



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 01:32 PM UTC

PDB ID : 6BQ1 / pdb_00006bq1
EMDB ID : EMD-7129
Title : Human PI4KIIIa lipid kinase complex
Authors : Lees, J.A.; Zhang, Y.; Oh, M.; Schauder, C.M.; Yu, X.; Baskin, J.; Dobbs, K.;
Notarangelo, L.D.; Camilli, P.D.; Walz, T.; Reinisch, K.M.
Deposited on : 2017-11-27
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

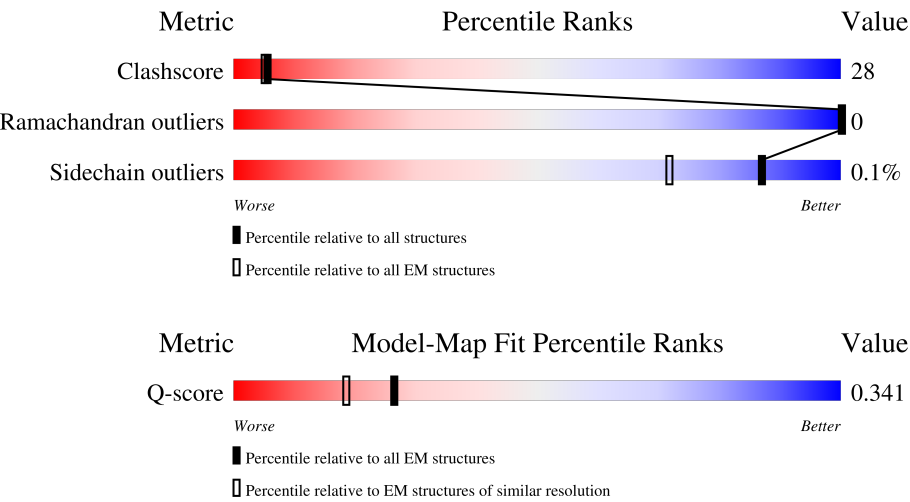
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	1647	14% 59% 31% 8%
2	B	863	37% 52% 32% 16%
2	F	863	35% 50% 34% 16%
3	C	292	44% 43% 47% 10%

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Mol	Chain	Length	Quality of chain
3	G	292	
4	E	1648	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	E4S	E	2201	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37217 atoms, of which 54 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 Phosphatidylinositol 4-kinase III alpha (PI4KA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1509	Total	C	N	O	S	0	0
			10673	6767	1872	1972	62		

- Molecule 2 is a protein called Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	728	Total	C	N	O	S	0	0
			5774	3670	1007	1065	32		
2	F	728	Total	C	N	O	S	0	0
			5774	3670	1007	1065	32		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q86TV6
B	-18	TYR	-	expression tag	UNP Q86TV6
B	-17	PRO	-	expression tag	UNP Q86TV6
B	-16	TYR	-	expression tag	UNP Q86TV6
B	-15	ASP	-	expression tag	UNP Q86TV6
B	-14	VAL	-	expression tag	UNP Q86TV6
B	-13	PRO	-	expression tag	UNP Q86TV6
B	-12	ASP	-	expression tag	UNP Q86TV6
B	-11	TYR	-	expression tag	UNP Q86TV6
B	-10	ALA	-	expression tag	UNP Q86TV6
B	-9	ALA	-	expression tag	UNP Q86TV6
B	-8	ILE	-	expression tag	UNP Q86TV6
B	-7	ALA	-	expression tag	UNP Q86TV6
B	-6	GLY	-	expression tag	UNP Q86TV6
B	-5	ALA	-	expression tag	UNP Q86TV6
B	-4	PRO	-	expression tag	UNP Q86TV6
B	-3	ASP	-	expression tag	UNP Q86TV6
B	-2	LEU	-	expression tag	UNP Q86TV6
B	-1	LYS	-	expression tag	UNP Q86TV6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q86TV6
F	-19	MET	-	expression tag	UNP Q86TV6
F	-18	TYR	-	expression tag	UNP Q86TV6
F	-17	PRO	-	expression tag	UNP Q86TV6
F	-16	TYR	-	expression tag	UNP Q86TV6
F	-15	ASP	-	expression tag	UNP Q86TV6
F	-14	VAL	-	expression tag	UNP Q86TV6
F	-13	PRO	-	expression tag	UNP Q86TV6
F	-12	ASP	-	expression tag	UNP Q86TV6
F	-11	TYR	-	expression tag	UNP Q86TV6
F	-10	ALA	-	expression tag	UNP Q86TV6
F	-9	ALA	-	expression tag	UNP Q86TV6
F	-8	ILE	-	expression tag	UNP Q86TV6
F	-7	ALA	-	expression tag	UNP Q86TV6
F	-6	GLY	-	expression tag	UNP Q86TV6
F	-5	ALA	-	expression tag	UNP Q86TV6
F	-4	PRO	-	expression tag	UNP Q86TV6
F	-3	ASP	-	expression tag	UNP Q86TV6
F	-2	LEU	-	expression tag	UNP Q86TV6
F	-1	LYS	-	expression tag	UNP Q86TV6
F	0	LEU	-	expression tag	UNP Q86TV6

- Molecule 3 is a protein called Protein FAM126A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	264	Total	C	N	O	S	0	0
			2091	1357	338	383	13		
3	G	264	Total	C	N	O	S	0	0
			2091	1357	338	383	13		

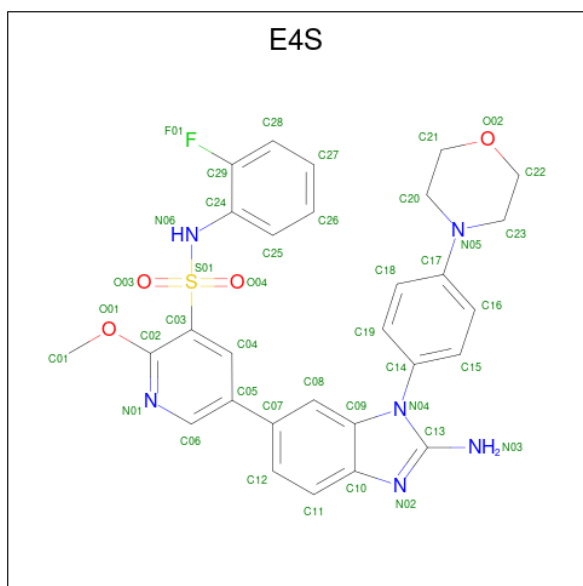
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9BYI3
C	-1	PRO	-	expression tag	UNP Q9BYI3
C	0	GLY	-	expression tag	UNP Q9BYI3
C	1	SER	-	expression tag	UNP Q9BYI3
G	-2	GLY	-	expression tag	UNP Q9BYI3
G	-1	PRO	-	expression tag	UNP Q9BYI3
G	0	GLY	-	expression tag	UNP Q9BYI3
G	1	SER	-	expression tag	UNP Q9BYI3

- Molecule 4 is a protein called Phosphatidylinositol 4-kinase III alpha (PI4KA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1510	Total	C	N	O	S	0	0
			10678	6770	1873	1973	62		

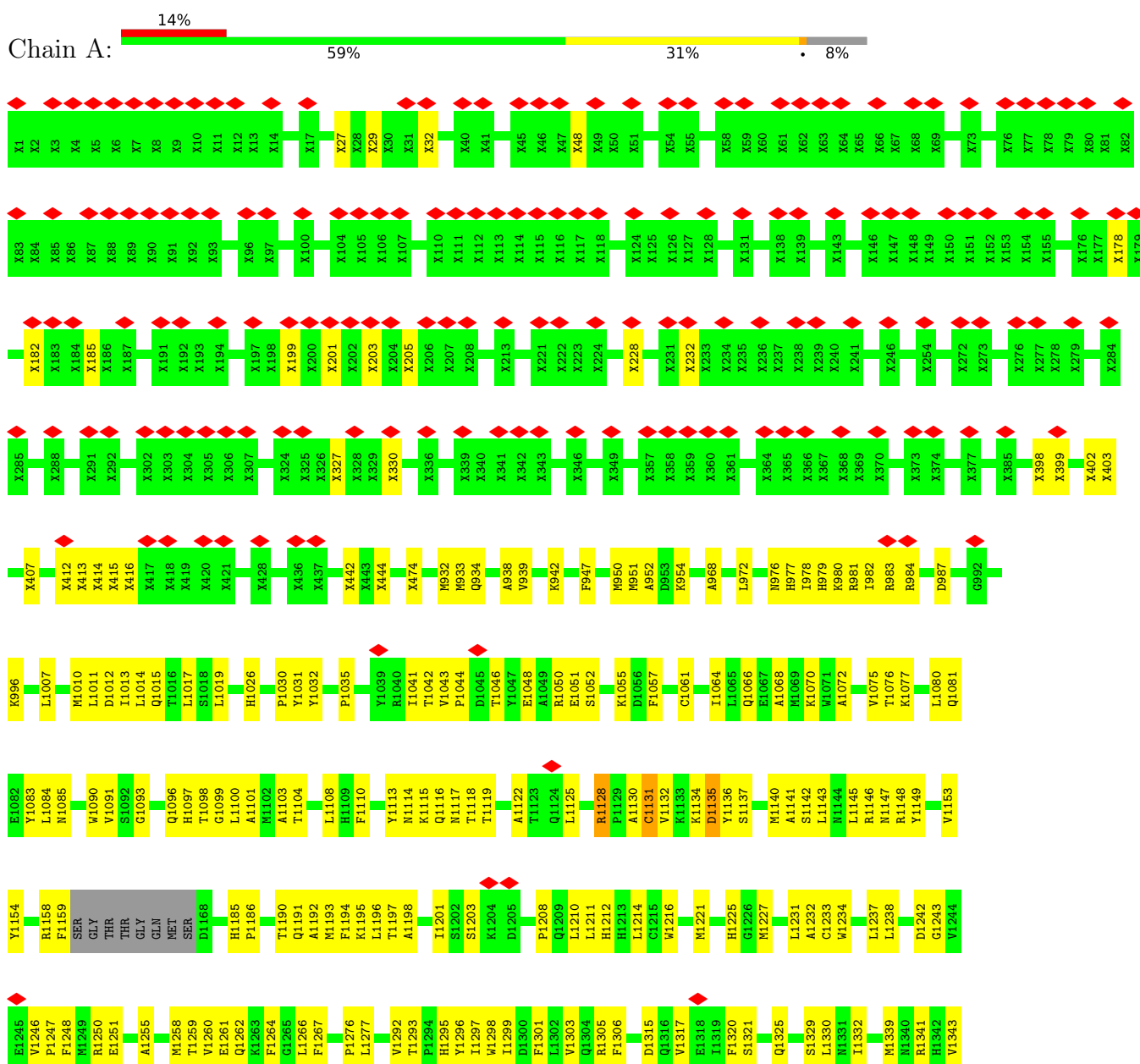
- Molecule 5 is 5-{2-amino-1-[4-(morpholin-4-yl)phenyl]-1H-benzimidazol-6-yl}-N-(2-fluorophenyl)-2-methoxypyridine-3-sulfonamide (CCD ID: E4S) (formula: C₂₉H₂₇FN₆O₄S).

