



## Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 04:07 pm BST

PDB ID : 7Z88  
EMDB ID : EMD-14546  
Title : DNA-PK in the intermediate state  
Authors : Liang, S.; Blundell, T.L.  
Deposited on : 2022-03-16  
Resolution : 3.33 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

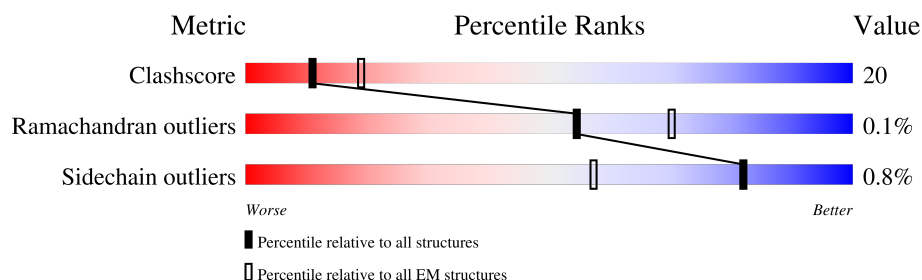
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.33 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4128	<div> <div>15%</div> <div>50%</div> <div>36%</div> <div>13%</div> </div>
2	B	609	<div> <div>10%</div> <div>46%</div> <div>33%</div> <div>20%</div> </div>
3	C	732	<div> <div>43%</div> <div>53%</div> <div>37%</div> <div>10%</div> </div>
4	D	26	<div> <div>12%</div> <div>50%</div> <div>50%</div> </div>
5	E	26	<div> <div>15%</div> <div>46%</div> <div>54%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 38754 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-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3599	Total	C	N	O	S	0	0
			28443	18257	4823	5179	184		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3937	2525	667	728	17		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	661	Total	C	N	O	S	0	0
			5274	3372	882	994	26		

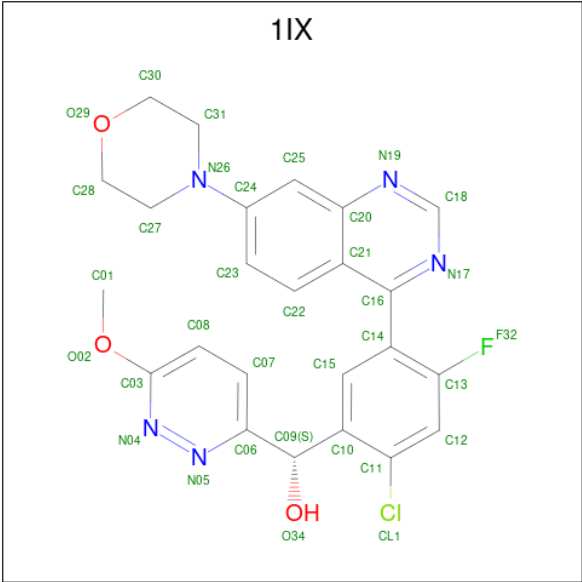
- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	26	Total	C	N	O	P	0	0
			526	250	92	158	26		

- Molecule 5 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	26	Total	C	N	O	P	0	0
			540	254	106	154	26		

- Molecule 6 is ( {S} )-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl ]-(6-methoxypyridazin-3-yl)methanol (three-letter code: 1IX) (formula: C<sub>24</sub>H<sub>21</sub>ClFN<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	Cl	F	N	O	0
			34	24	1	1	5	3	

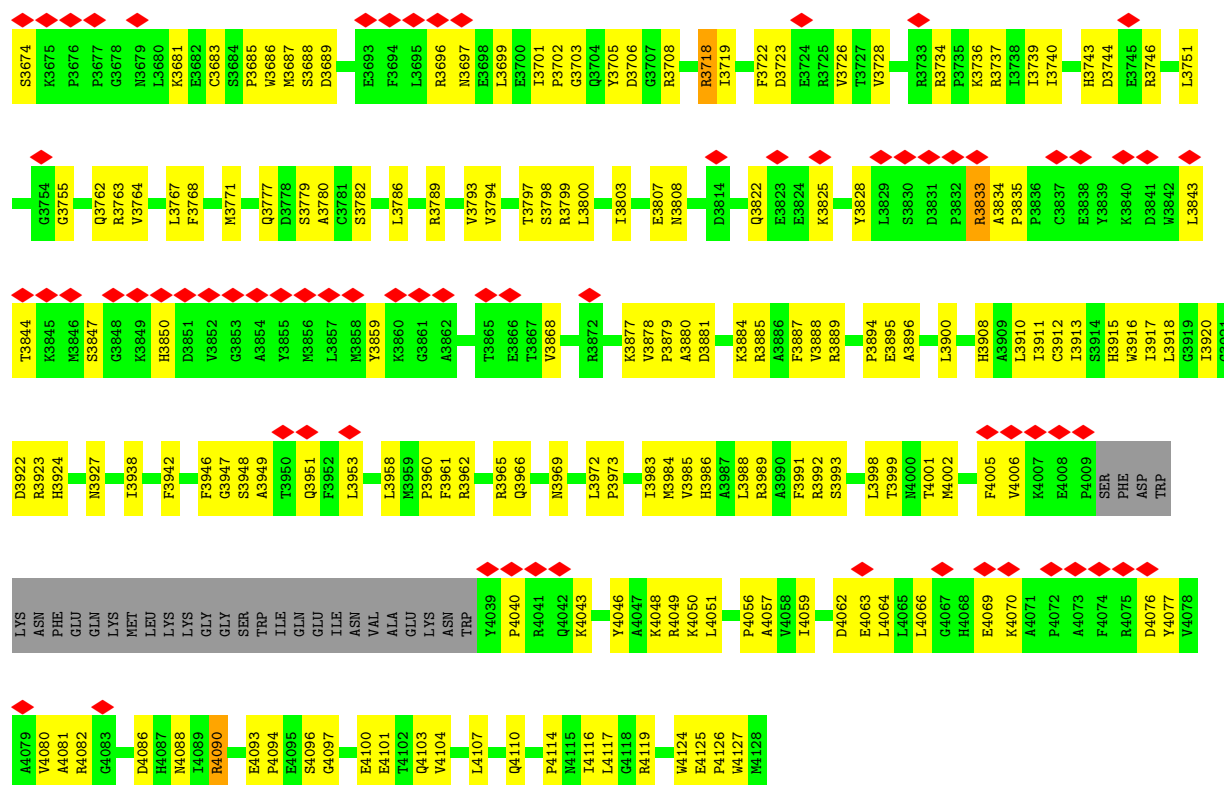




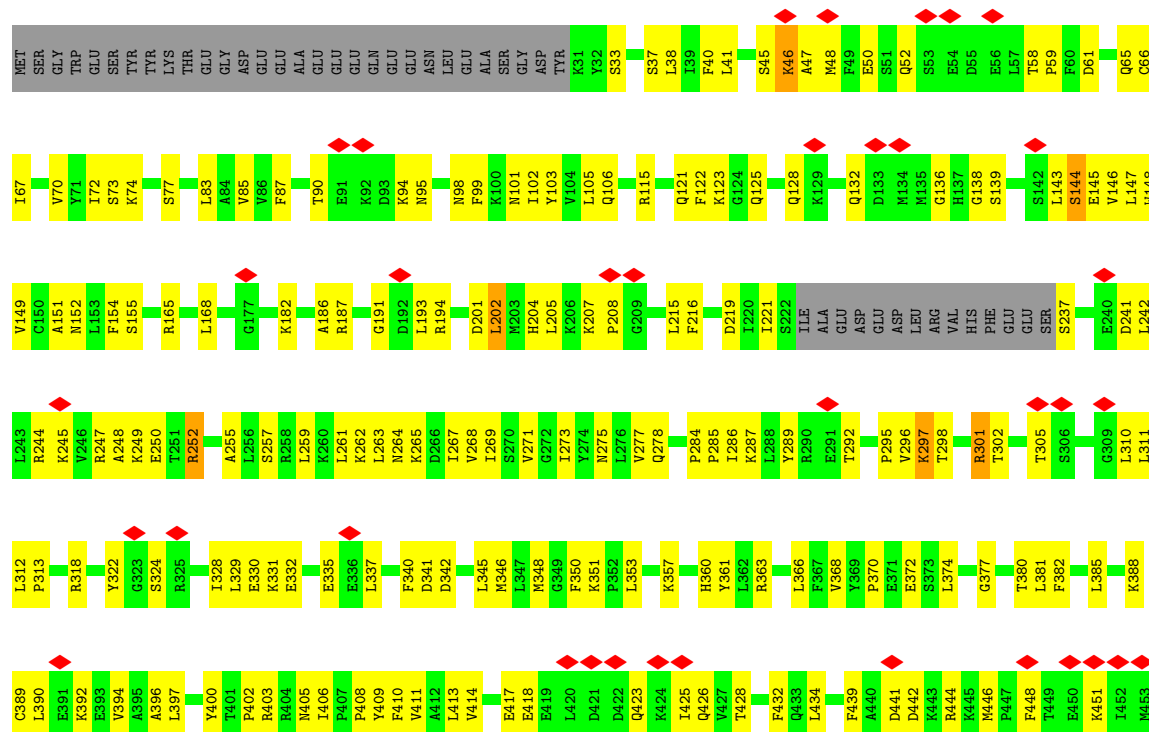
SER	VAL	ILE	N2574	Y2484	C2403	V2330	L2249	Y2160	VAL	GLU	C1947	T1965	S1800	L1717
GLY	ARG	ARG	P2575	R2485	R2404	M2331	S2250	S2166	HIS	ALA	A1945	T1968	S1801	I1718
PRO	ALA	ALA	M2576	D2486	V2405	E2332	P2252	L2251	ASP	ALA	I1949	T1969	Y1801	A1720
ASP	GLN	GLN	P2577	P2487	T2409	R2333	L2255	L2167	VAL	ASN	S1950	G1972	M1802	H1721
PHE	GLN	GLN	P2578	E2488	E2410	R2334	L2256	L2168	LEU	GLY	V1951	I1952	M1803	F1722
GLY	HIS	HIS	P2579	S2489	L2411	M2335	L2257	L2169	E2082	SER	K1875	K1876	F1805	P1723
LYS	ASP	ASP	E2490	E2490	Y2412	R2336	F2257	Q2170	L2083	ASP	I1876	I1877	M1806	M1724
ARG	PHE	PHE	T2491	T2491	Q2413	L2337	E2258	Q2171	E2084	PRO	V1879	V1880	Q1725	Q1726
LEU	THR	THR			Q2414	E2338	K2259	E2175	E2085	SER	L1959	L1960	S1726	S1727
CYS	LEU	LEU			S2417	L2341	F2260	N2176	M2086	TYR	K1886	K1887	D1808	R1727
PHE	LEU	LEU			K2418	C2342	P2265	N2177	D2087	MET	Y1881	Y1882	P1810	E1728
LEU	THR	THR			L2419			G2178	E2088	SER	L1884	L1885	P1811	F1729
PRO	GLN	GLN			F2420	V2345	K2268	G2179	L2089	SER	P1963	P1964	L1812	
GLY	THR	THR			V2421	A2346			R2090	SER	F1965	F1966	S1813	
ASP	ALA	ALA			Q2422				H2091	LEU	K1886	K1887	F1814	
GLU	ASP	ASP			V2423	K2350	V2272	I2182	E2092	SER	D1887	D1888	T1815	
VAL	GLY	GLY			V2424	Q2351	G2273	H2183	C2093	TYR	Y1890	Y1891	R1816	
ASP	ARG	ARG			H2426	H2352	L2275	Y2184	A2094	LEU	A1971	A1972	Q1817	
ASN	SER	SER			R2427	E2357	L2276	M2185	E2095	ASP	K1892	K1893	F1735	
VAL	PHE	PHE				D2358	L2277	V2186	P2096	ASP	H1890	H1891	R1736	
GLY	THR	THR				K2359		V2190	L2097	GLU	I1896	I1897	Y1739	
LYS	ASP	ASP				F2360	V2280		T2098	THR	A1973	A1974	V1740	
ALA	LEU	LEU				L2361	R2281	I2183	C2102	GLU	K1973	K1974	F1746	
GLY	THR	THR				V2362	L2282	Y2184	H2105	VAL	E1979	E1980	L1750	
ARG	GLY	GLY				C2363	P2283	G2198	R2106	GLN	Q1898	Q1899	L1828	
THR	LEU	LEU				L2364	L2284		S2107	GLN	F1900	F1901	H1829	
ASP	PRO	PRO				N2365	P2286	T2203	L2108	TYR	H1902	H1903	C1831	
LEU	LEU	LEU				V2367	P2287	G2204	GLY	VAL	I1905	I1906	S1832	
PRO	PRO	PRO				T2368	L2288	V2205	PRO	GLN	K1985	K1986	D1834	
PHE	PHE	PHE				K2369	P2289	K2207	GLN	SER	R1987	R1988	L1758	
VAL	VAL	VAL				S2370		D2208	GLN	TYR	E1907	E1908	L1759	
GLU	GLU	GLU				F2371	T2294	E2209	GLY	SER	L1911	L1912	L1836	
GLN	GLN	GLN				P2372		V2210	GLY	SER	N1989	N1990	R1837	
ALA	ALA	ALA				L2373	E2298	L2211	GLU	TYR	F1991	F1992	E1838	
SER	SER	SER				A2374	Y2299	L2212	ASP	SER	T1914	T1915	F1839	
PRO	PRO	PRO				D2376	A2302	L2216	VAL	SER	L1916	L1917	Q1770	
GLY	GLY	GLY				R2377	L2303		SER	GLN	I1918	I1919	S1841	
ASP	ASP	ASP				F2378	M2306	M2220	PRO	ASP	K1917	K1918	Q1771	
LEU	LEU	LEU				M2379	N2307		PRO	PRO	V1994	V1995	H1772	
LEU	LEU	LEU					L2307	F2224	ARG	ARG	GLU	GLU	V1773	
THR	THR	THR					S2308	H2225	THR	THR	D1921	D1922	E1776	
THR	THR	THR					F2309	D2226	PRO	PRO	F1923	F1924	L1777	
GLN	GLN	GLN					R2310	K2227	ALA	ALA	A1922	A1923	F1778	
THR	THR	THR					R2311	R2228	THR	THR	T1924	T1925	Q1779	
ALA	ALA	ALA					Y2312		ARG	ARG	L1924	L1925	S1780	
GLY	GLY	GLY					V2313	H2233	PHE	PHE	G1929	G1930	S1781	
ARG	ARG	ARG					E2314		ARG	ARG	L1932	L1933	R1854	
SER	SER	SER					V2315	T2237	ARG	ARG	Q1932	Q1933	F1782	
LEU	LEU	LEU					V2316	L2238	ARG	ARG	L1933	L1934	R1783	
GLY	GLY	GLY					V2317	K2239	GLN	GLN	I1933	I1934	R1784	
GLY	GLY	GLY					A2317		GLN	GLN	R1936	R1937	I1785	
ALA	ALA	ALA					A2318	V2242	ARG	ARG	R1937	R1938	A1786	
GLY	GLY	GLY					V2322		ASP	ASP	L1859	L1860	N1857	
VAL	VAL	VAL					K2246	K2247	THR	THR	E1859	E1860	R1787	
ALA	ALA	ALA					D2247	C2248	THR	THR	S1861	S1862	R1788	
GLN	GLN	GLN					L2327				Y1945	Y1946	D1864	

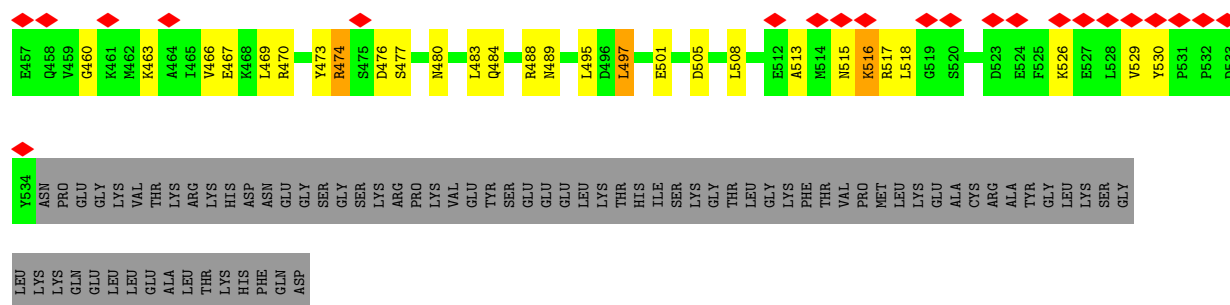




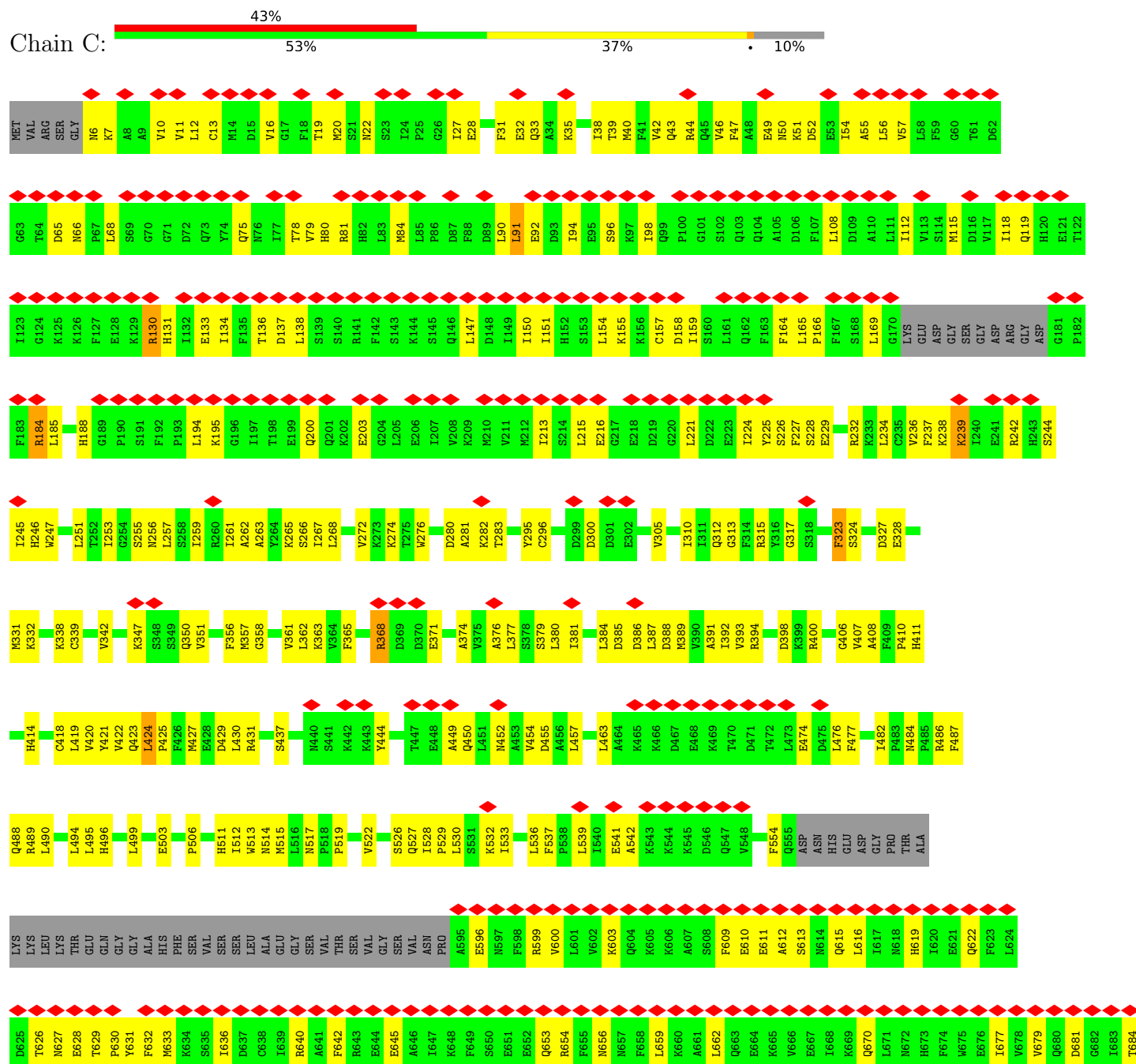


• Molecule 2: X-ray repair cross-complementing protein 6



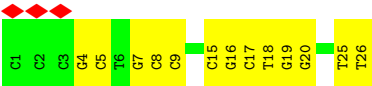


• Molecule 3: X-ray repair cross-complementing protein 5





• Molecule 4: DNA (26-MER)



• Molecule 5: DNA (26-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190498	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 ( $e^-/\text{\AA}^2$ )	47.22	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.648	Depositor
Minimum map value	-2.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	456.4, 456.4, 456.4	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1IX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.30	0/29016	0.53	1/39251 (0.0%)
2	B	0.32	0/4014	0.60	3/5408 (0.1%)
3	C	0.27	0/5374	0.50	2/7246 (0.0%)
4	D	0.56	0/587	0.91	0/902
5	E	0.56	0/607	0.86	0/936
All	All	0.31	0/39598	0.55	6/53743 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	2
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	424	LEU	CA-CB-CG	5.78	128.60	115.30
2	B	385	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	204	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	497	LEU	CA-CB-CG	5.34	127.57	115.30
2	B	202	LEU	CA-CB-CG	5.18	127.22	115.30
3	C	91	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	PRO	Peptide
1	A	1175	HIS	Peptide
1	A	3025	PRO	Peptide
1	A	3462	ARG	Peptide
2	B	252	ARG	Peptide
2	B	474	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28443	0	28622	1176	0
2	B	3937	0	4013	194	0
3	C	5274	0	5275	252	0
4	D	526	0	293	12	0
5	E	540	0	291	14	0
6	A	34	0	0	0	0
All	All	38754	0	38494	1577	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 20.

