:HG13	11:E:152:LEU:HD22	1.97	0.47
17:M:1329:ASP:OD1	17:M:1329:ASP:N	2.45	0.47
17:M:1435:GLN:H	17:M:1438:ILE:HD13	1.79	0.47
1:2:244:VAL:HG21	1:2:271:PHE:CE2	2.49	0.47
2:3:86:SER:N	6:7:215:TYR:O	2.47	0.47
4:5:464:LEU:HD11	4:5:509:ILE:HG21	1.96	0.47
9:C:33:ASN:HB2	9:C:36:ARG:HB3	1.97	0.47
9:C:121:ALA:HA	9:C:124:VAL:HG12	1.95	0.47
12:H:554:ILE:O	12:H:567:THR:HG23	2.14	0.47
15:K:62:PHE:HE2	15:K:134:LEU:HB3	1.79	0.47
15:K:454:HIS:O	15:K:457:THR:OG1	2.32	0.47
1:2:690:GLU:HB3	1:2:694:ARG:HH12	1.79	0.47
3:4:695:PRO:HG2	3:4:698:LEU:HB2	1.96	0.47
4:5:181:ILE:HD11	4:5:241:TYR:HB3	1.96	0.47
6:7:224:PRO:HA	6:7:240:THR:HG23	1.96	0.47
10:D:63:LEU:HD22	10:D:87:LEU:HD13	1.97	0.47
12:F:698:PHE:CG	12:F:744:PRO:HG3	2.49	0.47
12:G:576:GLU:HG3	12:G:594:LEU:HD23	1.97	0.47
15:K:272:SER:O	15:K:272:SER:OG	2.32	0.47
17:M:1668:MET:SD	17:M:1668:MET:N	2.88	0.47
18:N:553:HIS:CD2	18:N:619:LEU:HD21	2.49	0.47
2:3:199:SER:OG	2:3:201:HIS:NE2	2.44	0.47
3:4:532:GLU:CD	3:4:533:LEU:H	2.23	0.47
3:4:802:ILE:O	3:4:806:GLU:HG3	2.15	0.47
3:4:848:ASN:HD21	3:4:850:VAL:HB	1.79	0.47
3:4:882:SER:HA	3:4:922:GLY:O	2.15	0.47
4:5:561:ASN:ND2	4:5:563:GLU:OE2	2.47	0.47
4:5:642:GLU:OE2	4:5:643:ARG:N	2.47	0.47
4:5:753:TYR:CE2	4:5:757:LYS:HE3	2.49	0.47
22:5:802:AGS:O3G	22:5:802:AGS:O1B	2.33	0.47
6:7:21:ILE:HG12	6:7:117:PHE:HE1	1.78	0.47
6:7:80:ILE:HG21	6:7:117:PHE:CE2	2.50	0.47
6:7:364:LYS:HB2	13:I:47:DT:O4'	2.14	0.47
6:7:367:LYS:HG3	13:I:47:DT:C2	2.48	0.47
7:A:35:ASP:OD1	7:A:36:ILE:N	2.48	0.47
12:G:500:GLY:HA2	12:G:517:PHE:HA	1.97	0.47
12:G:510:GLN:NE2	12:G:529:GLU:OE2	2.48	0.47
13:I:43:DG:H2''	13:I:44:DT:H5''	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:176:LEU:HB2	15:K:260:ASN:ND2	2.29	0.47
15:K:414:LEU:HD22	15:K:473:VAL:CG2	2.44	0.47
15:K:716:ILE:O	15:K:720:ARG:HG3	2.14	0.47
17:M:1532:TYR:CD2	17:M:1640:LEU:HD12	2.50	0.47
17:M:1731:VAL:HG22	17:M:1906:TRP:HB2	1.96	0.47
17:M:1819:TRP:CD1	17:M:1825:ALA:HB2	2.49	0.47
18:N:416:ALA:O	18:N:420:ILE:HG12	2.15	0.47
3:4:925:ARG:HG2	3:4:926:SER:H	1.80	0.47
12:F:546:PHE:HE2	12:F:557:ARG:HD2	1.80	0.47
12:F:778:MET:HE2	12:F:829:ARG:HA	1.96	0.47
12:G:688:PHE:CE2	12:G:744:PRO:HB2	2.50	0.47
12:H:516:SER:OG	12:H:517:PHE:N	2.47	0.47
12:H:560:ASP:OD1	12:H:560:ASP:N	2.47	0.47
12:H:639:SER:HB3	12:H:653:ARG:HD2	1.96	0.47
16:L:48:ARG:HH12	16:L:51:GLN:HG2	1.80	0.47
4:5:302:ASN:HB3	4:5:324:ARG:HD3	1.97	0.47
5:6:118:PHE:HD1	5:6:161:ARG:HD2	1.80	0.47
5:6:323:GLN:NE2	5:6:328:THR:O	2.48	0.47
5:6:730:HIS:NE2	5:6:734:LEU:HD11	2.29	0.47
12:H:616:VAL:HG11	12:H:682:MET:HE1	1.97	0.47
12:H:892:ASP:O	12:H:896:THR:HG23	2.14	0.47
3:4:404:ASP:OD1	3:4:404:ASP:N	2.47	0.47
6:7:450:ILE:HG22	6:7:451:ARG:HG3	1.97	0.47
7:A:14:LYS:O	7:A:18:GLN:HG3	2.15	0.47
9:C:132:ALA:HA	9:C:135:LEU:HG	1.97	0.47
11:E:527:LEU:HD21	11:E:529:VAL:HG23	1.97	0.47
17:M:1536:PHE:HA	17:M:1539:LYS:HB3	1.97	0.47
18:N:66:PHE:CE1	18:N:80:ASP:HB3	2.49	0.47
18:N:178:GLN:NE2	18:N:531:ARG:HD2	2.30	0.47
4:5:53:ASN:HB3	4:5:58:ASN:O	2.14	0.46
6:7:547:SER:HA	6:7:556:THR:HA	1.96	0.46
7:A:133:GLU:OE2	10:D:189:ILE:HG12	2.16	0.46
9:C:52:ARG:HG3	9:C:114:LEU:HD11	1.97	0.46
12:F:729:TRP:NE1	12:F:734:GLY:O	2.40	0.46
17:M:1536:PHE:CD1	17:M:1640:LEU:HB3	2.51	0.46
18:N:11:LYS:HD2	18:N:11:LYS:HA	1.68	0.46
3:4:193:ASN:HA	3:4:196:ASN:HD21	1.80	0.46
3:4:233:MET:HE1	3:4:241:LEU:HB2	1.97	0.46
3:4:251:TYR:CD2	3:4:254:THR:HG23	2.51	0.46
3:4:896:ASP:OD1	3:4:896:ASP:N	2.48	0.46
4:5:211:CYS:SG	4:5:213:SER:O	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:519:MET:HE1	5:6:750:GLN:HG2	1.96	0.46
6:7:18:PHE:HE1	6:7:120:ALA:HB2	1.79	0.46
11:E:131:LEU:HA	11:E:134:ILE:HG22	1.96	0.46
12:G:549:SER:HA	12:G:578:ILE:HB	1.97	0.46
12:H:840:THR:O	12:H:845:GLY:N	2.49	0.46
17:M:1887:LYS:O	17:M:1891:THR:HG23	2.15	0.46
4:5:301:TYR:CE2	4:5:303:SER:HB2	2.51	0.46
5:6:777:TYR:OH	5:6:781:ARG:HD2	2.15	0.46
12:G:488:PHE:N	12:G:765:GLU:OE2	2.42	0.46
17:M:1593:GLN:OE1	17:M:1617:LEU:N	2.42	0.46
18:N:433:ILE:HG21	18:N:541:ILE:HD13	1.97	0.46
1:2:397:VAL:HG21	1:2:403:PRO:HB3	1.98	0.46
3:4:601:LEU:HD12	3:4:620:ALA:HB3	1.97	0.46
3:4:880:SER:CB	3:4:925:ARG:HG3	2.44	0.46
5:6:297:THR:HG22	5:6:359:VAL:HG12	1.98	0.46
7:A:178:TYR:O	18:N:18:ARG:NE	2.49	0.46
17:M:1809:ALA:O	17:M:1813:VAL:HG13	2.16	0.46
3:4:621:LEU:HD12	3:4:648:VAL:HG21	1.98	0.46
6:7:146:ARG:HD3	6:7:192:PHE:HE1	1.81	0.46
6:7:569:PRO:HG2	6:7:574:TYR:HB2	1.97	0.46
11:E:301:ARG:HA	12:F:505:VAL:HG11	1.96	0.46
11:E:305:SER:HB3	12:F:491:ARG:HG3	1.97	0.46
11:E:519:ILE:O	11:E:519:ILE:HG13	2.16	0.46
12:F:722:LEU:HD12	12:F:776:ILE:HA	1.98	0.46
18:N:53:TRP:HB3	18:N:54:ARG:NH2	2.31	0.46
3:4:448:SER:HB2	5:6:419:SER:HB2	1.97	0.46
5:6:326:LYS:HD3	5:6:410:LEU:HB3	1.98	0.46
6:7:106:ILE:HG22	6:7:113:PHE:CG	2.51	0.46
7:A:40:ILE:HG21	7:A:86:LEU:HD21	1.98	0.46
10:D:79:TYR:OH	10:D:84:MET:HG2	2.16	0.46
12:F:616:VAL:HG11	12:F:682:MET:SD	2.56	0.46
12:G:763:TRP:NE1	12:G:765:GLU:OE1	2.40	0.46
17:M:1584:ARG:HA	17:M:1584:ARG:HD2	1.53	0.46
18:N:45:VAL:O	18:N:49:ILE:HG22	2.16	0.46
1:2:564:VAL:HG13	5:6:669:HIS:NE2	2.31	0.46
3:4:745:GLU:O	3:4:748:THR:HG22	2.15	0.46
3:4:801:MET:HG2	3:4:829:ILE:HG13	1.97	0.46
6:7:82:LEU:HD23	6:7:85:ILE:HD12	1.98	0.46
6:7:291:GLN:NE2	6:7:292:ASN:OD1	2.49	0.46
6:7:527:ASP:OD1	6:7:527:ASP:N	2.49	0.46
12:F:493:TYR:CG	12:F:496:MET:HE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:709:LYS:HB3	12:F:715:GLU:HB3	1.97	0.46
12:H:478:PRO:HA	12:H:579:THR:HA	1.96	0.46
12:H:916:ASN:O	12:H:919:GLU:HG2	2.15	0.46
17:M:1801:GLU:O	17:M:1806:ASN:HB2	2.16	0.46
18:N:70:TRP:CD1	18:N:72:GLN:HE22	2.26	0.46
2:3:354:SER:HB3	2:3:717:LEU:HD12	1.97	0.46
2:3:367:LEU:HD23	2:3:656:LEU:HD21	1.98	0.46
6:7:504:ASP:OD1	6:7:505:GLU:N	2.48	0.46
11:E:271:TRP:CE3	11:E:318:LEU:HD11	2.51	0.46
15:K:505:LEU:HD21	15:K:542:LEU:HD22	1.96	0.46
1:2:309:LEU:HD11	1:2:320:VAL:HG11	1.97	0.46
1:2:511:ILE:HD11	1:2:683:VAL:HG22	1.97	0.46
3:4:352:CYS:SG	3:4:373:ARG:NH1	2.89	0.46
3:4:613:GLN:HG3	5:6:360:ARG:NH2	2.31	0.46
12:F:750:ASP:OD1	12:F:776:ILE:HG12	2.15	0.46
12:H:537:CYS:SG	12:H:538:PHE:N	2.89	0.46
15:K:62:PHE:CE2	15:K:134:LEU:HB3	2.51	0.46
17:M:1332:GLU:HB3	17:M:1335:VAL:HB	1.98	0.46
17:M:1532:TYR:CE2	17:M:1637:ASN:HA	2.51	0.46
3:4:774:TYR:CG	3:4:798:LEU:HD12	2.51	0.46
6:7:364:LYS:HA	6:7:367:LYS:CB	2.45	0.46
10:D:126:LEU:HD12	10:D:126:LEU:HA	1.81	0.46
10:D:277:MET:HE3	10:D:277:MET:HB3	1.80	0.46
11:E:434:VAL:HG11	11:E:502:LEU:HD11	1.97	0.46
15:K:713:PHE:O	15:K:716:ILE:HG22	2.17	0.46
17:M:1792:ARG:HG2	17:M:1796:LYS:NZ	2.31	0.46
18:N:671:ARG:HG2	18:N:686:GLU:HG2	1.98	0.46
9:C:51:ALA:HB1	9:C:74:LEU:HD21	1.98	0.45
9:C:116:SER:O	9:C:116:SER:OG	2.30	0.45
10:D:253:LYS:HA	10:D:253:LYS:HD2	1.77	0.45
11:E:396:LEU:HD22	11:E:401:LEU:HB2	1.98	0.45
12:F:592:THR:HG22	12:F:594:LEU:H	1.82	0.45
17:M:1691:GLU:HG3	17:M:1826:LYS:HE3	1.98	0.45
18:N:61:LYS:HA	18:N:64:GLU:HG2	1.98	0.45
3:4:323:ASP:OD2	6:7:302:THR:OG1	2.34	0.45
3:4:802:ILE:HD12	5:6:735:HIS:CD2	2.52	0.45
6:7:366:LEU:HD13	14:J:15:DC:H2"	1.98	0.45
2:3:312:ASN:O	2:3:313:THR:C	2.59	0.45
2:3:485:ALA:O	2:3:489:VAL:HG23	2.17	0.45
3:4:239:SER:HA	3:4:301:TYR:HD1	1.82	0.45
3:4:758:ILE:HG21	3:4:810:LYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:185:ASN:HB2	4:5:236:CYS:SG	2.56	0.45
5:6:187:ARG:HH12	15:K:252:THR:HG22	1.81	0.45
8:B:2:SER:O	10:D:145:ARG:NH2	2.32	0.45
9:C:97:LEU:HD11	9:C:127:LEU:HD21	1.98	0.45
11:E:82:LEU:HD23	11:E:121:TYR:HB2	1.97	0.45
11:E:561:ASP:N	11:E:561:ASP:OD1	2.49	0.45
12:F:727:GLU:HA	12:F:730:LYS:HG2	1.99	0.45
12:F:727:GLU:O	12:F:731:MET:HG2	2.16	0.45
17:M:1540:LYS:HE3	17:M:1552:ILE:HG22	1.96	0.45
17:M:1585:GLY:O	17:M:1587:GLN:HG2	2.17	0.45
18:N:604:LYS:HB3	18:N:604:LYS:HE2	1.70	0.45
1:2:190:LYS:HG2	1:2:200:GLN:HE22	1.81	0.45
6:7:410:VAL:HG13	6:7:411:TYR:HD1	1.80	0.45
7:A:33:HIS:ND1	7:A:36:ILE:HD12	2.31	0.45
8:B:100:ARG:HH21	8:B:101:LYS:NZ	2.13	0.45
12:F:616:VAL:HG21	12:F:682:MET:SD	2.56	0.45
12:H:486:PHE:HA	12:H:492:ARG:HB2	1.99	0.45
12:H:551:THR:H	12:H:572:LEU:HD22	1.81	0.45
15:K:52:LEU:O	15:K:56:LYS:HG2	2.16	0.45
1:2:190:LYS:HB3	1:2:190:LYS:HE3	1.57	0.45
1:2:803:PHE:CD1	1:2:804:PRO:HD2	2.52	0.45
2:3:259:GLN:HA	2:3:273:SER:HA	1.98	0.45
2:3:312:ASN:O	2:3:314:LEU:HG	2.16	0.45
3:4:379:PRO:O	15:K:228:MET:HE1	2.17	0.45
3:4:775:VAL:CA	3:4:779:LYS:NZ	2.80	0.45
6:7:106:ILE:HD12	6:7:204:PHE:CE2	2.51	0.45
9:C:129:LEU:O	9:C:133:GLN:HG2	2.17	0.45
11:E:506:ILE:HD12	11:E:548:LEU:HB2	1.99	0.45
12:H:620:ALA:HA	12:H:625:VAL:HA	1.99	0.45
12:H:622:ASN:OD1	12:H:623:TYR:N	2.50	0.45
12:H:707:LEU:HB3	12:H:710:TRP:HB3	1.97	0.45
15:K:354:SER:OG	15:K:356:ARG:O	2.33	0.45
15:K:774:GLY:HA2	15:K:778:ARG:HE	1.81	0.45
17:M:1800:ASP:O	17:M:1804:LYS:HG2	2.16	0.45
2:3:497:ILE:HG23	2:3:499:LYS:HE2	1.98	0.45
6:7:17:LEU:HD21	6:7:100:ASP:HB2	1.98	0.45
6:7:140:ASP:HA	6:7:143:LEU:HD12	1.98	0.45
16:L:99:ALA:O	16:L:103:PHE:N	2.48	0.45
17:M:2143:GLN:HE21	17:M:2210:PHE:HD1	1.63	0.45
2:3:444:ALA:HB1	2:3:457:LEU:HD22	1.98	0.45
7:A:165:VAL:HA	7:A:207:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:159:GLY:C	8:B:161:LYS:N	2.72	0.45
17:M:1499:PHE:HB3	17:M:1573:LEU:HD21	1.97	0.45
17:M:1636:VAL:HA	17:M:1639:VAL:HG22	1.99	0.45
18:N:65:GLN:HB3	18:N:84:VAL:HG13	1.98	0.45
1:2:344:CYS:SG	1:2:366:ASN:HB3	2.57	0.45
2:3:582:VAL:O	2:3:582:VAL:HG13	2.16	0.45
4:5:731:GLN:HG2	4:5:735:ARG:CZ	2.46	0.45
11:E:296:GLN:HG3	11:E:320:ILE:HD13	1.98	0.45
15:K:400:LYS:HA	15:K:400:LYS:HD3	1.64	0.45
17:M:1487:LEU:O	17:M:1487:LEU:HD23	2.17	0.45
17:M:1810:ASP:O	17:M:1811:LEU:C	2.58	0.45
1:2:190:LYS:CB	1:2:197:TRP:CZ3	2.98	0.45
5:6:519:MET:CE	5:6:750:GLN:HG2	2.46	0.45
6:7:333:ILE:HD13	6:7:351:VAL:HG11	1.97	0.45
6:7:366:LEU:HD21	14:J:16:DA:H5'	1.98	0.45
6:7:400:ARG:O	6:7:404:LEU:HG	2.16	0.45
6:7:501:PRO:HB2	6:7:504:ASP:OD1	2.16	0.45
12:G:560:ASP:OD1	12:G:560:ASP:N	2.48	0.45
12:H:897:ALA:O	12:H:901:ILE:HG12	2.17	0.45
3:4:544:LEU:HD21	3:4:581:VAL:HG23	1.98	0.45
9:C:161:ALA:HA	9:C:164:THR:HG22	1.99	0.45
12:F:631:SER:OG	12:F:634:HIS:ND1	2.38	0.45
12:G:883:LEU:N	12:G:913:LYS:HZ1	2.15	0.45
12:H:493:TYR:HA	12:H:503:SER:HA	1.98	0.45
12:H:506:LYS:HD3	12:H:511:TYR:CZ	2.52	0.45
13:I:35:DT:H3	14:J:27:DA:H61	1.64	0.45
17:M:1438:ILE:HD12	17:M:1438:ILE:H	1.82	0.45
18:N:490:LEU:HB3	18:N:491:TRP:CE3	2.48	0.45
2:3:367:LEU:HD11	2:3:382:LEU:HB2	1.98	0.44
3:4:268:VAL:O	3:4:272:MET:HG3	2.16	0.44
3:4:610:ASP:O	3:4:611:THR:OG1	2.30	0.44
5:6:666:ALA:C	5:6:668:ILE:H	2.26	0.44
7:A:91:ARG:HH11	7:A:91:ARG:HG2	1.82	0.44
12:G:704:LEU:HD23	12:G:704:LEU:HA	1.85	0.44
17:M:1593:GLN:CD	17:M:1617:LEU:H	2.24	0.44
2:3:478:MET:O	2:3:483:ARG:NH2	2.50	0.44
3:4:402:THR:OG1	3:4:404:ASP:OD1	2.28	0.44
6:7:255:VAL:HG21	6:7:258:ILE:HG13	1.99	0.44
6:7:545:THR:HG23	6:7:558:ASN:HA	1.98	0.44
17:M:1322:TRP:HB3	17:M:1338:VAL:HG13	1.99	0.44
18:N:503:LEU:HB3	18:N:504:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:615:GLN:NE2	1:2:616:ASP:OD1	2.51	0.44
4:5:236:CYS:O	4:5:240:PRO:HB3	2.16	0.44
6:7:81:ASP:HA	6:7:205:LYS:HB3	2.00	0.44
12:F:750:ASP:OD1	12:F:776:ILE:N	2.35	0.44
12:G:534:TYR:CG	12:G:546:PHE:HB3	2.52	0.44
15:K:773:VAL:HA	15:K:776:TYR:HB3	1.99	0.44
17:M:1319:ASN:H	17:M:1447:PHE:HB2	1.81	0.44
17:M:1454:ALA:HA	17:M:1457:LYS:HE3	1.99	0.44
17:M:1510:THR:HA	17:M:1559:GLU:HB2	1.99	0.44
18:N:63:LEU:HD12	18:N:64:GLU:N	2.32	0.44
18:N:447:MET:O	18:N:447:MET:HG2	2.16	0.44
3:4:445:ARG:NH2	3:4:448:SER:O	2.38	0.44
3:4:502:THR:O	3:4:506:LEU:HG	2.18	0.44
3:4:502:THR:HB	3:4:505:ASP:HB2	2.00	0.44
5:6:776:LYS:HA	5:6:776:LYS:HD3	1.66	0.44
6:7:311:GLN:HB2	6:7:340:VAL:HG13	1.99	0.44
6:7:414:LEU:O	6:7:418:ILE:HG12	2.17	0.44
9:C:36:ARG:HD3	9:C:37:PRO:O	2.17	0.44
11:E:619:LYS:HD2	11:E:633:ARG:HG3	1.99	0.44
12:H:621:GLN:N	12:H:624:ARG:O	2.37	0.44
12:H:688:PHE:CD2	12:H:746:ALA:HA	2.52	0.44
15:K:34:PRO:HB3	15:K:43:PRO:HB2	1.99	0.44
15:K:529:THR:HG22	15:K:533:MET:SD	2.57	0.44
15:K:686:GLU:N	15:K:689:SER:OG	2.51	0.44
2:3:462:MET:HE2	2:3:489:VAL:HB	1.98	0.44
3:4:618:SER:HB2	3:4:622:VAL:HG13	1.98	0.44
3:4:682:TYR:HB3	3:4:709:LEU:HD21	1.99	0.44
4:5:152:ASP:OD1	4:5:154:GLU:HG2	2.18	0.44
4:5:337:VAL:HG21	4:5:434:PRO:O	2.18	0.44
4:5:473:ASP:HA	4:5:517:THR:HG22	1.99	0.44
5:6:559:THR:HG22	5:6:563:ILE:O	2.18	0.44
6:7:586:LEU:HD12	6:7:590:LEU:HD23	2.00	0.44
7:A:30:PRO:O	7:A:31:MET:C	2.60	0.44
11:E:271:TRP:HE3	11:E:318:LEU:HD11	1.82	0.44