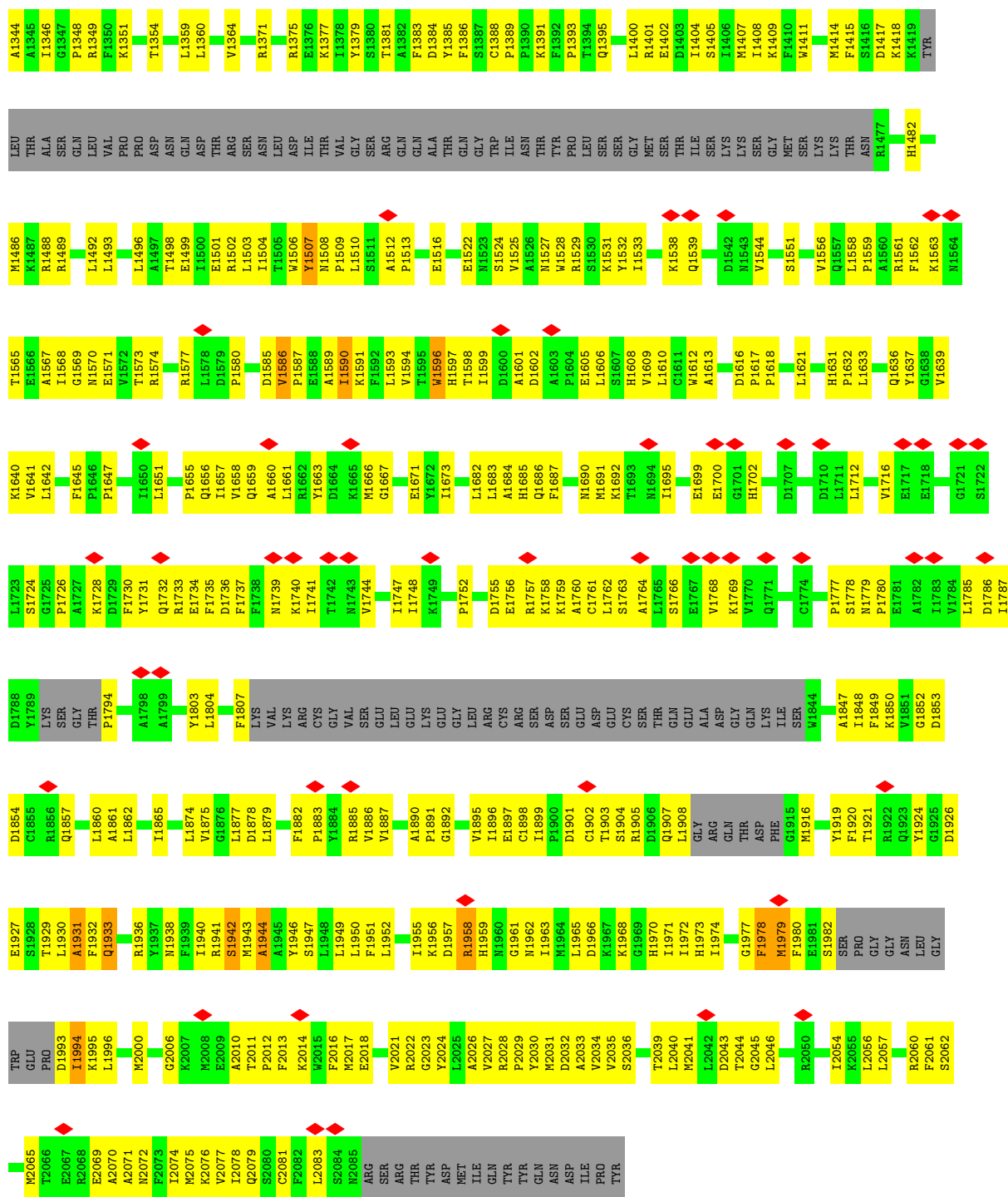


3 Residue-property plots

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

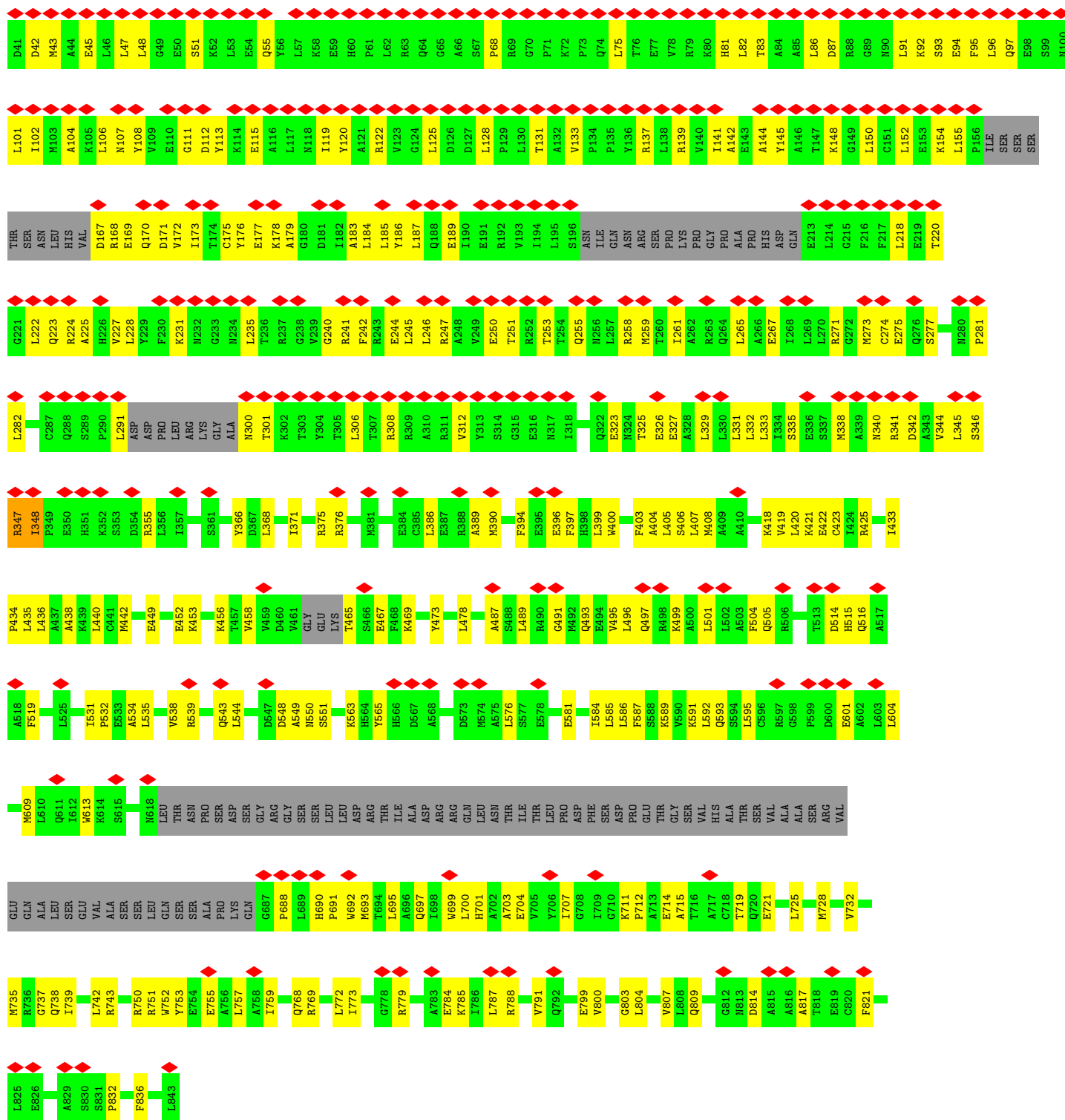
- Molecule 1: Phosphatidylinositol 4-kinase III alpha (PI4KA)