All (1577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:TYR:CE2	3:C:274:LYS:HG3	1.64	1.32
3:C:323:PHE:CE1	3:C:328:GLU:HB3	1.82	1.13
2:B:322:TYR:HE2	3:C:274:LYS:CG	1.68	1.05
1:A:2225:HIS:ND1	1:A:2226:PRO:HD2	1.72	1.04
1:A:3190:LEU:HB3	1:A:3235:LYS:HZ2	1.27	0.98
1:A:2458:VAL:HG21	1:A:2476:ILE:HD11	1.49	0.95
1:A:1023:SER:HA	1:A:1026:ARG:HE	1.35	0.92
1:A:1711:ARG:HE	1:A:1757:MET:HB3	1.35	0.91
1:A:2971:GLN:HA	1:A:2974:GLU:HG2	1.54	0.89
1:A:2548:PRO:HG3	1:A:2846:THR:HG22	1.54	0.89
1:A:2280:VAL:HG23	1:A:2285:LEU:HD12	1.54	0.89
2:B:322:TYR:CE2	3:C:274:LYS:NZ	2.43	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2402:LEU:HB2	1:A:2438:ILE:HG22	1.57	0.85
1:A:2421:VAL:HG13	1:A:2457:PRO:HG3	1.58	0.85
1:A:3630:ARG:NH1	1:A:3683:CYS:SG	2.50	0.85
3:C:532:LYS:O	3:C:536:LEU:HB2	1.77	0.85
2:B:322:TYR:CD2	3:C:274:LYS:NZ	2.45	0.84
1:A:3424:LEU:HD21	1:A:3443:PRO:HD3	1.59	0.84
1:A:752:LEU:HD23	1:A:792:ILE:HD11	1.60	0.82
1:A:4064:LEU:HD21	1:A:4077:TYR:HB3	1.61	0.82
1:A:1204:PRO:HB2	1:A:1275:THR:HG23	1.61	0.81
1:A:207:GLN:HE22	1:A:216:LYS:HB2	1.46	0.81
1:A:160:LEU:HD12	2:B:312:LEU:HD11	1.61	0.81
1:A:1892:LYS:HE2	1:A:1905:ILE:HG23	1.62	0.81
1:A:3681:LYS:HE3	1:A:3688:SER:HA	1.62	0.81
1:A:873:VAL:HG13	1:A:874:THR:H	1.46	0.80
1:A:3307:LEU:HD23	1:A:3330:LEU:HD23	1.62	0.80
1:A:3176:MET:SD	1:A:3249:GLN:NE2	2.55	0.79
2:B:144:SER:HB3	2:B:186:ALA:HA	1.63	0.79
1:A:380:ASP:HA	1:A:383:PHE:HB3	1.63	0.79
1:A:3190:LEU:HB3	1:A:3235:LYS:NZ	1.96	0.79
2:B:202:LEU:HD23	2:B:221:ILE:HD12	1.63	0.79
2:B:480:ASN:HD22	2:B:483:LEU:HB2	1.47	0.79
3:C:323:PHE:CE1	3:C:328:GLU:CB	2.66	0.79
2:B:48:MET:HA	2:B:59:PRO:HG2	1.63	0.78
1:A:3173:MET:SD	1:A:3782:SER:OG	2.41	0.78
3:C:56:LEU:H	3:C:81:ARG:HB3	1.49	0.78
1:A:3389:VAL:HG21	1:A:3416:LEU:HD22	1.63	0.78
1:A:1767:CYS:SG	1:A:1823:SER:OG	2.42	0.77
3:C:323:PHE:CD1	3:C:328:GLU:HB3	2.20	0.77
1:A:3718:ARG:H	1:A:3743:HIS:CD2	2.01	0.77
1:A:2177:ASN:HB3	1:A:2182:ILE:HG23	1.64	0.77
2:B:322:TYR:HE2	3:C:274:LYS:HG3	0.74	0.76
1:A:2459:VAL:HG21	1:A:2501:LEU:HD21	1.67	0.76
2:B:257:SER:HB3	2:B:259:LEU:HD13	1.66	0.76
1:A:1582:LEU:HG	1:A:1593:VAL:HG23	1.66	0.76
1:A:1437:TYR:HA	1:A:1445:ARG:HH22	1.51	0.75
1:A:1675:TYR:HD1	1:A:1695:LEU:HD22	1.52	0.75
1:A:605:THR:HG21	1:A:1076:LEU:HD21	1.70	0.74
1:A:1769:GLU:O	1:A:1822:ARG:NH1	2.20	0.74
1:A:1868:THR:HG22	1:A:1936:ARG:HH21	1.53	0.74
1:A:3231:ILE:HG23	1:A:3235:LYS:HZ3	1.51	0.74
3:C:411:HIS:CB	3:C:418:CYS:H	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3718:ARG:HE	1:A:3743:HIS:CD2	2.06	0.73
1:A:1933:LEU:H	1:A:1937:ARG:HH21	1.35	0.73
1:A:3506:LEU:HB2	1:A:3533:PHE:HZ	1.52	0.73
3:C:213:ILE:HD11	3:C:221:LEU:HB2	1.71	0.73
1:A:3951:GLN:HE21	1:A:4063:GLU:HA	1.54	0.73
1:A:1167:ASP:HA	1:A:1170:LYS:HB2	1.70	0.73
1:A:2475:ASN:HA	1:A:2478:MET:HE3	1.70	0.73
3:C:81:ARG:HH12	3:C:84:MET:H	1.37	0.72
1:A:9:ARG:HE	1:A:57:LEU:HG	1.53	0.72
1:A:396:PHE:HE2	1:A:438:LEU:HD11	1.55	0.72
1:A:1261:LEU:HD13	1:A:1337:VAL:HG12	1.70	0.72
1:A:2784:GLN:HG2	1:A:2785:ILE:HG12	1.71	0.72
1:A:4090:ARG:NH1	1:A:4110:GLN:HG3	2.05	0.72
1:A:3718:ARG:H	1:A:3743:HIS:HD2	1.36	0.71
2:B:297:LYS:HE3	3:C:296:CYS:SG	2.30	0.71
3:C:323:PHE:HE1	3:C:328:GLU:HB3	1.55	0.71
1:A:762:TYR:HD2	1:A:765:LEU:HB2	1.55	0.71
1:A:2859:GLN:NE2	1:A:2880:CYS:SG	2.63	0.71
1:A:2860:ASP:O	1:A:2864:GLN:NE2	2.23	0.71
2:B:488:ARG:HG2	2:B:501:GLU:HB2	1.72	0.71
3:C:457:LEU:HD11	3:C:530:LEU:HD23	1.70	0.71
2:B:312:LEU:HG	2:B:313:PRO:HD2	1.72	0.71
2:B:460:GLY:HA2	2:B:463:LYS:HD2	1.73	0.71
1:A:259:GLN:HB3	1:A:262:LEU:HD22	1.71	0.71
1:A:3231:ILE:HG23	1:A:3235:LYS:NZ	2.05	0.71
1:A:3378:TYR:OH	1:A:3426:LYS:NZ	2.24	0.71
1:A:1990:PHE:HD2	1:A:2182:ILE:HG22	1.56	0.71
1:A:2426:HIS:O	1:A:2432:GLN:NE2	2.24	0.71
3:C:65:ASP:H	3:C:78:THR:HG22	1.56	0.70
1:A:2507:ILE:HD11	1:A:2547:SER:CB	2.21	0.70
2:B:410:PHE:HE2	3:C:482:ILE:HD11	1.55	0.70
1:A:36:ARG:HH12	1:A:825:GLY:HA2	1.55	0.70
1:A:876:SER:HB2	1:A:880:MET:HG2	1.72	0.70
2:B:102:ILE:HG21	2:B:149:VAL:HG21	1.73	0.70
1:A:1832:SER:HB2	1:A:1836:LEU:HD22	1.74	0.70
3:C:533:ILE:HG23	3:C:537:PHE:CD2	2.26	0.70
1:A:1445:ARG:HH21	1:A:1507:CYS:HB3	1.57	0.70
1:A:2953:THR:HG22	1:A:2994:TRP:HE1	1.56	0.70
1:A:1361:LYS:HA	1:A:1364:CYS:HB2	1.73	0.70
2:B:61:ASP:O	2:B:65:GLN:HG2	1.92	0.70
1:A:3531:TYR:CD2	1:A:3532:PRO:HD3	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3917:ILE:HG13	1:A:3991:PHE:HD2	1.56	0.70
1:A:278:HIS:HB3	1:A:281:GLN:HG3	1.72	0.69
1:A:1198:LEU:HD23	1:A:1200:GLY:H	1.56	0.69
1:A:61:ARG:NH1	1:A:106:GLU:OE2	2.25	0.69
1:A:789:TYR:HA	1:A:792:ILE:HG22	1.74	0.69
1:A:3471:ILE:HA	1:A:3474:ARG:HD3	1.73	0.69
1:A:3763:ARG:NH2	1:A:4005:PHE:O	2.25	0.69
2:B:132:GLN:HA	2:B:136:GLY:HA2	1.73	0.69
3:C:391:ALA:HB3	3:C:408:ALA:HB3	1.73	0.69
1:A:36:ARG:HH22	1:A:825:GLY:H	1.38	0.69
1:A:4050:LYS:HD3	1:A:4059:ILE:HG21	1.74	0.69
3:C:411:HIS:CB	3:C:418:CYS:SG	2.81	0.69
1:A:65:LEU:HD12	1:A:85:ILE:HG23	1.73	0.69
1:A:880:MET:HA	1:A:883:TYR:HB2	1.76	0.68
1:A:1606:ARG:HG3	1:A:2042:GLN:HG2	1.75	0.68
2:B:388:LYS:HG3	3:C:454:VAL:HG23	1.74	0.68
1:A:1773:VAL:HG13	1:A:1774:MET:HG3	1.74	0.68
1:A:3880:ALA:HB1	1:A:3969:ASN:HD22	1.58	0.68
1:A:2251:ILE:HG12	1:A:2285:LEU:CD1	2.24	0.68
1:A:2510:LEU:O	1:A:2518:GLN:NE2	2.27	0.68
1:A:2952:ILE:HD13	1:A:2975:ALA:HB2	1.74	0.68
1:A:2958:LEU:HD11	1:A:4101:GLU:HG2	1.75	0.68
1:A:1718:ILE:O	1:A:1722:PHE:HB2	1.94	0.68
2:B:322:TYR:HD2	3:C:49:GLU:OE1	1.76	0.68
1:A:1783:ARG:HG2	1:A:1830:HIS:CD2	2.29	0.67
1:A:1836:LEU:HB3	1:A:1884:LEU:HD21	1.74	0.67
1:A:3786:LEU:HD22	1:A:3910:LEU:HD23	1.75	0.67
1:A:487:LEU:HD11	1:A:568:PHE:HE1	1.59	0.67
1:A:2224:PHE:HD2	1:A:2272:VAL:CG2	2.07	0.67
1:A:2511:ILE:HD13	1:A:2550:ILE:HG22	1.76	0.67
2:B:264:ASN:OD1	2:B:265:LYS:N	2.25	0.67
2:B:273:ILE:HG12	2:B:368:VAL:HG12	1.76	0.67
1:A:1142:HIS:CD2	1:A:1165:LEU:HB2	2.30	0.67
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.67	0.67
1:A:3361:GLU:HG3	1:A:3362:LEU:HG	1.76	0.67
1:A:3630:ARG:HB3	1:A:3633:ILE:HG22	1.76	0.67
3:C:10:VAL:HG12	3:C:131:HIS:HB3	1.75	0.67
1:A:1018:VAL:HG11	1:A:1066:LEU:HD11	1.77	0.67
1:A:3410:ILE:O	1:A:3414:MET:HG2	1.95	0.67
3:C:130:ARG:NH2	3:C:157:CYS:O	2.28	0.67
3:C:185:LEU:HB2	3:C:514:ASN:HD22	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1852:LYS:O	1:A:1854:ARG:NH1	2.28	0.66
2:B:40:PHE:HZ	2:B:70:VAL:HG11	1.59	0.66
2:B:248:ALA:O	2:B:249:LYS:NZ	2.22	0.66
1:A:1754:GLN:NE2	1:A:1788:ARG:HG2	2.10	0.66
2:B:296:VAL:HG21	3:C:295:TYR:HB3	1.78	0.66
1:A:1301:ILE:HD11	1:A:1334:LYS:HB2	1.78	0.65
1:A:1553:PHE:HE2	1:A:1558:TYR:HB2	1.61	0.65
1:A:984:TYR:HA	1:A:987:LEU:HB2	1.78	0.65
1:A:3577:GLN:HB3	1:A:3630:ARG:HE	1.61	0.65
2:B:409:TYR:HA	2:B:439:PHE:HZ	1.62	0.65
1:A:603:ILE:HG21	1:A:1083:ASN:HD22	1.61	0.65
1:A:915:THR:HA	1:A:934:LEU:HD11	1.77	0.65
1:A:3951:GLN:OE1	1:A:4043:LYS:NZ	2.29	0.65
3:C:27:ILE:HG13	3:C:28:GLU:H	1.61	0.65
1:A:1136:ARG:HH11	1:A:1136:ARG:HG3	1.60	0.65
1:A:2859:GLN:HE21	1:A:2876:VAL:HG13	1.59	0.65
1:A:2037:SER:O	1:A:2040:MET:HB2	1.97	0.65
3:C:463:LEU:HD23	3:C:477:PHE:HB3	1.79	0.65
1:A:899:ARG:NH2	1:A:2565:MET:O	2.30	0.65
1:A:918:ALA:O	1:A:927:LYS:NZ	2.29	0.65
1:A:997:ASN:HA	1:A:1043:GLN:HG2	1.78	0.65
1:A:1770:GLN:HA	1:A:1814:PHE:HZ	1.61	0.65
1:A:2957:LEU:HD21	1:A:2993:PHE:HZ	1.62	0.65
2:B:297:LYS:CE	3:C:296:CYS:SG	2.85	0.65
1:A:1004:GLN:HA	1:A:1007:VAL:HG12	1.79	0.64
1:A:2548:PRO:CG	1:A:2846:THR:HG22	2.25	0.64
1:A:3455:LYS:NZ	1:A:3489:SER:OG	2.30	0.64
1:A:3654:MET:HE1	1:A:3657:SER:H	1.62	0.64
2:B:451:LYS:NZ	3:C:414:HIS:O	2.27	0.64
2:B:335:GLU:O	2:B:405:ASN:ND2	2.30	0.64
3:C:339:CYS:SG	3:C:394:ARG:NH1	2.70	0.64
1:A:7:GLY:N	1:A:10:CYS:SG	2.70	0.64
1:A:1671:VAL:HG22	1:A:1675:TYR:CE2	2.32	0.64
1:A:1821:ASP:OD1	1:A:1875:LYS:NZ	2.27	0.64
2:B:301:ARG:HE	2:B:310:LEU:HD13	1.62	0.64
1:A:628:GLU:HG3	1:A:631:ARG:NH2	2.11	0.64
1:A:1335:CYS:HB3	1:A:1384:PHE:CE1	2.32	0.64
1:A:2887:PRO:HG2	1:A:3895:GLU:HG3	1.79	0.64
3:C:431:ARG:NH2	4:D:17:DC:OP2	2.29	0.64
1:A:264:ARG:HH12	5:E:37:DC:H4'	1.63	0.64
1:A:2126:MET:O	1:A:2130:HIS:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3455:LYS:NZ	1:A:3489:SER:O	2.30	0.64
1:A:4002:MET:O	1:A:4005:PHE:HB3	1.97	0.64
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.26	0.64
1:A:3137:GLU:OE2	1:A:3167:ARG:NH1	2.30	0.64
1:A:3297:VAL:HG23	1:A:3337:ILE:HG23	1.79	0.64
1:A:76:ILE:O	1:A:79:ARG:NH1	2.31	0.64
1:A:1708:GLU:OE1	1:A:1712:ARG:NH1	2.31	0.64
3:C:188:HIS:HB2	3:C:519:PRO:HG3	1.78	0.64
1:A:1686:LEU:HD21	1:A:1721:HIS:HB3	1.80	0.63
1:A:3170:ASP:OD2	1:A:3173:MET:HB2	1.97	0.63
3:C:131:HIS:NE2	3:C:133:GLU:OE2	2.29	0.63
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.79	0.63
1:A:396:PHE:CE2	1:A:438:LEU:HD11	2.34	0.63
1:A:1135:CYS:HA	1:A:1138:ILE:HG22	1.80	0.63
1:A:1716:GLN:HA	1:A:1719:VAL:HG12	1.80	0.63
1:A:2251:ILE:CD1	1:A:2285:LEU:HD13	2.28	0.63
1:A:3843:LEU:O	1:A:3847:SER:HB2	1.99	0.63
2:B:45:SER:N	2:B:48:MET:SD	2.64	0.63
2:B:489:ASN:ND2	3:C:331:MET:O	2.30	0.63
1:A:3962:ARG:NH1	1:A:4124:TRP:O	2.31	0.63
2:B:515:ASN:OD1	3:C:255:SER:N	2.32	0.63
1:A:1406:LEU:HD23	1:A:1415:LEU:HD22	1.80	0.63
1:A:1566:THR:HA	1:A:1569:THR:HG22	1.81	0.63
2:B:410:PHE:CE2	3:C:482:ILE:HD11	2.33	0.63
3:C:246:HIS:O	3:C:246:HIS:ND1	2.31	0.63
1:A:2832:ILE:HA	1:A:2835:LYS:HE3	1.81	0.62
3:C:659:LEU:HD12	3:C:662:LEU:HD21	1.81	0.62
5:E:34:DC:H4'	5:E:35:DG:H5'	1.80	0.62
1:A:631:ARG:HH11	1:A:668:LYS:HB3	1.63	0.62
1:A:665:GLY:HA2	1:A:668:LYS:HB2	1.80	0.62
1:A:2859:GLN:NE2	1:A:2876:VAL:HG13	2.14	0.62
1:A:185:HIS:CE1	1:A:188:GLU:H	2.17	0.62
1:A:3028:ASN:HA	1:A:3031:TRP:HD1	1.64	0.62
1:A:484:HIS:O	1:A:488:ILE:HG12	1.99	0.62
1:A:1572:LEU:HD21	1:A:1604:SER:HB2	1.80	0.62
1:A:2332:GLU:O	1:A:2334:LYS:NZ	2.31	0.62
1:A:3091:LEU:HD12	1:A:3142:ILE:HD12	1.82	0.62
1:A:3444:ALA:HB1	1:A:3479:THR:HG21	1.81	0.62
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.33	0.62
2:B:330:GLU:HG3	2:B:332:GLU:H	1.64	0.62
1:A:166:ILE:HD11	1:A:171:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1676:ILE:O	1:A:1680:ALA:HB2	1.98	0.62
1:A:1840:PHE:O	1:A:1844:VAL:HG23	1.99	0.62
1:A:2574:ASN:OD1	1:A:2784:GLN:N	2.33	0.62
1:A:2225:HIS:ND1	1:A:2226:PRO:CD	2.58	0.62
1:A:1098:GLN:O	1:A:1152:ARG:NH2	2.33	0.61
3:C:423:GLN:HG2	3:C:424:LEU:H	1.65	0.61
1:A:2962:ARG:O	1:A:2964:ASP:N	2.31	0.61
1:A:3232:ARG:HH11	1:A:3269:ARG:HE	1.45	0.61
1:A:3958:LEU:HD11	1:A:4081:ALA:HB2	1.81	0.61
2:B:41:LEU:HD21	2:B:146:VAL:HG22	1.81	0.61
2:B:426:GLN:NE2	2:B:428:THR:O	2.33	0.61
3:C:40:MET:HA	3:C:43:GLN:HE21	1.65	0.61
1:A:137:THR:HG23	1:A:138:PHE:CD1	2.35	0.61
1:A:2484:TYR:CE2	1:A:2498:ILE:HD11	2.35	0.61
2:B:241:ASP:HA	2:B:245:LYS:HE3	1.80	0.61
2:B:403:ARG:HG2	5:E:29:DG:H5'	1.81	0.61
1:A:349:ILE:HG23	1:A:350:ARG:HD2	1.82	0.61
1:A:1813:SER:HB2	1:A:1868:THR:HG21	1.82	0.61
1:A:3536:SER:HA	1:A:3539:SER:HB3	1.82	0.61
1:A:3755:GLY:HA2	1:A:3799:ARG:HG3	1.82	0.61
1:A:2823:PHE:CD2	1:A:2824:LYS:HG2	2.35	0.61
1:A:3917:ILE:HG13	1:A:3991:PHE:CD2	2.36	0.61
1:A:935:HIS:HD1	1:A:983:LEU:HD11	1.65	0.61
1:A:937:MET:O	1:A:941:MET:HG2	2.00	0.61
1:A:2255:LEU:HA	1:A:2258:GLU:HG3	1.81	0.61
1:A:886:TRP:HH2	1:A:915:THR:HG21	1.64	0.61
1:A:2346:ALA:O	1:A:2350:LYS:HG2	2.00	0.61
1:A:2376:ASP:OD1	1:A:2404:ARG:NE	2.24	0.61
3:C:44:ARG:HH12	3:C:234:LEU:HD13	1.66	0.61
1:A:1378:GLU:OE1	1:A:1447:ARG:NH2	2.34	0.60
1:A:1809:ASP:O	1:A:1816:ARG:NH1	2.33	0.60
1:A:2525:TRP:O	1:A:2531:LEU:HD13	2.01	0.60
3:C:136:THR:HG22	3:C:138:LEU:H	1.65	0.60
1:A:767:GLU:OE2	1:A:854:ARG:NH2	2.34	0.60
1:A:2464:HIS:CE1	1:A:2469:CYS:HG	2.19	0.60
1:A:1704:GLY:O	1:A:1708:GLU:HB2	2.01	0.60
1:A:2957:LEU:HD21	1:A:2993:PHE:CZ	2.35	0.60
1:A:3887:PHE:CD2	1:A:3900:LEU:HB3	2.37	0.60
2:B:473:TYR:HB3	3:C:350:GLN:HE21	1.65	0.60
1:A:524:TYR:HA	1:A:527:TYR:HD2	1.65	0.60
1:A:2133:LEU:HD12	1:A:2143:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2851:PHE:CE2	1:A:2853:PRO:HG2	2.37	0.60
1:A:3495:PHE:HB3	1:A:3502:MET:HE3	1.84	0.60
1:A:3915:HIS:HD2	1:A:3920:ILE:HG21	1.67	0.60
2:B:341:ASP:OD1	2:B:342:ASP:N	2.35	0.60
1:A:36:ARG:NH2	1:A:823:GLN:O	2.34	0.60
2:B:277:VAL:HB	3:C:357:MET:HE2	1.84	0.60
1:A:1298:LEU:HD11	1:A:1341:ILE:HD13	1.82	0.60
1:A:2464:HIS:ND1	1:A:2469:CYS:SG	2.75	0.60
1:A:3885:ARG:O	1:A:3889:ARG:HB2	2.01	0.60
1:A:2302:ALA:O	1:A:2306:ASN:ND2	2.35	0.60
1:A:2440:TYR:CD1	1:A:2476:ILE:HG22	2.37	0.60
1:A:2464:HIS:ND1	1:A:2465:PRO:O	2.30	0.60
1:A:1672:PHE:HA	1:A:1675:TYR:HD2	1.66	0.59
1:A:1014:LEU:O	1:A:1017:ILE:HG22	2.02	0.59
1:A:2417:SER:HB2	2:B:152:ASN:ND2	2.17	0.59
1:A:439:VAL:HG13	1:A:482:VAL:HG21	1.83	0.59
1:A:1491:ILE:HG21	1:A:1562:LEU:HD22	1.85	0.59
2:B:95:ASN:OD1	2:B:98:ASN:N	2.35	0.59
1:A:985:GLU:O	1:A:989:MET:HG2	2.03	0.59
1:A:2233:HIS:O	1:A:2237:ILE:HG13	2.02	0.59
3:C:357:MET:HE3	3:C:429:ASP:HB3	1.84	0.59
1:A:1162:SER:OG	1:A:1164:CYS:SG	2.61	0.59
1:A:886:TRP:CH2	1:A:915:THR:HG21	2.36	0.59
1:A:1186:LYS:O	1:A:1190:LEU:HD23	2.03	0.59
1:A:3911:ILE:O	1:A:3915:HIS:ND1	2.34	0.59
1:A:1626:TRP:HE1	1:A:1674:THR:HG21	1.68	0.59
1:A:2150:VAL:HG11	1:A:2168:LEU:HD21	1.84	0.59
1:A:2516:GLY:O	1:A:2520:ILE:HG13	2.03	0.59
1:A:3574:ALA:HB1	1:A:3687:MET:HG3	1.85	0.59
1:A:3833:ARG:HD3	1:A:3877:LYS:HD2	1.84	0.59
3:C:28:GLU:OE2	3:C:32:GLU:HB3	2.02	0.59
1:A:137:THR:HG23	1:A:138:PHE:HD1	1.67	0.59
1:A:1485:SER:O	1:A:1489:LYS:HG2	2.03	0.59
1:A:2480:ILE:O	1:A:2484:TYR:HB2	2.03	0.59
1:A:2507:ILE:CD1	1:A:2547:SER:CB	2.81	0.59
3:C:424:LEU:HD12	3:C:425:PRO:HD2	1.84	0.59
1:A:917:LEU:O	1:A:921:ALA:HB2	2.03	0.59
1:A:393:LYS:HA	1:A:397:LEU:HD13	1.85	0.58
1:A:424:LEU:O	1:A:471:LYS:NZ	2.36	0.58
1:A:1017:ILE:HG23	1:A:1018:VAL:HG13	1.85	0.58
1:A:1089:PHE:CE2	1:A:1100:VAL:HB	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2831:ASN:O	1:A:2835:LYS:HG3	2.04	0.58
1:A:2898:LEU:O	1:A:2899:ARG:HD3	2.04	0.58
1:A:1298:LEU:O	1:A:1370:ARG:NH2	2.36	0.58
1:A:1820:VAL:O	1:A:1825:LEU:HG	2.03	0.58
1:A:1261:LEU:HD11	1:A:1340:ARG:HE	1.68	0.58
1:A:1377:CYS:SG	1:A:1422:LYS:NZ	2.72	0.58
1:A:1018:VAL:HG12	1:A:1077:GLY:HA3	1.86	0.58
1:A:1342:MET:HG2	1:A:1402:LEU:HD22	1.86	0.58
1:A:178:LEU:HB3	1:A:196:LEU:HD21	1.86	0.58
1:A:1916:ILE:HD11	1:A:1955:VAL:HG11	1.85	0.58
1:A:862:LEU:HD13	1:A:866:ILE:HG22	1.85	0.58
1:A:3147:LYS:HB3	1:A:3150:ASN:HB2	1.85	0.58
1:A:4090:ARG:HH11	1:A:4110:GLN:HG3	1.67	0.58
2:B:37:SER:HG	2:B:154:PHE:HE1	1.51	0.58
2:B:263:LEU:HB2	2:B:267:ILE:HG13	1.86	0.58
3:C:57:VAL:HG12	3:C:79:VAL:HG13	1.86	0.58
3:C:513:TRP:O	3:C:517:ASN:ND2	2.28	0.58
1:A:895:ALA:HB1	1:A:902:LYS:HG2	1.84	0.58
1:A:762:TYR:CE2	1:A:764:PRO:HG2	2.39	0.58
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.86	0.58
2:B:305:THR:HB	2:B:311:LEU:HD21	1.84	0.58
3:C:11:VAL:HG22	3:C:55:ALA:HB3	1.86	0.58
3:C:385:ASP:OD1	3:C:386:ASP:N	2.37	0.58
1:A:459:ARG:HH21	1:A:544:ILE:HD11	1.67	0.57
1:A:2352:HIS:HB3	1:A:2360:PHE:HB2	1.86	0.57
1:A:424:LEU:C	1:A:424:LEU:HD23	2.24	0.57
1:A:899:ARG:NH1	1:A:2565:MET:SD	2.77	0.57
1:A:3414:MET:HE1	1:A:3461:ALA:HB2	1.84	0.57
1:A:3949:ALA:HA	1:A:3953:LEU:HD13	1.86	0.57
3:C:347:LYS:HA	3:C:389:MET:HA	1.85	0.57
1:A:1020:PRO:O	1:A:1022:ASP:N	2.37	0.57
1:A:1098:GLN:HB3	1:A:1152:ARG:HB2	1.85	0.57
1:A:3332:THR:HG22	1:A:3335:ARG:HH21	1.70	0.57
3:C:57:VAL:HA	3:C:80:HIS:H	1.69	0.57
3:C:533:ILE:HG23	3:C:537:PHE:HD2	1.67	0.57
1:A:491:CYS:O	1:A:622:ALA:HA	2.04	0.57
1:A:1044:ILE:O	1:A:1049:GLN:NE2	2.37	0.57
1:A:3880:ALA:HB2	1:A:3965:ARG:NH2	2.20	0.57
2:B:38:LEU:HB2	2:B:83:LEU:HD23	1.84	0.57
3:C:225:TYR:HB3	3:C:229:GLU:HG3	1.87	0.57
3:C:381:ILE:HG22	3:C:419:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:LEU:O	1:A:613:HIS:ND1	2.38	0.57
1:A:899:ARG:NH2	1:A:2568:MET:SD	2.71	0.57
1:A:919:LEU:HD21	1:A:968:VAL:HG23	1.86	0.57
1:A:2478:MET:HG2	1:A:2524:PHE:CD1	2.40	0.57
1:A:418:ALA:HB2	1:A:464:VAL:HG22	1.85	0.57
1:A:572:VAL:O	1:A:576:VAL:HG23	2.04	0.57
2:B:33:SER:HB3	5:E:32:DA:H5"	1.87	0.57
1:A:1774:MET:HB3	1:A:1777:LEU:HD12	1.87	0.57
1:A:1938:ARG:NH2	1:A:1981:LEU:O	2.34	0.57
1:A:3887:PHE:HD2	1:A:3900:LEU:HB3	1.68	0.57
1:A:1117:ASP:OD1	1:A:1118:GLU:N	2.33	0.56
1:A:415:GLN:HE21	1:A:460:ALA:HB2	1.70	0.56
1:A:855:VAL:O	1:A:859:LEU:HB2	2.05	0.56
1:A:1893:GLU:HB2	1:A:1896:ILE:HG12	1.88	0.56
1:A:1979:GLU:HG2	1:A:1984:LEU:HD11	1.88	0.56
1:A:3108:GLN:O	1:A:3112:GLN:HG3	2.05	0.56
1:A:409:GLN:N	1:A:409:GLN:OE1	2.38	0.56
1:A:532:ARG:O	1:A:536:SER:OG	2.23	0.56
1:A:575:ILE:O	1:A:579:LEU:HG	2.06	0.56
1:A:1711:ARG:NE	1:A:1757:MET:HB3	2.15	0.56
1:A:1963:GLN:N	1:A:1963:GLN:OE1	2.38	0.56
1:A:2093:CYS:HA	1:A:2096:PRO:HG2	1.88	0.56
1:A:3828:TYR:OH	1:A:4125:GLU:OE1	2.21	0.56
4:D:20:DG:N2	5:E:25:DC:O2	2.39	0.56
1:A:113:SER:HA	1:A:116:THR:HG22	1.86	0.56
1:A:2536:LEU:HD11	1:A:2820:MET:HB3	1.86	0.56
1:A:2572:TYR:CE2	1:A:2788:SER:HB3	2.41	0.56
1:A:3285:HIS:CE1	1:A:3329:LEU:HD22	2.41	0.56
2:B:65:GLN:OE1	2:B:123:LYS:HE3	2.06	0.56
1:A:427:VAL:HG12	1:A:429:GLU:H	1.71	0.56
1:A:1195:VAL:HG23	1:A:1196:PRO:HD3	1.88	0.56
1:A:2257:PHE:HA	1:A:2260:PHE:CZ	2.41	0.56
1:A:1157:PHE:HD2	1:A:1163:LEU:HD23	1.71	0.56
1:A:3407:ALA:O	1:A:3411:ASP:N	2.36	0.56
2:B:262:LYS:NZ	2:B:346:MET:HB3	2.21	0.56
3:C:66:ASN:ND2	3:C:68:LEU:O	2.32	0.56
1:A:940:PHE:O	1:A:944:LYS:HG2	2.06	0.56
1:A:1493:PRO:HG3	1:A:1501:PRO:HD3	1.88	0.56
2:B:165:ARG:NH1	2:B:201:ASP:OD2	2.39	0.56
2:B:275:ASN:ND2	2:B:278:GLN:OE1	2.39	0.56
1:A:1029:CYS:O	1:A:1033:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:THR:OG1	1:A:1735:ARG:NH1	2.39	0.56
1:A:3332:THR:HA	1:A:3335:ARG:HD3	1.88	0.56
1:A:3335:ARG:HG2	1:A:3419:PHE:CD2	2.41	0.56
1:A:3723:ASP:HB3	1:A:3739:ILE:HB	1.88	0.56
3:C:327:ASP:O	3:C:331:MET:HG2	2.05	0.56
3:C:384:LEU:HB3	3:C:410:PRO:HG3	1.88	0.56
1:A:1915:LEU:HD12	1:A:1918:LEU:HD11	1.88	0.56
3:C:351:VAL:HG21	3:C:407:VAL:HG21	1.88	0.56
4:D:4:DG:H2''	4:D:5:DC:H5''	1.88	0.56
1:A:185:HIS:HE1	1:A:188:GLU:HB2	1.71	0.55
1:A:1881:TYR:CD2	1:A:1951:VAL:HG12	2.41	0.55
1:A:2228:ARG:HD3	5:E:41:DG:H5'	1.87	0.55
1:A:3764:VAL:HG12	1:A:4005:PHE:HE2	1.70	0.55
1:A:3835:PRO:HD3	1:A:3877:LYS:HD3	1.87	0.55
1:A:931:CYS:O	1:A:984:TYR:OH	2.21	0.55
1:A:962:TYR:HA	1:A:965:THR:HG22	1.88	0.55
1:A:3577:GLN:O	1:A:3630:ARG:NH2	2.39	0.55
1:A:72:SER:O	1:A:75:SER:OG	2.22	0.55
1:A:1420:ARG:O	1:A:1424:THR:HB	2.06	0.55
1:A:2303:LEU:HA	1:A:2306:ASN:HD21	1.71	0.55
1:A:2331:MET:HG3	1:A:2371:PHE:CE1	2.41	0.55
1:A:3244:ASP:O	1:A:3248:LYS:HG2	2.06	0.55
1:A:3807:GLU:OE1	1:A:3808:ASN:ND2	2.39	0.55
3:C:347:LYS:HD2	3:C:388:ASP:HB3	1.88	0.55
1:A:2038:GLU:HG2	1:A:2042:GLN:HE22	1.72	0.55
1:A:2434:VAL:O	1:A:2438:ILE:HG23	2.07	0.55
1:A:2436:LEU:HA	1:A:2439:ILE:HG22	1.89	0.55
1:A:1282:LEU:HD22	1:A:1291:LEU:HD21	1.87	0.55
1:A:1419:LEU:HD13	1:A:1458:LEU:HD11	1.88	0.55
1:A:1649:LEU:HD11	1:A:1675:TYR:OH	2.06	0.55
1:A:1807:LYS:HZ1	1:A:1811:ARG:HH12	1.55	0.55
1:A:2224:PHE:HD2	1:A:2272:VAL:HG21	1.71	0.55
3:C:272:VAL:HG13	3:C:486:ARG:HH12	1.72	0.55
3:C:645:GLU:HG3	3:C:654:ARG:HH22	1.71	0.55
1:A:185:HIS:O	1:A:185:HIS:ND1	2.39	0.55
1:A:642:PHE:HE2	1:A:673:THR:HG1	1.54	0.55
1:A:865:GLN:HG2	1:A:3170:ASP:HB3	1.88	0.55
1:A:1107:TYR:CZ	1:A:1130:ALA:HB3	2.41	0.55
1:A:3048:LYS:HB3	1:A:3061:LEU:HD22	1.89	0.55
1:A:3472:ILE:HG21	1:A:3480:LEU:HD11	1.88	0.55
1:A:3786:LEU:HD21	1:A:3983:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:ASN:O	3:C:242:ARG:NH1	2.39	0.55
1:A:348:ILE:HB	1:A:362:ALA:HB2	1.88	0.55
1:A:2813:PHE:HZ	1:A:2836:LEU:HD22	1.71	0.55
1:A:3989:ARG:NH2	1:A:4100:GLU:OE1	2.36	0.55
2:B:85:VAL:HG23	2:B:105:LEU:HB3	1.89	0.55
1:A:3454:LEU:HD12	1:A:3462:ARG:HA	1.88	0.55
1:A:628:GLU:HG3	1:A:631:ARG:HH22	1.69	0.55
1:A:3045:ILE:HD11	1:A:3082:TYR:CD1	2.41	0.55
1:A:3512:VAL:HA	1:A:3515:GLN:HG3	1.89	0.55
1:A:7:GLY:N	1:A:10:CYS:HG	2.06	0.54
1:A:105:VAL:HA	1:A:147:PHE:CE1	2.42	0.54
1:A:2280:VAL:CG2	1:A:2285:LEU:HD12	2.33	0.54
1:A:3880:ALA:HB1	1:A:3969:ASN:ND2	2.21	0.54
3:C:54:ILE:O	3:C:81:ARG:NH1	2.40	0.54
3:C:259:ILE:HG21	3:C:377:LEU:HB3	1.89	0.54
3:C:363:LYS:HG2	3:C:420:VAL:HG12	1.89	0.54
1:A:43:VAL:HG12	1:A:818:LEU:HD21	1.89	0.54
1:A:756:PHE:HE1	1:A:770:LEU:HD22	1.72	0.54
1:A:909:VAL:HB	1:A:2807:GLN:HE21	1.72	0.54
1:A:3734:ARG:HB2	1:A:3734:ARG:NH1	2.22	0.54
1:A:3031:TRP:HB3	1:A:3074:GLN:HE21	1.73	0.54
1:A:112:THR:HG21	1:A:155:LYS:HE3	1.89	0.54
1:A:414:LEU:HG	1:A:442:GLN:NE2	2.22	0.54
1:A:466:LEU:HB2	1:A:560:LEU:HD22	1.89	0.54
1:A:1028:PHE:HA	1:A:1031:ARG:HD3	1.89	0.54
1:A:1075:ARG:NH2	1:A:1117:ASP:OD2	2.40	0.54
1:A:1649:LEU:O	1:A:1653:LEU:HG	2.07	0.54
1:A:1770:GLN:HA	1:A:1814:PHE:CZ	2.41	0.54
1:A:2358:ASP:OD1	1:A:2359:LYS:N	2.41	0.54
1:A:3422:GLN:NE2	1:A:3423:GLN:OE1	2.40	0.54
1:A:3529:ILE:O	1:A:3532:PRO:HD2	2.07	0.54
3:C:130:ARG:NH2	3:C:158:ASP:OD1	2.39	0.54
3:C:188:HIS:H	3:C:232:ARG:NH1	2.05	0.54
3:C:633:MET:HA	3:C:636:ILE:HG22	1.90	0.54
1:A:672:ILE:O	1:A:676:ASN:ND2	2.35	0.54
1:A:978:GLN:OE1	1:A:981:ARG:NH2	2.32	0.54
1:A:1963:GLN:HG2	1:A:2123:PRO:HG2	1.90	0.54
1:A:2265:PRO:HB3	1:A:2309:PHE:CG	2.42	0.54
1:A:3951:GLN:HE22	1:A:4066:LEU:HD23	1.73	0.54
1:A:1362:ASP:OD1	1:A:1363:LEU:N	2.39	0.54
1:A:1990:PHE:CD2	1:A:2182:ILE:HG22	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:VAL:HG11	1:A:2225:HIS:HE2	1.72	0.54
1:A:2182:ILE:HB	1:A:2185:MET:HB3	1.87	0.54
1:A:2363:CYS:O	1:A:2367:VAL:HG23	2.07	0.54
2:B:262:LYS:HZ3	2:B:346:MET:HB3	1.71	0.54
2:B:348:MET:HB2	2:B:397:LEU:HD23	1.90	0.54
1:A:528:VAL:HG11	1:A:632:GLU:CD	2.27	0.54
1:A:933:LEU:HD11	1:A:2794:LEU:HA	1.90	0.54
1:A:2458:VAL:O	1:A:2461:PHE:HB2	2.08	0.54
3:C:659:LEU:HD23	3:C:685:LEU:HD12	1.89	0.54
1:A:450:SER:O	1:A:453:MET:HG2	2.07	0.54
1:A:1515:LEU:HD11	1:A:1566:THR:OG1	2.08	0.54
1:A:2503:LYS:O	1:A:2507:ILE:HG12	2.07	0.54
2:B:403:ARG:HB2	2:B:406:ILE:HG13	1.88	0.54
1:A:43:VAL:O	1:A:95:LYS:NZ	2.41	0.54
2:B:418:GLU:OE2	3:C:437:SER:OG	2.23	0.54
3:C:28:GLU:OE1	3:C:33:GLN:HG3	2.07	0.54
1:A:73:LEU:HB2	1:A:117:LYS:HD3	1.90	0.54
1:A:1727:ARG:HD3	1:A:1773:VAL:HB	1.90	0.54
1:A:1986:ARG:HE	1:A:1988:TYR:HE1	1.55	0.54
1:A:2379:MET:O	1:A:2382:VAL:HG12	2.08	0.54
1:A:3183:ILE:HD12	1:A:3238:MET:HG2	1.89	0.54
1:A:107:ILE:HA	1:A:110:THR:HG22	1.88	0.53
1:A:142:ARG:HG3	1:A:143:LEU:HG	1.89	0.53
1:A:453:MET:O	1:A:457:CYS:N	2.35	0.53
1:A:3357:ARG:O	1:A:3361:GLU:N	2.39	0.53
1:A:2086:ASP:OD1	1:A:2087:GLU:N	2.39	0.53
1:A:2443:MET:HE1	1:A:2479:TRP:HB3	1.89	0.53
2:B:143:LEU:O	2:B:145:GLU:N	2.42	0.53
1:A:965:THR:O	1:A:969:LEU:HD23	2.08	0.53
1:A:2506:LEU:HD13	1:A:2524:PHE:CE2	2.44	0.53
1:A:3228:SER:HA	1:A:3231:ILE:HD12	1.90	0.53
3:C:188:HIS:CE1	3:C:232:ARG:HD3	2.44	0.53
1:A:1702:LEU:HD23	1:A:1706:SER:HB2	1.89	0.53
1:A:1969:GLU:N	1:A:1969:GLU:OE1	2.41	0.53
3:C:628:GLU:HB2	3:C:631:TYR:HD2	1.72	0.53
1:A:935:HIS:ND1	1:A:983:LEU:HD11	2.23	0.53
2:B:262:LYS:HB3	2:B:268:VAL:HG12	1.89	0.53
2:B:277:VAL:HB	3:C:357:MET:CE	2.38	0.53
5:E:20:DT:H2"	5:E:21:DG:C8	2.43	0.53
1:A:476:ARG:O	1:A:479:ILE:HG22	2.08	0.53
1:A:2190:VAL:HA	1:A:2193:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3859:TYR:HE1	1:A:4119:ARG:HG2	1.73	0.53
3:C:91:LEU:HD21	3:C:495:LEU:HD13	1.90	0.53
1:A:3357:ARG:HA	1:A:3360:LEU:HB2	1.90	0.53
1:A:3418:ASP:OD1	1:A:3419:PHE:N	2.41	0.53
1:A:935:HIS:CE1	1:A:987:LEU:HD21	2.44	0.53
1:A:1564:SER:O	1:A:1568:ASN:ND2	2.41	0.53
1:A:3843:LEU:O	1:A:3847:SER:CB	2.56	0.53
1:A:3868:VAL:HG22	1:A:4114:PRO:HB2	1.89	0.53
1:A:4057:ALA:HB1	1:A:4082:ARG:HA	1.90	0.53
1:A:4126:PRO:HD2	1:A:4127:TRP:CE3	2.44	0.53
2:B:143:LEU:HD23	2:B:182:LYS:HD3	1.91	0.53
3:C:386:ASP:OD1	3:C:387:LEU:N	2.42	0.53
1:A:1188:ILE:HD13	1:A:1269:THR:HG21	1.90	0.53
1:A:1414:ILE:O	1:A:1418:HIS:HB2	2.08	0.53
1:A:2426:HIS:CG	1:A:2427:ARG:H	2.27	0.53
1:A:2439:ILE:O	1:A:2443:MET:HB2	2.08	0.53
3:C:81:ARG:NH1	3:C:84:MET:SD	2.82	0.53
1:A:479:ILE:HA	1:A:482:VAL:HG12	1.91	0.53
1:A:571:SER:O	1:A:575:ILE:HG13	2.09	0.53
1:A:581:LEU:HB2	1:A:660:LEU:HD13	1.90	0.53
1:A:749:VAL:HG23	1:A:750:PRO:HD3	1.91	0.53