11:E:349:SER:OG	11:E:351:TRP:NE1	2.51	0.44
12:F:624:ARG:HA	12:F:642:GLU:HA	2.00	0.44
12:F:697:ILE:HB	12:F:705:LEU:HD12	2.00	0.44
12:H:843:ASN:C	12:H:843:ASN:HD22	2.25	0.44
17:M:1318:ALA:HA	17:M:1447:PHE:HD1	1.82	0.44
17:M:1486:TYR:CE2	17:M:1488:LEU:HD22	2.53	0.44
17:M:1863:ARG:HD2	17:M:1863:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:1968:LYS:HB3	17:M:1968:LYS:HE3	1.79	0.44
18:N:547:SER:HB3	18:N:645:THR:HG23	1.99	0.44
3:4:204:LYS:HE3	3:4:215:PHE:HB2	2.00	0.44
5:6:775:GLU:O	5:6:779:GLU:HG2	2.17	0.44
12:F:720:PRO:HG3	12:G:611:LYS:HB2	2.00	0.44
12:H:659:MET:HG3	12:H:684:ILE:HD11	1.99	0.44
12:H:818:PRO:O	12:H:822:ALA:N	2.41	0.44
12:H:910:LEU:O	12:H:914:ILE:HG12	2.17	0.44
15:K:414:LEU:O	15:K:415:PRO:C	2.61	0.44
2:3:171:LEU:HD11	2:3:180:VAL:HG21	1.99	0.44
2:3:576:TYR:OH	2:3:583:ARG:O	2.35	0.44
4:5:610:CYS:HB2	4:5:668:LEU:HD23	1.99	0.44
5:6:333:CYS:SG	5:6:338:CYS:HB3	2.58	0.44
15:K:210:ARG:HB3	15:K:289:ILE:HA	1.99	0.44
1:2:183:LEU:HD13	1:2:210:GLU:HG3	2.00	0.44
1:2:340:ASN:HB2	1:2:374:ARG:NH1	2.33	0.44
1:2:625:GLU:OE1	1:2:808:ARG:NE	2.35	0.44
1:2:792:ASP:OD2	1:2:864:TYR:OH	2.28	0.44
2:3:305:GLY:HA2	2:3:310:ASN:HB2	2.00	0.44
3:4:569:ASP:HB2	3:4:570:PRO:HD2	1.99	0.44
3:4:789:LYS:HB3	3:4:789:LYS:HE2	1.37	0.44
8:B:193:ARG:HD2	10:D:225:ASN:HB3	2.00	0.44
12:G:883:LEU:HB2	12:G:913:LYS:HD2	1.98	0.44
12:H:553:GLN:HG3	12:H:569:ILE:HD13	2.00	0.44
12:H:730:LYS:HA	12:H:734:GLY:HA2	1.99	0.44
12:H:774:MET:SD	12:H:775:GLU:N	2.91	0.44
14:J:30:DT:H2''	14:J:31:DC:H5'	1.99	0.44
15:K:194:ARG:HA	15:K:194:ARG:HD3	1.33	0.44
17:M:1324:VAL:HA	17:M:1661:CYS:HB3	2.00	0.44
18:N:352:ARG:NH1	18:N:637:SER:H	2.14	0.44
1:2:181:LEU:HD23	1:2:185:SER:CB	2.48	0.44
1:2:465:ASN:HD21	1:2:558:LYS:HE2	1.83	0.44
1:2:866:LEU:HD11	17:M:2073:ARG:HB2	2.00	0.44
3:4:393:ASP:O	3:4:420:TYR:HA	2.18	0.44
4:5:361:SER:HA	4:5:366:LEU:HD22	1.99	0.44
6:7:140:ASP:O	6:7:144:ASN:ND2	2.51	0.44
6:7:685:THR:C	6:7:687:ARG:N	2.75	0.44
8:B:157:LEU:HD22	9:C:136:ASN:HD21	1.83	0.44
11:E:349:SER:OG	11:E:352:ASN:ND2	2.51	0.44
12:F:597:PHE:HB3	12:F:610:GLU:HB3	2.00	0.44
12:G:743:TRP:CE3	12:G:764:PRO:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:92:LEU:HD12	15:K:178:ALA:HB1	2.00	0.44
2:3:118:PRO:HD2	2:3:177:ASN:O	2.18	0.43
2:3:159:GLY:O	2:3:592:VAL:N	2.37	0.43
2:3:519:VAL:N	2:3:532:ASN:O	2.45	0.43
3:4:795:THR:HG23	5:6:731:ILE:HD13	2.00	0.43
3:4:798:LEU:C	3:4:798:LEU:HD23	2.43	0.43
3:4:811:MET:HG2	3:4:812:LYS:N	2.33	0.43
4:5:734:ARG:O	4:5:737:PHE:HB3	2.17	0.43
9:C:3:TYR:CD2	10:D:218:MET:HG3	2.53	0.43
12:F:670:LYS:HD3	12:F:670:LYS:HA	1.89	0.43
12:G:711:ARG:HH21	12:G:839:ASP:HB3	1.83	0.43
12:H:870:PHE:CZ	12:H:910:LEU:HD11	2.53	0.43
15:K:420:ASN:OD1	15:K:420:ASN:N	2.51	0.43
15:K:455:SER:O	15:K:458:ASN:ND2	2.51	0.43
17:M:1819:TRP:CD1	17:M:1825:ALA:CB	3.00	0.43
17:M:2174:TYR:HE2	18:N:289:ASN:HD22	1.66	0.43
2:3:333:SER:HB3	2:3:336:VAL:HG22	1.99	0.43
3:4:265:PRO:HB3	3:4:325:LEU:HD13	2.01	0.43
4:5:252:ASP:OD1	4:5:252:ASP:N	2.51	0.43
4:5:737:PHE:O	4:5:737:PHE:CG	2.71	0.43
5:6:162:GLU:HG3	5:6:165:ALA:HB3	1.99	0.43
5:6:277:ARG:NE	5:6:363:GLU:OE2	2.49	0.43
7:A:32:TYR:CZ	7:A:37:ILE:HG13	2.53	0.43
11:E:26:GLN:NE2	11:E:79:ASN:OD1	2.51	0.43
11:E:615:GLU:HG3	11:E:616:THR:HG23	2.00	0.43
12:F:687:LEU:HD22	12:F:697:ILE:HD12	1.98	0.43
12:H:711:ARG:NH2	12:H:839:ASP:O	2.52	0.43
12:H:761:HIS:O	12:H:761:HIS:ND1	2.50	0.43
15:K:164:LYS:HB2	15:K:215:ILE:HD12	1.99	0.43
18:N:277:ARG:HD2	18:N:277:ARG:N	2.33	0.43
18:N:404:ALA:HB2	18:N:642:CYS:SG	2.57	0.43
1:2:333:GLN:HE22	1:2:355:SER:HA	1.83	0.43
3:4:447:ASN:OD1	3:4:450:GLN:N	2.46	0.43
3:4:775:VAL:HA	3:4:779:LYS:HZ1	1.83	0.43
6:7:264:GLN:HE21	6:7:294:THR:HB	1.83	0.43
6:7:409:ASP:OD1	6:7:409:ASP:N	2.49	0.43
12:H:701:ASP:N	12:H:701:ASP:OD1	2.47	0.43
15:K:212:VAL:HG23	15:K:213:ILE:HG23	1.99	0.43
1:2:191:ALA:CB	1:2:196:GLU:HG3	2.45	0.43
3:4:685:ASN:N	3:4:685:ASN:OD1	2.52	0.43
4:5:373:SER:O	4:5:373:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:500:GLY:HA2	12:H:518:PHE:HD1	1.84	0.43
15:K:743:ASP:OD1	16:L:84:SER:HB3	2.18	0.43
15:K:753:LEU:HD21	15:K:763:LEU:HD12	2.00	0.43
17:M:1918:SER:HB2	17:M:1939:TRP:NE1	2.34	0.43
2:3:435:ARG:HA	2:3:435:ARG:HD2	1.78	0.43
3:4:569:ASP:HB3	3:4:682:TYR:N	2.15	0.43
3:4:883:PHE:O	3:4:887:ILE:HG12	2.18	0.43
4:5:735:ARG:N	4:5:735:ARG:HH11	2.17	0.43
6:7:71:ALA:HB2	6:7:125:MET:HE3	2.00	0.43
6:7:364:LYS:HD2	6:7:367:LYS:HD2	2.00	0.43
6:7:396:ASP:OD1	6:7:396:ASP:N	2.52	0.43
6:7:720:VAL:O	6:7:724:LYS:HG2	2.18	0.43
12:H:823:ALA:CB	12:H:868:ARG:HD2	2.49	0.43
17:M:1689:TRP:CD1	17:M:1691:GLU:HB2	2.53	0.43
17:M:1806:ASN:HB3	17:M:1809:ALA:HB3	2.01	0.43
2:3:43:ARG:HE	2:3:47:VAL:HG13	1.83	0.43
2:3:406:LEU:HD23	2:3:546:LEU:HG	2.01	0.43
2:3:412:SER:O	2:3:412:SER:OG	2.34	0.43
4:5:106:ARG:NH2	8:B:107:THR:O	2.51	0.43
4:5:731:GLN:O	4:5:735:ARG:HD2	2.18	0.43
12:G:581:VAL:HG12	12:G:590:VAL:HG23	2.01	0.43
15:K:412:GLU:OE2	15:K:419:LEU:HB3	2.18	0.43
15:K:487:LEU:HD21	15:K:542:LEU:HA	2.01	0.43
17:M:2211:ASP:OD1	17:M:2211:ASP:N	2.45	0.43
1:2:605:LEU:HD23	1:2:647:ILE:HB	1.99	0.43
3:4:197:PHE:HB2	3:4:254:THR:HG21	2.01	0.43
3:4:690:GLU:N	3:4:690:GLU:OE1	2.52	0.43
4:5:286:VAL:HG11	4:5:292:VAL:HG11	2.01	0.43
4:5:602:TYR:OH	4:5:666:LEU:O	2.31	0.43
4:5:618:ALA:HB1	4:5:677:VAL:HG21	2.00	0.43
6:7:142:ILE:HG22	6:7:192:PHE:HZ	1.84	0.43
11:E:347:LYS:NZ	11:E:400:GLY:O	2.32	0.43
11:E:579:TYR:HB2	11:E:632:ILE:HG23	2.01	0.43
12:H:545:LEU:HA	12:H:556:TYR:HA	1.99	0.43
12:H:702:ASN:OD1	12:H:725:ASN:ND2	2.52	0.43
15:K:160:GLN:HA	15:K:163:TYR:CD2	2.53	0.43
17:M:1579:LYS:O	17:M:1582:GLU:HG3	2.18	0.43
17:M:1819:TRP:O	17:M:1821:GLN:N	2.51	0.43
1:2:485:ARG:NH2	1:2:769:TYR:OH	2.50	0.43
2:3:478:MET:HE2	2:3:478:MET:HB3	1.79	0.43
3:4:881:MET:SD	3:4:881:MET:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:633:LEU:HD22	4:5:648:ILE:HB	2.01	0.43
4:5:731:GLN:CD	18:N:294:GLY:HA3	2.44	0.43
12:F:621:GLN:HG3	12:F:622:ASN:H	1.84	0.43
12:F:870:PHE:CE2	12:F:882:ALA:HB1	2.53	0.43
12:G:482:ALA:HB3	12:G:496:MET:H	1.84	0.43
12:H:496:MET:SD	12:H:745:LEU:HD13	2.59	0.43
15:K:260:ASN:HB3	15:K:262:VAL:HG13	2.00	0.43
15:K:458:ASN:O	15:K:461:THR:OG1	2.36	0.43
17:M:1598:THR:HA	17:M:1601:LEU:HG	2.01	0.43
18:N:632:LEU:HD13	18:N:639:MET:HE1	2.00	0.43
3:4:195:ARG:HD3	3:4:199:MET:HE1	2.01	0.43
3:4:767:LYS:HA	5:6:732:VAL:HG11	2.00	0.43
4:5:343:TRP:C	4:5:348:MET:HE2	2.44	0.43
7:A:22:ARG:HA	7:A:22:ARG:HD3	1.62	0.43
7:A:33:HIS:O	7:A:37:ILE:HG12	2.18	0.43
7:A:155:LEU:HD21	10:D:145:ARG:HD3	2.01	0.43
8:B:36:LYS:HE2	12:F:848:TYR:HE1	1.84	0.43
12:F:859:ASN:OD1	12:F:890:LYS:HD2	2.19	0.43
12:H:827:TYR:CE1	12:H:866:LEU:HG	2.52	0.43
15:K:239:LEU:HD23	15:K:243:VAL:HG12	2.01	0.43
17:M:1385:ASN:OD1	17:M:1698:HIS:ND1	2.51	0.43
1:2:552:ILE:O	1:2:556:VAL:HG23	2.19	0.43
3:4:377:ASN:HD21	15:K:404:LYS:HD3	1.84	0.43
3:4:444:ILE:HG13	3:4:454:LYS:HB2	2.01	0.43
4:5:283:THR:O	4:5:284:ASN:C	2.61	0.43
5:6:186:ARG:HA	5:6:189:VAL:HG12	2.01	0.43
9:C:78:ASP:OD2	9:C:78:ASP:N	2.51	0.43
12:F:830:SER:OG	12:F:862:TYR:HB2	2.19	0.43
12:H:752:LEU:O	12:H:774:MET:N	2.50	0.43
17:M:1819:TRP:HD1	17:M:1825:ALA:HB2	1.83	0.43
1:2:672:PRO:HD3	4:5:528:GLY:HA3	2.01	0.42
3:4:561:ASP:OD1	3:4:562:ILE:N	2.48	0.42
3:4:646:HIS:CD2	3:4:698:LEU:HD13	2.54	0.42
6:7:672:LYS:O	6:7:672:LYS:HD3	2.18	0.42
6:7:690:LEU:HG	6:7:694:ARG:HH21	1.84	0.42
7:A:70:CYS:HB3	9:C:24:ILE:HD11	2.01	0.42
12:F:615:ILE:HG12	12:F:629:HIS:HD1	1.84	0.42
12:F:757:VAL:HG11	12:F:762:ILE:O	2.19	0.42
17:M:1865:GLN:HE22	17:M:1914:LYS:HE2	1.84	0.42
2:3:476:ASP:OD1	2:3:476:ASP:N	2.51	0.42
3:4:251:TYR:HE2	3:4:253:GLN:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:137:ASP:OD1	6:7:137:ASP:N	2.53	0.42
7:A:165:VAL:HG21	7:A:205:LEU:HD13	2.00	0.42
12:G:739:ASP:OD1	12:G:739:ASP:N	2.52	0.42
12:H:545:LEU:HD13	12:H:556:TYR:HB2	2.01	0.42
15:K:568:GLU:HG3	15:K:569:ARG:HG3	2.01	0.42
18:N:503:LEU:O	18:N:505:GLN:N	2.52	0.42
2:3:104:ARG:NH1	9:C:90:THR:OG1	2.53	0.42
2:3:166:LEU:HD13	2:3:171:LEU:HD12	2.01	0.42
3:4:884:ASN:O	3:4:888:LYS:NZ	2.52	0.42
4:5:349:PHE:CD1	4:5:357:PHE:HE2	2.37	0.42
7:A:11:LEU:HD23	7:A:11:LEU:HA	1.86	0.42
8:B:60:LEU:HD11	8:B:75:ILE:HD13	2.00	0.42
9:C:138:HIS:ND1	9:C:162:THR:HA	2.33	0.42
11:E:24:SER:OG	11:E:25:CYS:N	2.52	0.42
12:H:477:MET:HE3	12:H:678:ASN:O	2.19	0.42
15:K:195:THR:O	15:K:199:ASN:HB3	2.18	0.42
15:K:366:ILE:H	15:K:366:ILE:HG13	1.51	0.42
17:M:1489:HIS:ND1	17:M:1599:LYS:HE3	2.33	0.42
17:M:1511:ILE:HB	17:M:1558:PHE:HE1	1.85	0.42
17:M:1708:ASN:O	17:M:1712:ILE:HG23	2.19	0.42
17:M:1798:TRP:O	17:M:1809:ALA:HB1	2.18	0.42
18:N:416:ALA:HB2	18:N:689:ILE:HD13	2.01	0.42
3:4:445:ARG:HA	3:4:453:LEU:HD23	2.01	0.42
6:7:578:LEU:HD12	6:7:578:LEU:HA	1.93	0.42
8:B:58:LYS:HE2	8:B:58:LYS:HB2	1.81	0.42
12:F:688:PHE:CE1	12:F:744:PRO:HB2	2.54	0.42
12:F:895:LEU:O	12:F:899:VAL:HG23	2.18	0.42
15:K:62:PHE:CE1	15:K:75:ALA:HB2	2.52	0.42
15:K:78:VAL:HG13	15:K:83:ILE:HB	2.01	0.42
15:K:176:LEU:O	15:K:180:ILE:HG23	2.19	0.42
18:N:503:LEU:HD23	18:N:630:LEU:HD13	2.01	0.42
1:2:183:LEU:CD1	1:2:186:LEU:HD12	2.49	0.42
2:3:132:LEU:O	2:3:136:MET:HG2	2.18	0.42
2:3:313:THR:HG23	2:3:315:ILE:HG23	2.01	0.42
3:4:846:ASP:N	3:4:846:ASP:OD1	2.50	0.42
4:5:723:PRO:HB2	4:5:726:TRP:CE3	2.55	0.42
5:6:321:VAL:HG11	5:6:330:PRO:HD3	2.01	0.42
6:7:82:LEU:CD2	6:7:106:ILE:HD11	2.45	0.42
6:7:228:ARG:NH2	6:7:326:HIS:HB3	2.35	0.42
7:A:71:GLN:HA	9:C:27:LEU:HD21	2.02	0.42
8:B:173:LEU:HD12	8:B:173:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:145:ASP:HB3	11:E:254:GLN:OE1	2.20	0.42
11:E:155:GLN:HE21	11:E:240:TYR:HB2	1.84	0.42
12:H:499:VAL:O	12:H:518:PHE:N	2.45	0.42
15:K:595:THR:HA	15:K:598:VAL:HG12	2.02	0.42
15:K:598:VAL:HA	15:K:601:VAL:HG22	2.01	0.42
15:K:667:MET:SD	15:K:672:ILE:HD11	2.59	0.42
17:M:2069:ILE:O	17:M:2073:ARG:HG2	2.19	0.42
18:N:356:LEU:HA	18:N:359:ILE:HG22	2.01	0.42
1:2:866:LEU:HD11	17:M:2073:ARG:CB	2.49	0.42
2:3:305:GLY:O	2:3:307:ASN:N	2.52	0.42
3:4:273:ASP:OD2	15:K:356:ARG:NH1	2.41	0.42
6:7:436:LEU:HD21	6:7:477:SER:HB2	2.02	0.42
6:7:664:TYR:CD2	6:7:689:LEU:HD11	2.54	0.42
7:A:81:ARG:HD3	9:C:49:TRP:CD1	2.54	0.42
7:A:97:LEU:HD23	7:A:97:LEU:HA	1.87	0.42
11:E:388:LEU:HD23	11:E:388:LEU:HA	1.81	0.42
12:H:568:LYS:NZ	12:H:604:GLY:O	2.46	0.42
12:H:621:GLN:HG3	12:H:622:ASN:H	1.84	0.42
15:K:546:THR:O	15:K:550:GLN:HB2	2.20	0.42
17:M:1411:LYS:HB3	17:M:1411:LYS:HE3	1.44	0.42
17:M:1906:TRP:CZ3	17:M:1921:ALA:HB2	2.54	0.42
18:N:399:PHE:HB2	18:N:675:TYR:HB3	2.00	0.42
1:2:189:VAL:HG22	1:2:197:TRP:CG	2.55	0.42
1:2:422:GLU:OE2	1:2:458:ARG:NH2	2.49	0.42
2:3:244:GLU:OE2	6:7:112:HIS:ND1	2.48	0.42
2:3:256:ILE:HD13	2:3:278:LEU:HD11	2.01	0.42
5:6:312:ASP:O	5:6:315:ARG:NH1	2.46	0.42
5:6:529:LEU:HD22	5:6:751:LEU:HD13	2.02	0.42
6:7:710:ILE:HA	6:7:713:VAL:HG22	2.02	0.42
9:C:96:ASP:HA	9:C:168:LYS:HB3	2.01	0.42
11:E:243:GLN:N	11:E:607:MET:HE1	2.34	0.42
15:K:683:ARG:H	15:K:683:ARG:HG2	1.65	0.42
17:M:1376:ILE:C	17:M:1378:LYS:H	2.27	0.42
2:3:305:GLY:C	2:3:307:ASN:N	2.77	0.42
2:3:680:VAL:HG12	6:7:613:ALA:HB1	2.02	0.42
3:4:400:GLN:HE21	3:4:412:PRO:HG2	1.83	0.42
3:4:796:ARG:CZ	3:4:796:ARG:HB3	2.49	0.42
6:7:419:ALA:HB3	6:7:429:LYS:HE2	2.02	0.42
6:7:667:LEU:HA	6:7:670:ASP:OD2	2.20	0.42
10:D:125:PRO:O	10:D:129:MET:HG3	2.20	0.42
12:F:595:GLY:HA2	12:F:614:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:659:MET:HE1	12:F:701:ASP:OD1	2.20	0.42
12:G:598:ARG:H	12:G:598:ARG:HG3	1.68	0.42
12:G:669:LYS:HD3	12:G:669:LYS:HA	1.84	0.42
12:H:703:THR:HA	12:H:722:LEU:O	2.20	0.42
15:K:449:PHE:O	15:K:453:LEU:HG	2.19	0.42
17:M:1336:LEU:HD23	17:M:1434:HIS:HB2	2.02	0.42
17:M:1450:LYS:HA	17:M:1450:LYS:HD3	1.88	0.42
18:N:22:TYR:O	18:N:23:ARG:C	2.63	0.42
1:2:241:SER:HB3	1:2:413:ASP:OD1	2.20	0.42
20:3:1001:ADP:O1B	4:5:651:ARG:NH2	2.47	0.42
4:5:369:ILE:HD12	4:5:592:SER:HA	2.02	0.42
5:6:368:ILE:HD11	5:6:374:PRO:HB3	2.01	0.42
6:7:157:ARG:NH2	15:K:370:ASP:OD1	2.53	0.42
11:E:32:SER:HB3	11:E:86:PHE:HD1	1.85	0.42
11:E:123:LEU:HD21	11:E:255:ILE:HD11	2.01	0.42
12:G:640:LEU:HD23	12:G:651:TYR:HB2	2.02	0.42
15:K:154:GLY:HA2	15:K:157:LYS:HE3	2.02	0.42
15:K:384:ASP:HB3	15:K:387:ILE:HG12	2.01	0.42
16:L:94:PHE:O	16:L:97:LEU:HG	2.19	0.42
18:N:25:LEU:HD13	18:N:25:LEU:HA	1.89	0.42
18:N:455:SER:O	18:N:512:PHE:HE2	2.01	0.42
1:2:268:LEU:HD23	1:2:268:LEU:HA	1.84	0.42
1:2:866:LEU:HD23	1:2:866:LEU:HA	1.91	0.42
3:4:443:PRO:HB2	3:4:453:LEU:HD22	2.01	0.42