• Molecule 2: Tetratricopeptide repeat protein 7B

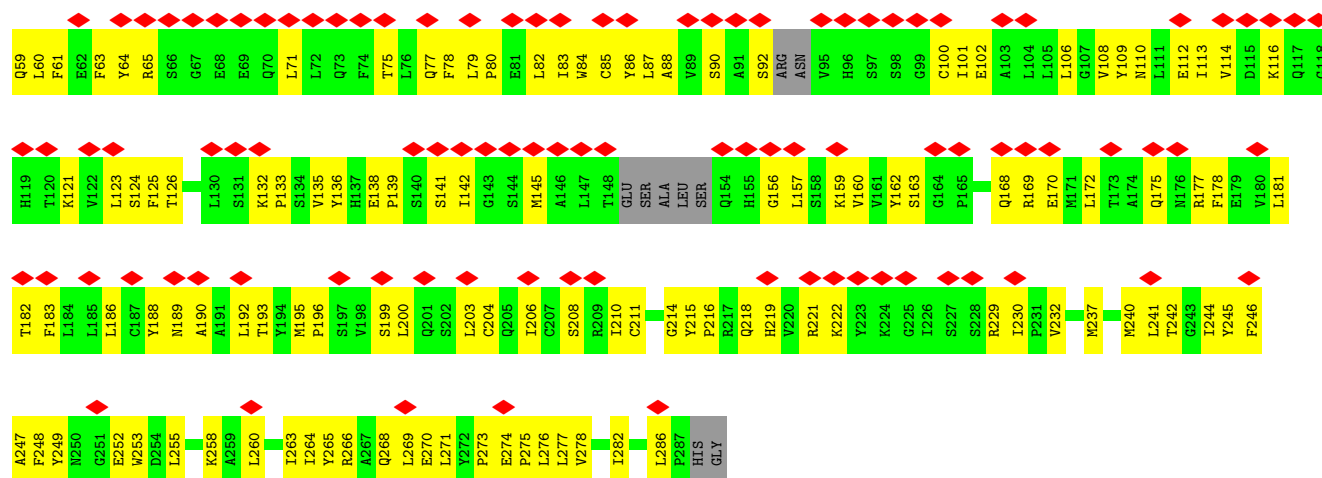




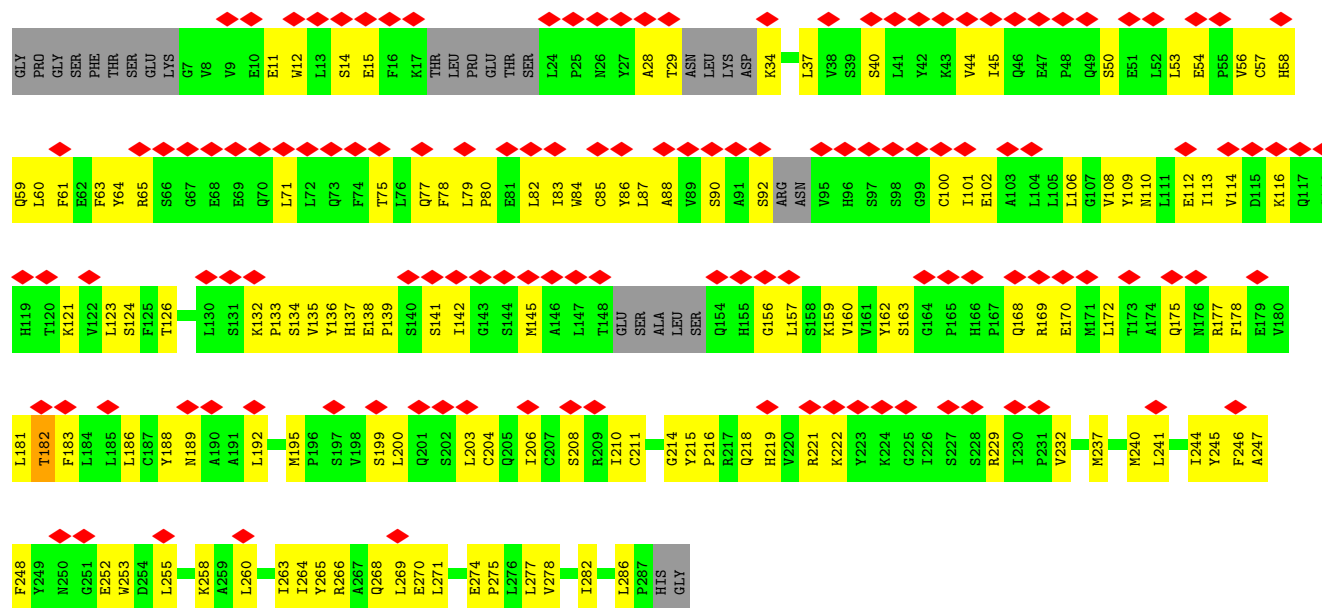
• Molecule 2: Tetratricopeptide repeat protein 7B



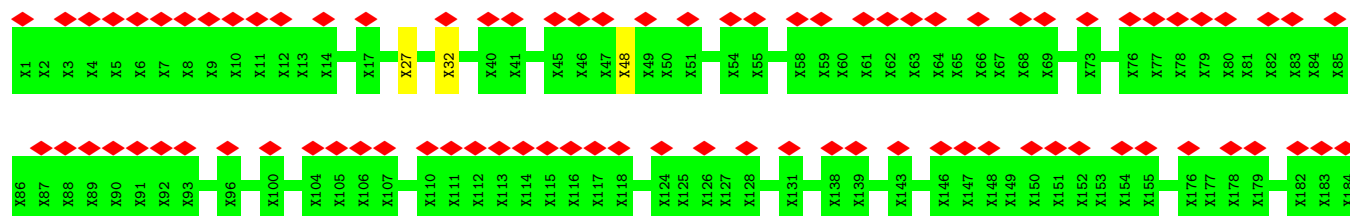




• Molecule 3: Protein FAM126A



• Molecule 4: Phosphatidylinositol 4-kinase III alpha (PI4KA)





A2071	N2072	F2073	I2074	M2075	K2076	V2077	I2078	Q2079	L2083	S2084	N2085	ARG	SER	ARG	THR	TYR	MET	ILE	GLN	TYR	ASN	ASP	ILE	PRO	TYR																														
K1995	L1996	M2000	G2006	K2007	M2008	E2009	A2010	T2011	P2012	F2013	K2014	W2015	F2016	M2017	E2018	V2021	R2022	G2023	V2024	L2025	A2026	V2027	R2028	P2029	V2030	M2031	D2032	A2033	V2034	V2035	S2036	T2039	L2040	M2041	L2042	D2043	T2044	G2045	L2046	R2050	I2054	K2055	L2056	L2057	R2060	F2061	S2062	M2065	E2069	A2070					
T1929	L1930	A1931	F1932	R1936	Y1937	M1938	F1939	I1940	R1941	S1942	M1943	A1944	A1945	Y1946	S1947	L1948	L1949	L1950	F1951	L1952	L1953	Q1954	I1955	K1956	D1957	R1958	H1959	I1963	M1964	L1965	K1968	G1969	H1970	I1971	I1972	H1973	I1974	G1977	F1978	M1979	F1980	E1981	S1982	SER	PRO	GLY	GLY	ASN	LEU	GLY	TRP	GLU	PRO	D1993	I1994
Q1857	L1860	A1861	L1862	I1865	F1868	L1874	S1875	G1876	L1877	D1878	L1879	F1882	P1883	Y1884	R1885	V1886	V1887	A1890	P1891	G1892	V1895	I1896	E1897	C1898	I1899	C1902	T1903	S1904	R1905	D1906	Q1907	L1908	GLY	ARG	GLN	THR	ASP	PHE	G1915	M1916	Y1919	F1920	T1921	R1922	Q1923	Y1924	G1925	D1926	E1927	S1928					
Y1789	LYS	SER	GLY	THR	P1794	A1799	Y1803	L1804	F1807	LYS	VAL	LYS	ARG	CYS	GLY	VAL	SER	GLU	LEU	GLU	LYS	GLY	LEU	ARG	CYS	ARG	SER	ASP	SER	GLU	ASP	GLU	ALA	ASP	GLY	GLN	LYS	ILE	SER	W1844	A1847	I1848	F1849	K1850	V1851	G1852	D1853	D1854							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64104	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	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	38461	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: E4S