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.42	0.53
1:A:1297:PHE:CZ	1:A:1337:VAL:HG23	2.44	0.53
1:A:1334:LYS:NZ	1:A:1382:ILE:O	2.26	0.53
1:A:3478:GLU:OE1	1:A:3479:THR:OG1	2.16	0.53
1:A:10:CYS:SG	1:A:14:ARG:NH2	2.82	0.52
1:A:2476:ILE:O	1:A:2480:ILE:HG13	2.09	0.52
1:A:3578:LEU:HG	1:A:3736:LYS:HD2	1.91	0.52
1:A:3961:PHE:HE1	1:A:4107:LEU:HG	1.74	0.52
3:C:232:ARG:HA	3:C:515:MET:SD	2.49	0.52
1:A:1013:ILE:HD11	1:A:1029:CYS:HA	1.90	0.52
1:A:2548:PRO:HG3	1:A:2846:THR:CG2	2.35	0.52
1:A:3988:LEU:O	1:A:3992:ARG:HG2	2.09	0.52
1:A:275:PHE:HE2	1:A:319:PHE:HB2	1.74	0.52
1:A:1335:CYS:HA	1:A:1338:VAL:HG12	1.92	0.52
2:B:476:ASP:HB3	3:C:427:MET:SD	2.50	0.52
3:C:679:VAL:HG12	3:C:705:LEU:HD21	1.90	0.52
1:A:1302:ALA:HB3	1:A:1370:ARG:HH12	1.74	0.52
1:A:1802:TYR:CZ	1:A:1843:ILE:HD12	2.45	0.52
1:A:1851:LEU:HB3	1:A:1918:LEU:HD13	1.91	0.52
3:C:244:SER:O	3:C:245:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2357:GLU:HG2	1:A:2385:LEU:HD11	1.91	0.52
1:A:2420:PHE:CE1	1:A:2438:ILE:HD11	2.45	0.52
2:B:480:ASN:O	2:B:484:GLN:HG2	2.10	0.52
1:A:204:LEU:HD23	1:A:251:PHE:CD2	2.44	0.52
1:A:256:ILE:HB	1:A:300:TRP:HZ3	1.74	0.52
1:A:1407:LYS:HG3	1:A:1463:LEU:HD11	1.91	0.52
1:A:3028:ASN:HA	1:A:3031:TRP:CD1	2.45	0.52
1:A:3946:PHE:HE2	1:A:4006:VAL:HB	1.74	0.52
2:B:46:LYS:HD2	2:B:47:ALA:HB2	1.92	0.52
1:A:415:GLN:NE2	1:A:460:ALA:HB2	2.24	0.52
1:A:797:ASP:OD1	1:A:798:GLY:N	2.42	0.52
1:A:2257:PHE:HB2	1:A:2299:TYR:CE2	2.44	0.52
1:A:3147:LYS:HE3	1:A:3149:GLY:H	1.75	0.52
1:A:433:PRO:HB2	1:A:2047:THR:HG23	1.92	0.52
1:A:1147:LYS:O	1:A:1151:ARG:NH2	2.41	0.52
1:A:1675:TYR:CD1	1:A:1695:LEU:HD22	2.40	0.52
1:A:1847:ALA:HA	1:A:1850:VAL:HG12	1.92	0.52
1:A:2251:ILE:CD1	1:A:2285:LEU:CD1	2.88	0.52
1:A:2933:ILE:HD12	1:A:3121:LEU:HD13	1.91	0.52
3:C:323:PHE:HE1	3:C:328:GLU:CB	2.16	0.52
3:C:328:GLU:O	3:C:332:LYS:HB3	2.10	0.52
3:C:449:ALA:HA	3:C:452:ASN:HD21	1.74	0.52
3:C:522:VAL:O	3:C:526:SER:HB3	2.10	0.52
1:A:295:GLU:O	1:A:299:LYS:HG2	2.10	0.52
1:A:650:SER:O	1:A:654:ILE:HD12	2.09	0.52
1:A:1105:VAL:HG23	1:A:1171:TRP:CZ2	2.44	0.52
1:A:2503:LYS:HD2	1:A:2525:TRP:HH2	1.74	0.52
1:A:3113:ASN:O	1:A:3117:ILE:HD12	2.10	0.52
1:A:3358:ARG:HA	1:A:3361:GLU:HG2	1.92	0.52
2:B:143:LEU:O	2:B:146:VAL:N	2.29	0.52
2:B:372:GLU:OE1	2:B:377:GLY:N	2.43	0.52
1:A:215:PRO:HB2	1:A:217:LEU:HD22	1.92	0.52
1:A:1118:GLU:HB3	1:A:1121:LEU:HB2	1.91	0.52
1:A:2931:ARG:NH2	1:A:3043:TYR:OH	2.42	0.52
1:A:2977:ASN:O	1:A:2979:GLN:NE2	2.42	0.52
1:A:3033:GLU:O	1:A:3035:PHE:N	2.42	0.52
1:A:3502:MET:HB2	1:A:3514:VAL:HG21	1.91	0.52
1:A:3969:ASN:HA	1:A:3972:LEU:HD22	1.91	0.52
1:A:440:VAL:CG1	1:A:482:VAL:HG23	2.40	0.51
1:A:911:LEU:HD21	1:A:961:LEU:HD21	1.92	0.51
1:A:2085:MET:SD	1:A:2090:ARG:HG2	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3281:CYS:HB3	1:A:3329:LEU:HD13	1.92	0.51
3:C:31:PHE:HE2	3:C:98:ILE:HD12	1.75	0.51
1:A:444:ASP:OD2	1:A:489:ARG:NH1	2.43	0.51
1:A:1178:ARG:O	1:A:1184:ARG:NH2	2.41	0.51
1:A:1355:GLY:O	1:A:1358:LEU:HG	2.09	0.51
1:A:2121:ASP:HA	1:A:2160:TYR:HE2	1.75	0.51
1:A:2857:CYS:O	1:A:2861:ILE:HG12	2.10	0.51
1:A:3649:SER:O	1:A:3653:ARG:NH1	2.41	0.51
2:B:261:LEU:HD11	2:B:269:ILE:HD12	1.92	0.51
3:C:185:LEU:HB2	3:C:514:ASN:ND2	2.24	0.51
1:A:146:GLU:OE2	1:A:146:GLU:N	2.43	0.51
1:A:424:LEU:O	1:A:424:LEU:HD23	2.11	0.51
1:A:1418:HIS:O	1:A:1421:GLU:HG2	2.11	0.51
1:A:1872:GLY:O	1:A:1876:ILE:HG13	2.11	0.51
1:A:2823:PHE:HD2	1:A:2824:LYS:HG2	1.73	0.51
1:A:2987:THR:HG22	1:A:2989:ALA:H	1.76	0.51
1:A:3030:ILE:HD12	1:A:3041:LEU:HD13	1.92	0.51
1:A:3443:PRO:HB3	1:A:3471:ILE:HG21	1.92	0.51
1:A:3798:SER:O	1:A:3799:ARG:HB2	2.11	0.51
2:B:59:PRO:HB2	2:B:205:LEU:HD13	1.91	0.51
2:B:66:CYS:SG	2:B:242:LEU:HD22	2.50	0.51
3:C:266:SER:OG	3:C:267:ILE:N	2.44	0.51
1:A:235:THR:HG22	1:A:281:GLN:HE22	1.75	0.51
1:A:1783:ARG:HG2	1:A:1830:HIS:NE2	2.25	0.51
1:A:3577:GLN:HB3	1:A:3630:ARG:NE	2.25	0.51
1:A:3844:THR:HG22	1:A:3850:HIS:HA	1.91	0.51
3:C:251:LEU:HB2	3:C:259:ILE:HB	1.91	0.51
1:A:32:HIS:NE2	1:A:84:GLU:OE1	2.44	0.51
1:A:437:HIS:HB2	1:A:2047:THR:HG21	1.91	0.51
1:A:526:ASP:OD1	1:A:526:ASP:N	2.44	0.51
1:A:1249:SER:HB3	1:A:1326:GLU:HB3	1.93	0.51
1:A:1841:SER:O	1:A:1898:GLN:NE2	2.43	0.51
1:A:3356:ALA:O	1:A:3360:LEU:N	2.36	0.51
1:A:3923:ARG:O	1:A:4124:TRP:NE1	2.43	0.51
3:C:315:ARG:NH2	3:C:317:GLY:O	2.42	0.51
1:A:1089:PHE:CZ	1:A:1099:PHE:HB2	2.46	0.51
1:A:3619:ASP:N	1:A:3619:ASP:OD1	2.44	0.51
1:A:3767:LEU:HD13	1:A:3918:LEU:HD22	1.92	0.51
1:A:3960:PRO:HB2	1:A:3961:PHE:CD1	2.45	0.51
2:B:204:HIS:HB3	2:B:237:SER:N	2.26	0.51
1:A:2182:ILE:HG13	1:A:2186:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2280:VAL:O	1:A:2285:LEU:HB2	2.10	0.51
2:B:463:LYS:O	2:B:467:GLU:HG2	2.10	0.51
1:A:3992:ARG:HB3	1:A:4051:LEU:O	2.11	0.51
2:B:345:LEU:HD21	2:B:434:LEU:HD21	1.92	0.51
1:A:603:ILE:HG12	1:A:1083:ASN:HB3	1.92	0.51
1:A:1294:VAL:HB	1:A:1341:ILE:CD1	2.41	0.51
1:A:2101:VAL:HG12	1:A:2156:VAL:HG21	1.93	0.51
1:A:2409:THR:HG23	1:A:2410:GLU:OE1	2.11	0.51
1:A:3510:GLN:HE22	1:A:3513:ALA:HB2	1.76	0.51
3:C:39:THR:O	3:C:43:GLN:HG2	2.11	0.51
4:D:18:DT:H2''	4:D:19:DG:C8	2.46	0.51
1:A:1651:LYS:O	1:A:1655:ILE:HG12	2.11	0.51
1:A:1723:PRO:HD2	1:A:1739:TYR:CE1	2.45	0.51
1:A:2550:ILE:HG13	1:A:2550:ILE:O	2.11	0.51
2:B:318:ARG:HH22	2:B:331:LYS:HE2	1.76	0.51
2:B:350:PHE:HB3	2:B:394:VAL:HG22	1.93	0.51
1:A:1887:ASP:OD1	1:A:1888:ASP:N	2.43	0.50
2:B:298:THR:HB	3:C:295:TYR:CD1	2.46	0.50
2:B:467:GLU:O	2:B:470:ARG:HG2	2.11	0.50
3:C:35:LYS:NZ	3:C:94:ILE:O	2.44	0.50
3:C:81:ARG:NH1	3:C:84:MET:H	2.08	0.50
1:A:101:ALA:HB1	1:A:143:LEU:HD22	1.94	0.50
1:A:451:PRO:O	1:A:452:LYS:HG2	2.11	0.50
1:A:3506:LEU:HA	1:A:3511:ALA:HB1	1.92	0.50
1:A:3670:MET:O	1:A:3674:SER:HB3	2.11	0.50
2:B:301:ARG:NE	2:B:310:LEU:HD13	2.25	0.50
1:A:144:MET:CE	1:A:185:HIS:HB2	2.41	0.50
1:A:267:VAL:HG21	3:C:554:PHE:HZ	1.76	0.50
1:A:636:GLU:HA	1:A:679:LYS:NZ	2.27	0.50
1:A:1093:GLU:HA	1:A:1096:VAL:HG22	1.92	0.50
1:A:4080:VAL:HG12	1:A:4116:ILE:HG22	1.92	0.50
2:B:518:LEU:HD23	3:C:256:ASN:HD21	1.76	0.50
3:C:684:THR:HG21	3:C:701:ALA:HA	1.94	0.50
1:A:3768:PHE:HE2	1:A:3942:PHE:CZ	2.29	0.50
2:B:340:PHE:CG	2:B:408:PRO:HD3	2.47	0.50
3:C:19:THR:O	3:C:22:ASN:ND2	2.33	0.50
1:A:662:LEU:HD23	1:A:662:LEU:H	1.77	0.50
1:A:1249:SER:OG	1:A:1326:GLU:OE1	2.23	0.50
1:A:2310:VAL:HG23	1:A:2310:VAL:O	2.12	0.50
1:A:3049:LEU:O	1:A:3053:LEU:HD23	2.12	0.50
3:C:40:MET:HG3	3:C:488:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:CYS:SG	1:A:131:LEU:HB2	2.52	0.50
1:A:1139:GLU:HB2	1:A:1197:LEU:HD11	1.93	0.50
1:A:3706:ASP:OD1	1:A:3706:ASP:N	2.43	0.50
2:B:411:VAL:HG21	2:B:434:LEU:HD22	1.94	0.50
3:C:115:MET:O	3:C:119:GLN:HG3	2.12	0.50
1:A:204:LEU:HD12	1:A:220:LEU:HD12	1.92	0.50
1:A:250:ASN:O	1:A:254:LYS:HG3	2.12	0.50
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.84	0.50
1:A:1668:PHE:O	1:A:1672:PHE:HD2	1.94	0.50
1:A:1747:LEU:HD21	1:A:1781:SER:HB3	1.94	0.50
1:A:1875:LYS:O	1:A:1879:VAL:HG23	2.12	0.50
1:A:2872:ASP:HB3	1:A:2875:ALA:HB3	1.94	0.50
1:A:3299:THR:OG1	1:A:3302:LYS:NZ	2.45	0.50
1:A:3355:LYS:O	1:A:3358:ARG:HB2	2.10	0.50
1:A:3596:LEU:HD11	1:A:3606:ILE:HB	1.93	0.50
2:B:255:ALA:HB3	5:E:30:DG:H4'	1.94	0.50
3:C:238:LYS:O	3:C:239:LYS:HG3	2.12	0.50
3:C:376:ALA:O	3:C:379:SER:OG	2.25	0.50
1:A:2824:LYS:O	1:A:2829:LYS:HG3	2.11	0.50
1:A:3535:ILE:HD13	1:A:3798:SER:HB3	1.94	0.50
1:A:3922:ASP:OD1	1:A:3924:HIS:NE2	2.45	0.50
2:B:286:ILE:O	3:C:313:GLY:N	2.33	0.50
3:C:232:ARG:HA	3:C:515:MET:HE1	1.94	0.50
1:A:977:ASP:HB2	1:A:980:THR:HG22	1.93	0.50
1:A:2402:LEU:HB2	1:A:2438:ILE:CG2	2.36	0.50
1:A:3335:ARG:NH1	1:A:3418:ASP:OD1	2.45	0.50
1:A:105:VAL:HA	1:A:147:PHE:HE1	1.75	0.49
1:A:346:TYR:HA	1:A:349:ILE:HG22	1.94	0.49
1:A:1105:VAL:O	1:A:1109:GLU:HG2	2.12	0.49
1:A:1675:TYR:CE1	1:A:1699:PHE:HE1	2.30	0.49
1:A:3233:SER:HA	1:A:3272:TRP:HZ2	1.77	0.49
1:A:3462:ARG:HE	1:A:3708:ARG:NH2	2.10	0.49
2:B:473:TYR:CD1	3:C:392:ILE:HG13	2.46	0.49
3:C:184:ARG:HG2	3:C:185:LEU:N	2.27	0.49
3:C:276:TRP:HZ2	3:C:494:LEU:HD11	1.77	0.49
1:A:859:LEU:HD21	1:A:870:LEU:HD13	1.94	0.49
1:A:2840:PHE:CE2	1:A:2868:LEU:HD21	2.47	0.49
1:A:2841:ASN:O	1:A:2845:ASN:ND2	2.33	0.49
1:A:3834:ALA:HA	1:A:3877:LYS:HD3	1.94	0.49
3:C:527:GLN:HA	3:C:530:LEU:HD12	1.94	0.49
1:A:1014:LEU:O	1:A:1017:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:VAL:CG2	1:A:1196:PRO:HD3	2.42	0.49
1:A:2268:LYS:HD2	1:A:2314:GLU:OE2	2.11	0.49
1:A:3268:THR:HG23	1:A:3269:ARG:HG3	1.93	0.49
1:A:3726:VAL:HG11	1:A:3736:LYS:HD3	1.94	0.49
1:A:3744:ASP:HB2	1:A:3746:ARG:HE	1.77	0.49
3:C:381:ILE:HG21	3:C:419:LEU:HB2	1.93	0.49
1:A:87:LYS:O	1:A:91:ILE:HG12	2.12	0.49
1:A:355:ASN:OD1	1:A:356:ASN:N	2.42	0.49
1:A:1759:LEU:HD12	1:A:1797:LEU:HD22	1.92	0.49
1:A:2256:ILE:HG22	1:A:2276:LEU:HD13	1.93	0.49
1:A:3062:LEU:HD12	1:A:3062:LEU:H	1.76	0.49
1:A:3334:TYR:HB2	1:A:3381:ALA:HB2	1.95	0.49
1:A:3420:CYS:SG	1:A:3445:LEU:HD22	2.52	0.49
2:B:40:PHE:CZ	2:B:70:VAL:HG11	2.44	0.49
2:B:360:HIS:HA	3:C:267:ILE:HD12	1.93	0.49
2:B:441:ASP:OD2	3:C:44:ARG:NH2	2.46	0.49
3:C:640:ARG:HH21	3:C:681:ASP:HB3	1.77	0.49
1:A:1379:PRO:O	1:A:1384:PHE:HB2	2.12	0.49
1:A:3316:LEU:HD22	1:A:3323:PHE:HD1	1.77	0.49
1:A:86:LEU:HD21	1:A:114:VAL:HG11	1.94	0.49
1:A:202:GLY:O	1:A:206:THR:HG23	2.13	0.49
1:A:524:TYR:HA	1:A:527:TYR:CD2	2.47	0.49
1:A:1618:LEU:O	1:A:1622:ILE:HG12	2.13	0.49
1:A:2085:MET:HG3	1:A:2090:ARG:HG2	1.93	0.49
1:A:3118:ASP:OD1	1:A:3119:VAL:N	2.44	0.49
2:B:473:TYR:HB3	3:C:350:GLN:NE2	2.25	0.49
3:C:151:ILE:HD12	3:C:215:LEU:HD13	1.95	0.49
1:A:115:TYR:HB2	1:A:127:ALA:HB1	1.94	0.49
1:A:252:VAL:O	1:A:256:ILE:HG12	2.13	0.49
1:A:1736:PHE:O	1:A:1740:VAL:HG23	2.12	0.49
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	1.95	0.49
3:C:90:LEU:O	3:C:94:ILE:HG13	2.12	0.49
1:A:373:CYS:HA	1:A:376:ILE:HG22	1.93	0.49
1:A:1138:ILE:HG13	1:A:1141:LYS:HE3	1.95	0.49
1:A:1970:LYS:HD2	1:A:1970:LYS:O	2.13	0.49
1:A:2205:VAL:HB	1:A:2208:ASP:HB3	1.94	0.49
1:A:3699:LEU:HD12	1:A:3719:ILE:HG21	1.95	0.49
1:A:4046:TYR:CZ	1:A:4062:ASP:HB3	2.47	0.49
3:C:33:GLN:HB3	3:C:227:PHE:HB3	1.94	0.49
3:C:356:PHE:CG	3:C:422:VAL:HG11	2.48	0.49
3:C:457:LEU:HD13	3:C:533:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1432:CYS:HB3	1:A:1486:LEU:HD22	1.95	0.49
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.94	0.49
1:A:1613:HIS:O	1:A:1617:LYS:HG3	2.12	0.49
1:A:2239:LYS:HA	1:A:2242:VAL:HG12	1.95	0.49
1:A:3468:LEU:HA	1:A:3471:ILE:HG22	1.93	0.49
1:A:3767:LEU:O	1:A:3771:MET:HG3	2.12	0.49
1:A:4069:GLU:O	1:A:4070:LYS:HG2	2.11	0.49
1:A:450:SER:OG	1:A:453:MET:SD	2.71	0.49
1:A:1932:GLN:H	1:A:1937:ARG:NH2	2.11	0.49
1:A:3499:ILE:O	1:A:3503:VAL:HG22	2.12	0.49
2:B:77:SER:OG	2:B:249:LYS:HB2	2.12	0.49
2:B:247:ARG:HH21	2:B:488:ARG:HG3	1.77	0.49
1:A:1142:HIS:CE1	1:A:1146:ASN:HA	2.48	0.48
1:A:1820:VAL:HA	1:A:1824:LEU:HG	1.95	0.48
1:A:1881:TYR:CE1	1:A:1889:VAL:HG11	2.48	0.48
1:A:2933:ILE:HG22	1:A:2933:ILE:O	2.13	0.48
3:C:323:PHE:HE1	3:C:328:GLU:CA	2.25	0.48
1:A:919:LEU:HD11	1:A:968:VAL:HG23	1.95	0.48
1:A:1249:SER:CB	1:A:1326:GLU:HB3	2.43	0.48
1:A:3465:PHE:O	1:A:3469:LEU:HG	2.13	0.48
1:A:3734:ARG:HB2	1:A:3734:ARG:HH11	1.78	0.48
3:C:39:THR:HA	3:C:42:VAL:HG22	1.95	0.48
4:D:16:DG:H2'	4:D:17:DC:C6	2.48	0.48
1:A:858:MET:HA	1:A:861:SER:HB2	1.95	0.48
1:A:1271:ILE:HG22	1:A:1276:VAL:HG23	1.96	0.48
1:A:2182:ILE:O	1:A:2186:VAL:HG23	2.13	0.48
1:A:2414:GLN:O	1:A:2418:LYS:HG2	2.13	0.48
1:A:3141:PHE:CD1	1:A:3189:PHE:HB3	2.48	0.48
1:A:3143:SER:O	1:A:3146:SER:OG	2.24	0.48
1:A:3144:PHE:O	1:A:3150:ASN:ND2	2.45	0.48
2:B:48:MET:SD	2:B:48:MET:N	2.87	0.48
2:B:73:SER:O	2:B:77:SER:HB3	2.12	0.48
2:B:106:GLN:HB3	2:B:115:ARG:NH1	2.28	0.48
1:A:152:LEU:HA	1:A:155:LYS:NZ	2.29	0.48
1:A:235:THR:CG2	1:A:281:GLN:HE22	2.26	0.48
1:A:297:LEU:HB3	1:A:316:LEU:HD12	1.94	0.48
1:A:1389:VAL:HG13	1:A:1390:GLN:N	2.29	0.48
1:A:1470:SER:OG	1:A:1477:HIS:HA	2.14	0.48
1:A:1505:LEU:HD23	1:A:1505:LEU:H	1.77	0.48
1:A:2923:TRP:CH2	1:A:3973:PRO:HB2	2.49	0.48
1:A:2972:TYR:O	1:A:2976:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ASP:OD1	2:B:242:LEU:N	2.46	0.48
2:B:529:VAL:HG23	2:B:530:TYR:HD1	1.78	0.48
1:A:208:MET:HE1	1:A:255:ALA:HB2	1.95	0.48
1:A:1107:TYR:OH	1:A:1127:CYS:HA	2.13	0.48
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.13	0.48
1:A:3916:TRP:CD1	1:A:3960:PRO:HB3	2.49	0.48
2:B:297:LYS:HE2	3:C:296:CYS:SG	2.53	0.48
2:B:363:ARG:NH2	2:B:363:ARG:HB3	2.28	0.48
3:C:632:PHE:HB3	3:C:677:ILE:HD13	1.94	0.48
3:C:688:LYS:HE3	3:C:694:SER:H	1.79	0.48
1:A:439:VAL:O	1:A:443:ILE:HG12	2.14	0.48
1:A:1058:SER:HA	1:A:1061:LYS:HG3	1.95	0.48
1:A:2440:TYR:HD1	1:A:2476:ILE:HG22	1.77	0.48
1:A:3055:GLY:O	1:A:3056:GLU:HG3	2.14	0.48
1:A:3448:GLU:HB3	1:A:3452:LYS:HE2	1.93	0.48
2:B:297:LYS:O	2:B:297:LYS:HG2	2.12	0.48
2:B:392:LYS:NZ	3:C:455:ASP:OD1	2.44	0.48
3:C:338:LYS:HB3	3:C:398:ASP:HA	1.96	0.48
3:C:411:HIS:CB	3:C:418:CYS:N	2.74	0.48
1:A:101:ALA:HB2	1:A:143:LEU:HD13	1.96	0.48
1:A:455:LEU:O	1:A:459:ARG:HG2	2.13	0.48
1:A:1886:LYS:HB2	1:A:1890:HIS:CD2	2.48	0.48
1:A:1920:TYR:O	1:A:1924:THR:OG1	2.23	0.48
3:C:387:LEU:CD2	3:C:389:MET:HG3	2.43	0.48
3:C:511:HIS:O	3:C:515:MET:HG2	2.13	0.48
3:C:528:ILE:HB	3:C:529:PRO:HD3	1.96	0.48
1:A:1649:LEU:HD21	1:A:1675:TYR:CE1	2.48	0.48
1:A:1876:ILE:HG22	1:A:1880:MET:CE	2.44	0.48
1:A:3026:ASP:N	1:A:3026:ASP:OD1	2.47	0.48
1:A:3090:TYR:HD2	1:A:3098:ARG:HB3	1.79	0.48
1:A:629:PHE:O	1:A:633:ILE:HG12	2.14	0.48
1:A:1668:PHE:HB3	1:A:1669:PRO:HD3	1.95	0.48
1:A:1864:ASP:O	1:A:1868:THR:HG23	2.14	0.48
1:A:2398:LEU:HA	1:A:2401:VAL:HG22	1.96	0.48
1:A:3133:GLN:HG2	1:A:3182:ILE:HD11	1.96	0.48
1:A:3550:LYS:O	1:A:3553:GLU:HG3	2.14	0.48
2:B:145:GLU:O	2:B:148:TRP:HB3	2.14	0.48
3:C:155:LYS:NZ	3:C:216:GLU:OE1	2.45	0.48
3:C:653:GLN:HA	3:C:656:ASN:HD21	1.77	0.48
1:A:92:PHE:HA	1:A:95:LYS:HB3	1.95	0.48
1:A:1616:LEU:O	1:A:1620:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2528:GLU:O	1:A:2529:THR:OG1	2.27	0.48
3:C:44:ARG:HD3	3:C:237:PHE:CZ	2.49	0.48
3:C:194:LEU:O	3:C:195:LYS:HE2	2.14	0.48
1:A:1389:VAL:HG13	1:A:1390:GLN:H	1.79	0.47
1:A:1484:LEU:HD21	1:A:1531:LEU:HD12	1.94	0.47
1:A:1685:ASP:O	1:A:1689:LYS:HG3	2.14	0.47
1:A:3685:PRO:O	1:A:3689:ASP:N	2.44	0.47
1:A:1772:HIS:H	1:A:1822:ARG:HH22	1.62	0.47
1:A:2412:TYR:HE2	1:A:2454:LEU:HG	1.80	0.47
1:A:3737:ARG:HB3	1:A:3751:LEU:HD23	1.95	0.47
5:E:34:DC:H1'	5:E:35:DG:C8	2.49	0.47
1:A:1301:ILE:HG23	1:A:1302:ALA:H	1.78	0.47
1:A:2286:PRO:HG2	1:A:2288:TYR:CD1	2.49	0.47
1:A:2341:LEU:H	1:A:2341:LEU:HD23	1.79	0.47
1:A:3053:LEU:HD22	1:A:3092:LEU:HD11	1.97	0.47
1:A:3496:ILE:HG21	1:A:3705:TYR:HB3	1.97	0.47
1:A:3654:MET:SD	1:A:3655:LYS:N	2.88	0.47
2:B:368:VAL:CG2	2:B:432:PHE:HB2	2.44	0.47
3:C:253:ILE:HB	3:C:257:LEU:HB3	1.97	0.47
1:A:267:VAL:HG21	3:C:554:PHE:CZ	2.50	0.47
1:A:1893:GLU:O	1:A:1897:ASN:ND2	2.47	0.47
1:A:1919:CYS:SG	1:A:1920:TYR:N	2.87	0.47
1:A:3281:CYS:SG	1:A:3307:LEU:HD21	2.54	0.47
1:A:3417:ALA:HB1	1:A:3446:VAL:HG13	1.96	0.47
1:A:3558:ILE:O	1:A:3562:LEU:N	2.44	0.47
2:B:442:ASP:O	3:C:267:ILE:HA	2.14	0.47
3:C:229:GLU:HB3	3:C:232:ARG:HH21	1.79	0.47
3:C:371:GLU:HB3	3:C:374:ALA:HB2	1.97	0.47
1:A:1696:LEU:O	1:A:1700:THR:HG23	2.15	0.47
1:A:2546:TYR:CD2	1:A:2548:PRO:HD3	2.49	0.47
1:A:3172:LYS:HA	1:A:3779:SER:HB2	1.95	0.47
1:A:3534:ILE:HG13	1:A:3535:ILE:HG13	1.96	0.47
2:B:366:LEU:HB2	2:B:434:LEU:HB2	1.96	0.47
3:C:688:LYS:HB3	3:C:694:SER:HB2	1.97	0.47
1:A:765:LEU:HA	1:A:768:VAL:HG12	1.97	0.47
1:A:2572:TYR:N	1:A:2573:PRO:HD3	2.29	0.47
1:A:3086:LEU:HB3	1:A:3102:TYR:CD2	2.50	0.47
1:A:3356:ALA:HA	1:A:3359:ILE:HD12	1.95	0.47
1:A:3728:VAL:HG12	1:A:3736:LYS:HE3	1.96	0.47
1:A:3960:PRO:HB2	1:A:3961:PHE:HD1	1.79	0.47
2:B:289:TYR:HD2	2:B:292:THR:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:VAL:HA	2:B:469:LEU:HB2	1.96	0.47
1:A:111:CYS:HA	1:A:114:VAL:HG12	1.96	0.47
1:A:385:TYR:CE1	1:A:389:ILE:HD11	2.49	0.47
1:A:624:ILE:O	1:A:627:VAL:HG22	2.14	0.47
1:A:631:ARG:NH1	1:A:668:LYS:HD3	2.30	0.47
1:A:750:PRO:HA	1:A:753:GLN:HG2	1.97	0.47
1:A:873:VAL:HG13	1:A:874:THR:N	2.23	0.47
1:A:901:MET:HG3	1:A:903:PRO:HD3	1.96	0.47
1:A:1067:ALA:O	1:A:1075:ARG:HG2	2.14	0.47
1:A:1325:GLN:NE2	1:A:1326:GLU:HG3	2.30	0.47
1:A:1952:ILE:O	1:A:1955:VAL:HG22	2.14	0.47
1:A:2377:ARG:HG3	1:A:2378:PHE:CD1	2.49	0.47
1:A:2433:LYS:NZ	1:A:2437:ASP:OD1	2.47	0.47
1:A:2547:SER:HA	1:A:2548:PRO:HD2	1.52	0.47
1:A:2840:PHE:HE2	1:A:2868:LEU:HD21	1.80	0.47
1:A:3120:LEU:HD13	1:A:3896:ALA:HA	1.96	0.47
1:A:3296:GLN:O	1:A:3300:VAL:HG12	2.14	0.47
1:A:3351:ILE:HG13	1:A:3351:ILE:O	2.14	0.47
1:A:3522:THR:O	1:A:3526:PRO:HB3	2.15	0.47
1:A:3558:ILE:HA	1:A:3561:LYS:HG2	1.96	0.47
2:B:517:ARG:NH1	2:B:517:ARG:HB2	2.30	0.47
3:C:27:ILE:HG13	3:C:28:GLU:N	2.29	0.47
1:A:475:LEU:HD23	1:A:475:LEU:H	1.80	0.47
1:A:941:MET:HE3	1:A:961:LEU:HD22	1.97	0.47
1:A:1539:SER:HA	1:A:1552:HIS:HA	1.95	0.47
1:A:1861:SER:O	1:A:1865:THR:HG23	2.15	0.47
1:A:1947:CYS:O	1:A:1951:VAL:HG13	2.14	0.47
1:A:2574:ASN:O	1:A:2576:MET:N	2.47	0.47
1:A:3498:TRP:HH2	1:A:4001:THR:HG23	1.80	0.47
3:C:246:HIS:CG	3:C:368:ARG:HH22	2.32	0.47
1:A:399:GLN:HG3	1:A:400:THR:HG23	1.97	0.47
1:A:2563:LEU:O	1:A:2566:THR:HG22	2.15	0.47
1:A:2956:ALA:HB2	1:A:2971:GLN:HG3	1.97	0.47
1:A:3018:SER:OG	1:A:3040:TYR:OH	2.28	0.47
1:A:3469:LEU:HD22	1:A:3510:GLN:NE2	2.29	0.47
1:A:3567:VAL:HG11	1:A:3697:ASN:HB2	1.96	0.47
2:B:125:GLN:OE1	2:B:128:GLN:NE2	2.48	0.47
3:C:96:SER:O	3:C:96:SER:OG	2.28	0.47
4:D:8:DC:H4'	4:D:9:DC:OP1	2.14	0.47
1:A:189:MET:HB2	1:A:192:ASN:OD1	2.15	0.47
1:A:1129:ASP:O	1:A:1132:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:ILE:O	1:A:1225:GLU:HG2	2.13	0.47
1:A:1267:TYR:O	1:A:1271:ILE:HG12	2.15	0.47
1:A:1592:MET:O	1:A:1596:VAL:HG23	2.15	0.47
1:A:1690:GLY:HA2	1:A:1693:VAL:HG22	1.97	0.47
1:A:1714:LEU:O	1:A:1718:ILE:HG12	2.15	0.47
1:A:2182:ILE:HG13	1:A:2182:ILE:O	2.14	0.47
1:A:2401:VAL:O	1:A:2405:VAL:HG13	2.15	0.47
1:A:2436:LEU:HD21	1:A:2458:VAL:HG23	1.96	0.47
1:A:2885:GLN:O	1:A:2888:VAL:HG22	2.14	0.47
1:A:2967:GLU:HA	1:A:2970:LYS:HB2	1.97	0.47
1:A:3335:ARG:HG2	1:A:3419:PHE:HD2	1.80	0.47
2:B:513:ALA:O	2:B:516:LYS:HG3	2.14	0.47
1:A:204:LEU:HD11	1:A:224:LEU:HG	1.96	0.46
1:A:1294:VAL:HB	1:A:1341:ILE:HD12	1.97	0.46
1:A:2166:SER:O	1:A:2170:GLN:HG2	2.15	0.46
1:A:2420:PHE:HA	1:A:2423:VAL:HG12	1.97	0.46
1:A:3277:VAL:HG21	1:A:3311:ASN:HD22	1.80	0.46
1:A:3307:LEU:HA	1:A:3311:ASN:HD21	1.80	0.46
1:A:4096:SER:OG	1:A:4097:GLY:N	2.47	0.46
2:B:45:SER:HB3	2:B:48:MET:HE1	1.97	0.46
3:C:689:GLU:HG3	3:C:691:ALA:HB3	1.97	0.46
1:A:266:ALA:N	1:A:268:PRO:HD2	2.31	0.46
1:A:1760:GLU:HA	1:A:1804:MET:HE1	1.98	0.46
1:A:3006:ALA:HB1	1:A:3008:TRP:CE2	2.50	0.46
1:A:3179:TRP:O	1:A:3183:ILE:HG12	2.15	0.46
1:A:3793:VAL:HG13	1:A:3803:ILE:HG12	1.96	0.46
2:B:269:ILE:CD1	2:B:381:LEU:HD11	2.46	0.46
3:C:92:GLU:OE1	3:C:499:LEU:HD22	2.15	0.46
1:A:862:LEU:HD13	1:A:866:ILE:CG2	2.46	0.46
2:B:361:TYR:OH	3:C:422:VAL:HG13	2.16	0.46
3:C:496:HIS:CG	3:C:506:PRO:HG3	2.50	0.46
5:E:37:DC:H2"	5:E:38:DA:H5"	1.98	0.46
1:A:2091:HIS:CG	1:A:2091:HIS:O	2.69	0.46
1:A:2786:LYS:HG3	1:A:2787:HIS:H	1.80	0.46
1:A:3134:ALA:O	1:A:3138:ILE:HG12	2.16	0.46
1:A:3822:GLN:HA	1:A:3825:LYS:HG2	1.96	0.46
2:B:330:GLU:HG3	2:B:332:GLU:N	2.30	0.46
1:A:477:ASN:O	1:A:480:SER:OG	2.33	0.46
1:A:1224:PHE:HB3	1:A:1266:CYS:SG	2.55	0.46
1:A:1428:ILE:HD13	1:A:1468:LEU:HD11	1.98	0.46
1:A:2392:VAL:O	1:A:2396:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3532:PRO:O	1:A:3536:SER:N	2.37	0.46
2:B:351:LYS:CG	3:C:463:LEU:HB2	2.46	0.46
1:A:11:SER:HB2	1:A:38:LEU:HD21	1.98	0.46
1:A:1604:SER:HB2	1:A:1618:LEU:HD21	1.98	0.46
1:A:3274:VAL:HA	1:A:3277:VAL:HG12	1.97	0.46
1:A:2268:LYS:HG2	1:A:2312:TYR:CD2	2.51	0.46
1:A:3138:ILE:HD12	1:A:3189:PHE:HZ	1.80	0.46
1:A:3183:ILE:HG13	1:A:3242:MET:HB2	1.98	0.46
3:C:46:VAL:HG13	3:C:47:PHE:HD1	1.81	0.46
3:C:609:PHE:CD2	3:C:610:GLU:HG2	2.51	0.46
1:A:240:GLU:HG2	1:A:241:ASP:H	1.81	0.46
1:A:579:LEU:HD21	1:A:2036:LEU:HD12	1.98	0.46
1:A:935:HIS:O	1:A:939:MET:HG2	2.16	0.46
1:A:1409:SER:HB2	1:A:1410:PRO:HD2	1.98	0.46
1:A:3632:PHE:O	1:A:3636:PHE:CB	2.64	0.46
1:A:9:ARG:NE	1:A:57:LEU:HG	2.26	0.46
1:A:367:GLY:HA3	1:A:416:SER:HA	1.98	0.46
1:A:1210:ASP:O	1:A:1213:LYS:HG3	2.16	0.46
1:A:1590:THR:HA	1:A:1593:VAL:HG12	1.97	0.46
1:A:1657:SER:OG	1:A:1658:SER:N	2.49	0.46
1:A:1726:SER:OG	1:A:1727:ARG:N	2.48	0.46
1:A:2155:GLU:CD	1:A:2155:GLU:H	2.19	0.46
1:A:4064:LEU:CD2	1:A:4077:TYR:HB3	2.38	0.46
2:B:302:THR:HG23	2:B:311:LEU:HB2	1.97	0.46
3:C:56:LEU:O	3:C:81:ARG:N	2.44	0.46
3:C:265:LYS:HD3	3:C:268:LEU:HD13	1.98	0.46
1:A:338:LEU:HD21	1:A:373:CYS:SG	2.55	0.46
1:A:569:VAL:HA	1:A:572:VAL:HG12	1.98	0.46
1:A:959:TYR:HD2	1:A:963:LYS:HD2	1.81	0.46
1:A:2038:GLU:O	1:A:2041:SER:N	2.49	0.46
2:B:337:LEU:HD11	3:C:490:LEU:HD12	1.97	0.46
1:A:821:ALA:HB1	1:A:829:VAL:HG23	1.99	0.45
1:A:973:ALA:O	1:A:981:ARG:HG3	2.16	0.45
1:A:1298:LEU:CD2	1:A:1368:LEU:HA	2.46	0.45
1:A:1689:LYS:O	1:A:1693:VAL:N	2.40	0.45
1:A:1689:LYS:HA	1:A:1692:ALA:HB3	1.98	0.45
1:A:2038:GLU:CG	1:A:2042:GLN:HE22	2.28	0.45
1:A:2571:ASP:C	1:A:2573:PRO:HD3	2.35	0.45
1:A:3045:ILE:HD11	1:A:3082:TYR:CE1	2.50	0.45
1:A:3580:ASN:O	1:A:3583:LEU:HG	2.15	0.45
1:A:3606:ILE:HG21	1:A:3655:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3780:ALA:HB1	1:A:3986:HIS:ND1	2.32	0.45
2:B:187:ARG:HB2	2:B:187:ARG:CZ	2.46	0.45
1:A:166:ILE:HB	1:A:170:VAL:CG2	2.46	0.45
1:A:623:PHE:O	1:A:627:VAL:HG13	2.17	0.45
1:A:645:TRP:CZ3	1:A:1505:LEU:HD13	2.51	0.45
1:A:1297:PHE:HZ	1:A:1337:VAL:HG23	1.80	0.45
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.49	0.45
1:A:1945:TYR:HE1	1:A:1966:LEU:HA	1.81	0.45
1:A:3100:LYS:O	1:A:3103:ILE:HG22	2.16	0.45
1:A:3385:LEU:HD21	1:A:3416:LEU:HA	1.99	0.45
1:A:3699:LEU:HB2	1:A:3719:ILE:CG2	2.47	0.45
1:A:3789:ARG:HB3	1:A:3938:ILE:HG23	1.99	0.45
2:B:219:ASP:N	2:B:219:ASP:OD1	2.48	0.45
2:B:322:TYR:CE2	3:C:274:LYS:CG	2.59	0.45
1:A:873:VAL:CG1	1:A:874:THR:H	2.23	0.45
1:A:1034:ARG:HA	1:A:1085:ILE:HG22	1.98	0.45
1:A:2091:HIS:O	1:A:2091:HIS:ND1	2.50	0.45
1:A:2528:GLU:OE2	1:A:2533:SER:OG	2.26	0.45
1:A:3128:LYS:HA	1:A:3128:LYS:HD2	1.76	0.45
1:A:3409:VAL:HG22	1:A:3413:TYR:CE2	2.52	0.45
1:A:3462:ARG:HD3	1:A:3497:SER:OG	2.15	0.45
1:A:3908:HIS:NE2	1:A:3912:CYS:SG	2.89	0.45
1:A:4126:PRO:HD2	1:A:4127:TRP:CZ3	2.52	0.45
2:B:72:ILE:HD11	2:B:495:LEU:HD21	1.98	0.45
2:B:261:LEU:CD1	2:B:269:ILE:HD12	2.47	0.45
3:C:154:LEU:HD22	3:C:159:ILE:HD11	1.99	0.45
3:C:496:HIS:CE1	3:C:503:GLU:HB2	2.51	0.45
1:A:344:GLN:O	1:A:348:ILE:HG12	2.16	0.45
1:A:439:VAL:CG1	1:A:482:VAL:HG21	2.47	0.45
1:A:565:TYR:OH	1:A:634:LEU:HD22	2.17	0.45
1:A:3091:LEU:HD22	1:A:3188:PHE:CE2	2.51	0.45
1:A:3708:ARG:HA	1:A:3708:ARG:HD3	1.54	0.45
1:A:3880:ALA:HB2	1:A:3965:ARG:HH21	1.79	0.45
1:A:3889:ARG:HG2	1:A:3889:ARG:HH21	1.81	0.45
2:B:94:LYS:H	2:B:103:TYR:HA	1.80	0.45
3:C:362:LEU:HD12	3:C:421:TYR:CD2	2.52	0.45
1:A:176:GLU:HG3	1:A:225:LYS:HG3	1.98	0.45
1:A:320:LEU:HD22	1:A:345:PHE:HZ	1.80	0.45
1:A:1801:VAL:HA	1:A:1804:MET:HE3	1.99	0.45
1:A:2216:LEU:O	1:A:2220:MET:HG3	2.17	0.45
1:A:2844:LEU:HD11	1:A:2871:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3496:ILE:HD12	1:A:3496:ILE:H	1.80	0.45
1:A:3681:LYS:HD2	1:A:3722:PHE:HB3	1.97	0.45
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	1.98	0.45
1:A:4049:ARG:HB3	1:A:4059:ILE:HD11	1.99	0.45
2:B:297:LYS:NZ	2:B:297:LYS:HB3	2.25	0.45
3:C:164:PHE:CE2	3:C:236:VAL:HG12	2.52	0.45
1:A:440:VAL:HG13	1:A:482:VAL:HG23	1.97	0.45
1:A:1178:ARG:HE	1:A:1180:GLN:NE2	2.14	0.45
1:A:1356:TRP:HA	1:A:1359:LEU:HD13	1.97	0.45
1:A:1965:PHE:O	1:A:1966:LEU:HB2	2.16	0.45
1:A:2251:ILE:CG1	1:A:2285:LEU:CD1	2.94	0.45
1:A:2486:ASP:O	1:A:2488:GLU:N	2.49	0.45
1:A:3172:LYS:NZ	1:A:3777:GLN:HG3	2.32	0.45
1:A:3281:CYS:SG	1:A:3285:HIS:CE1	3.10	0.45
1:A:3506:LEU:HB2	1:A:3533:PHE:CZ	2.42	0.45
1:A:4116:ILE:HG13	1:A:4117:LEU:HD12	1.97	0.45