3:4:601:LEU:HA	3:4:620:ALA:HB3	2.02	0.42
3:4:780:MET:HE3	3:4:780:MET:HB3	1.88	0.42
5:6:340:ASN:OD1	5:6:343:PHE:HB2	2.20	0.42
5:6:508:LEU:HD12	5:6:508:LEU:HA	1.93	0.42
6:7:149:ARG:HA	6:7:152:ARG:HD3	2.01	0.42
6:7:402:MET:O	6:7:406:THR:HG23	2.19	0.42
22:7:903:AGS:O2B	22:7:903:AGS:S1G	2.78	0.42
11:E:618:ALA:HB2	17:M:2027:LEU:HD13	2.01	0.42
12:F:843:ASN:C	12:F:843:ASN:HD22	2.27	0.42
12:G:506:LYS:HG2	12:G:511:TYR:HD1	1.84	0.42
12:H:554:ILE:O	12:H:567:THR:HA	2.20	0.42
12:H:868:ARG:NH1	12:H:872:SER:HB2	2.35	0.42
17:M:1383:LEU:O	17:M:1385:ASN:ND2	2.52	0.42
17:M:1718:PHE:HE1	17:M:1844:LEU:HD22	1.85	0.42
18:N:88:ILE:HG22	18:N:92:LYS:HE2	2.02	0.42
1:2:390:LEU:HD23	1:2:390:LEU:HA	1.93	0.41
1:2:585:ILE:HG13	1:2:586:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:111:TRP:HZ2	9:C:90:THR:HG23	1.84	0.41
3:4:689:THR:OG1	3:4:690:GLU:OE1	2.30	0.41
3:4:696:PRO:N	3:4:697:PRO:HD2	2.34	0.41
7:A:24:ASN:ND2	7:A:26:ASP:OD1	2.53	0.41
7:A:87:LEU:HD21	10:D:194:VAL:HG21	2.02	0.41
11:E:127:ARG:HA	11:E:127:ARG:NE	2.34	0.41
12:G:610:GLU:OE2	12:G:653:ARG:NH2	2.53	0.41
15:K:292:TYR:O	15:K:295:LYS:NZ	2.33	0.41
15:K:752:ARG:HA	15:K:755:LYS:HE2	2.01	0.41
17:M:1372:LYS:HG2	17:M:1405:SER:HB3	2.01	0.41
17:M:1500:SER:HB3	17:M:1511:ILE:HG12	2.02	0.41
17:M:1676:TYR:HA	17:M:1794:MET:HE1	2.02	0.41
17:M:1707:LEU:HD23	17:M:1707:LEU:HA	1.88	0.41
3:4:433:ILE:HG22	3:4:468:LYS:HA	2.01	0.41
3:4:886:LEU:HD23	3:4:886:LEU:HA	1.94	0.41
4:5:564:ARG:CZ	4:5:568:ILE:HD11	2.50	0.41
5:6:737:LYS:HA	5:6:737:LYS:HD3	1.43	0.41
6:7:230:ILE:HD11	6:7:241:VAL:HG12	2.00	0.41
6:7:265:CYS:SG	6:7:288:GLU:HB3	2.60	0.41
10:D:63:LEU:HB2	10:D:87:LEU:HD11	2.00	0.41
10:D:176:SER:O	10:D:180:ILE:HG12	2.20	0.41
11:E:105:ILE:O	11:E:115:SER:OG	2.33	0.41
11:E:127:ARG:HH12	11:E:129:TRP:HE1	1.67	0.41
11:E:404:ILE:HD13	11:E:404:ILE:HA	1.94	0.41
12:G:526:TYR:HE2	12:G:557:ARG:HH21	1.69	0.41
17:M:1730:VAL:O	17:M:1870:THR:OG1	2.31	0.41
18:N:532:ILE:HD11	18:N:541:ILE:HD11	2.02	0.41
1:2:235:GLY:HA3	1:2:283:TYR:CE2	2.55	0.41
1:2:434:TYR:HB2	1:2:447:PHE:CZ	2.54	0.41
3:4:616:LEU:HB3	5:6:362:GLN:HE22	1.85	0.41
3:4:635:ASP:HB3	3:4:675:ALA:HB1	2.02	0.41
4:5:724:ILE:HG23	17:M:1842:LYS:HE2	2.03	0.41
12:G:597:PHE:HB3	12:G:610:GLU:HB3	2.02	0.41
12:H:883:LEU:HD13	12:H:913:LYS:HD2	2.01	0.41
15:K:87:ASP:C	15:K:90:PRO:HD2	2.45	0.41
3:4:193:ASN:OD1	3:4:253:GLN:NE2	2.54	0.41
5:6:403:VAL:CG2	5:6:450:TYR:HB3	2.50	0.41
6:7:364:LYS:HA	6:7:367:LYS:HB3	2.02	0.41
7:A:28:ASN:HD22	7:A:29:LEU:N	2.18	0.41
11:E:416:ARG:NH1	11:E:489:VAL:HG21	2.36	0.41
11:E:473:TRP:CH2	11:E:542:PRO:HD3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:523:ARG:HD2	11:E:524:ILE:HG13	2.03	0.41
12:F:652:LYS:HA	12:F:652:LYS:HD3	1.76	0.41
15:K:243:VAL:HG13	15:K:248:ILE:HG21	2.03	0.41
18:N:91:MET:HE2	18:N:91:MET:HB2	1.96	0.41
1:2:402:LEU:HD23	1:2:402:LEU:HA	1.88	0.41
6:7:79:ILE:HD13	6:7:203:TYR:HB2	2.02	0.41
12:F:703:THR:HG22	12:F:723:ASP:HA	2.01	0.41
12:F:766:PHE:HB3	12:F:767:PRO:HD3	2.03	0.41
12:H:554:ILE:HG21	12:H:566:TRP:HZ3	1.85	0.41
13:I:54:DT:H6	13:I:54:DT:H2'	1.69	0.41
15:K:414:LEU:CD1	15:K:473:VAL:HG11	2.47	0.41
17:M:2132:ARG:HG3	17:M:2133:CYS:N	2.36	0.41
18:N:62:PHE:CE2	18:N:81:GLN:HA	2.56	0.41
1:2:190:LYS:NZ	15:K:25:ALA:HB1	2.35	0.41
1:2:215:LEU:HD12	1:2:274:VAL:HG12	2.02	0.41
1:2:798:ILE:HB	4:5:560:HIS:ND1	2.36	0.41
4:5:455:ARG:NH1	4:5:460:ARG:O	2.53	0.41
5:6:381:LEU:HD23	5:6:456:ALA:HB3	2.03	0.41
5:6:777:TYR:CZ	5:6:781:ARG:HD2	2.55	0.41
6:7:601:LEU:H	6:7:601:LEU:HD23	1.86	0.41
12:H:750:ASP:OD1	12:H:776:ILE:HG12	2.21	0.41
17:M:1419:ASN:OD1	17:M:1425:GLY:HA2	2.21	0.41
17:M:1816:LEU:O	17:M:1817:ALA:C	2.62	0.41
18:N:528:ASN:HB3	18:N:529:PRO:HD3	2.01	0.41
1:2:335:LYS:HB3	1:2:381:VAL:HG13	2.02	0.41
1:2:342:LEU:HD12	1:2:372:PRO:HB2	2.02	0.41
2:3:308:GLN:HB2	4:5:209:ARG:CZ	2.51	0.41
3:4:298:THR:HG21	15:K:347:LYS:HG2	2.03	0.41
3:4:870:MET:HB3	3:4:874:LYS:HZ1	1.85	0.41
4:5:414:LEU:HD23	4:5:554:PHE:HB2	2.03	0.41
4:5:429:VAL:HA	4:5:432:VAL:HG12	2.02	0.41
4:5:683:LEU:HD23	4:5:683:LEU:HA	1.89	0.41
4:5:723:PRO:HB2	4:5:726:TRP:HE3	1.85	0.41
5:6:720:ASN:HB3	5:6:723:ILE:HB	2.02	0.41
6:7:64:MET:HE1	6:7:124:ASN:HB3	2.02	0.41
6:7:130:LYS:O	6:7:132:ILE:HD12	2.20	0.41
6:7:228:ARG:NH2	6:7:327:ILE:O	2.53	0.41
7:A:29:LEU:HG	7:A:93:ARG:CZ	2.51	0.41
12:G:507:ASN:C	12:G:509:GLU:H	2.29	0.41
12:G:648:LYS:HE3	12:G:648:LYS:HB3	1.85	0.41
12:H:833:LEU:HD23	12:H:836:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:284:ILE:HD13	15:K:284:ILE:HA	1.92	0.41
17:M:1375:LEU:HB2	17:M:1403:PRO:HG3	2.01	0.41
17:M:1580:LEU:O	17:M:1583:GLU:HB3	2.21	0.41
17:M:1799:TRP:CZ2	17:M:1803:LEU:HD21	2.55	0.41
18:N:400:VAL:HG21	18:N:424:LEU:HD11	2.03	0.41
18:N:452:ILE:O	18:N:453:SER:C	2.64	0.41
1:2:511:ILE:HG23	1:2:541:LEU:HD22	2.03	0.41
1:2:585:ILE:HG13	1:2:586:THR:N	2.35	0.41
3:4:561:ASP:OD2	3:4:670:SER:OG	2.32	0.41
4:5:421:ALA:HA	22:5:802:AGS:O1A	2.20	0.41
6:7:311:GLN:HB3	6:7:335:VAL:CG2	2.50	0.41
6:7:524:ASP:OD1	6:7:525:GLU:N	2.53	0.41
12:G:728:ILE:HB	12:G:740:ILE:HB	2.03	0.41
15:K:89:LEU:O	15:K:93:ILE:HG12	2.21	0.41
17:M:1912:MET:HG3	17:M:2064:LEU:HD21	2.03	0.41
18:N:81:GLN:O	18:N:85:LYS:HG3	2.20	0.41
1:2:435:ASP:OD1	1:2:435:ASP:N	2.54	0.41
1:2:519:LEU:HD23	1:2:519:LEU:HA	1.93	0.41
1:2:707:HIS:ND1	1:2:708:PRO:HD2	2.36	0.41
2:3:21:PHE:HE1	2:3:127:LYS:HD3	1.85	0.41
2:3:384:MET:HG3	2:3:403:ILE:O	2.20	0.41
3:4:269:ILE:HD13	3:4:269:ILE:HA	1.96	0.41
3:4:365:ILE:N	5:6:438:THR:O	2.52	0.41
3:4:522:LEU:O	3:4:526:ILE:HG12	2.20	0.41
3:4:695:PRO:HA	3:4:696:PRO:HD3	2.00	0.41
3:4:888:LYS:HA	3:4:888:LYS:HD3	1.88	0.41
5:6:321:VAL:HG21	5:6:330:PRO:HD3	2.03	0.41
6:7:682:GLY:HA2	6:7:724:LYS:HZ3	1.85	0.41
11:E:71:TYR:CE1	11:E:98:ILE:HD11	2.56	0.41
12:F:491:ARG:HE	12:F:505:VAL:HB	1.86	0.41
12:G:520:VAL:HG13	12:G:522:ARG:H	1.86	0.41
12:G:615:ILE:HG12	12:G:629:HIS:CE1	2.56	0.41
12:G:895:LEU:O	12:G:899:VAL:HG23	2.21	0.41
12:H:568:LYS:NZ	12:H:606:PRO:HD3	2.36	0.41
12:H:696:CYS:HA	12:H:705:LEU:O	2.21	0.41
12:H:748:ALA:O	12:H:751:THR:OG1	2.25	0.41
13:I:31:DG:H2'	13:I:32:DA:C8	2.56	0.41
15:K:565:PHE:HZ	15:K:602:LEU:HD21	1.85	0.41
17:M:1796:LYS:HE3	17:M:1796:LYS:HB2	1.63	0.41
18:N:37:GLY:HA3	18:N:76:GLY:HA3	2.03	0.41
18:N:94:ARG:HB3	18:N:164:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:269:THR:HG21	18:N:282:PHE:HD1	1.85	0.41
18:N:397:HIS:O	18:N:677:PRO:HD2	2.21	0.41
2:3:371:ILE:HD12	2:3:414:ALA:HB1	2.03	0.41
2:3:372:TYR:CD2	2:3:561:ILE:HG12	2.55	0.41
3:4:325:LEU:HA	3:4:325:LEU:HD12	1.87	0.41
3:4:512:VAL:HG21	3:4:746:PHE:HE2	1.85	0.41
4:5:54:ILE:HD11	4:5:98:ALA:HB1	2.02	0.41
5:6:734:LEU:HD21	5:6:742:ILE:HD11	2.01	0.41
6:7:339:LEU:O	6:7:342:SER:OG	2.23	0.41
7:A:130:TYR:O	7:A:133:GLU:HG3	2.21	0.41
12:F:560:ASP:N	12:F:560:ASP:OD1	2.54	0.41
12:F:910:LEU:HA	12:F:913:LYS:HG2	2.02	0.41
17:M:1377:GLU:C	17:M:1379:SER:H	2.29	0.41
17:M:1563:PHE:HA	17:M:1568:LYS:HB3	2.03	0.41
18:N:41:LEU:HD23	18:N:41:LEU:HA	1.92	0.41
18:N:607:LEU:HD23	18:N:607:LEU:HA	1.78	0.41
18:N:620:ARG:HA	18:N:620:ARG:HD2	1.93	0.41
18:N:633:CYS:HB3	18:N:634:PRO:HD3	2.03	0.41
3:4:573:SER:O	3:4:574:LYS:C	2.63	0.40
4:5:183:CYS:SG	4:5:240:PRO:HB2	2.61	0.40
4:5:638:LEU:HD23	4:5:638:LEU:HA	1.92	0.40
5:6:304:LEU:HD21	5:6:307:ALA:HB2	2.02	0.40
6:7:460:GLY:HA2	6:7:600:MET:O	2.21	0.40
6:7:662:GLN:HA	6:7:665:ILE:HD12	2.03	0.40
6:7:726:SER:HA	6:7:729:GLN:HG3	2.02	0.40
7:A:64:ASP:OD1	7:A:67:VAL:HG12	2.21	0.40
7:A:149:ILE:HA	10:D:137:LYS:HD2	2.03	0.40
12:G:585:PRO:O	12:G:602:GLN:NE2	2.54	0.40
15:K:732:SER:O	15:K:736:LYS:NZ	2.46	0.40
15:K:753:LEU:HD12	15:K:760:PHE:CD1	2.56	0.40
1:2:370:LYS:HD2	1:2:370:LYS:HA	1.78	0.40
1:2:384:ASN:HB2	1:2:412:ALA:HA	2.03	0.40
3:4:545:PHE:O	3:4:755:LYS:NZ	2.54	0.40
3:4:550:LYS:HD2	3:4:550:LYS:HA	1.70	0.40
3:4:801:MET:HE2	3:4:801:MET:HB2	1.97	0.40
4:5:605:TYR:CZ	4:5:609:LYS:HG3	2.56	0.40
4:5:755:LEU:HD22	4:5:760:THR:HG21	2.03	0.40
5:6:153:ILE:HD12	5:6:265:ILE:HG23	2.03	0.40
5:6:612:VAL:HG11	5:6:668:ILE:HG21	2.03	0.40
6:7:367:LYS:HD3	6:7:367:LYS:C	2.46	0.40
6:7:498:MET:SD	6:7:498:MET:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:742:VAL:HG22	12:F:756:LEU:HD22	2.02	0.40
12:G:629:HIS:O	12:G:637:SER:N	2.54	0.40
12:G:717:LYS:HE2	12:H:648:LYS:HE2	2.03	0.40
12:H:517:PHE:CG	12:H:523:PHE:HB3	2.56	0.40
15:K:700:VAL:HB	15:K:704:ALA:HB3	2.03	0.40
17:M:2045:LEU:HD23	17:M:2045:LEU:HA	1.93	0.40
17:M:2216:CYS:HB2	18:N:491:TRP:HZ2	1.86	0.40
18:N:89:GLN:CD	18:N:159:GLU:HB3	2.45	0.40
18:N:412:LYS:HB3	18:N:412:LYS:HE2	1.93	0.40
2:3:572:LEU:HB2	4:5:613:ARG:HH11	1.86	0.40
3:4:749:MET:HG3	3:4:753:TYR:CE2	2.56	0.40
5:6:532:SER:HB2	5:6:745:PRO:HG2	2.02	0.40
6:7:664:TYR:CG	6:7:689:LEU:HD11	2.56	0.40
11:E:236:VAL:O	11:E:239:GLU:HG3	2.21	0.40
11:E:390:ILE:H	11:E:390:ILE:HD12	1.86	0.40
11:E:622:ILE:HG12	11:E:630:ILE:HG22	2.02	0.40
14:J:26:DC:H2"	14:J:27:DA:C8	2.56	0.40
17:M:1503:LYS:HD2	17:M:1503:LYS:HA	1.86	0.40
18:N:394:LEU:HD23	18:N:397:HIS:CD2	2.56	0.40
2:3:115:LEU:HD22	2:3:164:HIS:HD2	1.85	0.40
2:3:253:HIS:CE1	2:3:277:ILE:HG23	2.56	0.40
3:4:180:ILE:HB	3:4:183:THR:OG1	2.21	0.40
3:4:260:GLN:O	3:4:264:TYR:N	2.37	0.40
3:4:601:LEU:HD11	3:4:631:ILE:HD12	2.04	0.40
4:5:276:MET:CE	4:5:294:ILE:HG21	2.52	0.40
5:6:776:LYS:HD2	5:6:828:TYR:CD2	2.56	0.40
6:7:284:CYS:SG	6:7:289:CYS:CB	3.10	0.40
6:7:401:VAL:HB	6:7:637:LYS:HG2	2.03	0.40
9:C:24:ILE:HA	9:C:25:PRO:HD3	1.85	0.40
12:H:624:ARG:HG3	12:H:642:GLU:OE1	2.21	0.40
12:H:711:ARG:HH21	12:H:843:ASN:HB3	1.87	0.40
15:K:341:LYS:HB3	15:K:341:LYS:HE2	1.88	0.40
17:M:1675:LEU:C	17:M:1794:MET:HE1	2.46	0.40
1:2:190:LYS:HD3	15:K:25:ALA:HA	2.03	0.40
1:2:300:PHE:CE1	1:2:317:LEU:HD23	2.56	0.40
2:3:99:SER:HB2	2:3:158:LYS:HE2	2.04	0.40
2:3:100:LEU:HD23	2:3:100:LEU:HA	1.89	0.40
2:3:446:VAL:HG21	2:3:499:LYS:HG3	2.03	0.40
3:4:367:GLU:HG3	5:6:441:ARG:HD2	2.04	0.40
3:4:622:VAL:O	3:4:623:LEU:HB2	2.22	0.40
4:5:66:GLU:OE2	4:5:142:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:146:ARG:HD3	6:7:192:PHE:CE1	2.57	0.40
9:C:162:THR:O	9:C:166:LEU:HG	2.22	0.40
11:E:130:ASN:ND2	11:E:132:ASP:OD1	2.55	0.40
18:N:228:ARG:HG3	18:N:350:GLU:HG3	2.02	0.40
18:N:268:ILE:HD13	18:N:268:ILE:HA	1.94	0.40
18:N:435:GLN:NE2	18:N:642:CYS:SG	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	658/868 (76%)	632 (96%)	26 (4%)	0	100	100
2	3	639/971 (66%)	605 (95%)	33 (5%)	1 (0%)	43	71
3	4	684/933 (73%)	646 (94%)	35 (5%)	3 (0%)	30	58
4	5	663/775 (86%)	632 (95%)	29 (4%)	2 (0%)	36	64
5	6	605/1017 (60%)	579 (96%)	26 (4%)	0	100	100
6	7	633/845 (75%)	584 (92%)	47 (7%)	2 (0%)	36	64
7	A	196/208 (94%)	181 (92%)	14 (7%)	1 (0%)	24	54
8	B	191/213 (90%)	182 (95%)	9 (5%)	0	100	100
9	C	167/194 (86%)	160 (96%)	7 (4%)	0	100	100
10	D	237/294 (81%)	229 (97%)	8 (3%)	0	100	100
11	E	560/650 (86%)	544 (97%)	16 (3%)	0	100	100
12	F	429/927 (46%)	407 (95%)	22 (5%)	0	100	100
12	G	417/927 (45%)	393 (94%)	24 (6%)	0	100	100
12	H	415/927 (45%)	385 (93%)	30 (7%)	0	100	100
15	K	644/1238 (52%)	620 (96%)	21 (3%)	3 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	L	92/317 (29%)	89 (97%)	3 (3%)	0	100	100
17	M	799/2222 (36%)	745 (93%)	52 (6%)	2 (0%)	36	64
18	N	524/689 (76%)	491 (94%)	33 (6%)	0	100	100
All	All	8553/14215 (60%)	8104 (95%)	435 (5%)	14 (0%)	44	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	5	346	VAL
15	K	417	SER
3	4	780	MET
7	A	22	ARG
17	M	1406	VAL
3	4	574	LYS
4	5	338	GLU
6	7	682	GLY
6	7	683	GLN
17	M	1820	VAL
15	K	420	ASN
3	4	882	SER
2	3	304	GLY
15	K	369	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	579/770 (75%)	572 (99%)	7 (1%)	63	75
2	3	551/835 (66%)	541 (98%)	10 (2%)	51	70
3	4	621/848 (73%)	596 (96%)	25 (4%)	28	56
4	5	605/688 (88%)	598 (99%)	7 (1%)	63	75
5	6	535/886 (60%)	532 (99%)	3 (1%)	78	81
6	7	550/753 (73%)	549 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A	182/193 (94%)	174 (96%)	8 (4%)	25	54
8	B	184/198 (93%)	182 (99%)	2 (1%)	65	76
9	C	156/173 (90%)	156 (100%)	0	100	100
10	D	234/279 (84%)	234 (100%)	0	100	100
11	E	509/586 (87%)	509 (100%)	0	100	100
12	F	382/825 (46%)	382 (100%)	0	100	100
12	G	370/825 (45%)	370 (100%)	0	100	100
12	H	368/825 (45%)	361 (98%)	7 (2%)	50	70
15	K	600/1125 (53%)	591 (98%)	9 (2%)	57	73
16	L	87/285 (30%)	87 (100%)	0	100	100
17	M	720/2014 (36%)	701 (97%)	19 (3%)	40	65
18	N	474/629 (75%)	472 (100%)	2 (0%)	84	84
All	All	7707/12737 (60%)	7607 (99%)	100 (1%)	59	74