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	0.39	0/8500	0.65	21/11506 (0.2%)
2	B	0.27	0/5877	0.44	4/7948 (0.1%)
2	F	0.27	0/5877	0.46	6/7948 (0.1%)
3	C	0.23	0/2140	0.45	1/2903 (0.0%)
3	G	0.23	0/2140	0.43	0/2903
4	E	0.39	0/8500	0.65	15/11506 (0.1%)
All	All	0.33	0/33034	0.56	47/44714 (0.1%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1994	ILE	N-CA-C	11.60	123.31	110.21
4	E	1979	MET	N-CA-C	9.46	121.19	111.07
4	E	1702	HIS	N-CA-C	-9.12	101.34	111.28
4	E	1586	VAL	CB-CA-C	-8.17	105.69	114.35
1	A	1586	VAL	CB-CA-C	-8.01	105.86	114.35
2	F	348	ILE	CA-C-N	-7.70	110.96	118.97
2	F	348	ILE	C-N-CA	-7.70	110.96	118.97
4	E	1950	LEU	N-CA-C	-7.56	103.04	111.28
1	A	1956	LYS	N-CA-C	7.37	121.57	112.58
1	A	978	ILE	N-CA-C	7.30	118.07	110.62
2	F	327	GLU	N-CA-C	7.20	119.12	111.28
2	F	348	ILE	N-CA-C	6.97	123.94	108.88
4	E	1699	GLU	N-CA-C	6.89	118.58	111.14
1	A	1958	ARG	N-CA-C	6.77	119.44	108.34
1	A	1590	ILE	N-CA-C	6.58	116.72	110.53
4	E	1507	TYR	N-CA-C	6.54	120.47	112.23
4	E	1698	ASP	N-CA-C	6.50	118.55	109.31
1	A	1933	GLN	N-CA-C	6.48	118.34	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1507	TYR	N-CA-C	6.42	120.32	112.23
2	B	348	ILE	N-CA-C	6.29	122.47	108.88
4	E	1590	ILE	N-CA-C	6.26	116.41	110.53
1	A	1962	ASN	N-CA-C	-6.25	105.65	113.28
1	A	1979	MET	N-CA-C	6.21	117.72	111.07
2	F	349	PRO	N-CA-C	-6.19	104.62	113.47
1	A	1944	ALA	N-CA-C	-5.92	104.83	111.28
2	B	347	ARG	N-CA-C	-5.76	104.91	111.07
3	C	230	ILE	N-CA-CB	5.70	118.24	111.23
4	E	980	LYS	N-CA-C	-5.68	105.46	112.90
4	E	1586	VAL	N-CA-C	5.67	120.83	112.61
1	A	1586	VAL	N-CA-C	5.64	120.78	112.61
1	A	1931	ALA	N-CA-C	5.55	117.01	111.07
1	A	1596	TRP	CA-C-N	5.52	132.08	121.54
1	A	1596	TRP	C-N-CA	5.52	132.08	121.54
4	E	1596	TRP	CA-C-N	5.52	132.08	121.54
4	E	1596	TRP	C-N-CA	5.52	132.08	121.54
1	A	1942	SER	N-CA-C	5.51	116.97	111.07
2	B	348	ILE	CA-C-N	-5.49	112.97	119.84
2	B	348	ILE	C-N-CA	-5.49	112.97	119.84
4	E	1956	LYS	N-CA-C	5.46	122.44	110.80
1	A	1131	CYS	N-CA-C	-5.45	104.13	111.54
1	A	1978	PHE	N-CA-C	-5.30	102.28	109.54
1	A	1128	ARG	CA-C-N	-5.10	113.47	119.84
1	A	1128	ARG	C-N-CA	-5.10	113.47	119.84
2	F	325	THR	N-CA-C	-5.10	105.42	111.69
1	A	980	LYS	N-CA-C	-5.06	105.47	111.69
1	A	1135	ASP	N-CA-C	-5.06	106.95	112.72
4	E	1699	GLU	CB-CA-C	-5.02	102.97	110.90

There are no chirality outliers.

There are no planarity outliers.

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	10673	0	8799	634	0
2	B	5774	0	5852	267	0
2	F	5774	0	5852	279	0
3	C	2091	0	2096	158	0
3	G	2091	0	2096	136	0
4	E	10678	0	8800	635	0
5	A	41	27	0	3	0
5	E	41	27	0	3	0
All	All	37163	54	33495	1951	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 28.