2:B:58:THR:HG23	2:B:61:ASP:H	1.81	0.45
2:B:446:MET:HB2	2:B:448:PHE:CE1	2.51	0.45
3:C:342:VAL:HG22	3:C:393:VAL:HG22	1.99	0.45
1:A:125:ILE:HB	1:A:126:PRO:HD3	1.97	0.45
1:A:459:ARG:HH22	1:A:545:LEU:HD11	1.80	0.45
1:A:1432:CYS:HB3	1:A:1486:LEU:CD2	2.46	0.45
1:A:3011:LEU:HD11	1:A:3043:TYR:HD1	1.82	0.45
2:B:470:ARG:NH2	3:C:347:LYS:HB3	2.31	0.45
3:C:627:ASN:HD22	3:C:632:PHE:HZ	1.64	0.45
4:D:18:DT:H3	5:E:26:DA:H2	1.65	0.45
1:A:2575:PRO:HD3	1:A:2787:HIS:HB2	1.98	0.45
1:A:3407:ALA:HA	1:A:3410:ILE:HG12	1.99	0.45
1:A:3413:TYR:CD1	1:A:3449:LYS:HB3	2.52	0.45
1:A:3496:ILE:O	1:A:3499:ILE:HG22	2.17	0.45
2:B:263:LEU:HD11	2:B:269:ILE:HD11	1.99	0.45
3:C:226:SER:OG	3:C:228:SER:OG	2.30	0.45
3:C:357:MET:CE	3:C:429:ASP:HB3	2.45	0.45
1:A:1090:ARG:HD3	1:A:1137:ILE:HG21	1.98	0.45
2:B:191:GLY:HA2	2:B:194:ARG:HG2	1.98	0.45
1:A:1088:GLU:C	1:A:1090:ARG:H	2.21	0.45
1:A:1626:TRP:CH2	1:A:1649:LEU:HD13	2.52	0.45
1:A:1779:GLN:HB3	1:A:1783:ARG:HH12	1.82	0.45
1:A:1983:ASP:OD1	1:A:1986:ARG:N	2.50	0.45
1:A:1988:TYR:CZ	1:A:2088:LEU:HD21	2.52	0.45
1:A:2224:PHE:CD2	1:A:2272:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2980:ASP:OD1	1:A:2981:TRP:N	2.43	0.45
1:A:3126:LEU:O	1:A:3130:GLN:HG3	2.17	0.45
1:A:3658:ASP:OD1	1:A:3658:ASP:N	2.49	0.45
3:C:347:LYS:HD3	3:C:387:LEU:HD21	1.99	0.45
3:C:484:ASN:HB3	3:C:487:PHE:CD1	2.51	0.45
1:A:1190:LEU:HD12	1:A:1194:PHE:CE2	2.52	0.44
1:A:1433:ALA:H	1:A:1436:LEU:HD21	1.82	0.44
1:A:2920:VAL:O	1:A:2924:VAL:HG23	2.16	0.44
1:A:3455:LYS:HA	1:A:3490:VAL:HG23	1.99	0.44
1:A:3514:VAL:HG23	1:A:3514:VAL:O	2.17	0.44
1:A:3531:TYR:O	1:A:3535:ILE:HD12	2.18	0.44
1:A:3660:ASN:HD22	1:A:3663:THR:HG21	1.82	0.44
1:A:4088:ASN:HB3	1:A:4090:ARG:HG2	1.99	0.44
3:C:200:GLN:O	3:C:203:GLU:HG3	2.17	0.44
3:C:519:PRO:O	3:C:522:VAL:HG22	2.17	0.44
1:A:712:LYS:O	1:A:716:VAL:HG23	2.17	0.44
1:A:1839:PHE:O	1:A:1843:ILE:HG12	2.17	0.44
1:A:2953:THR:O	1:A:2957:LEU:HD23	2.18	0.44
1:A:3911:ILE:HG23	1:A:3915:HIS:CE1	2.52	0.44
1:A:3951:GLN:HG2	1:A:4063:GLU:O	2.18	0.44
2:B:87:PHE:HE2	2:B:105:LEU:HD22	1.82	0.44
2:B:242:LEU:HD23	2:B:242:LEU:O	2.17	0.44
4:D:15:DC:H42	5:E:28:DC:H42	1.65	0.44
1:A:303:HIS:ND1	1:A:305:ASN:HB2	2.31	0.44
1:A:400:THR:HB	1:A:404:ASP:HB3	2.00	0.44
1:A:619:ASP:OD2	1:A:2035:THR:HB	2.17	0.44
1:A:671:SER:HA	1:A:674:VAL:HG12	1.98	0.44
1:A:1589:ASN:HB3	1:A:1592:MET:HB2	1.98	0.44
1:A:1888:ASP:N	1:A:1888:ASP:OD1	2.49	0.44
1:A:2182:ILE:O	1:A:2186:VAL:N	2.41	0.44
1:A:2338:GLU:O	1:A:2342:CYS:HB2	2.17	0.44
1:A:3495:PHE:O	1:A:3499:ILE:N	2.50	0.44
2:B:351:LYS:HG3	3:C:463:LEU:HB2	1.99	0.44
3:C:147:LEU:O	3:C:150:ILE:HG12	2.17	0.44
4:D:25:DT:H2"	4:D:26:DT:H5"	1.98	0.44
1:A:212:VAL:HG12	1:A:213:ARG:HB2	1.99	0.44
1:A:238:MET:HE2	1:A:246:ARG:NH1	2.32	0.44
1:A:1605:PHE:HB2	1:A:1655:ILE:HD11	2.00	0.44
2:B:423:GLN:HG3	2:B:425:ILE:HG23	1.98	0.44
2:B:526:LYS:HA	2:B:530:TYR:CZ	2.53	0.44
3:C:362:LEU:HB2	3:C:421:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HG13	1:A:127:ALA:HB2	2.00	0.44
1:A:134:LEU:HD21	1:A:147:PHE:CE1	2.52	0.44
1:A:363:ILE:HD12	1:A:413:PHE:CE1	2.52	0.44
1:A:670:LEU:HA	1:A:673:THR:HG22	1.99	0.44
1:A:1504:ASP:N	1:A:1507:CYS:SG	2.88	0.44
1:A:1804:MET:HA	1:A:1807:LYS:HZ2	1.82	0.44
1:A:1832:SER:CB	1:A:1836:LEU:HD22	2.45	0.44
1:A:2183:HIS:O	1:A:2187:VAL:HG23	2.16	0.44
1:A:2251:ILE:HD13	1:A:2285:LEU:HD13	2.00	0.44
1:A:2365:ASN:O	1:A:2369:LYS:HG3	2.18	0.44
1:A:3297:VAL:HG21	1:A:3341:LEU:HD11	1.99	0.44
2:B:439:PHE:CD1	3:C:484:ASN:HA	2.52	0.44
3:C:305:VAL:HG21	3:C:310:ILE:HD11	2.00	0.44
1:A:100:ILE:HB	1:A:138:PHE:HZ	1.82	0.44
1:A:1720:ALA:HA	3:C:596:GLU:HG2	1.99	0.44
1:A:1788:ARG:HA	1:A:1788:ARG:HD3	1.63	0.44
1:A:1896:ILE:HG13	1:A:1897:ASN:N	2.32	0.44
1:A:2459:VAL:HG11	1:A:2501:LEU:CD2	2.48	0.44
1:A:2472:GLN:O	1:A:2476:ILE:HG23	2.18	0.44
1:A:2952:ILE:HD11	1:A:2971:GLN:HB2	2.00	0.44
2:B:207:LYS:HB3	2:B:208:PRO:HD3	1.99	0.44
3:C:398:ASP:OD1	3:C:400:ARG:N	2.45	0.44
1:A:793:LEU:N	1:A:794:PRO:HD2	2.33	0.44
1:A:1360:LYS:HE2	1:A:1362:ASP:OD2	2.18	0.44
1:A:1807:LYS:NZ	1:A:1811:ARG:HH12	2.15	0.44
1:A:1991:PRO:O	1:A:2184:TYR:HD1	2.00	0.44
1:A:2274:ILE:HD12	1:A:2318:ALA:HB3	2.00	0.44
2:B:284:PRO:HA	2:B:285:PRO:HD3	1.83	0.44
2:B:350:PHE:HB3	2:B:394:VAL:CG2	2.47	0.44
3:C:13:CYS:SG	3:C:134:ILE:HA	2.58	0.44
3:C:365:PHE:CD1	3:C:418:CYS:HB3	2.53	0.44
3:C:450:GLN:O	3:C:454:VAL:HG22	2.18	0.44
3:C:512:ILE:O	3:C:515:MET:HB2	2.17	0.44
1:A:162:LEU:HD12	1:A:163:LYS:O	2.18	0.44
1:A:657:SER:O	1:A:661:PRO:HA	2.18	0.44
1:A:759:GLY:O	1:A:760:LEU:HB2	2.18	0.44
1:A:1990:PHE:HZ	1:A:2088:LEU:HD12	1.83	0.44
1:A:2034:SER:N	1:A:2037:SER:HG	2.15	0.44
1:A:2958:LEU:HD11	1:A:4101:GLU:CG	2.44	0.44
1:A:3282:ARG:HA	1:A:3285:HIS:ND1	2.33	0.44
1:A:3503:VAL:CG2	1:A:3532:PRO:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3686:TRP:HH2	1:A:3699:LEU:HD11	1.81	0.44
1:A:3916:TRP:HH2	1:A:4103:GLN:HE21	1.66	0.44
3:C:155:LYS:HE3	3:C:215:LEU:CD1	2.48	0.44
1:A:1059:LEU:O	1:A:1062:ARG:HG2	2.18	0.44
1:A:1766:LEU:HB2	1:A:1778:PHE:CE2	2.53	0.44
1:A:1828:LEU:HB3	1:A:1879:VAL:HG11	2.00	0.44
1:A:2225:HIS:C	1:A:2227:LYS:H	2.21	0.44
1:A:2987:THR:O	1:A:2991:LYS:HG3	2.18	0.44
1:A:3137:GLU:OE2	1:A:3186:ARG:NH2	2.51	0.44
1:A:3552:LYS:HE3	1:A:3552:LYS:HB2	1.90	0.44
1:A:3567:VAL:HG13	1:A:3568:ILE:N	2.33	0.44
2:B:121:GLN:HG3	2:B:122:PHE:CE1	2.53	0.44
2:B:244:ARG:HG3	2:B:245:LYS:N	2.33	0.44
2:B:252:ARG:HH11	3:C:431:ARG:HE	1.64	0.44
2:B:409:TYR:HA	2:B:439:PHE:CZ	2.47	0.44
3:C:50:ASN:OD1	3:C:52:ASP:HB2	2.18	0.44
1:A:100:ILE:HB	1:A:138:PHE:CZ	2.52	0.43
1:A:180:LEU:O	1:A:184:VAL:HG22	2.18	0.43
1:A:759:GLY:C	1:A:761:SER:H	2.20	0.43
1:A:2105:HIS:CE1	1:A:2156:VAL:HA	2.53	0.43
1:A:3285:HIS:HE1	1:A:3329:LEU:HD22	1.80	0.43
2:B:444:ARG:CZ	3:C:268:LEU:HD21	2.48	0.43
2:B:451:LYS:HD2	2:B:451:LYS:HA	1.83	0.43
3:C:532:LYS:O	3:C:536:LEU:CB	2.58	0.43
1:A:121:ALA:HA	1:A:124:LYS:HB2	1.99	0.43
1:A:1268:ASN:HD21	1:A:1343:GLU:HG3	1.82	0.43
1:A:3309:GLU:HG2	1:A:3310:ASN:N	2.33	0.43
1:A:3595:GLU:O	1:A:3602:ASN:ND2	2.42	0.43
2:B:357:LYS:HG2	2:B:360:HIS:CD2	2.52	0.43
1:A:436:GLU:O	1:A:440:VAL:HG13	2.18	0.43
1:A:913:ARG:HD2	1:A:913:ARG:HA	1.76	0.43
1:A:1488:TYR:CE2	1:A:1531:LEU:HD22	2.54	0.43
1:A:1638:PRO:C	1:A:1640:GLU:H	2.22	0.43
1:A:1970:LYS:HA	1:A:1971:PRO:HD3	1.85	0.43
1:A:2277:LEU:HA	1:A:2280:VAL:HG12	2.00	0.43
2:B:360:HIS:ND1	3:C:267:ILE:HD11	2.33	0.43
2:B:515:ASN:ND2	3:C:256:ASN:OD1	2.51	0.43
3:C:599:ARG:HD3	3:C:599:ARG:HA	1.73	0.43
1:A:238:MET:SD	1:A:245:SER:HB3	2.58	0.43
1:A:323:VAL:O	1:A:327:VAL:HG12	2.18	0.43
1:A:1007:VAL:O	1:A:1011:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:LEU:CD1	1:A:1341:ILE:HD13	2.48	0.43
1:A:1679:LEU:HD23	1:A:1689:LYS:HD3	2.00	0.43
1:A:3353:GLU:HB2	1:A:3355:LYS:NZ	2.33	0.43
2:B:380:THR:HG22	3:C:444:TYR:HA	2.01	0.43
3:C:165:LEU:HD12	3:C:166:PRO:O	2.18	0.43
3:C:312:GLN:NE2	3:C:324:SER:O	2.51	0.43
3:C:526:SER:O	3:C:529:PRO:HD2	2.19	0.43
1:A:118:ASP:OD1	1:A:123:CYS:HB2	2.19	0.43
1:A:160:LEU:HD22	1:A:175:TYR:HE1	1.84	0.43
1:A:413:PHE:O	1:A:417:VAL:HG23	2.18	0.43
1:A:1975:LEU:O	1:A:1976:LEU:HD23	2.19	0.43
1:A:3240:MET:SD	1:A:3279:SER:OG	2.66	0.43
1:A:566:ASP:O	1:A:570:LYS:HG3	2.19	0.43
1:A:1124:ILE:HG13	1:A:1125:GLN:OE1	2.19	0.43
1:A:1488:TYR:CD2	1:A:1531:LEU:HD13	2.53	0.43
1:A:1775:GLU:O	1:A:1779:GLN:HG2	2.19	0.43
1:A:2286:PRO:HG2	1:A:2288:TYR:CE1	2.54	0.43
1:A:2546:TYR:CE1	1:A:2854:PHE:CZ	3.07	0.43
1:A:3410:ILE:HA	1:A:3413:TYR:HB2	2.01	0.43
1:A:3835:PRO:HG2	1:A:3878:VAL:HG13	2.00	0.43
1:A:3913:ILE:HD11	1:A:3988:LEU:HB2	2.00	0.43
2:B:41:LEU:HD12	2:B:41:LEU:HA	1.88	0.43
2:B:138:GLY:O	2:B:139:SER:OG	2.33	0.43
3:C:247:TRP:HE3	3:C:263:ALA:HB3	1.83	0.43
3:C:700:GLU:HA	3:C:703:LYS:HG2	2.00	0.43
1:A:275:PHE:HZ	1:A:286:LEU:HD11	1.83	0.43
1:A:624:ILE:O	1:A:628:GLU:OE1	2.36	0.43
1:A:1150:LYS:HA	1:A:1150:LYS:HD2	1.78	0.43
1:A:1153:LEU:HD12	1:A:1154:PRO:HD2	2.01	0.43
1:A:1759:LEU:HD23	1:A:1759:LEU:HA	1.86	0.43
1:A:1868:THR:HG22	1:A:1936:ARG:NH2	2.28	0.43
1:A:2555:LEU:HD13	1:A:2806:LYS:HA	1.99	0.43
1:A:3089:LEU:HA	1:A:3092:LEU:HD12	2.00	0.43
2:B:361:TYR:HE1	3:C:422:VAL:HG22	1.84	0.43
2:B:389:CYS:HA	2:B:394:VAL:HG12	2.01	0.43
2:B:396:ALA:HB3	2:B:413:LEU:HB2	2.01	0.43
2:B:477:SER:O	2:B:477:SER:OG	2.31	0.43
3:C:357:MET:O	3:C:357:MET:HG3	2.18	0.43
1:A:1479:VAL:O	1:A:1482:GLU:HG3	2.18	0.43
1:A:1719:VAL:HG23	3:C:631:TYR:CE1	2.54	0.43
1:A:2372:PRO:O	1:A:2374:LEU:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2478:MET:HG2	1:A:2524:PHE:CE1	2.53	0.43
1:A:2567:SER:HA	1:A:2572:TYR:OH	2.18	0.43
1:A:2888:VAL:HG12	1:A:3894:PRO:HG2	2.01	0.43
1:A:3441:ALA:HB1	1:A:3444:ALA:HB3	2.00	0.43
1:A:3575:LEU:HB2	1:A:3800:LEU:HD21	2.00	0.43
1:A:3701:ILE:HA	1:A:3702:PRO:HD3	1.83	0.43
3:C:75:GLN:OE1	3:C:75:GLN:N	2.52	0.43
1:A:18:THR:OG1	1:A:27:ALA:HB1	2.18	0.43
1:A:112:THR:O	1:A:116:THR:N	2.43	0.43
1:A:115:TYR:CE1	1:A:124:LYS:HE3	2.53	0.43
1:A:1290:LEU:O	1:A:1294:VAL:HG13	2.19	0.43
1:A:1626:TRP:NE1	1:A:1674:THR:HG21	2.32	0.43
1:A:1839:PHE:O	1:A:1842:THR:OG1	2.31	0.43
1:A:2317:ALA:HB1	1:A:2366:LYS:NZ	2.34	0.43
1:A:2516:GLY:O	1:A:2520:ILE:N	2.45	0.43
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.73	0.43
2:B:52:GLN:OE1	2:B:207:LYS:HG2	2.19	0.43
2:B:247:ARG:HE	2:B:488:ARG:NH1	2.16	0.43
3:C:276:TRP:CZ2	3:C:494:LEU:HD11	2.53	0.43
1:A:132:ILE:HG13	1:A:177:LEU:HD13	2.00	0.43
1:A:851:ILE:O	1:A:855:VAL:HG23	2.19	0.43
1:A:1223:THR:HG23	1:A:1224:PHE:CD1	2.53	0.43
1:A:1676:ILE:O	1:A:1680:ALA:CB	2.67	0.43
1:A:2207:LYS:O	1:A:2211:LEU:HD23	2.18	0.43
1:A:2386:LEU:O	1:A:2394:LYS:HE3	2.19	0.43
1:A:2967:GLU:O	1:A:2971:GLN:NE2	2.47	0.43
1:A:3155:VAL:HG23	1:A:3156:PRO:HD3	2.01	0.43
1:A:3947:GLY:O	1:A:4043:LYS:NZ	2.51	0.43
2:B:151:ALA:HB2	2:B:193:LEU:HD11	1.99	0.43
1:A:939:MET:HA	1:A:942:LEU:HG	2.00	0.42
1:A:1291:LEU:HA	1:A:1294:VAL:HG22	2.01	0.42
1:A:1834:ASP:OD1	1:A:1835:ALA:N	2.52	0.42
1:A:1988:TYR:CE2	1:A:2088:LEU:HD11	2.54	0.42
1:A:2503:LYS:HD2	1:A:2525:TRP:CH2	2.52	0.42
1:A:3057:ALA:C	1:A:3059:GLN:H	2.22	0.42
3:C:115:MET:HA	3:C:118:ILE:HD12	2.01	0.42
3:C:147:LEU:O	3:C:151:ILE:HG12	2.18	0.42
3:C:463:LEU:HD21	3:C:477:PHE:HD2	1.84	0.42
1:A:54:GLN:HA	1:A:57:LEU:HB3	2.01	0.42
1:A:429:GLU:OE1	1:A:1591:LYS:HD3	2.18	0.42
1:A:614:PRO:HG3	1:A:620:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:SER:HB2	1:A:880:MET:CG	2.45	0.42
1:A:1553:PHE:CD2	1:A:1554:SER:N	2.88	0.42
1:A:1579:VAL:HB	1:A:1583:MET:HE3	2.01	0.42
1:A:1597:LEU:HD11	1:A:1622:ILE:HG21	2.01	0.42
1:A:1775:GLU:OE2	1:A:1779:GLN:NE2	2.51	0.42
1:A:2331:MET:HG3	1:A:2371:PHE:HE1	1.82	0.42
1:A:3122:HIS:O	1:A:3123:GLN:HB3	2.19	0.42
1:A:3666:LEU:HD12	1:A:3666:LEU:HA	1.91	0.42
1:A:3916:TRP:O	1:A:4050:LYS:HE3	2.19	0.42
4:D:7:DG:H1	5:E:37:DC:H42	1.65	0.42
1:A:9:ARG:HB2	1:A:57:LEU:HD11	2.01	0.42
1:A:648:SER:O	1:A:652:GLU:OE1	2.38	0.42
1:A:1667:SER:O	1:A:1671:VAL:HG12	2.19	0.42
1:A:3151:LEU:HD21	1:A:3196:LYS:HD3	2.02	0.42
2:B:328:ILE:O	2:B:329:LEU:HD12	2.19	0.42
3:C:380:LEU:O	3:C:384:LEU:HD23	2.19	0.42
3:C:474:GLU:N	3:C:474:GLU:OE1	2.52	0.42
3:C:610:GLU:HA	3:C:613:SER:HB3	2.01	0.42
1:A:766:ALA:O	1:A:770:LEU:HD23	2.18	0.42
1:A:835:LYS:HA	1:A:835:LYS:HD2	1.75	0.42
1:A:1136:ARG:HG3	1:A:1136:ARG:NH1	2.32	0.42
1:A:1880:MET:HB3	1:A:1884:LEU:HD12	2.00	0.42
1:A:2251:ILE:HD11	1:A:2285:LEU:CD1	2.49	0.42
1:A:2257:PHE:CZ	1:A:2294:ILE:HD13	2.55	0.42
1:A:2326:ILE:O	1:A:2330:VAL:HG22	2.19	0.42
1:A:2426:HIS:CG	1:A:2427:ARG:N	2.87	0.42
1:A:2436:LEU:HA	1:A:2436:LEU:HD23	1.90	0.42
1:A:3946:PHE:O	1:A:3948:SER:N	2.52	0.42
1:A:4093:GLU:OE1	1:A:4094:PRO:HD2	2.19	0.42
3:C:44:ARG:HD3	3:C:237:PHE:CE2	2.54	0.42
3:C:356:PHE:O	3:C:358:GLY:N	2.53	0.42
3:C:365:PHE:O	3:C:377:LEU:HD11	2.20	0.42
3:C:653:GLN:HG2	3:C:654:ARG:N	2.35	0.42
1:A:248:ILE:O	1:A:252:VAL:HG23	2.19	0.42
1:A:793:LEU:HB3	1:A:870:LEU:HA	2.01	0.42
1:A:1212:LEU:HD12	1:A:1212:LEU:HA	1.89	0.42
1:A:1779:GLN:O	1:A:1783:ARG:HG3	2.20	0.42
2:B:255:ALA:C	2:B:257:SER:H	2.23	0.42
3:C:280:ASP:OD2	3:C:283:THR:OG1	2.30	0.42
1:A:182:GLY:HA2	1:A:189:MET:SD	2.60	0.42
1:A:259:GLN:HG2	1:A:262:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:LYS:O	1:A:1061:LYS:HG3	2.19	0.42
1:A:1538:LEU:O	1:A:1552:HIS:HA	2.19	0.42
1:A:1563:PHE:O	1:A:1565:GLU:N	2.52	0.42
1:A:1582:LEU:HD23	1:A:1597:LEU:HD13	2.02	0.42
1:A:1671:VAL:O	1:A:1674:THR:OG1	2.24	0.42
1:A:1933:LEU:H	1:A:1937:ARG:NH2	2.11	0.42
1:A:3139:GLN:O	1:A:3142:ILE:HG22	2.19	0.42
1:A:3669:LYS:HA	1:A:3672:LYS:HG2	2.01	0.42
2:B:152:ASN:HA	2:B:155:SER:HB3	2.01	0.42
2:B:400:TYR:CZ	2:B:402:PRO:HB3	2.55	0.42
1:A:327:VAL:HG23	1:A:334:HIS:HB3	2.01	0.42
1:A:424:LEU:HD21	1:A:428:PRO:HD3	2.01	0.42
1:A:446:PHE:HD1	1:A:457:CYS:HG	1.68	0.42
1:A:1431:LEU:HD13	1:A:1451:VAL:HG11	2.02	0.42
1:A:1591:LYS:HE3	1:A:1591:LYS:HB2	1.88	0.42
1:A:1668:PHE:CD1	1:A:1672:PHE:CE2	3.08	0.42
1:A:2318:ALA:O	1:A:2322:VAL:HG12	2.20	0.42
1:A:2879:GLY:O	1:A:2883:SER:HB3	2.20	0.42
1:A:3443:PRO:HB3	1:A:3471:ILE:CG2	2.50	0.42
3:C:281:ALA:O	3:C:282:LYS:HG2	2.20	0.42
3:C:463:LEU:O	3:C:476:LEU:HB3	2.20	0.42
3:C:616:LEU:HD13	3:C:642:PHE:CE2	2.53	0.42
3:C:619:HIS:O	3:C:622:GLN:HG2	2.20	0.42
1:A:73:LEU:HD12	1:A:74:ASN:N	2.34	0.42
1:A:166:ILE:HB	1:A:170:VAL:HG23	2.00	0.42
1:A:183:GLU:HB2	1:A:229:SER:O	2.20	0.42
1:A:656:GLN:O	1:A:660:LEU:N	2.35	0.42
1:A:896:VAL:O	1:A:903:PRO:HD2	2.20	0.42
1:A:915:THR:OG1	1:A:968:VAL:HG21	2.20	0.42
1:A:1339:VAL:HG13	1:A:1398:VAL:HG11	2.02	0.42
1:A:1622:ILE:HD11	1:A:1652:ILE:HG12	2.02	0.42
1:A:1672:PHE:CE1	1:A:1702:LEU:HD21	2.54	0.42
1:A:2143:ARG:HG2	1:A:2171:LEU:HD13	2.02	0.42
1:A:3344:GLU:HB2	1:A:3348:LEU:HD23	2.02	0.42
1:A:3484:THR:HA	1:A:3487:ILE:HG22	2.00	0.42
1:A:3703:GLY:HA2	1:A:3794:VAL:HG21	2.02	0.42
2:B:249:LYS:O	2:B:250:GLU:HG3	2.20	0.42
3:C:12:LEU:HD13	3:C:38:ILE:HG13	2.01	0.42
3:C:600:VAL:HA	3:C:603:LYS:HE2	2.02	0.42
4:D:25:DT:H2''	4:D:26:DT:C5'	2.50	0.42
1:A:1301:ILE:HG23	1:A:1302:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:LEU:HD12	1:A:1463:LEU:O	2.19	0.42
1:A:1675:TYR:CZ	1:A:1699:PHE:CE1	3.08	0.42
1:A:1750:LEU:HG	1:A:1785:ILE:HD11	2.00	0.42
1:A:2150:VAL:HG23	1:A:2157:PHE:CE1	2.55	0.42
1:A:2203:THR:HG21	1:A:2247:ASP:HB2	2.02	0.42
1:A:3232:ARG:HG2	1:A:3272:TRP:HH2	1.85	0.42
1:A:3568:ILE:O	1:A:3572:ILE:HG13	2.20	0.42
1:A:3762:GLN:HG3	1:A:3793:VAL:O	2.20	0.42
1:A:3998:LEU:O	1:A:4002:MET:HG3	2.19	0.42
2:B:215:LEU:HD22	2:B:216:PHE:HD1	1.84	0.42
2:B:252:ARG:HD2	3:C:431:ARG:NE	2.35	0.42
2:B:271:VAL:CG2	2:B:368:VAL:HB	2.50	0.42
2:B:353:LEU:HD21	2:B:414:VAL:HG13	2.02	0.42
3:C:406:GLY:HA2	3:C:424:LEU:HB2	2.02	0.42
1:A:789:TYR:CD2	1:A:866:ILE:HG23	2.55	0.42
1:A:1382:ILE:HD11	1:A:1384:PHE:CE2	2.55	0.42
1:A:1695:LEU:HD13	1:A:1699:PHE:HD1	1.85	0.42
1:A:1814:PHE:O	1:A:1817:GLN:HG3	2.20	0.42
1:A:2476:ILE:HG21	1:A:2476:ILE:HD13	1.85	0.42
1:A:2575:PRO:HD2	1:A:2785:ILE:O	2.19	0.42
1:A:2786:LYS:HG3	1:A:2787:HIS:N	2.35	0.42
1:A:2978:LYS:HE2	1:A:2981:TRP:CE3	2.55	0.42
1:A:3005:LEU:HG	1:A:3007:GLU:OE1	2.20	0.42
1:A:3236:PHE:CE1	1:A:3262:LEU:HD21	2.55	0.42
1:A:3913:ILE:HB	1:A:3984:MET:SD	2.60	0.42
1:A:3985:VAL:CG2	1:A:4104:VAL:HG11	2.50	0.42
2:B:41:LEU:HB3	2:B:168:LEU:HD12	2.01	0.42
1:A:792:ILE:HG23	1:A:793:LEU:HD22	2.02	0.41
1:A:1299:GLU:HA	1:A:1367:HIS:HD2	1.84	0.41
1:A:2225:HIS:C	1:A:2227:LYS:N	2.73	0.41
1:A:2547:SER:O	1:A:2549:LYS:N	2.53	0.41
1:A:3535:ILE:HD11	1:A:3797:THR:OG1	2.20	0.41
1:A:3879:PRO:O	1:A:3966:GLN:NE2	2.50	0.41
2:B:77:SER:O	2:B:250:GLU:HA	2.20	0.41
2:B:363:ARG:NH1	4:D:18:DT:OP1	2.53	0.41
3:C:261:ILE:HD13	3:C:377:LEU:CD2	2.50	0.41
3:C:300:ASP:OD1	3:C:300:ASP:N	2.53	0.41
1:A:1018:VAL:CG1	1:A:1077:GLY:HA3	2.50	0.41
1:A:1448:LEU:HA	1:A:1451:VAL:HG12	2.01	0.41
1:A:1487:VAL:HG11	1:A:1515:LEU:HD23	2.01	0.41
1:A:1641:THR:O	1:A:1645:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1787:ARG:HA	1:A:1831:CYS:SG	2.59	0.41
1:A:2788:SER:O	1:A:2792:THR:HG22	2.21	0.41
1:A:3316:LEU:HD13	1:A:3323:PHE:HE1	1.85	0.41
1:A:3999:THR:HB	1:A:4048:LYS:NZ	2.34	0.41
2:B:473:TYR:HD1	3:C:392:ILE:HG13	1.84	0.41
3:C:81:ARG:HH12	3:C:84:MET:N	2.13	0.41
3:C:165:LEU:HD23	3:C:224:ILE:HD11	2.02	0.41
1:A:2281:MET:O	1:A:2283:ASN:O	2.38	0.41
1:A:2327:LEU:HD11	1:A:2345:VAL:HG11	2.02	0.41
1:A:3006:ALA:HB1	1:A:3008:TRP:CZ2	2.56	0.41
1:A:3113:ASN:O	1:A:3116:SER:OG	2.35	0.41
1:A:3332:THR:O	1:A:3336:ILE:HG13	2.20	0.41
2:B:74:LYS:HD3	2:B:83:LEU:HD11	2.01	0.41
2:B:143:LEU:HG	2:B:182:LYS:HB3	2.02	0.41
3:C:629:THR:OG1	3:C:630:PRO:HD3	2.20	0.41
1:A:42:CYS:SG	1:A:88:PHE:HE1	2.44	0.41
1:A:1165:LEU:HD23	1:A:1165:LEU:O	2.20	0.41
1:A:1922:ALA:C	1:A:1924:THR:H	2.23	0.41
1:A:2093:CYS:O	1:A:2097:LEU:HB2	2.20	0.41
1:A:2307:MET:SD	1:A:2345:VAL:HG23	2.60	0.41
1:A:2368:THR:HA	1:A:2371:PHE:O	2.21	0.41
1:A:3244:ASP:OD1	1:A:3247:ARG:NH2	2.49	0.41
1:A:3283:LEU:O	1:A:3287:ARG:HG2	2.20	0.41
1:A:4056:PRO:HG3	1:A:4107:LEU:HD13	2.02	0.41
2:B:67:ILE:HD13	2:B:85:VAL:HG12	2.02	0.41
3:C:16:VAL:HG12	3:C:31:PHE:HE1	1.86	0.41
1:A:630:CYS:O	1:A:634:LEU:N	2.50	0.41
1:A:1366:THR:HG23	1:A:1418:HIS:NE2	2.36	0.41
1:A:1760:GLU:OE2	1:A:1800:SER:HB2	2.21	0.41
1:A:2220:MET:SD	1:A:2252:PRO:HG2	2.60	0.41
1:A:2358:ASP:O	1:A:2362:VAL:HG23	2.21	0.41
1:A:2837:LEU:HD12	1:A:2868:LEU:HA	2.02	0.41
1:A:3061:LEU:H	1:A:3061:LEU:HD23	1.85	0.41
1:A:3110:PHE:HD1	1:A:3128:LYS:HE3	1.85	0.41
1:A:3575:LEU:HB3	1:A:3800:LEU:HD11	2.02	0.41
1:A:3699:LEU:HD23	1:A:3699:LEU:HA	1.94	0.41
3:C:20:MET:SD	3:C:137:ASP:HB2	2.61	0.41
1:A:377:ASN:C	1:A:379:LYS:H	2.23	0.41
1:A:1031:ARG:O	1:A:1034:ARG:HG2	2.19	0.41
1:A:1344:PHE:HA	1:A:1347:THR:HG22	2.02	0.41
1:A:2398:LEU:O	1:A:2401:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2884:LEU:HD13	1:A:3116:SER:OG	2.20	0.41
1:A:3132:VAL:HA	1:A:3135:LEU:HG	2.03	0.41
1:A:3859:TYR:HB3	1:A:4076:ASP:CB	2.50	0.41
2:B:146:VAL:HG13	2:B:147:LEU:N	2.35	0.41
2:B:287:LYS:O	2:B:295:PRO:HA	2.20	0.41
2:B:473:TYR:CE2	2:B:474:ARG:HG3	2.55	0.41
2:B:505:ASP:OD1	2:B:508:LEU:N	2.54	0.41
3:C:457:LEU:HD22	3:C:533:ILE:CD1	2.51	0.41
1:A:238:MET:HE2	1:A:246:ARG:HH11	1.86	0.41
1:A:816:SER:N	1:A:819:SER:OG	2.53	0.41
1:A:1064:TYR:OH	1:A:1099:PHE:O	2.23	0.41
1:A:1198:LEU:HG	1:A:1199:PRO:HD2	2.02	0.41
1:A:1538:LEU:HG	1:A:1555:HIS:CB	2.51	0.41
1:A:1911:LEU:HA	1:A:1914:THR:OG1	2.19	0.41
1:A:2091:HIS:C	1:A:2093:CYS:H	2.23	0.41
1:A:2252:PRO:HB2	1:A:2255:LEU:HD21	2.02	0.41
1:A:2327:LEU:O	1:A:2331:MET:HG2	2.20	0.41
1:A:3259:LEU:HB3	1:A:3276:TRP:CZ2	2.56	0.41
1:A:3354:ASP:O	1:A:3357:ARG:HG2	2.20	0.41
2:B:267:ILE:HG13	2:B:267:ILE:O	2.20	0.41
2:B:322:TYR:CD2	3:C:49:GLU:OE1	2.66	0.41
2:B:324:SER:O	2:B:324:SER:OG	2.36	0.41
2:B:329:LEU:HD22	3:C:276:TRP:CH2	2.56	0.41
2:B:374:LEU:O	3:C:542:ALA:HB3	2.21	0.41
3:C:261:ILE:HD12	3:C:262:ALA:H	1.85	0.41
1:A:131:LEU:HD22	1:A:177:LEU:HD21	2.03	0.41
1:A:784:VAL:O	1:A:787:PRO:HD2	2.21	0.41
1:A:1018:VAL:HG23	1:A:1018:VAL:O	2.21	0.41
1:A:1441:ALA:HA	1:A:1445:ARG:HD2	2.02	0.41
1:A:2088:LEU:O	1:A:2094:MET:HE3	2.21	0.41
1:A:2534:ASN:O	1:A:2535:THR:OG1	2.31	0.41
1:A:3227:ILE:O	1:A:3231:ILE:HG13	2.21	0.41
1:A:3384:HIS:O	1:A:3387:GLU:HG2	2.21	0.41
1:A:3881:ASP:OD1	1:A:3884:LYS:HB3	2.20	0.41
1:A:3951:GLN:NE2	1:A:4066:LEU:HD23	2.36	0.41
2:B:361:TYR:CE1	3:C:361:VAL:HG22	2.55	0.41
1:A:71:LYS:HE2	1:A:71:LYS:HB3	1.82	0.41
1:A:115:TYR:HE2	1:A:159:GLU:OE2	2.03	0.41
1:A:863:GLY:O	1:A:867:ASN:HB2	2.21	0.41
1:A:911:LEU:CD2	1:A:961:LEU:HD21	2.50	0.41
1:A:924:ARG:O	1:A:928:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:LEU:HD22	1:A:1337:VAL:HG21	2.02	0.41
1:A:1330:TYR:CE2	1:A:1334:LYS:HD3	2.56	0.41
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	2.03	0.41
1:A:1423:ILE:HD11	1:A:1467:ILE:HG21	2.02	0.41
1:A:2402:LEU:HA	1:A:2405:VAL:HG13	2.03	0.41
1:A:2454:LEU:HD23	1:A:2454:LEU:HA	1.83	0.41
1:A:2546:TYR:CE1	1:A:2854:PHE:CE2	3.09	0.41
1:A:2810:SER:OG	1:A:2857:CYS:SG	2.61	0.41
1:A:2880:CYS:HB3	1:A:2886:GLN:HA	2.02	0.41
1:A:2931:ARG:HD2	1:A:2939:LEU:HD21	2.03	0.41
1:A:3722:PHE:CE2	1:A:3740:ILE:HG22	2.56	0.41
1:A:3951:GLN:NE2	1:A:4063:GLU:OE1	2.53	0.41
2:B:95:ASN:HD21	2:B:99:PHE:H	1.68	0.41
2:B:244:ARG:CZ	2:B:245:LYS:HE2	2.50	0.41
2:B:370:PRO:HD3	2:B:382:PHE:CE1	2.56	0.41
2:B:497:LEU:O	2:B:497:LEU:HD12	2.20	0.41
3:C:430:LEU:HD23	3:C:430:LEU:H	1.86	0.41
1:A:488:ILE:HG23	1:A:2036:LEU:HG	2.02	0.41
1:A:880:MET:C	1:A:883:TYR:H	2.23	0.41
1:A:1436:LEU:O	1:A:1445:ARG:NH1	2.53	0.41
1:A:1723:PRO:HG3	1:A:1729:PHE:CE2	2.56	0.41
2:B:50:GLU:HG3	2:B:52:GLN:H	1.86	0.41
2:B:477:SER:N	3:C:427:MET:SD	2.76	0.41
3:C:539:LEU:HD23	3:C:539:LEU:H	1.86	0.41
1:A:852:ARG:HG2	1:A:3111:MET:CE	2.51	0.40
1:A:1068:LEU:HD13	1:A:1155:ARG:NH2	2.36	0.40
1:A:2978:LYS:NZ	1:A:2986:PRO:HD3	2.36	0.40
1:A:2990:GLU:HA	1:A:2993:PHE:HB3	2.03	0.40
1:A:3642:LYS:HE3	1:A:3643:HIS:CE1	2.56	0.40
1:A:4086:ASP:OD1	1:A:4086:ASP:N	2.54	0.40
2:B:90:THR:O	2:B:101:ASN:HA	2.21	0.40
2:B:252:ARG:CZ	3:C:431:ARG:HH21	2.34	0.40
3:C:43:GLN:HA	3:C:46:VAL:HG12	2.03	0.40
3:C:408:ALA:HB1	3:C:419:LEU:HG	2.03	0.40
3:C:611:GLU:HG3	3:C:612:ALA:N	2.36	0.40
3:C:612:ALA:O	3:C:615:GLN:HG2	2.21	0.40
3:C:626:THR:OG1	3:C:628:GLU:OE1	2.26	0.40
1:A:207:GLN:NE2	1:A:216:LYS:HE2	2.36	0.40
1:A:331:ALA:HA	1:A:334:HIS:HB2	2.04	0.40
1:A:1717:LEU:HD23	1:A:1746:PHE:HZ	1.85	0.40
1:A:2953:THR:HG22	1:A:2994:TRP:NE1	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3003:ASN:OD1	1:A:3046:ARG:NH1	2.54	0.40
1:A:3147:LYS:HG3	1:A:3150:ASN:H	1.85	0.40
1:A:3552:LYS:HA	1:A:3555:VAL:HG22	2.03	0.40
1:A:3568:ILE:HD13	1:A:3699:LEU:HD23	2.04	0.40
1:A:3570:ASP:OD1	1:A:3686:TRP:NE1	2.54	0.40
2:B:470:ARG:HB3	3:C:389:MET:HE3	2.03	0.40
3:C:169:LEU:HD21	3:C:226:SER:HB3	2.03	0.40
3:C:184:ARG:HG2	3:C:185:LEU:H	1.85	0.40
3:C:188:HIS:ND1	3:C:232:ARG:HD3	2.37	0.40
1:A:9:ARG:HH11	1:A:57:LEU:HA	1.86	0.40
1:A:185:HIS:HE1	1:A:188:GLU:CB	2.33	0.40
1:A:464:VAL:O	1:A:468:LEU:HG	2.22	0.40
1:A:1141:LYS:HE3	1:A:1142:HIS:HB2	2.03	0.40
1:A:1876:ILE:HG22	1:A:1880:MET:HE1	2.03	0.40
1:A:1915:LEU:HA	1:A:1918:LEU:HG	2.03	0.40
1:A:2315:VAL:HG13	1:A:2316:TYR:N	2.35	0.40
2:B:264:ASN:HB3	3:C:530:LEU:HD22	2.02	0.40
3:C:7:LYS:HB2	3:C:51:LYS:O	2.21	0.40
3:C:108:LEU:O	3:C:112:ILE:HG12	2.20	0.40
3:C:422:VAL:HG12	3:C:423:GLN:O	2.20	0.40
3:C:539:LEU:HG	3:C:541:GLU:HB2	2.04	0.40
1:A:364:ARG:NH2	1:A:415:GLN:OE1	2.54	0.40
1:A:723:ASP:OD1	1:A:723:ASP:N	2.52	0.40
1:A:959:TYR:CD2	1:A:963:LYS:HD2	2.57	0.40
1:A:1089:PHE:HE1	1:A:1099:PHE:HD2	1.70	0.40
1:A:1597:LEU:HA	1:A:1597:LEU:HD12	1.87	0.40
1:A:1920:TYR:CE2	1:A:1965:PHE:HA	2.56	0.40
1:A:2098:THR:O	1:A:2102:LYS:HG3	2.22	0.40
1:A:2447:LYS:HB2	1:A:2450:GLU:OE1	2.21	0.40
1:A:2927:ALA:HB2	1:A:2942:ILE:HD11	2.04	0.40
1:A:2970:LYS:HA	1:A:2970:LYS:HD2	1.92	0.40
1:A:3104:GLN:O	1:A:3108:GLN:OE1	2.39	0.40
1:A:3628:PHE:CD1	1:A:3685:PRO:HD2	2.56	0.40
1:A:3993:SER:O	1:A:3993:SER:OG	2.30	0.40
1:A:4006:VAL:HG22	1:A:4040:PRO:HB3	2.03	0.40
2:B:390:LEU:HD22	2:B:417:GLU:CD	2.42	0.40
5:E:33:DT:H2''	5:E:34:DC:H5'	2.03	0.40
1:A:737:PRO:C	1:A:739:ASN:H	2.24	0.40
1:A:1433:ALA:N	1:A:1436:LEU:HD21	2.37	0.40
1:A:1448:LEU:HA	1:A:1448:LEU:HD23	1.94	0.40
1:A:1725:GLN:NE2	1:A:1728:GLU:OE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1945:TYR:CE2	1:A:1949:ILE:HD11	2.57	0.40
1:A:1951:VAL:O	1:A:1955:VAL:N	2.55	0.40
1:A:2417:SER:HB2	2:B:152:ASN:HD22	1.87	0.40
1:A:2563:LEU:HD11	1:A:2808:LEU:HD21	2.04	0.40
1:A:3259:LEU:HD11	1:A:3279:SER:HB2	2.04	0.40
1:A:3762:GLN:HA	1:A:3793:VAL:HB	2.04	0.40
3:C:155:LYS:HE2	3:C:155:LYS:HA	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3555/4128 (86%)	3157 (89%)	395 (11%)	3 (0%)	51	82
2	B	486/609 (80%)	418 (86%)	67 (14%)	1 (0%)	47	78
3	C	653/732 (89%)	585 (90%)	68 (10%)	0	100	100
All	All	4694/5469 (86%)	4160 (89%)	530 (11%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2548	PRO
1	A	1021	VAL
2	B	144	SER
1	A	1020	PRO