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	183	LEU
1	2	188	ASN
1	2	189	VAL
1	2	190	LYS
1	2	193	SER
1	2	194	TYR
1	2	868	HIS
2	3	277	ILE
2	3	280	ASP
2	3	281	ASP
2	3	282	LEU
2	3	301	LEU
2	3	306	MET
2	3	309	SER
2	3	313	THR
2	3	314	LEU
2	3	315	ILE
3	4	572	THR
3	4	573	SER
3	4	574	LYS
3	4	705	VAL

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Mol	Chain	Res	Type
3	4	707	LEU
3	4	708	VAL
3	4	709	LEU
3	4	710	ASP
3	4	772	ARG
3	4	777	MET
3	4	779	LYS
3	4	780	MET
3	4	782	ASP
3	4	789	LYS
3	4	791	ILE
3	4	792	THR
3	4	796	ARG
3	4	797	GLN
3	4	802	ILE
3	4	866	SER
3	4	867	ARG
3	4	869	ILE
3	4	873	LEU
3	4	874	LYS
3	4	880	SER
4	5	212	LEU
4	5	335	SER
4	5	338	GLU
4	5	341	SER
4	5	348	MET
4	5	732	THR
4	5	735	ARG
5	6	731	ILE
5	6	736	MET
5	6	737	LYS
6	7	685	THR
7	A	14	LYS
7	A	15	ARG
7	A	18	GLN
7	A	22	ARG
7	A	25	GLN
7	A	26	ASP
7	A	28	ASN
7	A	29	LEU
8	B	158	LYS
8	B	160	LEU