All (1951) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1932:PHE:CZ	1:A:1936:ARG:HD3	1.30	1.60
4:E:1696:TYR:CD1	4:E:1701:GLY:HA2	1.34	1.58
4:E:1860:LEU:HD22	4:E:1979:MET:CE	1.50	1.40
1:A:1404:ILE:HD12	1:A:1507:TYR:CE2	1.55	1.40
1:A:1932:PHE:CE2	1:A:1936:ARG:HD3	1.55	1.38
3:C:178:PHE:CD1	3:C:181:LEU:HD12	1.57	1.37
1:A:1404:ILE:CD1	1:A:1507:TYR:HE2	1.36	1.35
4:E:1860:LEU:CD2	4:E:1979:MET:HE1	1.56	1.33
1:A:1860:LEU:HD22	1:A:1979:MET:CE	1.56	1.33
3:C:177:ARG:O	3:C:181:LEU:HG	1.26	1.31
4:E:1404:ILE:HD12	4:E:1507:TYR:CE2	1.66	1.29
4:E:1404:ILE:CD1	4:E:1507:TYR:HE2	1.45	1.28
3:G:178:PHE:CD1	3:G:181:LEU:HD12	1.70	1.27
1:A:1860:LEU:CD2	1:A:1979:MET:HE1	1.67	1.23
1:A:1932:PHE:CZ	1:A:1936:ARG:CD	2.20	1.23
4:E:1696:TYR:CD1	4:E:1701:GLY:CA	2.20	1.23
4:E:1955:ILE:HD12	4:E:1959:HIS:CD2	1.70	1.23
3:G:177:ARG:O	3:G:181:LEU:HG	1.35	1.21
1:A:1932:PHE:CE2	1:A:1936:ARG:CD	2.28	1.17
1:A:182:UNK:CB	1:A:201:UNK:CB	2.23	1.16
1:A:1950:LEU:HD23	1:A:1955:ILE:HD13	1.26	1.16
4:E:933:MET:HE1	4:E:981:ARG:HD2	1.17	1.16
1:A:1590:ILE:HA	1:A:1612:TRP:CZ3	1.83	1.12
1:A:933:MET:HE1	1:A:981:ARG:HD2	1.29	1.10
3:C:60:LEU:HD22	3:C:75:THR:HG22	1.34	1.10
1:A:1632:PRO:HG2	2:B:345:LEU:HD13	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:SER:CB	2:B:355:ARG:HH11	1.66	1.08
4:E:1666:MET:HG2	2:F:347:ARG:HG2	1.11	1.07
1:A:1098:THR:HG23	4:E:1131:CYS:HB2	1.35	1.06
4:E:1950:LEU:HB3	4:E:1994:ILE:HD12	1.34	1.06
1:A:1950:LEU:HG	1:A:1955:ILE:HG21	1.36	1.06
4:E:1666:MET:CG	2:F:347:ARG:HG2	1.84	1.06
4:E:1590:ILE:HD11	4:E:1594:VAL:HG21	1.38	1.04
4:E:1590:ILE:HG13	4:E:1594:VAL:HG23	1.37	1.04
1:A:1699:GLU:HB3	1:A:1702:HIS:HD2	1.20	1.04
3:G:60:LEU:HD22	3:G:75:THR:HG22	1.34	1.04
2:B:587:PHE:CD1	2:B:701:HIS:CE1	2.46	1.04
4:E:1404:ILE:HD12	4:E:1507:TYR:HE2	0.88	1.04
4:E:1666:MET:HG2	2:F:347:ARG:CG	1.87	1.04
4:E:1865:ILE:HG12	4:E:1949:LEU:HD23	1.39	1.03
1:A:933:MET:HE1	1:A:981:ARG:CD	1.87	1.03
1:A:1108:LEU:HD22	4:E:1108:LEU:HD22	1.40	1.03
3:C:178:PHE:CD1	3:C:181:LEU:CD1	2.40	1.03
4:E:1955:ILE:HD12	4:E:1959:HIS:HD2	1.21	1.03
2:F:346:SER:HB2	2:F:355:ARG:NH1	1.74	1.02
2:F:587:PHE:CD1	2:F:701:HIS:CE1	2.46	1.02
4:E:933:MET:HE1	4:E:981:ARG:CD	1.89	1.02
2:F:346:SER:CB	2:F:355:ARG:HH11	1.71	1.02
2:B:346:SER:HB2	2:B:355:ARG:NH1	1.75	1.01
3:G:211:CYS:O	3:G:266:ARG:HD2	1.61	1.01
4:E:1696:TYR:HD1	4:E:1701:GLY:HA2	1.19	1.00
1:A:1860:LEU:HD22	1:A:1979:MET:HE1	1.01	0.99
1:A:1590:ILE:HA	1:A:1612:TRP:HZ3	1.20	0.98
1:A:1699:GLU:HB3	1:A:1702:HIS:CD2	1.99	0.98
4:E:1590:ILE:HG13	4:E:1612:TRP:HZ3	1.25	0.97
3:C:178:PHE:HD1	3:C:181:LEU:CD1	1.76	0.97
1:A:1632:PRO:CG	2:B:345:LEU:HD13	1.94	0.96
4:E:185:UNK:CB	4:E:205:UNK:CB	2.42	0.96
1:A:1404:ILE:CD1	1:A:1507:TYR:CE2	2.27	0.96
1:A:182:UNK:CB	1:A:201:UNK:CA	2.43	0.95
4:E:1590:ILE:HG13	4:E:1594:VAL:CG2	1.97	0.94
1:A:1404:ILE:HD12	1:A:1507:TYR:HE2	0.77	0.94
4:E:933:MET:CE	4:E:981:ARG:HD2	1.97	0.94
3:G:83:ILE:O	3:G:87:LEU:HB3	1.68	0.94
3:C:83:ILE:O	3:C:87:LEU:HB3	1.68	0.93
4:E:1404:ILE:CD1	4:E:1507:TYR:CE2	2.36	0.93
1:A:1339:MET:HE1	1:A:1349:ARG:HA	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1586:VAL:CG1	4:E:1613:ALA:HB3	1.99	0.93
1:A:1590:ILE:CA	1:A:1612:TRP:HZ3	1.82	0.93
1:A:1929:THR:O	1:A:1933:GLN:HG3	1.68	0.93
4:E:1586:VAL:HG13	4:E:1613:ALA:HB3	1.50	0.93
1:A:1131:CYS:SG	4:E:1101:ALA:HB3	2.09	0.93
4:E:1339:MET:HE1	4:E:1349:ARG:HA	1.48	0.92
1:A:1277:LEU:HD23	1:A:1618:PRO:HG2	1.51	0.92
4:E:1590:ILE:CG1	4:E:1612:TRP:HZ3	1.83	0.92
3:G:60:LEU:HD22	3:G:75:THR:CG2	2.00	0.92
2:B:346:SER:CB	2:B:355:ARG:NH1	2.32	0.92
1:A:933:MET:CE	1:A:981:ARG:HD2	2.00	0.92
3:C:211:CYS:O	3:C:266:ARG:HD2	1.69	0.91
4:E:1590:ILE:CD1	4:E:1594:VAL:HG21	1.99	0.91
2:F:408:MET:HE1	2:F:436:LEU:HB3	1.52	0.91
3:C:60:LEU:HD22	3:C:75:THR:CG2	2.00	0.91
2:B:408:MET:HE1	2:B:436:LEU:HB3	1.53	0.91
1:A:1671:GLU:OE1	2:B:348:ILE:HD11	1.71	0.91
3:G:60:LEU:CD2	3:G:75:THR:CG2	2.49	0.91
3:C:82:LEU:O	3:C:86:TYR:HB3	1.70	0.90
4:E:1667:GLY:HA3	2:F:347:ARG:O	1.69	0.90
1:A:1128:ARG:HD3	4:E:1051:GLU:HG3	1.51	0.90
3:G:82:LEU:O	3:G:86:TYR:HB3	1.70	0.90
4:E:1112:GLY:O	4:E:1135:ASP:OD1	1.90	0.90
1:A:1905:ARG:HB3	1:A:1961:GLY:HA2	1.53	0.90
3:C:60:LEU:CD2	3:C:75:THR:CG2	2.49	0.89
1:A:1699:GLU:HG3	1:A:1700:GLU:H	1.38	0.89
3:G:178:PHE:CD1	3:G:181:LEU:CD1	2.56	0.89
4:E:1277:LEU:HD23	4:E:1618:PRO:HG2	1.51	0.89
4:E:1696:TYR:CE1	4:E:1701:GLY:CA	2.56	0.89
1:A:1804:LEU:HA	1:A:1848:ILE:HG22	1.54	0.89
1:A:1131:CYS:HB2	4:E:1098:THR:HG23	1.55	0.89
4:E:1565:THR:HG22	4:E:1567:ALA:H	1.38	0.89
1:A:1565:THR:HG22	1:A:1567:ALA:H	1.38	0.89
1:A:1946:TYR:O	1:A:1950:LEU:HD13	1.71	0.88
3:G:178:PHE:HD1	3:G:181:LEU:HD12	1.16	0.88
4:E:1585:ASP:OD1	4:E:1589:ALA:HB2	1.74	0.88
4:E:1955:ILE:CD1	4:E:1959:HIS:HD2	1.85	0.88
1:A:1865:ILE:HG12	1:A:1949:LEU:HD23	1.53	0.88
1:A:1586:VAL:HG23	1:A:1587:PRO:HD3	1.56	0.88
4:E:1696:TYR:CE1	4:E:1701:GLY:HA2	2.08	0.88
4:E:1950:LEU:CB	4:E:1994:ILE:HD12	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1250:ARG:HH22	2:F:781:SER:HB3	1.38	0.87
1:A:1590:ILE:CA	1:A:1612:TRP:CZ3	2.56	0.86
3:G:211:CYS:O	3:G:266:ARG:CD	2.23	0.86
4:E:1954:GLN:HG2	4:E:2060:ARG:CZ	2.05	0.86
3:C:84:TRP:O	3:C:88:ALA:HB3	1.76	0.86
4:E:1804:LEU:HA	4:E:1848:ILE:HG22	1.54	0.85
1:A:1950:LEU:HG	1:A:1955:ILE:CG2	2.05	0.85
1:A:1344:ALA:HA	1:A:1395:GLN:HE21	1.40	0.85
1:A:977:HIS:O	1:A:983:ARG:HD3	1.75	0.85
3:G:84:TRP:O	3:G:88:ALA:HB3	1.76	0.85
4:E:1590:ILE:CG1	4:E:1594:VAL:CG2	2.54	0.85
4:E:1344:ALA:HA	4:E:1395:GLN:HE21	1.40	0.84
1:A:1978:PHE:HD1	1:A:1982:SER:CB	1.91	0.84
3:C:178:PHE:HD1	3:C:181:LEU:HD12	1.02	0.84
2:F:346:SER:HB2	2:F:355:ARG:HH11	1.29	0.84
1:A:1052:SER:HA	1:A:1055:LYS:HE2	1.59	0.84
3:C:178:PHE:CE1	3:C:181:LEU:HD12	2.12	0.84
1:A:1122:ALA:HB3	1:A:1125:LEU:HD23	1.60	0.84