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3121/3671 (85%)	3099 (99%)	22 (1%)	84	91
2	B	439/548 (80%)	435 (99%)	4 (1%)	78	88
3	C	585/649 (90%)	578 (99%)	7 (1%)	71	84
All	All	4145/4868 (85%)	4112 (99%)	33 (1%)	82	90

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	LYS
1	A	1026	ARG
1	A	1051	LYS
1	A	1141	LYS
1	A	1213	LYS
1	A	1771	GLN
1	A	1784	ARG
1	A	1806	ARG
1	A	1970	LYS
1	A	2225	HIS
1	A	2311	ARG
1	A	2365	ASN
1	A	2899	ARG
1	A	2978	LYS
1	A	3159	ARG
1	A	3264	LYS
1	A	3289	ARG
1	A	3642	LYS
1	A	3696	ARG
1	A	3718	ARG
1	A	3833	ARG
1	A	4090	ARG
2	B	46	LYS
2	B	297	LYS
2	B	301	ARG
2	B	516	LYS
3	C	130	ARG
3	C	184	ARG
3	C	239	LYS
3	C	323	PHE

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Mol	Chain	Res	Type
3	C	368	ARG
3	C	489	ARG
3	C	670	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	281	GLN
1	A	1083	ASN
1	A	1830	HIS
1	A	1890	HIS
1	A	2306	ASN
1	A	2432	GLN
1	A	2518	GLN
1	A	2807	GLN
1	A	2859	GLN
1	A	2864	GLN
1	A	3510	GLN
1	A	3743	HIS
1	A	3969	ASN
2	B	480	ASN
3	C	43	GLN
3	C	452	ASN
3	C	488	GLN
3	C	511	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	1IX	A	4201	-	37,38,38	2.25	10 (27%)	50,54,54	2.00	18 (36%)