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Mol	Chain	Res	Type
12	H	551	THR
12	H	553	GLN
12	H	554	ILE
12	H	555	GLN
12	H	557	ARG
12	H	629	HIS
12	H	631	SER
15	K	76	MET
15	K	192	LEU
15	K	194	ARG
15	K	197	ARG
15	K	366	ILE
15	K	368	THR
15	K	414	LEU
15	K	416	ASN
15	K	419	LEU
17	M	1408	LEU
17	M	1411	LYS
17	M	1415	THR
17	M	1416	SER
17	M	1583	GLU
17	M	1584	ARG
17	M	1796	LYS
17	M	1797	GLU
17	M	1800	ASP
17	M	1803	LEU
17	M	1804	LYS
17	M	1805	GLU
17	M	1806	ASN
17	M	1810	ASP
17	M	1812	LEU
17	M	1815	SER
17	M	1816	LEU
17	M	1818	SER
17	M	1819	TRP
18	N	25	LEU
18	N	26	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	188	ASN

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Mol	Chain	Res	Type
1	2	290	HIS
1	2	366	ASN
1	2	615	GLN
1	2	748	GLN
1	2	849	GLN
2	3	269	GLN
2	3	310	ASN
2	3	312	ASN
2	3	487	HIS
2	3	677	ASN
3	4	196	ASN
3	4	218	ASN
3	4	253	GLN
3	4	387	ASN
3	4	576	GLN
3	4	613	GLN
3	4	895	GLN
3	4	912	GLN
4	5	198	ASN
4	5	543	GLN
4	5	731	GLN
4	5	758	HIS
5	6	156	GLN
5	6	335	ASN
5	6	434	ASN
5	6	730	HIS
5	6	814	ASN
6	7	16	ASN
6	7	68	GLN
6	7	144	ASN
6	7	210	ASN
6	7	412	ASN
6	7	622	HIS
6	7	669	GLN
6	7	683	GLN
7	A	24	ASN
7	A	28	ASN
7	A	82	ASN
7	A	175	GLN
8	B	8	GLN
8	B	196	HIS
9	C	101	ASN

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Mol	Chain	Res	Type
9	C	136	ASN
10	D	225	ASN
10	D	231	HIS
11	E	26	GLN
11	E	114	GLN
11	E	133	ASN
11	E	345	ASN
11	E	352	ASN
11	E	395	ASN
12	F	548	GLN
12	F	843	ASN
12	F	852	ASN
12	F	887	HIS
12	F	891	GLN
12	F	916	ASN
12	G	573	GLN
12	G	725	ASN
12	G	916	ASN
12	H	565	ASN
12	H	680	ASN
12	H	877	GLN
12	H	916	ASN
15	K	159	HIS
15	K	454	HIS
15	K	541	ASN
15	K	658	ASN
15	K	677	ASN
17	M	1473	ASN
17	M	1587	GLN
17	M	1648	HIS
17	M	1723	ASN
17	M	1785	ASN
17	M	1865	GLN
17	M	1877	ASN
17	M	1883	GLN
17	M	1940	GLN
17	M	2022	GLN
17	M	2030	GLN
17	M	2138	ASN
17	M	2143	GLN
18	N	81	GLN
18	N	236	GLN

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Mol	Chain	Res	Type
18	N	435	GLN
18	N	594	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	ADP	3	1001	21	28,29,29	1.37	5 (17%)	43,45,45	1.81	8 (18%)
22	AGS	7	903	21	32,33,33	0.54	1 (3%)	45,52,52	0.65	1 (2%)
22	AGS	6	1103	21	32,33,33	0.59	1 (3%)	45,52,52	0.75	1 (2%)
20	ADP	2	902	21	28,29,29	1.37	5 (17%)	43,45,45	1.74	7 (16%)
22	AGS	5	802	21	32,33,33	0.73	1 (3%)	45,52,52	0.77	1 (2%)

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
20	ADP	3	1001	21	-	2/16/32/32	0/3/3/3
22	AGS	7	903	21	-	5/21/38/38	0/3/3/3
22	AGS	6	1103	21	-	4/21/38/38	0/3/3/3
20	ADP	2	902	21	-	2/16/32/32	0/3/3/3
22	AGS	5	802	21	-	7/21/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	1001	ADP	C5-C4	4.29	1.46	1.39
20	2	902	ADP	C5-C4	4.29	1.46	1.39
20	2	902	ADP	C5-N7	-2.65	1.34	1.39
20	3	1001	ADP	C5-N7	-2.61	1.34	1.39
20	2	902	ADP	C5-C6	2.37	1.47	1.41
20	3	1001	ADP	C5-C6	2.33	1.47	1.41
20	3	1001	ADP	C8-N7	2.22	1.36	1.31
20	2	902	ADP	C4-N9	-2.21	1.33	1.37
20	2	902	ADP	C8-N7	2.16	1.35	1.31
22	7	903	AGS	PG-S1G	2.13	1.95	1.90
20	3	1001	ADP	C4-N9	-2.09	1.33	1.37
22	6	1103	AGS	PG-S1G	2.07	1.95	1.90
22	5	802	AGS	PG-S1G	2.06	1.95	1.90

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	1001	ADP	C5-C4-N3	-5.80	118.73	126.72
20	2	902	ADP	C5-C4-N3	-5.51	119.13	126.72
20	3	1001	ADP	N3-C4-N9	4.69	135.14	127.17
22	5	802	AGS	PB-O3B-PG	-4.47	116.81	133.17
20	2	902	ADP	N3-C4-N9	4.39	134.64	127.17
22	6	1103	AGS	PB-O3B-PG	-4.22	117.71	133.17
20	3	1001	ADP	C2-N3-C4	3.61	120.64	111.83
22	7	903	AGS	PB-O3B-PG	-3.49	120.40	133.17
20	2	902	ADP	C2-N3-C4	3.49	120.34	111.83
20	2	902	ADP	C4-C5-N7	-3.22	106.90	110.58
20	3	1001	ADP	C4-C5-N7	-3.21	106.91	110.58
20	3	1001	ADP	N3-C2-N1	-3.16	123.80	128.58
20	2	902	ADP	N3-C2-N1	-3.10	123.89	128.58
20	3	1001	ADP	C4-N9-C8	2.77	108.65	105.74
20	2	902	ADP	C4-N9-C8	2.66	108.53	105.74
20	3	1001	ADP	C5-N7-C8	2.37	107.18	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	902	ADP	C5'-N7'-C8	2.33	107.11	103.45
20	3	1001	ADP	C3'-C2'-C1'	2.02	105.28	101.46

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	2	902	ADP	C5'-O5'-PA-O3A
20	3	1001	ADP	C5'-O5'-PA-O2A
20	3	1001	ADP	C5'-O5'-PA-O3A
22	5	802	AGS	PB-O3B-PG-O2G
22	5	802	AGS	PB-O3B-PG-O3G
22	5	802	AGS	C5'-O5'-PA-O1A
22	5	802	AGS	C5'-O5'-PA-O3A
22	6	1103	AGS	C5'-O5'-PA-O1A
22	6	1103	AGS	C5'-O5'-PA-O3A
22	7	903	AGS	PB-O3B-PG-O2G
22	7	903	AGS	PB-O3B-PG-O3G
22	7	903	AGS	C5'-O5'-PA-O1A
22	5	802	AGS	PB-O3A-PA-O1A
22	6	1103	AGS	PB-O3A-PA-O1A
20	2	902	ADP	C5'-O5'-PA-O1A
22	5	802	AGS	C5'-O5'-PA-O2A
22	6	1103	AGS	C5'-O5'-PA-O2A
22	7	903	AGS	PA-O3A-PB-O1B
22	7	903	AGS	PA-O3A-PB-O2B
22	5	802	AGS	PB-O3A-PA-O2A

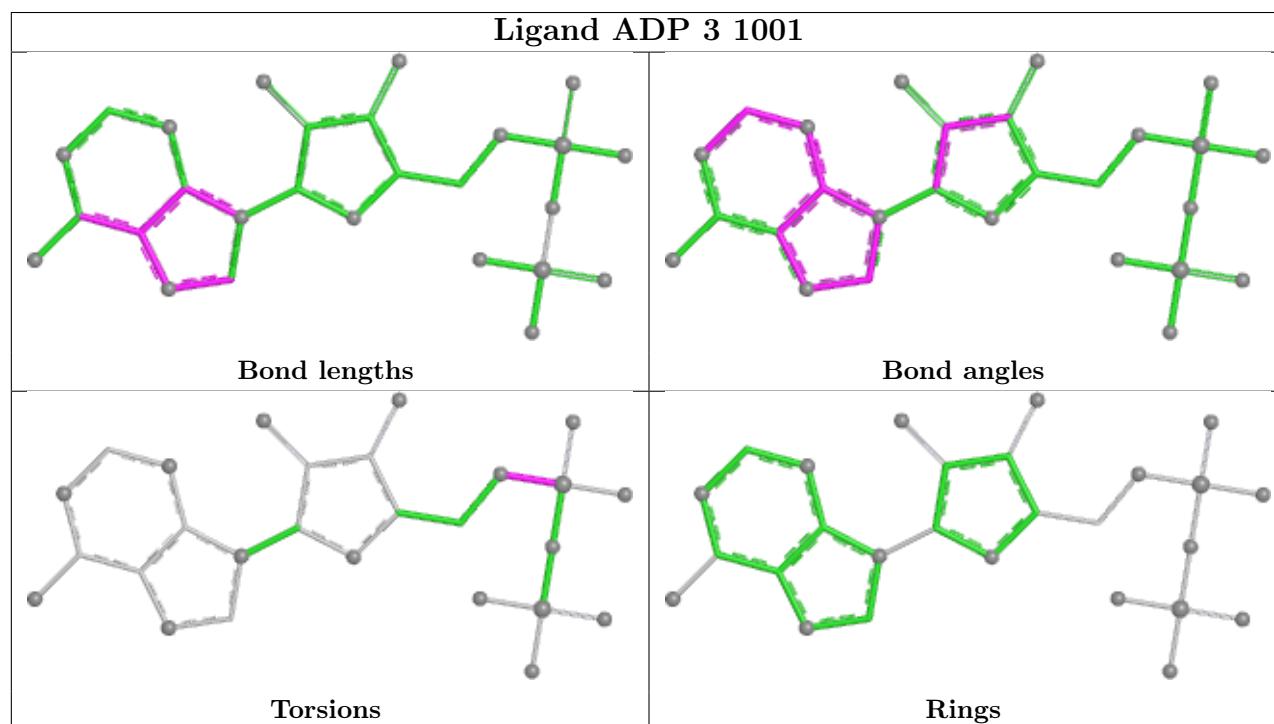
There are no ring outliers.

5 monomers are involved in 9 short contacts:

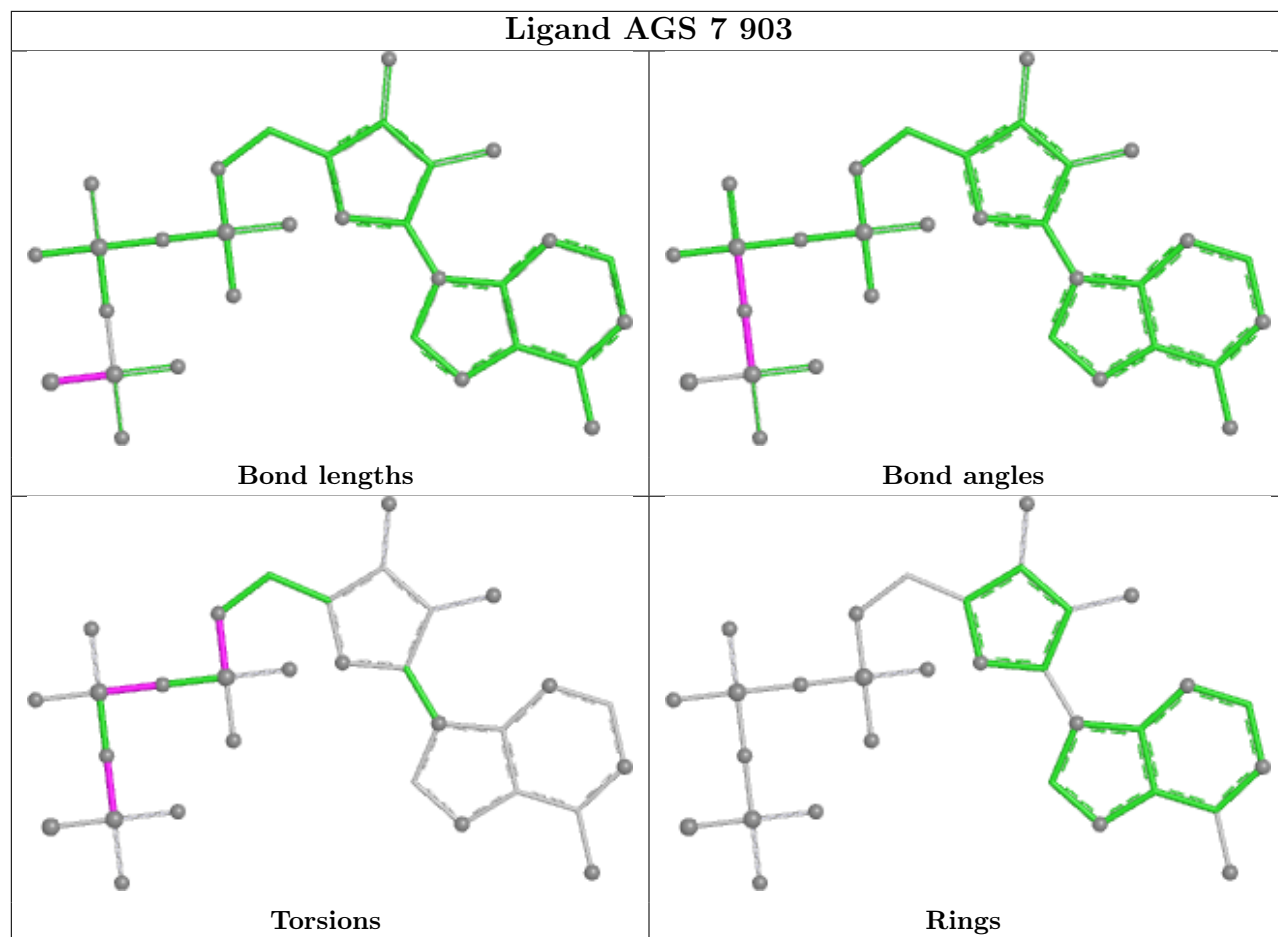
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	1001	ADP	1	0
22	7	903	AGS	1	0
22	6	1103	AGS	2	0
20	2	902	ADP	2	0
22	5	802	AGS	3	0