1:A:1134:LYS:HG3	1:A:1136:TYR:CE2	2.12	0.83
4:E:1052:SER:HA	4:E:1055:LYS:HE2	1.59	0.83
1:A:1400:LEU:CD2	1:A:1507:TYR:CD2	2.61	0.83
1:A:1651:LEU:HD11	1:A:1686:GLN:HG3	1.60	0.83
4:E:1122:ALA:HB3	4:E:1125:LEU:HD23	1.60	0.83
3:C:211:CYS:O	3:C:266:ARG:CD	2.26	0.83
1:A:1944:ALA:HB2	1:A:2016:PHE:CD1	2.14	0.82
4:E:1666:MET:HA	2:F:347:ARG:HG2	1.61	0.82
2:F:319:PHE:H	3:G:134:SER:HA	1.43	0.82
3:G:274:GLU:HG2	3:G:275:PRO:HD3	1.62	0.82
4:E:1586:VAL:CG1	4:E:1613:ALA:CB	2.57	0.82
2:B:346:SER:HB3	2:B:355:ARG:HH11	1.44	0.82
3:C:274:GLU:HG2	3:C:275:PRO:HD3	1.62	0.82
4:E:1950:LEU:HB3	4:E:1994:ILE:CD1	2.10	0.81
1:A:1860:LEU:HB3	1:A:1979:MET:HE1	1.60	0.81
1:A:1978:PHE:HD1	1:A:1982:SER:HB2	1.43	0.81
4:E:1651:LEU:HD11	4:E:1686:GLN:HG3	1.61	0.81
4:E:1666:MET:HA	2:F:347:ARG:CG	2.09	0.81
2:F:587:PHE:CD1	2:F:701:HIS:HE1	1.98	0.81
1:A:1994:ILE:H	1:A:1994:ILE:HD12	1.43	0.81
4:E:977:HIS:O	4:E:983:ARG:HD3	1.79	0.81
2:F:142:ALA:HA	2:F:145:TYR:HD2	1.46	0.81
2:B:274:CYS:HB3	3:C:192:LEU:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:THR:HG23	4:E:1131:CYS:CB	2.11	0.81
1:A:1963:ILE:CD1	1:A:1995:LYS:HD2	2.10	0.81
4:E:1860:LEU:HD22	4:E:1979:MET:HE1	0.85	0.81
3:G:178:PHE:HD1	3:G:181:LEU:CD1	1.93	0.81
2:B:142:ALA:HA	2:B:145:TYR:HD2	1.46	0.80
1:A:1944:ALA:HA	1:A:2016:PHE:CE1	2.16	0.80
1:A:474:UNK:CB	1:A:981:ARG:NH1	2.45	0.80
1:A:1666:MET:HG2	2:B:347:ARG:HG2	1.61	0.80
4:E:1507:TYR:C	4:E:1509:PRO:HD3	2.05	0.80
1:A:933:MET:HE1	1:A:981:ARG:HB2	1.64	0.80
1:A:976:ASN:OD1	1:A:1017:LEU:HD11	1.83	0.80
3:G:178:PHE:CE1	3:G:181:LEU:HD12	2.16	0.80
3:C:178:PHE:CE1	3:C:181:LEU:CD1	2.65	0.79
1:A:1507:TYR:C	1:A:1509:PRO:HD3	2.08	0.79
1:A:1684:ALA:HA	1:A:1687:PHE:HD2	1.47	0.79
4:E:1684:ALA:HA	4:E:1687:PHE:HD2	1.47	0.79
4:E:1586:VAL:HG23	4:E:1587:PRO:HD3	1.64	0.79
2:B:587:PHE:CD1	2:B:701:HIS:ND1	2.50	0.79
2:F:587:PHE:CD1	2:F:701:HIS:ND1	2.50	0.79
1:A:1192:ALA:HA	1:A:1195:LYS:HZ1	1.47	0.79
1:A:1101:ALA:HB3	4:E:1131:CYS:SG	2.22	0.79
1:A:1932:PHE:CE2	1:A:1936:ARG:NE	2.50	0.79
2:B:37:LEU:HB3	2:B:38:ILE:HD12	1.65	0.79
1:A:1153:VAL:HG21	1:A:1198:ALA:HB3	1.65	0.78
4:E:1696:TYR:CE1	4:E:1701:GLY:HA3	2.18	0.78
1:A:1101:ALA:HB1	4:E:1136:TYR:HB2	1.64	0.78
1:A:2065:MET:HE2	1:A:2069:GLU:HG3	1.64	0.78
4:E:1958:ARG:O	4:E:1959:HIS:CG	2.36	0.78
1:A:933:MET:HE1	1:A:981:ARG:CB	2.14	0.78
4:E:1726:PRO:O	4:E:1730:PHE:HB2	1.84	0.78
1:A:1944:ALA:CA	1:A:2016:PHE:CE1	2.67	0.78
1:A:1978:PHE:CD1	1:A:1982:SER:HB2	2.18	0.78
2:B:587:PHE:HD1	2:B:701:HIS:ND1	1.82	0.78
1:A:1943:MET:HB3	1:A:1971:ILE:HG21	1.65	0.77
2:B:587:PHE:CD1	2:B:701:HIS:HE1	1.98	0.77
1:A:1132:VAL:O	1:A:1134:LYS:HG2	1.85	0.77
2:F:346:SER:HA	2:F:355:ARG:HG3	1.66	0.77
1:A:1586:VAL:HG12	1:A:1613:ALA:CB	2.15	0.77
1:A:1924:TYR:HB3	1:A:1931:ALA:HB1	1.66	0.77
1:A:2034:VAL:HG12	1:A:2057:LEU:HD21	1.67	0.77
2:B:405:LEU:HB2	3:C:277:LEU:HD13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1726:PRO:O	1:A:1730:PHE:HB2	1.84	0.77
1:A:1861:ALA:HB2	1:A:1979:MET:HB2	1.64	0.77
4:E:1130:ALA:O	4:E:1131:CYS:HB3	1.83	0.77
4:E:1932:PHE:O	4:E:1936:ARG:HB2	1.85	0.77
4:E:1955:ILE:CD1	4:E:1959:HIS:CD2	2.58	0.77
4:E:2065:MET:HE2	4:E:2069:GLU:HG3	1.64	0.77
2:F:587:PHE:HD1	2:F:701:HIS:ND1	1.82	0.77
4:E:2034:VAL:HG12	4:E:2057:LEU:HD21	1.67	0.77
1:A:1098:THR:CG2	4:E:1131:CYS:HB2	2.15	0.77
4:E:1153:VAL:HG21	4:E:1198:ALA:HB3	1.66	0.77
4:E:1191:GLN:HG2	4:E:1195:LYS:HE3	1.67	0.77
4:E:1590:ILE:HG13	4:E:1612:TRP:CZ3	2.16	0.77
4:E:1400:LEU:CD2	4:E:1507:TYR:CD2	2.67	0.76
4:E:1886:VAL:HG22	4:E:1896:ILE:HG22	1.67	0.76
1:A:1055:LYS:HB3	4:E:1128:ARG:HA	1.67	0.76
1:A:1860:LEU:HD22	1:A:1979:MET:HE2	1.63	0.76
4:E:1666:MET:CB	2:F:347:ARG:HG2	2.14	0.76
1:A:1904:SER:HB2	1:A:1907:GLN:HG2	1.68	0.76
1:A:1950:LEU:CG	1:A:1955:ILE:HG21	2.13	0.76
4:E:1904:SER:HB2	4:E:1907:GLN:HG2	1.68	0.76
2:F:37:LEU:HB3	2:F:38:ILE:HD12	1.65	0.76
4:E:1590:ILE:CB	4:E:1612:TRP:CZ3	2.68	0.76
4:E:1667:GLY:CA	2:F:347:ARG:O	2.34	0.76
1:A:1077:LYS:O	1:A:1081:GLN:HB2	1.86	0.76
1:A:1259:THR:HG23	1:A:1264:PHE:HB2	1.68	0.76
4:E:1954:GLN:CG	4:E:2060:ARG:CZ	2.63	0.76
1:A:1418:LYS:HE2	1:A:1486:MET:HE1	1.67	0.76
1:A:1735:PHE:O	1:A:1739:ASN:HB2	1.86	0.76
1:A:1266:LEU:HD21	1:A:1339:MET:HE3	1.68	0.75
1:A:1860:LEU:CD2	1:A:1979:MET:CE	2.43	0.75
3:C:112:GLU:O	3:C:116:LYS:NZ	2.20	0.75
4:E:1640:LYS:HE2	2:F:425:ARG:HH22	1.51	0.75
4:E:1077:LYS:O	4:E:1081:GLN:HB2	1.86	0.75
4:E:1860:LEU:HD22	4:E:1979:MET:HE2	1.66	0.75
2:B:83:THR:O	2:B:87:ASP:HB2	1.87	0.75
2:F:83:THR:O	2:F:87:ASP:HB2	1.87	0.75
1:A:1191:GLN:HG2	1:A:1195:LYS:HE3	1.67	0.75
4:E:1418:LYS:HE2	4:E:1486:MET:HE1	1.67	0.75
1:A:1944:ALA:HB2	1:A:2016:PHE:CE1	2.21	0.74
4:E:1266:LEU:HD21	4:E:1339:MET:HE3	1.68	0.74
1:A:1886:VAL:HG22	1:A:1896:ILE:HG22	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:241:LEU:HD21	3:G:263:ILE:HG21	1.69	0.74
1:A:1699:GLU:HG3	1:A:1700:GLU:N	2.02	0.74
2:B:346:SER:HA	2:B:355:ARG:HG3	1.67	0.74
2:B:712:PRO:HB2	2:B:743:ARG:HE	1.52	0.74
1:A:182:UNK:CB	1:A:201:UNK:C	2.66	0.74
1:A:1667:GLY:N	2:B:347:ARG:O	2.20	0.74
4:E:1590:ILE:CG1	4:E:1594:VAL:HG21	2.16	0.74
4:E:1926:ASP:OD1	4:E:1927:GLU:HG3	1.87	0.74
1:A:1371:ARG:O	1:A:1375:ARG:HB2	1.88	0.74
4:E:1371:ARG:O	4:E:1375:ARG:HB2	1.88	0.74
4:E:1655:PRO:O	4:E:1659:GLN:NE2	2.20	0.74
3:G:60:LEU:CD2	3:G:75:THR:HG22	2.12	0.74
3:G:112:GLU:O	3:G:116:LYS:NZ	2.20	0.74
3:G:237:MET:HA	3:G:240:MET:HG2	1.69	0.74
4:E:1259:THR:HG23	4:E:1264:PHE:HB2	1.68	0.74
3:C:84:TRP:O	3:C:88:ALA:CB	2.36	0.74
4:E:1735:PHE:O	4:E:1739:ASN:HB2	1.86	0.74
4:E:1954:GLN:HG3	4:E:2060:ARG:NH2	2.03	0.73
1:A:1598:THR:HG22	1:A:1599:ILE:HG23	1.70	0.73
4:E:1590:ILE:HB	4:E:1612:TRP:CE3	2.22	0.73
1:A:1593:LEU:HB3	1:A:1612:TRP:HH2	1.53	0.73
1:A:1993:ASP:HB3	1:A:2081:CYS:SG	2.29	0.73