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
6	1IX	A	4201	-	-	0/18/26/26	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4201	1IX	C14-C16	6.37	1.56	1.49
6	A	4201	1IX	C12-C13	5.77	1.47	1.37
6	A	4201	1IX	C11-CL1	4.25	1.83	1.73
6	A	4201	1IX	C21-C20	-3.50	1.36	1.42
6	A	4201	1IX	C24-N26	3.36	1.48	1.38
6	A	4201	1IX	C25-C20	3.12	1.46	1.41
6	A	4201	1IX	C15-C14	2.37	1.43	1.39
6	A	4201	1IX	C14-C13	-2.36	1.35	1.39
6	A	4201	1IX	C20-N19	-2.24	1.33	1.37
6	A	4201	1IX	C15-C10	2.11	1.43	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4201	1IX	C21-C16-N17	-5.35	119.52	123.04
6	A	4201	1IX	C18-N19-C20	4.50	121.60	115.40
6	A	4201	1IX	C21-C20-N19	-4.21	118.34	122.83
6	A	4201	1IX	N19-C18-N17	-4.21	122.10	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4201	1IX	C15-C10-C11	3.23	120.30	117.12
6	A	4201	1IX	C25-C20-N19	2.89	121.26	117.97
6	A	4201	1IX	C03-N04-N05	2.79	122.76	118.45
6	A	4201	1IX	C16-C21-C20	2.64	118.47	115.88
6	A	4201	1IX	C12-C11-C10	-2.63	119.27	122.41
6	A	4201	1IX	C11-C12-C13	2.51	120.18	118.59
6	A	4201	1IX	C27-N26-C24	2.40	124.58	118.09
6	A	4201	1IX	C30-C31-N26	2.30	114.26	110.02
6	A	4201	1IX	C23-C24-N26	-2.26	118.27	121.38
6	A	4201	1IX	C01-O02-C03	-2.23	113.87	117.36
6	A	4201	1IX	C12-C13-C14	-2.16	120.24	123.64
6	A	4201	1IX	C15-C14-C13	2.03	118.99	116.15
6	A	4201	1IX	C14-C16-N17	2.02	119.01	115.38
6	A	4201	1IX	C28-C27-N26	2.02	113.74	110.02