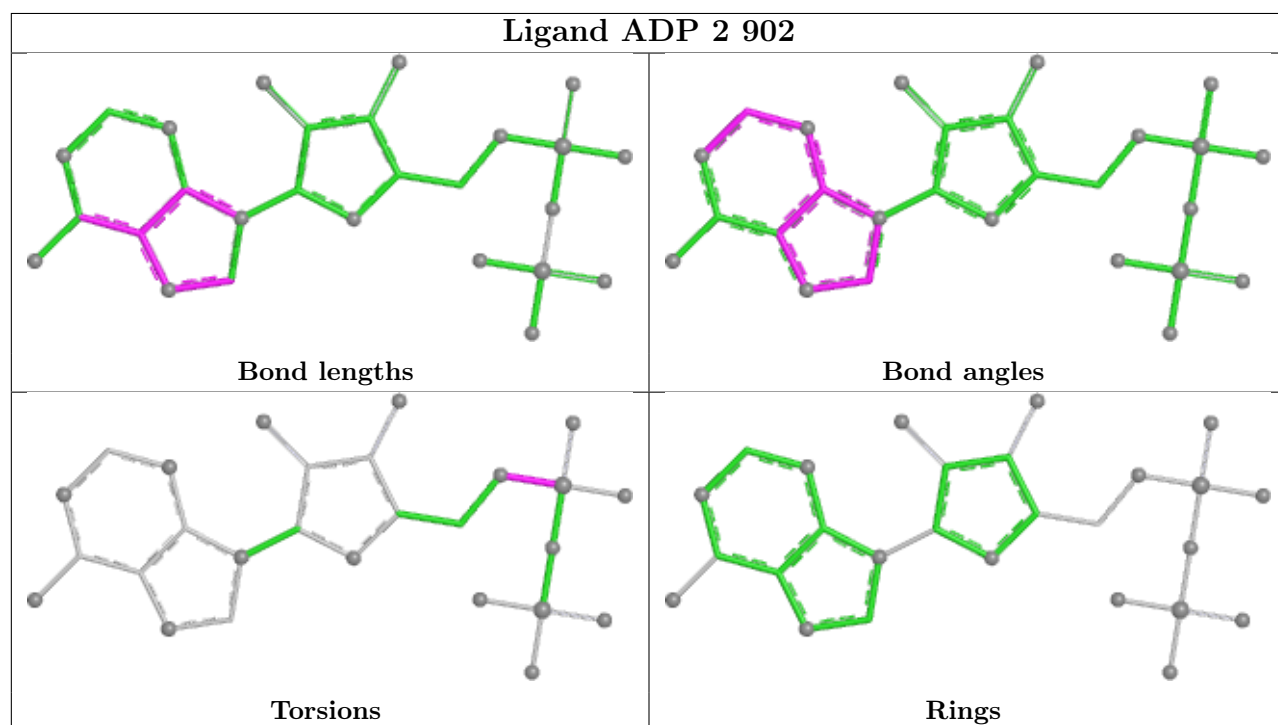
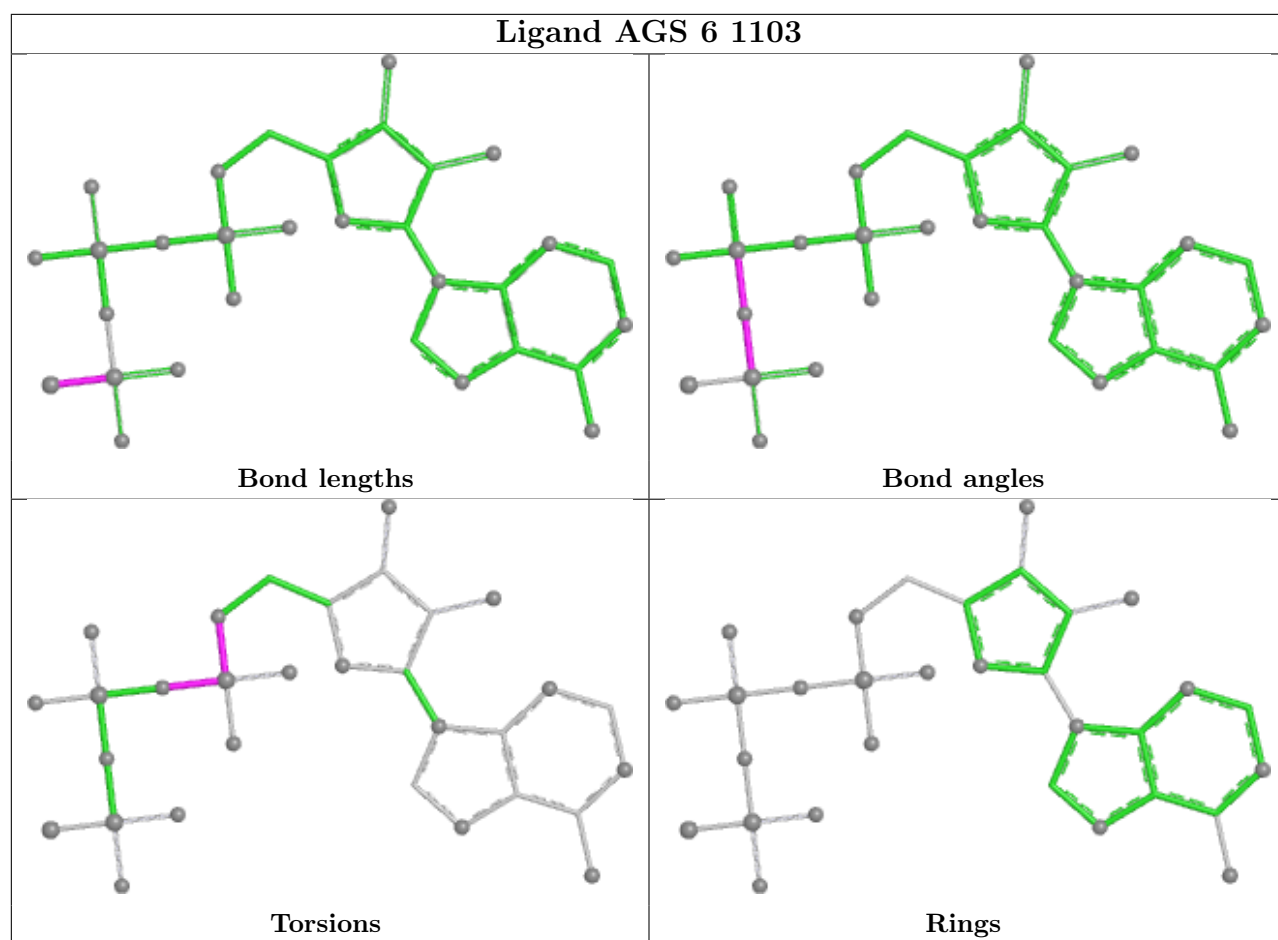
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

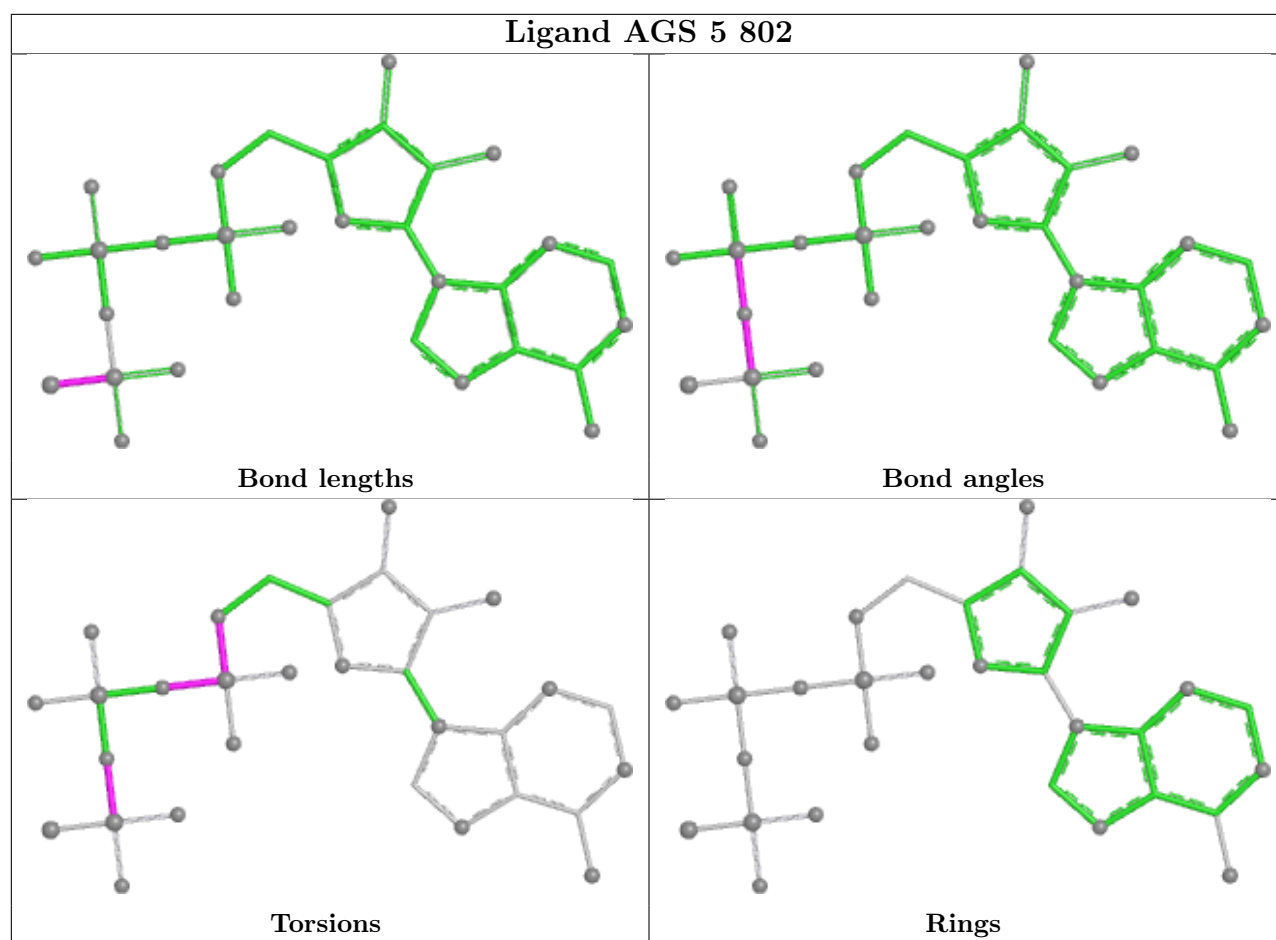
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 AGS 7 903







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.

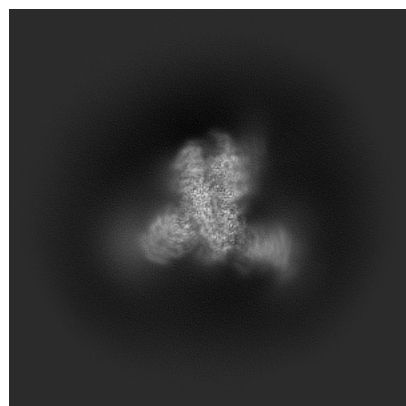
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37211. These allow visual inspection of the internal detail of the map and identification of artifacts.

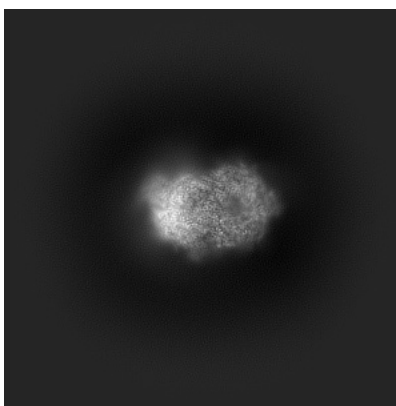
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

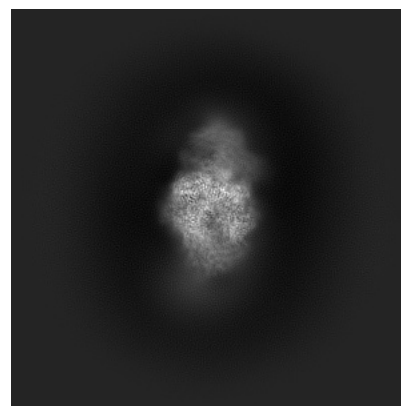
6.1.1 Primary map



X

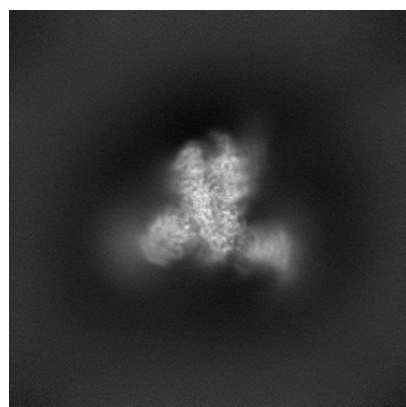


Y

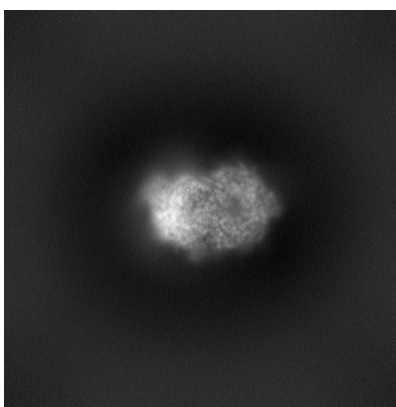


Z

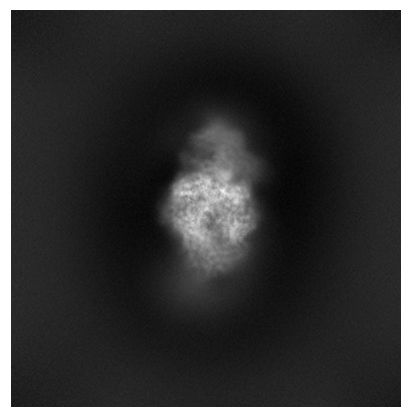
6.1.2 Raw map



X



Y

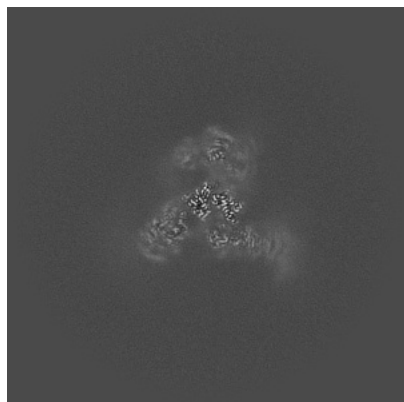


Z

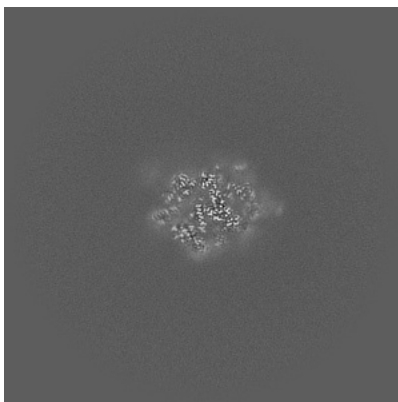
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

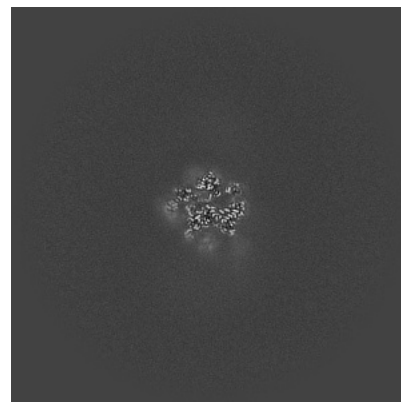
6.2.1 Primary map



X Index: 270

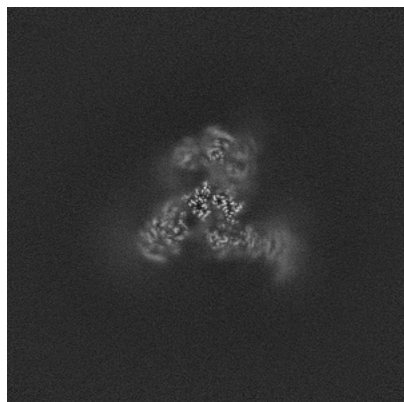


Y Index: 270

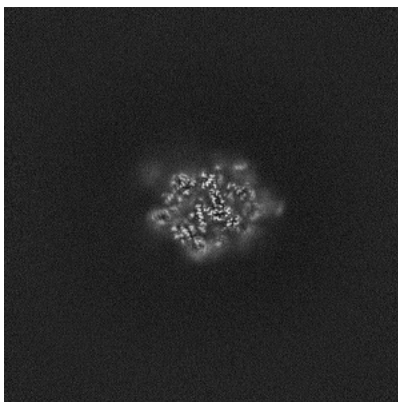


Z Index: 270

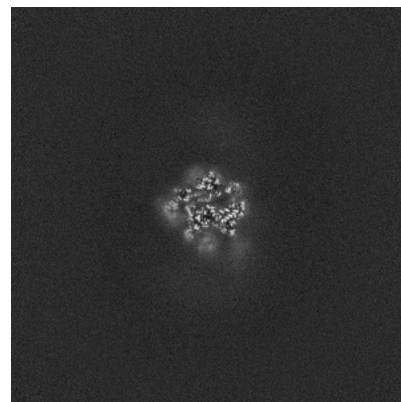
6.2.2 Raw map



X Index: 270



Y Index: 270

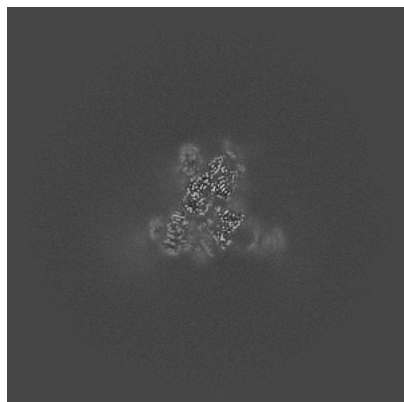


Z Index: 270

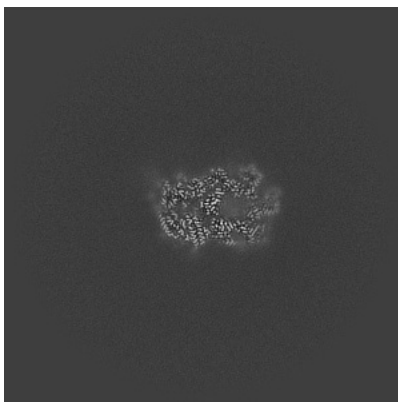
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