3:C:237:MET:HA	3:C:240:MET:HG2	1.69	0.73
3:C:241:LEU:HD21	3:C:263:ILE:HG21	1.69	0.73
2:F:587:PHE:CE1	2:F:701:HIS:CE1	2.76	0.73
1:A:1667:GLY:HA3	2:B:347:ARG:O	1.88	0.73
3:G:84:TRP:O	3:G:88:ALA:CB	2.36	0.73
1:A:1655:PRO:O	1:A:1659:GLN:NE2	2.20	0.73
1:A:1946:TYR:O	1:A:1950:LEU:CD1	2.37	0.73
1:A:1916:MET:HE3	1:A:1965:LEU:HD23	1.71	0.73
2:B:587:PHE:CE1	2:B:701:HIS:CE1	2.76	0.73
1:A:413:UNK:O	1:A:416:UNK:N	2.22	0.73
2:B:587:PHE:HD1	2:B:701:HIS:CE1	2.05	0.73
4:E:414:UNK:O	4:E:417:UNK:N	2.21	0.73
1:A:1586:VAL:CG1	1:A:1613:ALA:CB	2.66	0.73
3:C:177:ARG:O	3:C:181:LEU:CG	2.22	0.73
1:A:1994:ILE:HD12	1:A:1994:ILE:N	2.04	0.72
1:A:1920:PHE:HE2	1:A:1932:PHE:CD1	2.06	0.72
2:B:241:ARG:NH1	2:B:244:GLU:OE1	2.22	0.72
3:C:113:ILE:HG13	3:C:114:VAL:HG23	1.72	0.72
2:F:241:ARG:NH1	2:F:244:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:712:PRO:HB2	2:F:743:ARG:HE	1.52	0.72
1:A:1586:VAL:CG2	1:A:1587:PRO:HD3	2.19	0.72
1:A:1586:VAL:CG1	1:A:1613:ALA:HB3	2.20	0.72
4:E:1916:MET:HE3	4:E:1965:LEU:HD23	1.71	0.72
1:A:1667:GLY:CA	2:B:347:ARG:O	2.38	0.72
1:A:2028:ARG:NH1	1:A:2065:MET:O	2.22	0.72
4:E:1261:GLU:OE2	2:F:489:LEU:HG	1.88	0.72
4:E:1636:GLN:HG2	2:F:394:PHE:HD1	1.54	0.72
4:E:2028:ARG:NH1	4:E:2065:MET:O	2.22	0.72
1:A:1586:VAL:HG12	1:A:1613:ALA:HB3	1.71	0.72
4:E:1611:CYS:HB3	2:F:418:LYS:HB3	1.72	0.72
2:B:246:LEU:HD21	2:B:261:ILE:HG23	1.72	0.71
3:C:106:LEU:HD11	3:C:169:ARG:HB3	1.72	0.71
1:A:933:MET:CE	1:A:981:ARG:HB2	2.20	0.71
1:A:1926:ASP:OD1	1:A:1927:GLU:HG3	1.90	0.71
2:F:185:LEU:O	2:F:189:GLU:HB2	1.90	0.71
2:F:246:LEU:HD21	2:F:261:ILE:HG23	1.72	0.71
4:E:1250:ARG:NE	2:F:785:LYS:HB2	2.06	0.71
4:E:1950:LEU:HD22	4:E:1955:ILE:HG21	1.72	0.71
4:E:1598:THR:HG22	4:E:1599:ILE:HG23	1.70	0.71
1:A:178:UNK:O	1:A:201:UNK:CB	2.38	0.71
4:E:1861:ALA:HB2	4:E:1979:MET:HB2	1.71	0.71
1:A:1586:VAL:HG23	1:A:1587:PRO:CD	2.21	0.71
2:F:51:SER:O	2:F:55:GLN:HB2	1.91	0.71
3:G:86:TYR:OH	3:G:100:CYS:N	2.24	0.71
2:B:51:SER:O	2:B:55:GLN:HB2	1.91	0.70
4:E:1185:HIS:HD2	4:E:1186:PRO:HD2	1.56	0.70
4:E:1732:GLN:NE2	4:E:1736:ASP:OD2	2.24	0.70
1:A:1404:ILE:HD13	1:A:1507:TYR:HE2	1.51	0.70
4:E:408:UNK:CB	4:E:413:UNK:CB	2.70	0.70
4:E:1955:ILE:HD12	4:E:1959:HIS:NE2	2.06	0.70
3:G:113:ILE:HG13	3:G:114:VAL:HG23	1.72	0.70
2:B:185:LEU:O	2:B:189:GLU:HB2	1.90	0.70
1:A:1732:GLN:NE2	1:A:1736:ASP:OD2	2.24	0.70
1:A:1926:ASP:OD1	1:A:1927:GLU:N	2.25	0.70
1:A:1996:LEU:HA	1:A:2000:MET:CE	2.22	0.70
1:A:1860:LEU:CG	1:A:1979:MET:HE1	2.21	0.70
1:A:1963:ILE:HG22	1:A:1971:ILE:HD11	1.73	0.70
4:E:1590:ILE:CG1	4:E:1612:TRP:CZ3	2.71	0.70
3:G:106:LEU:HD11	3:G:169:ARG:HB3	1.72	0.70
1:A:1185:HIS:HD2	1:A:1186:PRO:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1860:LEU:CB	1:A:1979:MET:HE1	2.22	0.70
2:B:587:PHE:HD1	2:B:701:HIS:HD1	1.40	0.70
4:E:1586:VAL:HG13	4:E:1613:ALA:CB	2.19	0.69
2:B:591:LYS:NZ	2:B:704:GLU:OE1	2.26	0.69
4:E:1369:THR:HG21	2:F:755:GLU:HA	1.72	0.69
1:A:1128:ARG:HD3	4:E:1051:GLU:CG	2.21	0.69
4:E:1593:LEU:HB3	4:E:1612:TRP:HH2	1.57	0.69
2:F:33:LEU:HA	2:F:37:LEU:HD12	1.74	0.69
1:A:1499:GLU:OE2	1:A:1561:ARG:NE	2.25	0.69
4:E:1192:ALA:HA	4:E:1195:LYS:HZ1	1.56	0.69
2:F:591:LYS:NZ	2:F:704:GLU:OE1	2.26	0.69
2:B:291:LEU:HD23	3:C:193:THR:HG21	1.73	0.69
4:E:1489:ARG:O	4:E:1493:LEU:HD13	1.93	0.69
1:A:1590:ILE:HG13	1:A:1594:VAL:CG2	2.22	0.69
1:A:1916:MET:HE3	1:A:1965:LEU:CD2	2.23	0.69
3:C:86:TYR:OH	3:C:100:CYS:N	2.24	0.69
4:E:2075:MET:HA	4:E:2078:ILE:HG22	1.75	0.69
3:G:178:PHE:CE1	3:G:181:LEU:CD1	2.76	0.69
1:A:407:UNK:CB	1:A:412:UNK:CB	2.70	0.68
1:A:1978:PHE:CD1	1:A:1982:SER:CB	2.74	0.68
4:E:1666:MET:CA	2:F:347:ARG:HG2	2.23	0.68
4:E:1916:MET:HE3	4:E:1965:LEU:CD2	2.23	0.68
4:E:1938:ASN:HB3	4:E:1970:HIS:CD2	2.28	0.68
4:E:1963:ILE:HG22	4:E:1971:ILE:HD11	1.73	0.68
2:F:228:LEU:HD23	2:F:231:LYS:HD2	1.75	0.68
1:A:1938:ASN:HB3	1:A:1970:HIS:CD2	2.28	0.68
2:B:33:LEU:HA	2:B:37:LEU:HD12	1.74	0.68
2:B:228:LEU:HD23	2:B:231:LYS:HD2	1.75	0.68
4:E:1590:ILE:HB	4:E:1612:TRP:CZ3	2.28	0.68
1:A:1590:ILE:CB	1:A:1612:TRP:HZ3	2.06	0.68
4:E:449:UNK:CB	4:E:939:VAL:HG11	2.24	0.68
1:A:1946:TYR:HB3	1:A:1973:HIS:CE1	2.28	0.68
4:E:1994:ILE:HG22	4:E:1995:LYS:N	2.08	0.68
2:F:587:PHE:HD1	2:F:701:HIS:HD1	1.40	0.68
1:A:1114:ASN:HB3	1:A:1135:ASP:HB3	1.73	0.68
1:A:1489:ARG:O	1:A:1493:LEU:HD13	1.93	0.68
4:E:1571:GLU:OE1	4:E:1574:ARG:NH1	2.25	0.68
1:A:1014:LEU:HD21	1:A:1098:THR:HG22	1.74	0.68
1:A:1081:GLN:HE22	1:A:1142:SER:HB2	1.59	0.68
4:E:939:VAL:HA	4:E:942:LYS:HZ3	1.59	0.68
4:E:1954:GLN:HG2	4:E:2060:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1014:LEU:HD21	4:E:1098:THR:HG22	1.74	0.68
4:E:1590:ILE:HA	4:E:1612:TRP:CZ3	2.29	0.68
1:A:2075:MET:HA	1:A:2078:ILE:HG22	1.75	0.68
2:B:531:ILE:HB	2:B:532:PRO:HD3	1.76	0.68
2:F:531:ILE:HB	2:F:532:PRO:HD3	1.76	0.68
4:E:1952:LEU:C	4:E:1953:LEU:HD23	2.20	0.67
2:F:346:SER:HB3	2:F:355:ARG:HH11	1.59	0.67
1:A:182:UNK:CB	1:A:201:UNK:HA	2.24	0.67
1:A:1671:GLU:OE1	2:B:348:ILE:CD1	2.43	0.67
1:A:1932:PHE:O	1:A:1936:ARG:CB	2.43	0.67
4:E:1610:LEU:HB3	2:F:400:TRP:HH2	1.60	0.67
2:B:11:GLU:O	2:B:15:GLU:HB2	1.94	0.67
4:E:1943:MET:HE1	4:E:2000:MET:HG2	1.76	0.67
1:A:1571:GLU:OE1	1:A:1574:ARG:NH1	2.25	0.67
2:F:133:VAL:HG13	2:F:137:ARG:HD3	1.77	0.67
1:A:1994:ILE:H	1:A:1994:ILE:CD1	2.07	0.67
4:E:1978:PHE:CD1	4:E:1982:SER:HB2	2.30	0.67
2:B:323:GLU:OE2	2:B:325:THR:HB	1.95	0.67
4:E:1696:TYR:CG	4:E:1701:GLY:HA2	2.21	0.67
2:F:11:GLU:O	2:F:15:GLU:HB2	1.94	0.67
4:E:1227:MET:CB	4:E:1297:ILE:HD11	2.24	0.66
4:E:2072:ASN:O	4:E:2076:LYS:HB2	1.95	0.66
1:A:1227:MET:CB	1:A:1297:ILE:HD11	2.24	0.66
2:B:125:LEU:HD22	2:B:141:ILE:HG23	1.78	0.66
4:E:414:UNK:O	4:E:415:UNK:C	2.42	0.66
4:E:1590:ILE:CB	4:E:1612:TRP:HZ3	2.06	0.66
1:A:199:UNK:O	1:A:203:UNK:N	2.28	0.66
2:B:728:MET:HE3	2:B:759:ILE:HD11	1.76	0.66