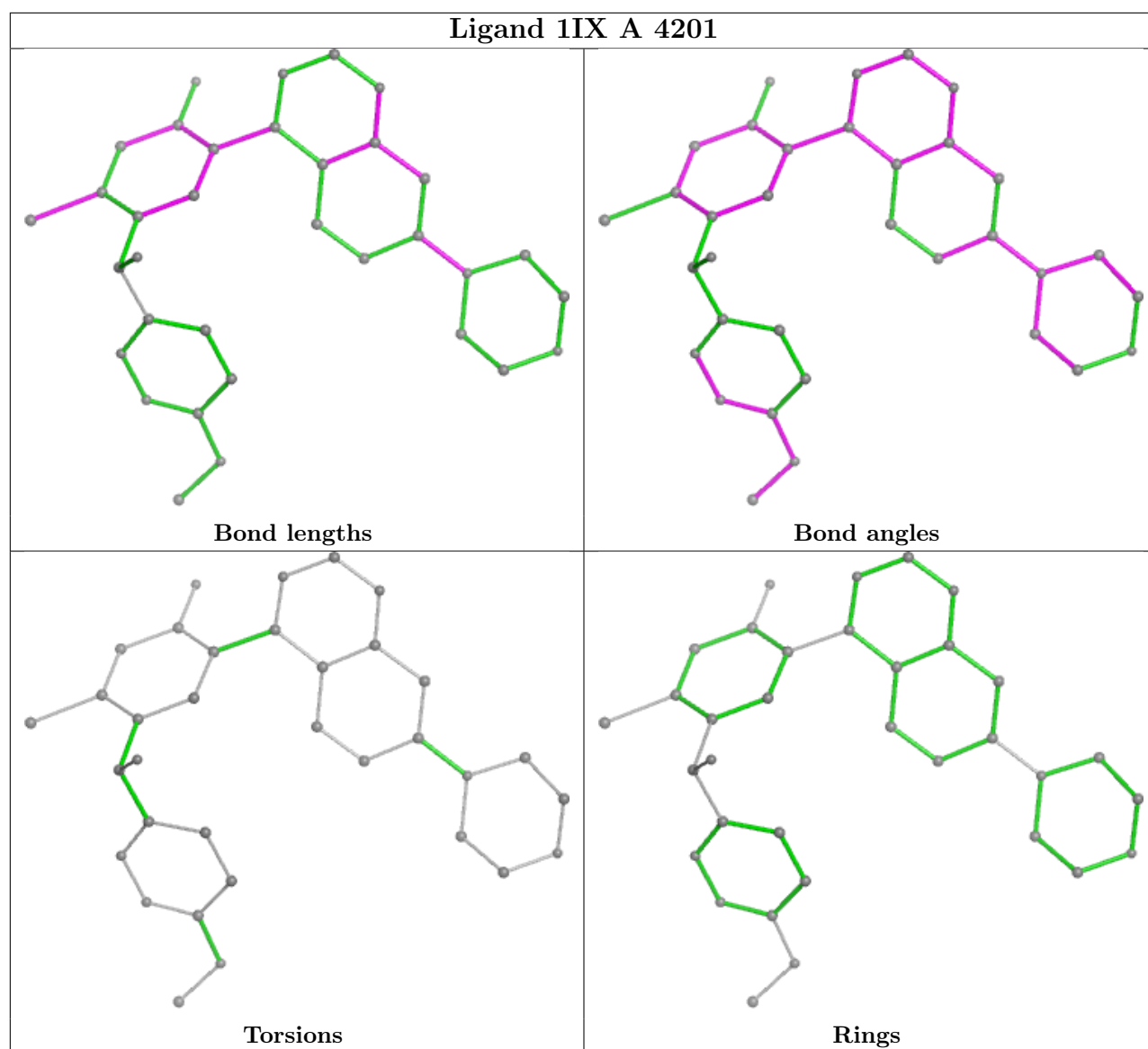
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

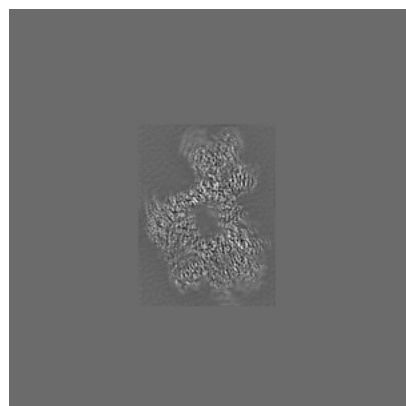
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14546. 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

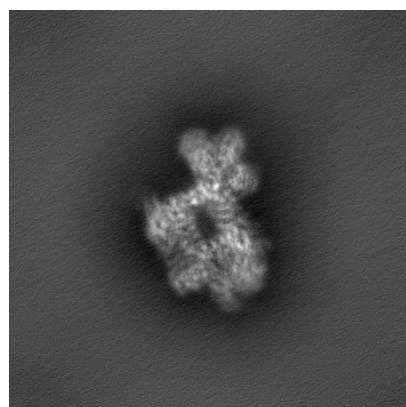


Y

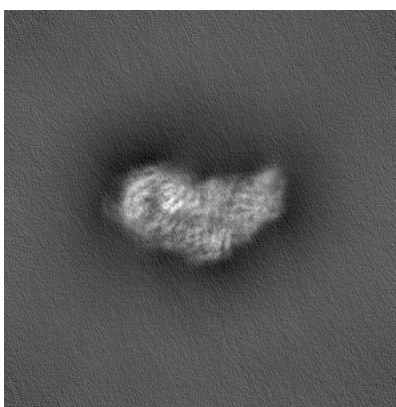


Z

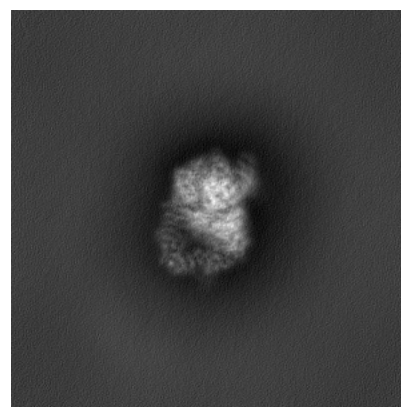
#### 6.1.2 Raw map



X



Y

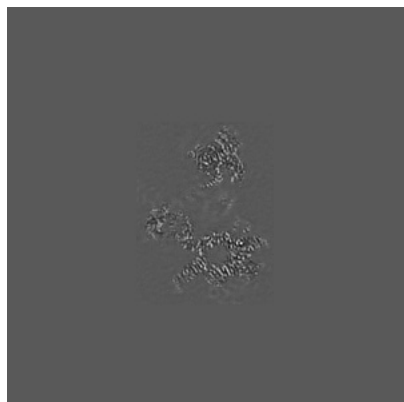


Z

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

## 6.2 Central slices [i](#)

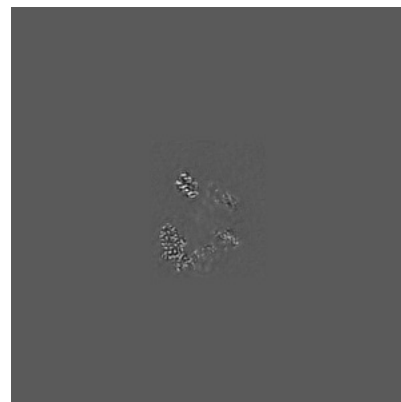
### 6.2.1 Primary map



X Index: 175

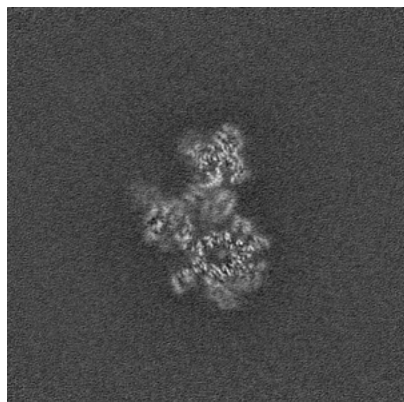


Y Index: 175

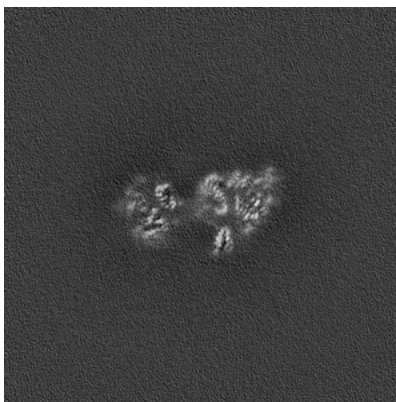


Z Index: 175

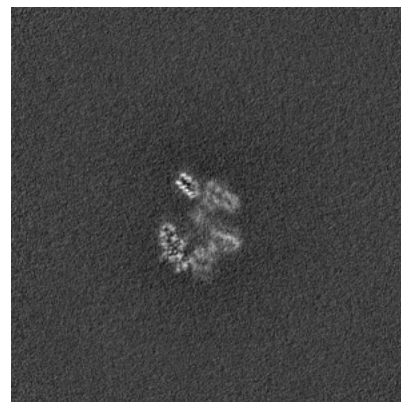
### 6.2.2 Raw map



X Index: 175



Y Index: 175

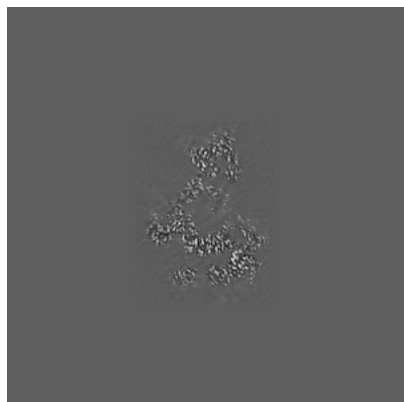


Z Index: 175

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

## 6.3 Largest variance slices [i](#)

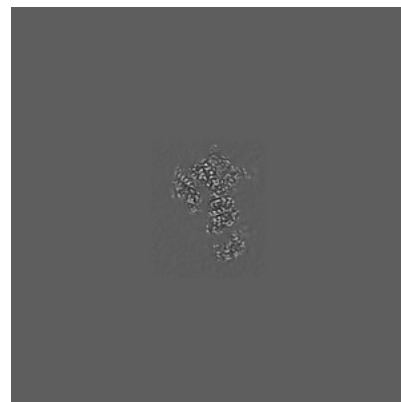
### 6.3.1 Primary map



X Index: 182

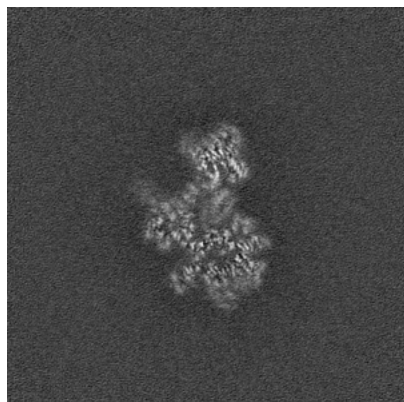


Y Index: 194

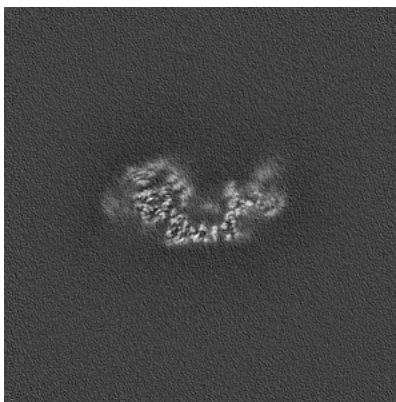


Z Index: 143

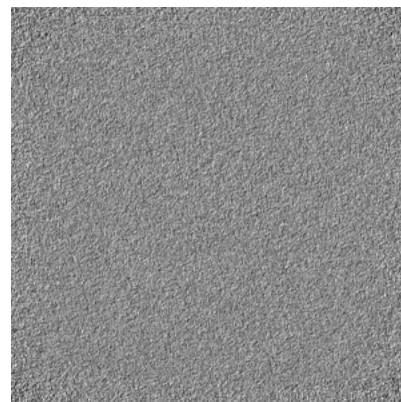
### 6.3.2 Raw map



X Index: 177



Y Index: 197

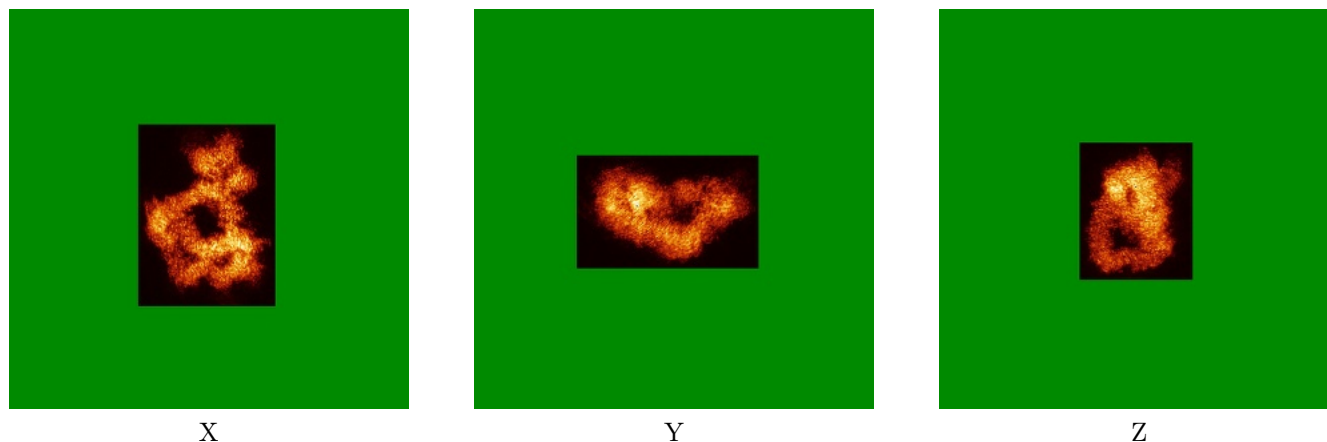


Z Index: 0

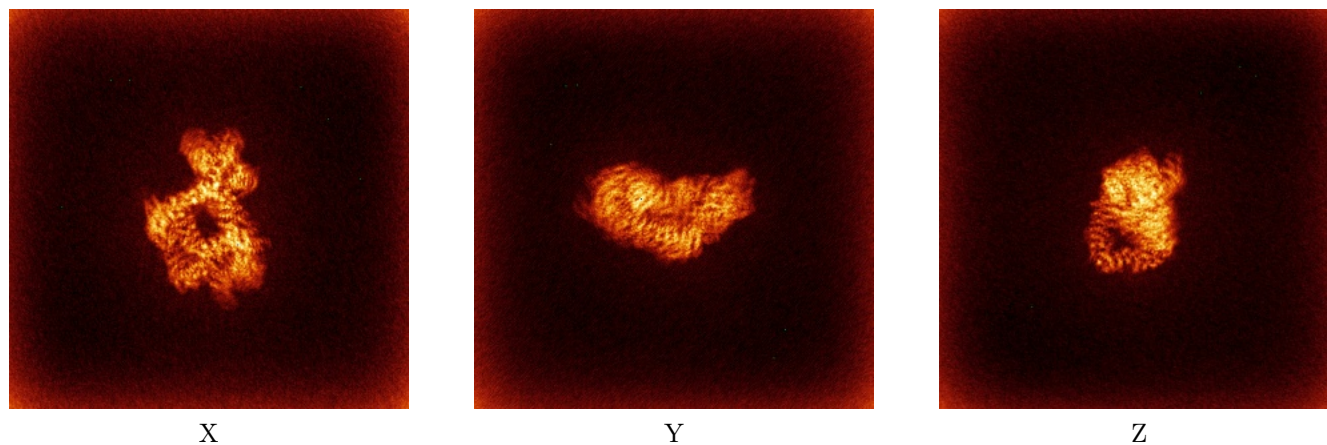
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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



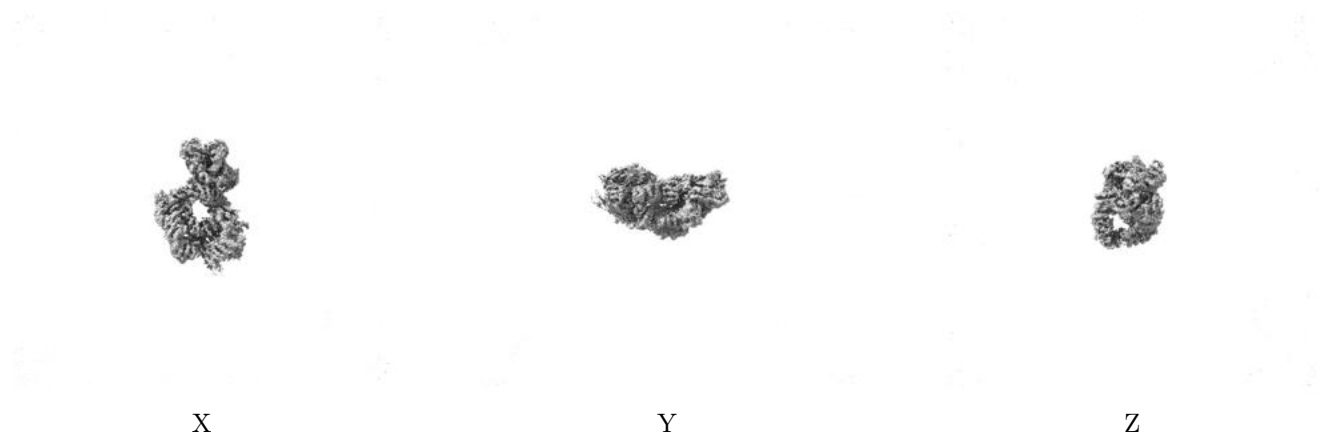
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