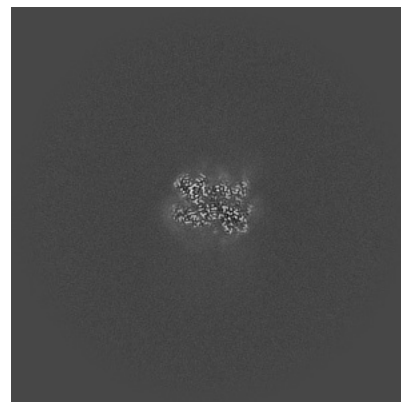
6.3.1 Primary map



X Index: 247

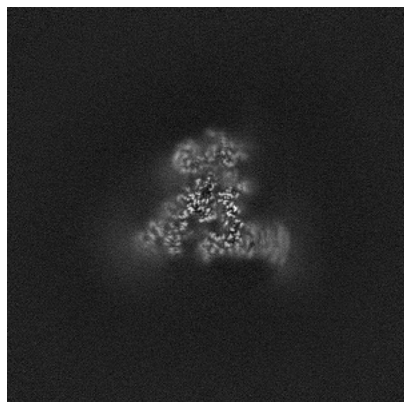


Y Index: 292

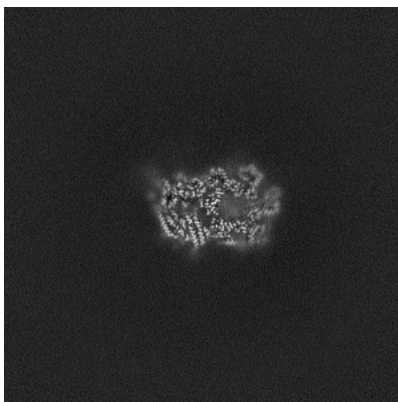


Z Index: 287

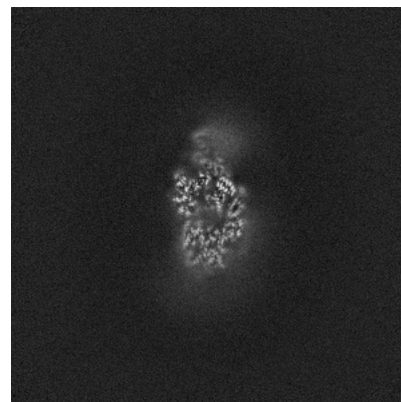
6.3.2 Raw map



X Index: 260



Y Index: 292

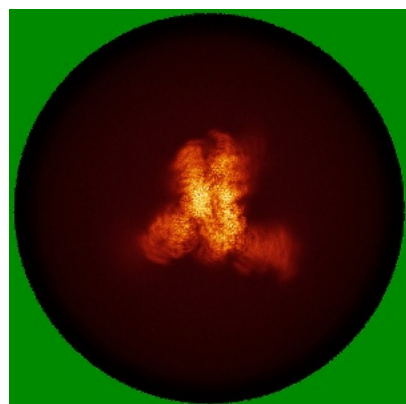


Z Index: 237

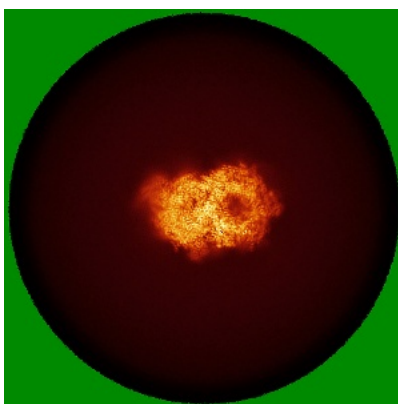
The images above show the largest variance slices of the map in three orthogonal directions.

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

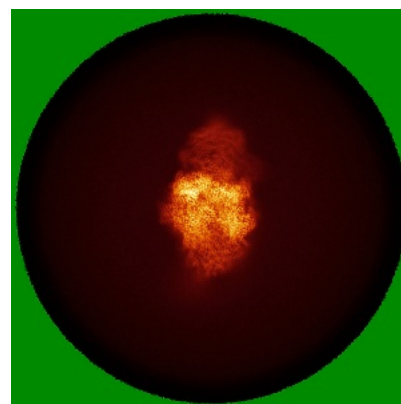
6.4.1 Primary map



X

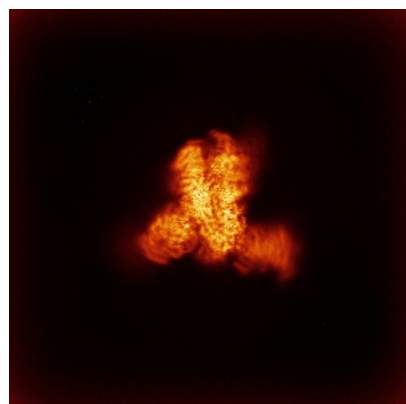


Y

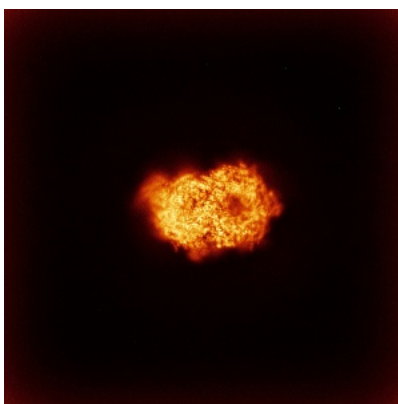


Z

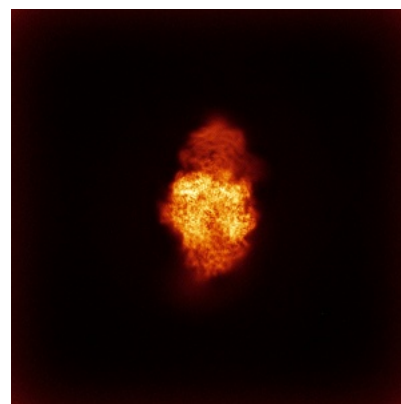
6.4.2 Raw map



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 0.35. 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.

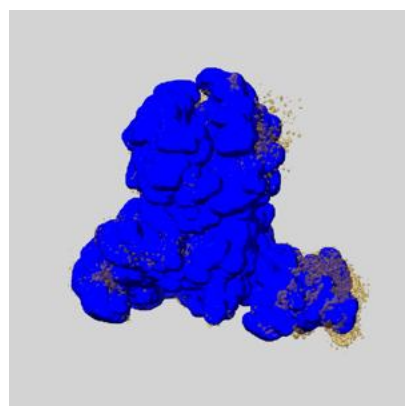
6.6 Mask visualisation [i](#)

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

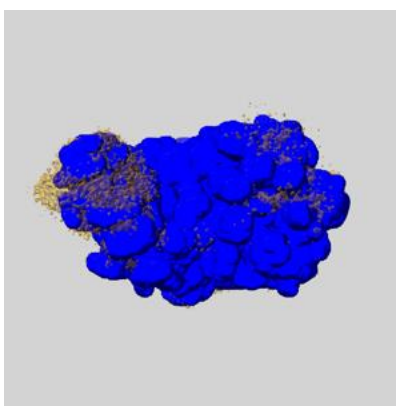
A mask typically either:

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

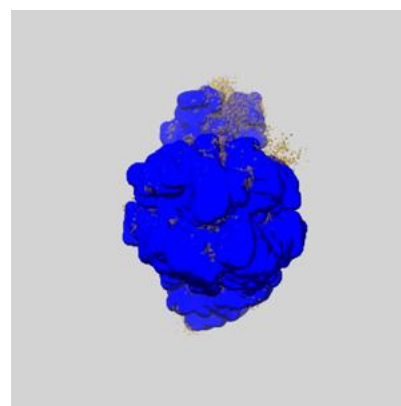
6.6.1 emd_37211_msk_1.map [i](#)



X



Y

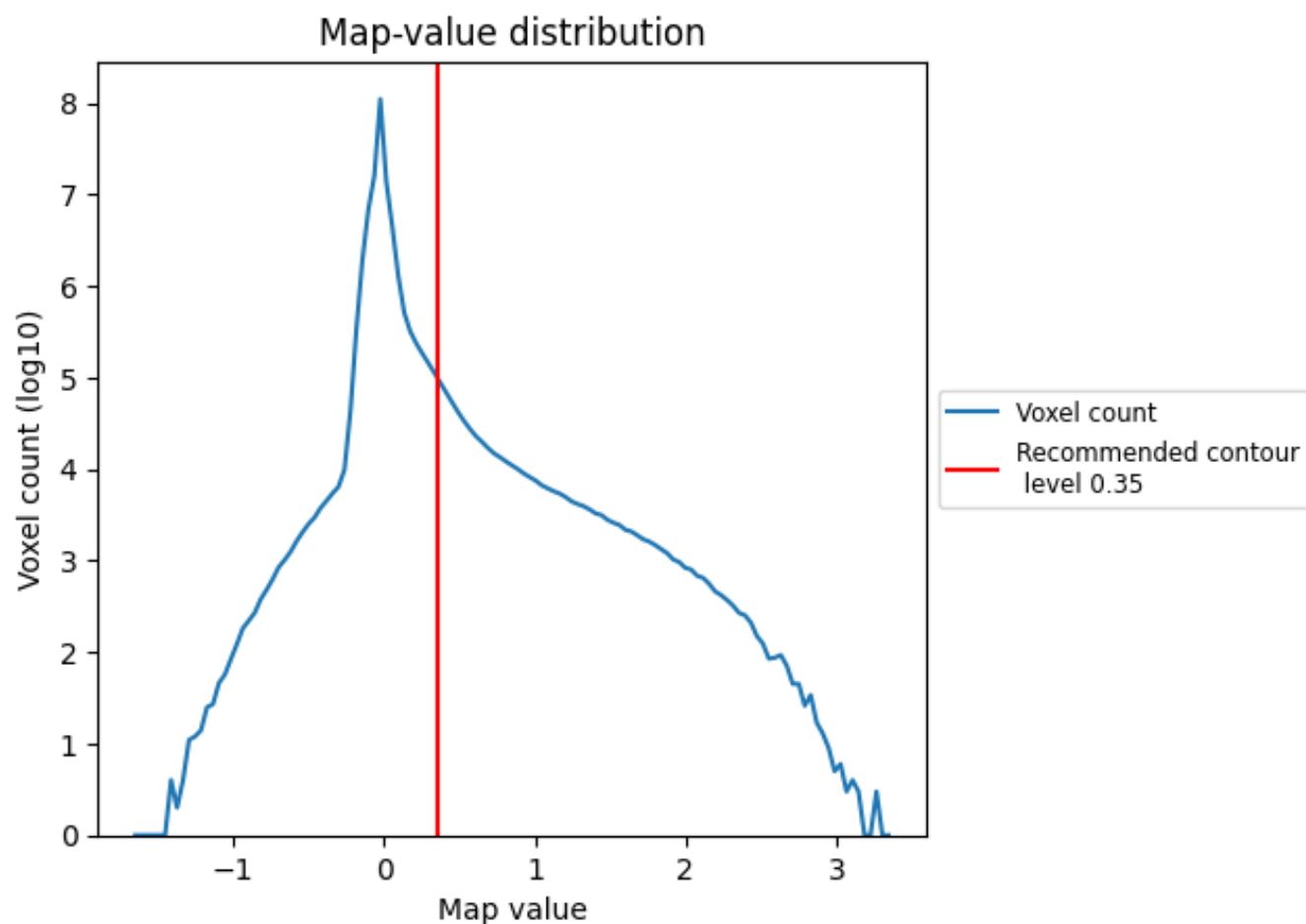


Z

7 Map analysis [i](#)

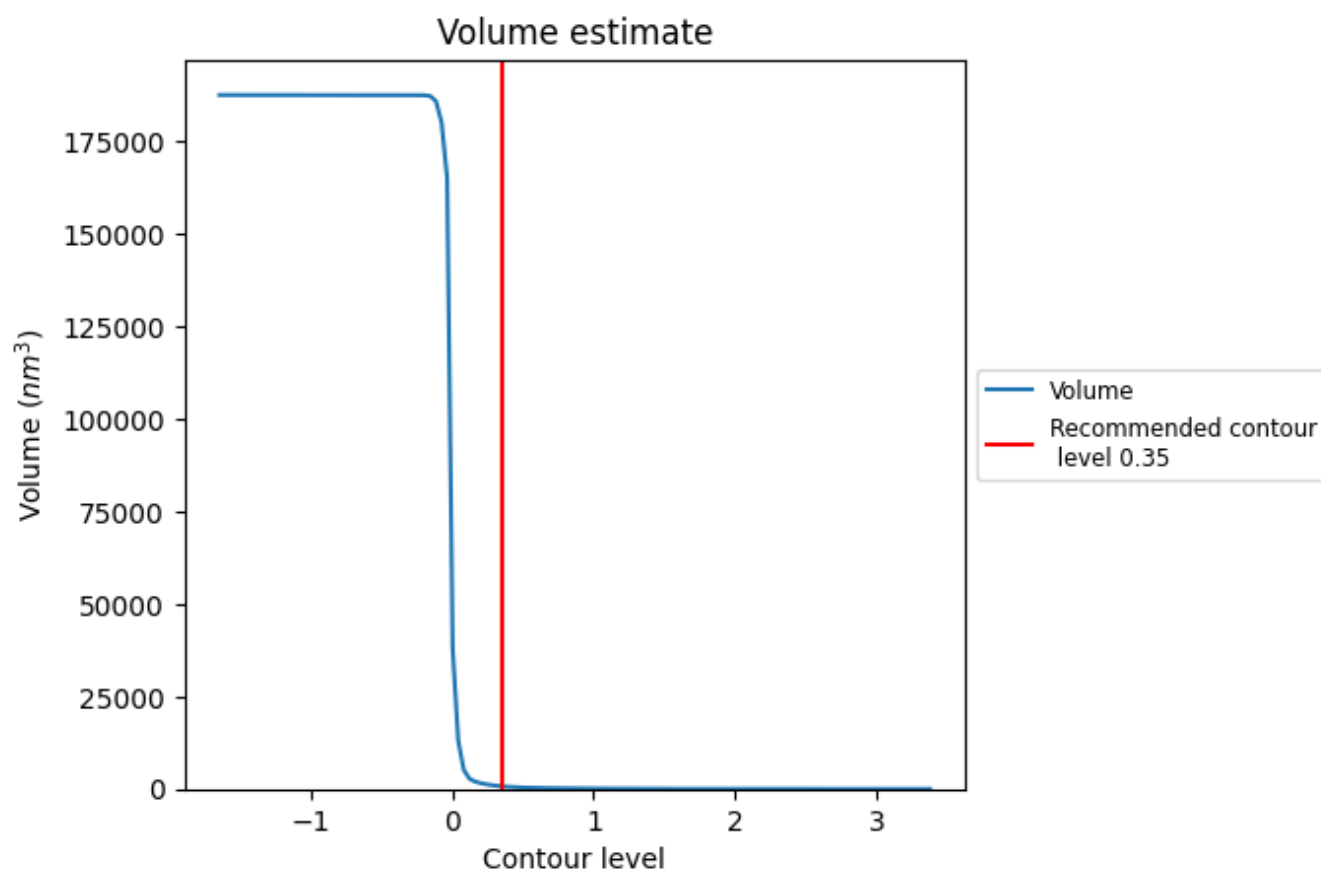
This section contains the results of statistical analysis of the map.

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.

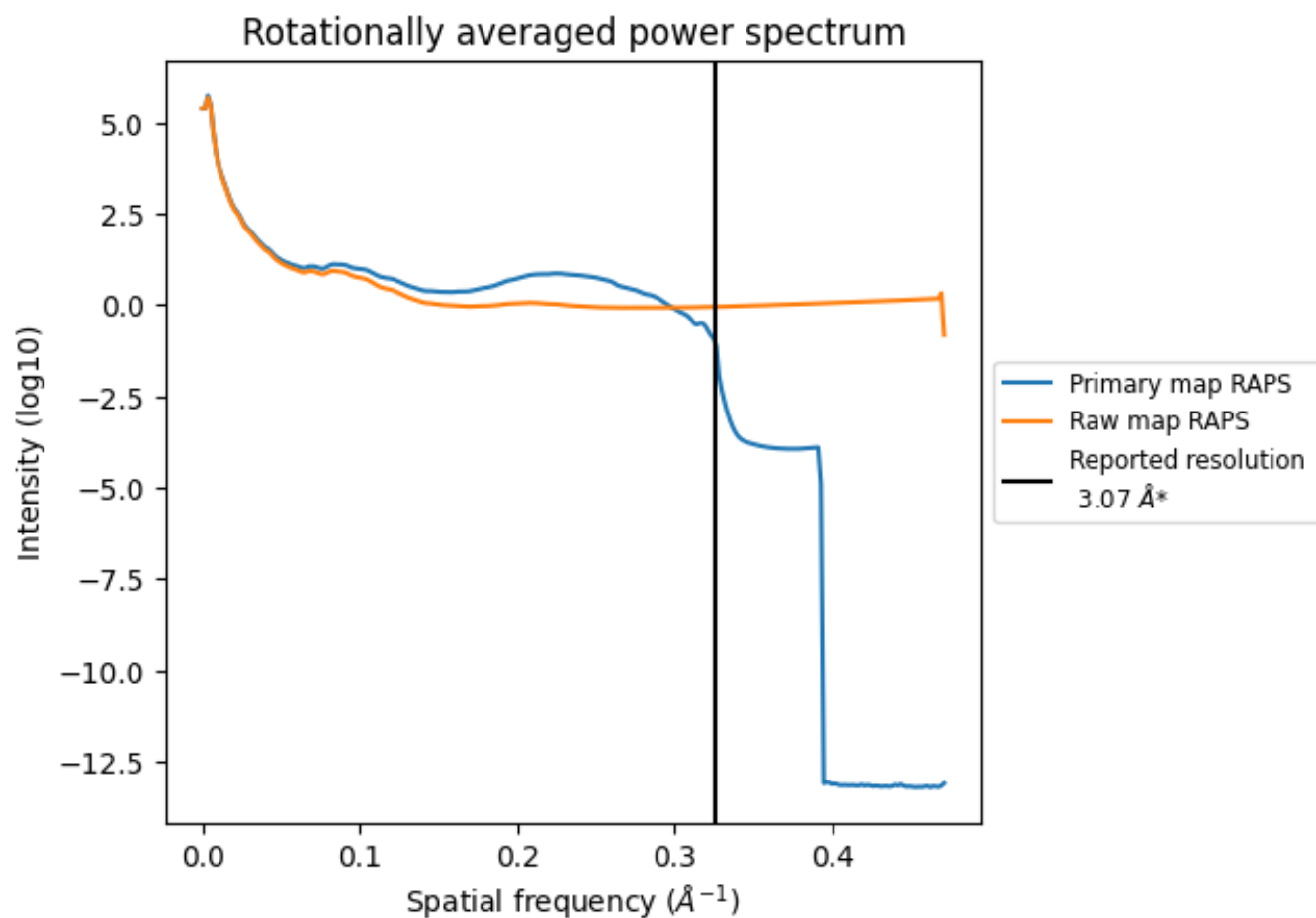
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 720 nm^3 ; this corresponds to an approximate mass of 651 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 ⓘ

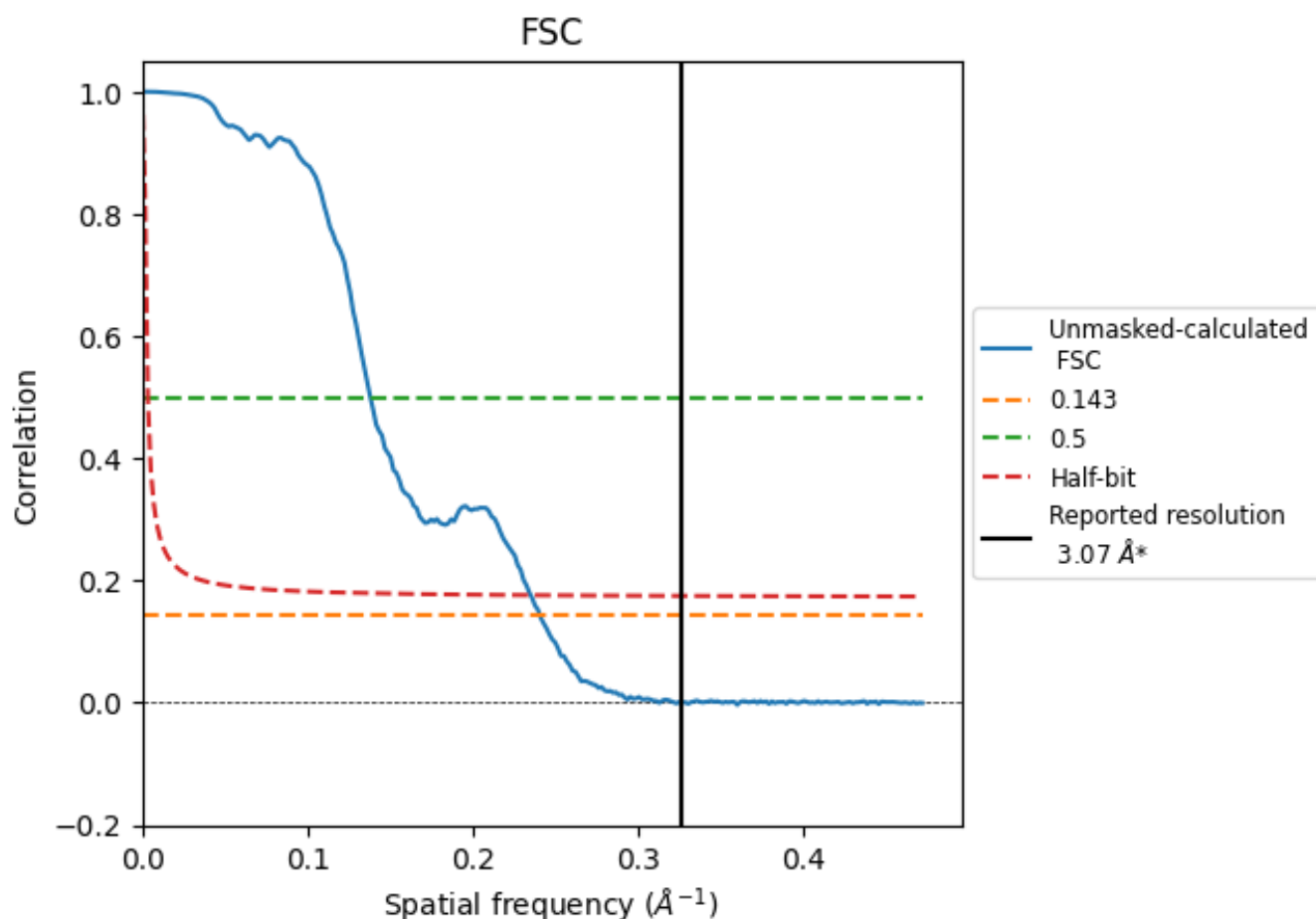


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

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 $0.326 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

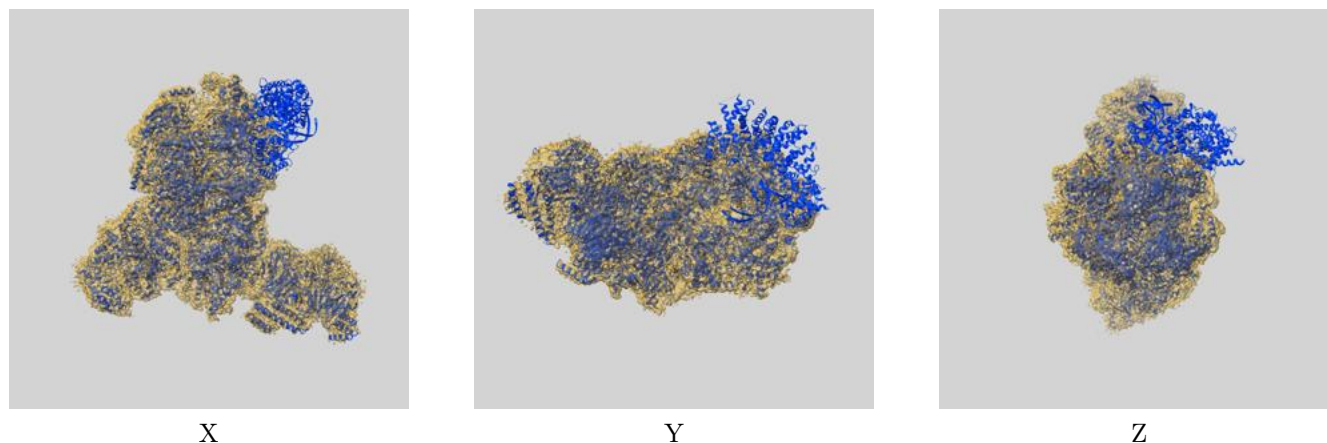
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.25	4.26

*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 4.16 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

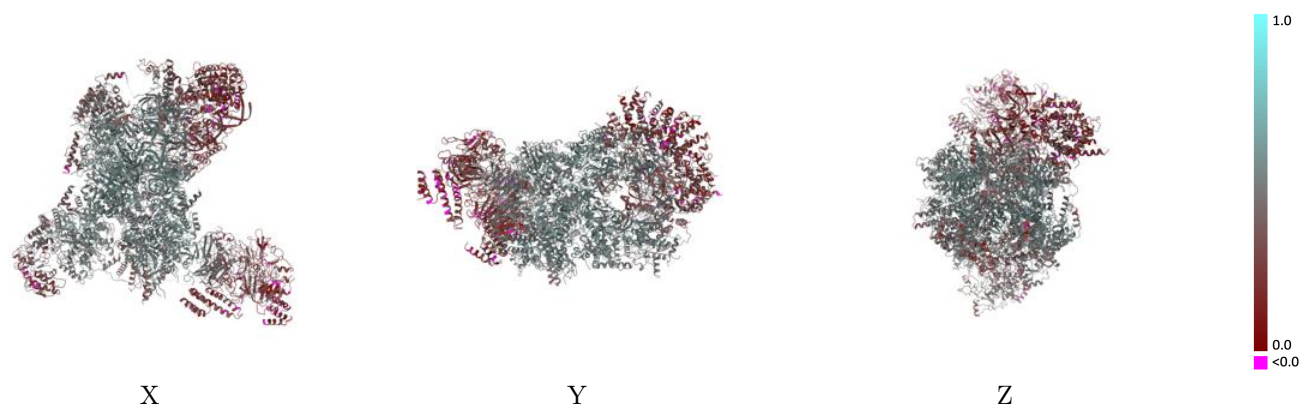
This section contains information regarding the fit between EMDB map EMD-37211 and PDB model 8KG6. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



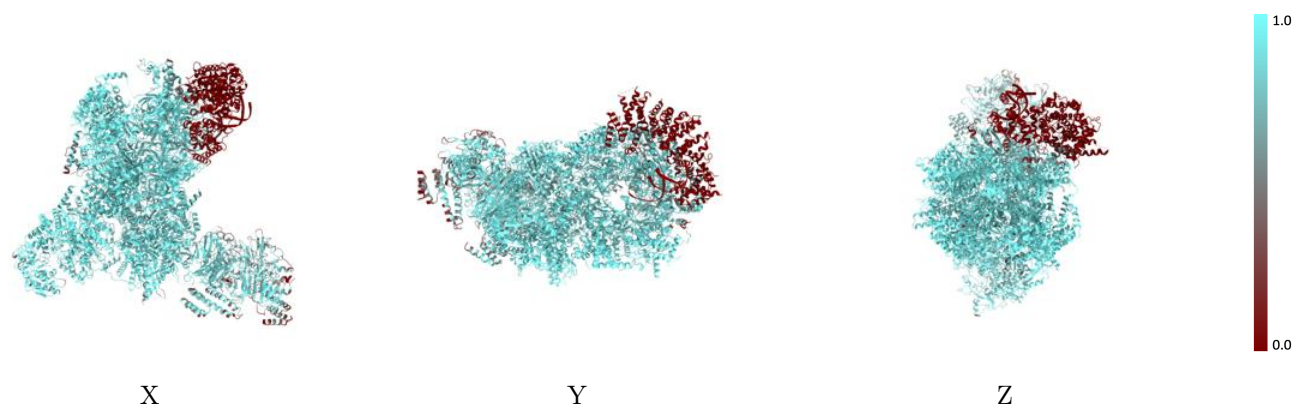
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



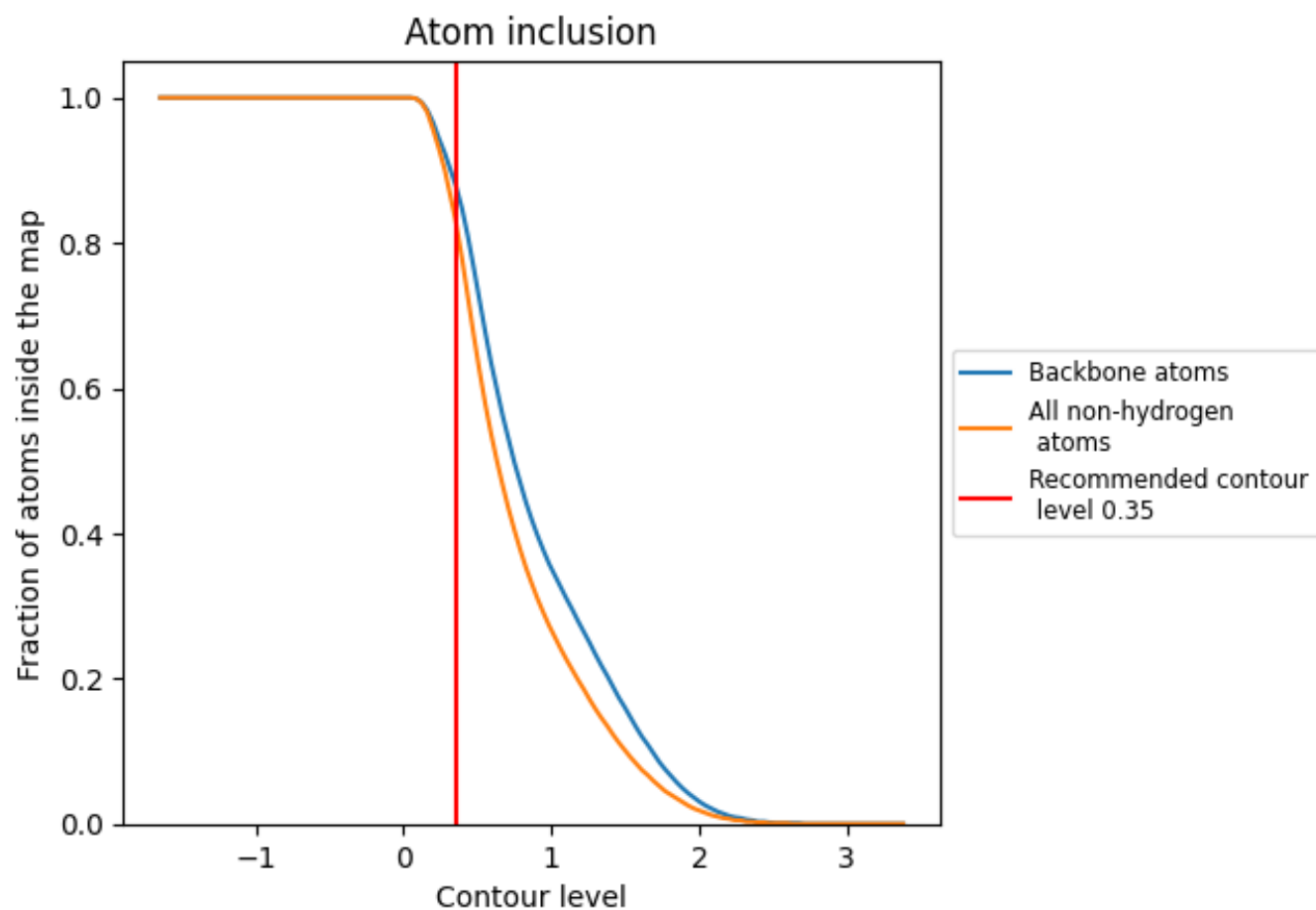
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.4370
2	 0.9600	 0.5330
3	 0.9710	 0.5320
4	 0.8990	 0.4220
5	 0.9520	 0.5310
6	 0.9560	 0.4970
7	 0.9270	 0.4400
A	 0.9430	 0.4760
B	 0.9780	 0.5500
C	 0.9720	 0.5130
D	 0.9390	 0.5040
E	 0.9510	 0.5140
F	 0.8350	 0.4000
G	 0.6860	 0.2220
H	 0.7200	 0.2670
I	 0.5890	 0.3550
J	 0.3650	 0.3120
K	 0.0790	 0.2590
L	 0.0250	 0.2590
M	 0.9310	 0.4300
N	 0.9420	 0.4680