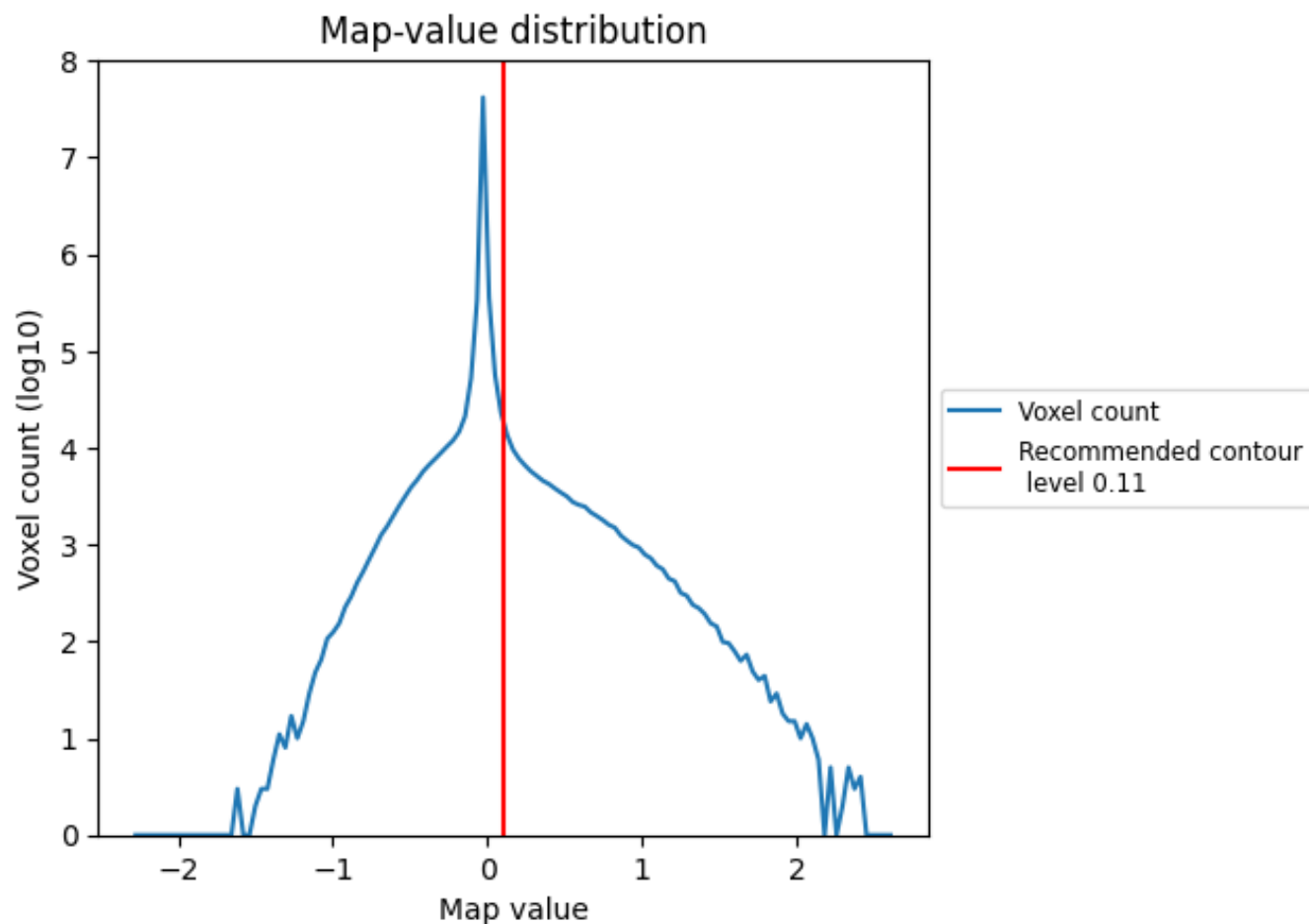
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

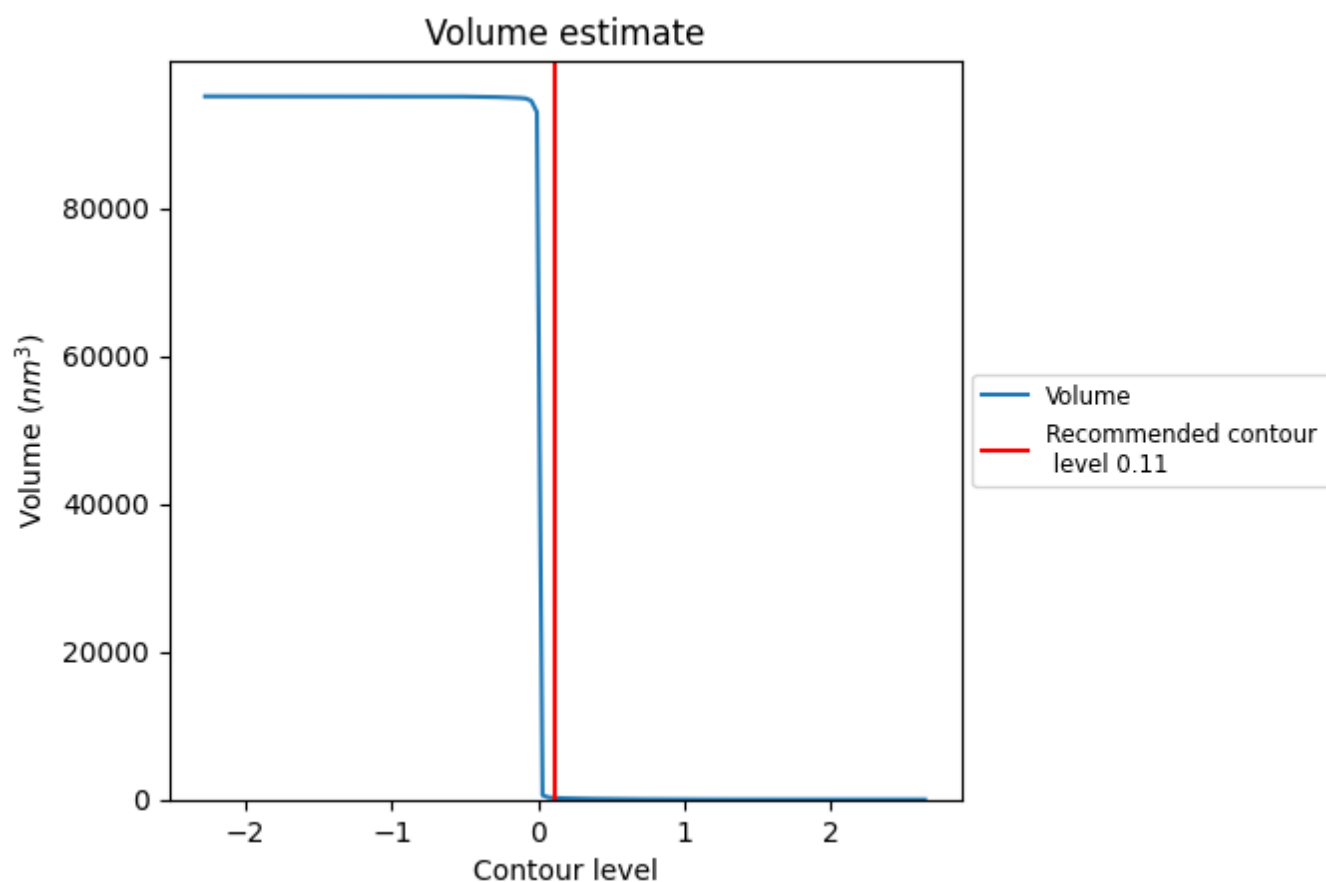
### 7.1 Map-value distribution [i](#)



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



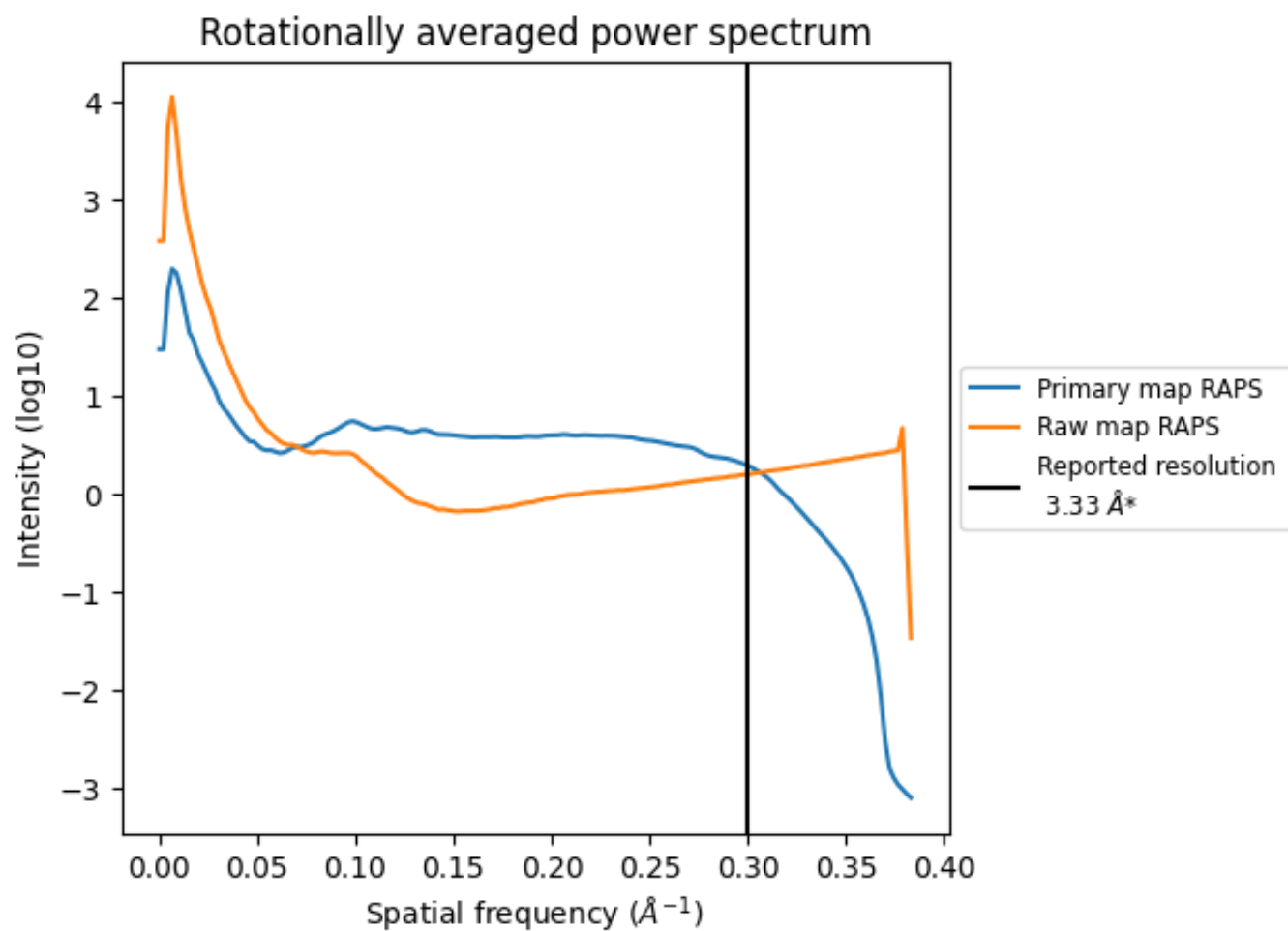
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm<sup>3</sup>; this corresponds to an approximate mass of 207 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 ⓘ

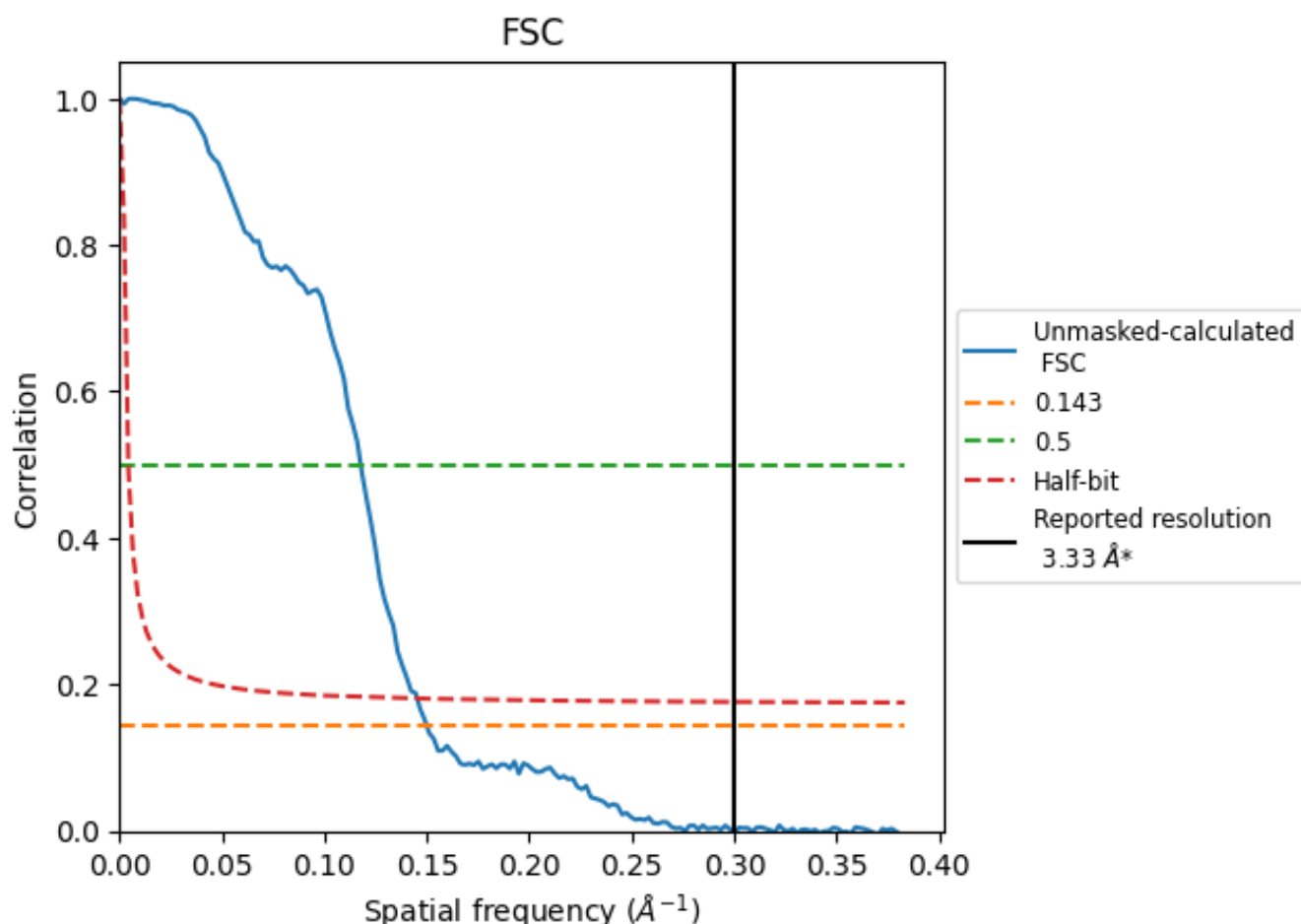


\*Reported resolution corresponds to spatial frequency of 0.300  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.300  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

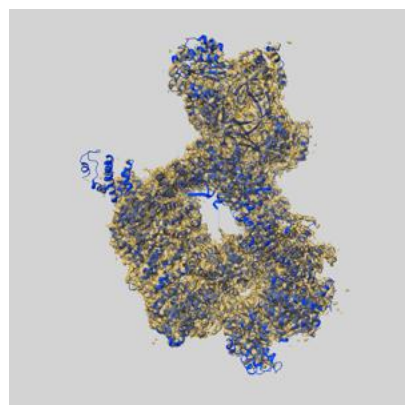
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.67	8.49	6.88

\*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 6.67 differs from the reported value 3.33 by more than 10 %

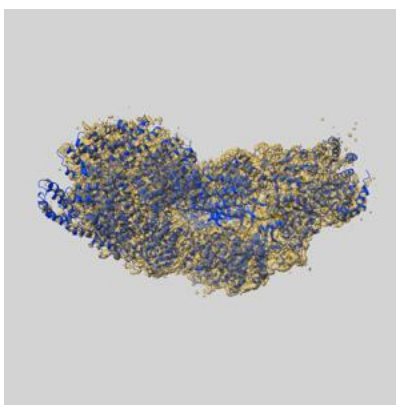
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14546 and PDB model 7Z88. Per-residue inclusion information can be found in section 3 on page 5.

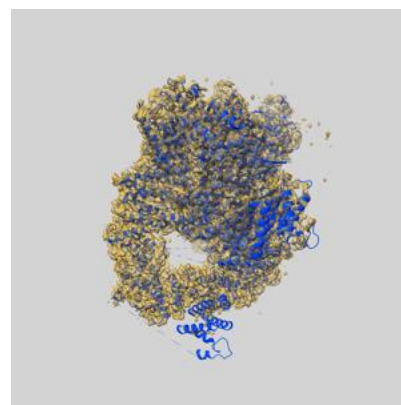
### 9.1 Map-model overlay [i](#)



X



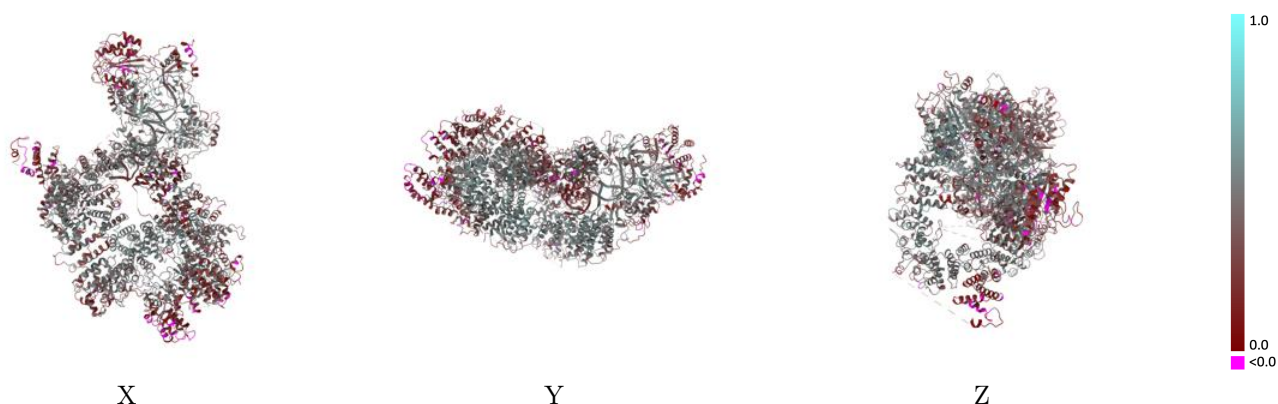
Y



Z

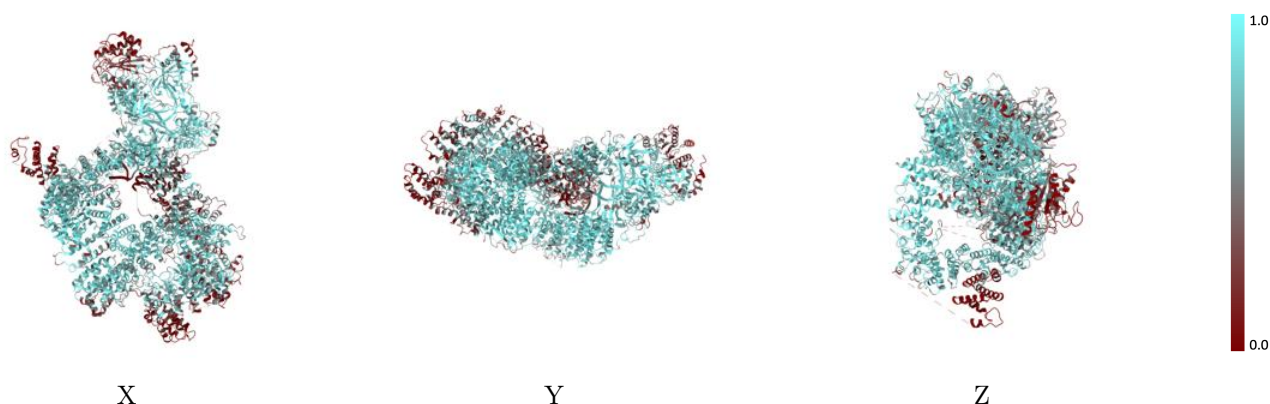
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



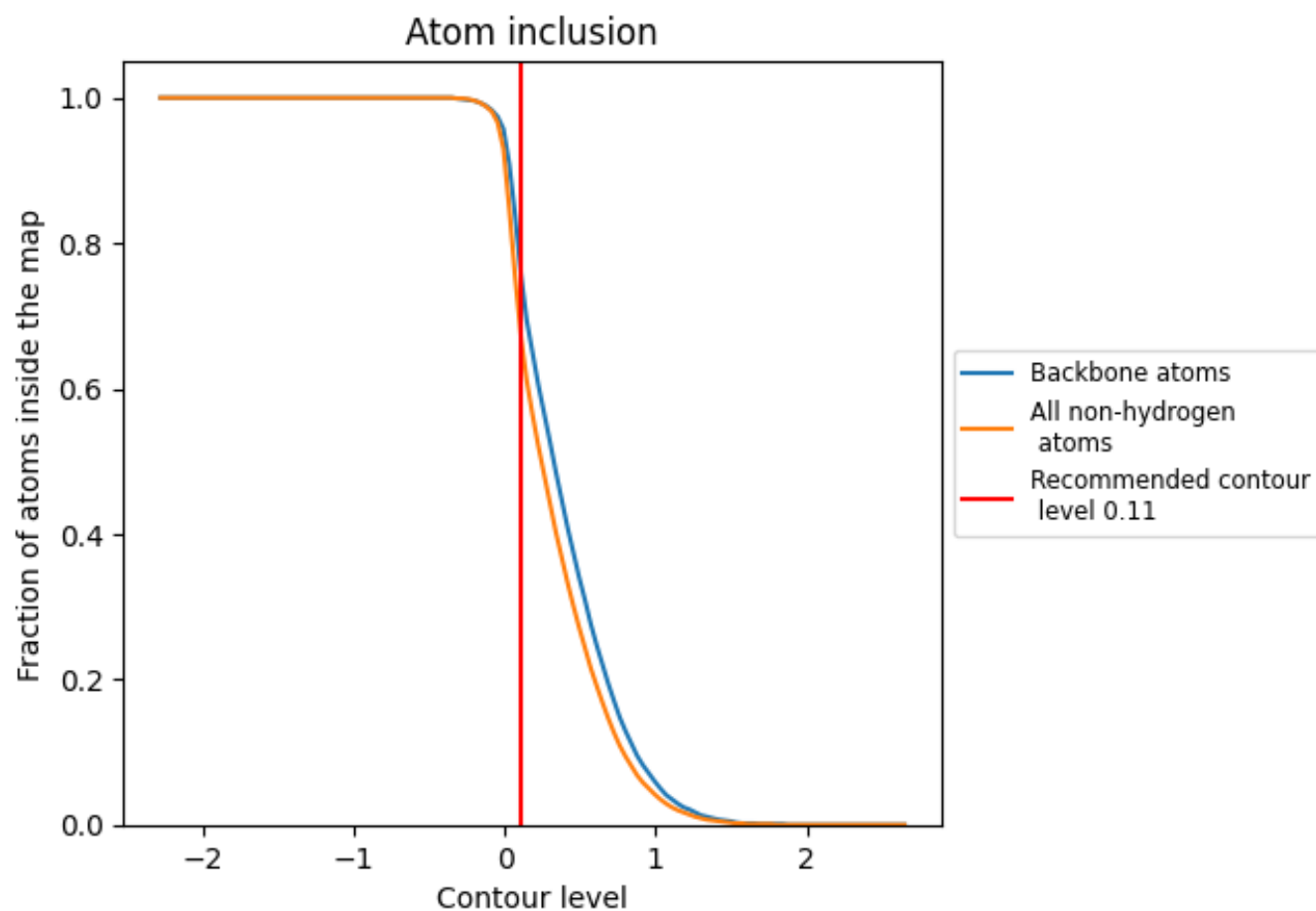
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6700	<div></div> 0.3890
A	<div></div> 0.7000	<div></div> 0.4010
B	<div></div> 0.7340	<div></div> 0.4110
C	<div></div> 0.4540	<div></div> 0.3040
D	<div></div> 0.7450	<div></div> 0.4420
E	<div></div> 0.6940	<div></div> 0.3990