1:A:1924:TYR:O	1:A:1931:ALA:HB3	1.95	0.66
3:C:60:LEU:CD2	3:C:75:THR:HG22	2.12	0.66
4:E:1369:THR:HG23	4:E:1370:ILE:N	2.11	0.66
1:A:1944:ALA:CB	1:A:2016:PHE:CE1	2.79	0.66
4:E:979:HIS:O	4:E:983:ARG:HG2	1.95	0.66
4:E:1590:ILE:CG1	4:E:1594:VAL:HG23	2.15	0.66
4:E:1860:LEU:CG	4:E:1979:MET:HE1	2.25	0.66
4:E:976:ASN:ND2	4:E:1013:ILE:CG2	2.58	0.66
2:F:125:LEU:HD22	2:F:141:ILE:HG23	1.78	0.66
2:F:323:GLU:OE2	2:F:325:THR:HB	1.95	0.66
1:A:1131:CYS:SG	4:E:1101:ALA:CB	2.83	0.66
1:A:2072:ASN:O	1:A:2076:LYS:HB2	1.95	0.66
2:B:346:SER:HB2	2:B:355:ARG:HH12	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:ILE:O	3:C:210:ILE:HG23	1.96	0.66
2:F:728:MET:HE3	2:F:759:ILE:HD11	1.76	0.66
2:B:133:VAL:HG13	2:B:137:ARG:HD3	1.77	0.66
2:B:271:ARG:HD2	3:C:249:TYR:CG	2.31	0.66
2:F:465:THR:HG23	2:F:467:GLU:H	1.61	0.65
4:E:1779:ASN:HD21	4:E:1897:GLU:HG3	1.61	0.65
4:E:1958:ARG:O	4:E:1959:HIS:ND1	2.29	0.65
4:E:1081:GLN:HE22	4:E:1142:SER:HB2	1.59	0.65
1:A:1882:PHE:CE2	1:A:1899:ILE:HG12	2.32	0.65
1:A:2024:TYR:HE2	1:A:2070:ALA:HB1	1.61	0.65
4:E:1882:PHE:CE2	4:E:1899:ILE:HG12	2.32	0.65
4:E:1212:HIS:ND1	4:E:1251:GLU:OE2	2.29	0.65
4:E:1926:ASP:OD1	4:E:1927:GLU:N	2.30	0.65
1:A:1212:HIS:ND1	1:A:1251:GLU:OE2	2.29	0.65
1:A:1544:VAL:HG22	1:A:1558:LEU:HD23	1.78	0.65
4:E:1752:PRO:HA	4:E:1755:ASP:OD2	1.97	0.65
3:C:126:THR:HG22	3:C:159:LYS:HA	1.79	0.65
4:E:1499:GLU:OE2	4:E:1561:ARG:NE	2.25	0.65
4:E:1544:VAL:HG22	4:E:1558:LEU:HD23	1.78	0.65
1:A:1691:MET:O	1:A:1695:ILE:HD12	1.97	0.65
1:A:1752:PRO:HA	1:A:1755:ASP:OD2	1.97	0.65
4:E:1586:VAL:HG23	4:E:1587:PRO:CD	2.27	0.65
4:E:1586:VAL:CG2	4:E:1587:PRO:HD3	2.26	0.65
3:G:126:THR:HG22	3:G:159:LYS:HA	1.79	0.65
1:A:1944:ALA:HA	1:A:2016:PHE:CZ	2.32	0.65
4:E:1586:VAL:HG12	4:E:1613:ALA:C	2.22	0.65
4:E:1994:ILE:CG2	4:E:1995:LYS:N	2.60	0.64
1:A:1590:ILE:CB	1:A:1612:TRP:CZ3	2.80	0.64
1:A:1905:ARG:CB	1:A:1961:GLY:HA2	2.26	0.64
2:B:465:THR:HG23	2:B:467:GLU:H	1.61	0.64
2:F:267:GLU:O	2:F:271:ARG:HG2	1.98	0.64
2:B:397:PHE:HZ	2:B:433:ILE:HD11	1.62	0.64
2:B:267:GLU:O	2:B:271:ARG:HG2	1.98	0.64
2:F:152:LEU:HD13	2:F:171:ASP:HB3	1.80	0.64
4:E:2024:TYR:HE2	4:E:2070:ALA:HB1	1.61	0.64
1:A:1748:ILE:HG12	1:A:1758:LYS:HB3	1.80	0.64
1:A:1276:PRO:HD3	1:A:1874:LEU:HD22	1.80	0.64
4:E:1748:ILE:HG12	4:E:1758:LYS:HB3	1.80	0.64
1:A:1131:CYS:CB	4:E:1098:THR:HG23	2.26	0.64
1:A:1779:ASN:HD21	1:A:1897:GLU:HG3	1.61	0.64
1:A:1804:LEU:CA	1:A:1848:ILE:HG22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1276:PRO:HD3	4:E:1874:LEU:HD22	1.80	0.64
1:A:1974:ILE:HG21	5:A:2201:E4S:C05	2.28	0.64
3:C:109:TYR:HE1	3:C:183:PHE:HB2	1.63	0.64
4:E:1404:ILE:HD13	4:E:1507:TYR:HE2	1.55	0.64
4:E:1524:SER:HA	4:E:1527:ASN:HD22	1.63	0.64
1:A:1524:SER:HA	1:A:1527:ASN:HD22	1.63	0.63
4:E:1655:PRO:HA	4:E:1690:ASN:ND2	2.13	0.63
4:E:1952:LEU:O	4:E:1953:LEU:HD23	1.98	0.63
3:G:206:ILE:O	3:G:210:ILE:HG23	1.96	0.63
1:A:1655:PRO:HA	1:A:1690:ASN:ND2	2.13	0.63
4:E:1860:LEU:HB3	4:E:1979:MET:HE1	1.80	0.63
2:F:86:LEU:HD23	2:F:96:LEU:HD22	1.81	0.63
1:A:1134:LYS:HG3	1:A:1136:TYR:CZ	2.33	0.63
4:E:1932:PHE:O	4:E:1936:ARG:CB	2.46	0.63
1:A:1585:ASP:OD1	1:A:1589:ALA:HB2	1.97	0.63
2:B:152:LEU:HD13	2:B:171:ASP:HB3	1.80	0.63
1:A:1250:ARG:HE	2:B:785:LYS:HD3	1.62	0.63
4:E:1956:LYS:HG3	4:E:1982:SER:OG	1.98	0.63
3:G:216:PRO:HA	3:G:219:HIS:ND1	2.13	0.63
1:A:1400:LEU:HD21	1:A:1507:TYR:CD2	2.32	0.63
1:A:1632:PRO:HG3	2:B:345:LEU:HD13	1.81	0.63
4:E:1344:ALA:HA	4:E:1395:GLN:NE2	2.13	0.63
4:E:1691:MET:O	4:E:1695:ILE:HD12	1.97	0.63
4:E:1886:VAL:CG2	4:E:1896:ILE:HG22	2.29	0.63
2:F:397:PHE:HZ	2:F:433:ILE:HD11	1.62	0.63
4:E:1954:GLN:CG	4:E:2060:ARG:NH2	2.62	0.63
3:C:216:PRO:HA	3:C:219:HIS:ND1	2.13	0.63
2:F:167:ASP:OD2	2:F:170:GLN:N	2.31	0.63
1:A:27:UNK:HA	2:B:821:PHE:CD2	2.34	0.62
4:E:1957:ASP:HB2	4:E:1993:ASP:O	1.99	0.62
4:E:2021:VAL:HG12	4:E:2074:ILE:HG23	1.81	0.62
2:F:173:ILE:O	2:F:177:GLU:HB2	1.98	0.62
1:A:2032:ASP:O	1:A:2036:SER:HB3	1.99	0.62
1:A:413:UNK:O	1:A:414:UNK:C	2.42	0.62
1:A:976:ASN:ND2	1:A:1013:ILE:HG21	2.14	0.62
4:E:1631:HIS:HD2	4:E:1632:PRO:HD2	1.64	0.62
2:B:544:LEU:HD13	3:C:229:ARG:NH2	2.14	0.62
4:E:1405:SER:OG	4:E:1409:LYS:NZ	2.33	0.62
4:E:1804:LEU:CA	4:E:1848:ILE:HG22	2.27	0.62
1:A:1349:ARG:NH2	1:A:1381:THR:O	2.32	0.62
1:A:1963:ILE:HD13	1:A:1995:LYS:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1586:VAL:HG12	4:E:1613:ALA:HB3	1.80	0.62
2:F:131:THR:HA	2:F:308:ARG:HH11	1.64	0.62
2:F:184:LEU:HD11	2:F:245:LEU:HD23	1.81	0.62
1:A:1632:PRO:HG2	2:B:345:LEU:CD1	2.21	0.62
1:A:2021:VAL:HG12	1:A:2074:ILE:HG23	1.81	0.62
2:B:131:THR:HA	2:B:308:ARG:HH11	1.64	0.62
2:B:173:ILE:O	2:B:177:GLU:HB2	1.98	0.62
3:C:63:PHE:HD2	3:C:75:THR:HG21	1.64	0.62
3:G:63:PHE:HD2	3:G:75:THR:HG21	1.64	0.62
2:B:184:LEU:HD11	2:B:245:LEU:HD23	1.81	0.62
4:E:1250:ARG:HE	2:F:785:LYS:HB2	1.64	0.62
4:E:1349:ARG:NH2	4:E:1381:THR:O	2.32	0.62
3:G:109:TYR:HE1	3:G:183:PHE:HB2	1.63	0.62
1:A:1529:ARG:HA	1:A:1532:TYR:CE2	2.35	0.62
1:A:1344:ALA:HA	1:A:1395:GLN:NE2	2.13	0.62
2:B:86:LEU:HD23	2:B:96:LEU:HD22	1.81	0.62
2:B:167:ASP:OD2	2:B:170:GLN:N	2.31	0.62
3:C:116:LYS:NZ	3:C:121:LYS:HB2	2.15	0.62
2:F:330:LEU:HD11	3:G:137:HIS:HE1	1.64	0.62
3:G:116:LYS:NZ	3:G:121:LYS:HB2	2.15	0.62
1:A:1405:SER:OG	1:A:1409:LYS:NZ	2.33	0.61
4:E:1527:ASN:O	4:E:1531:LYS:HG2	1.99	0.61
1:A:1077:LYS:O	1:A:1081:GLN:CB	2.48	0.61
1:A:1227:MET:HB3	1:A:1297:ILE:HD11	1.81	0.61
1:A:1886:VAL:CG2	1:A:1896:ILE:HG22	2.29	0.61
4:E:1130:ALA:O	4:E:1131:CYS:CB	2.48	0.61
4:E:1666:MET:HA	2:F:347:ARG:CB	2.30	0.61
1:A:1586:VAL:CG1	1:A:1613:ALA:HB1	2.30	0.61
4:E:1401:ARG:HH22	4:E:1516:GLU:HB2	1.65	0.61
4:E:2032:ASP:O	4:E:2036:SER:HB3	1.99	0.61
2:F:323:GLU:OE2	2:F:326:GLU:HG3	2.00	0.61
1:A:1527:ASN:O	1:A:1531:LYS:HG2	1.99	0.61
1:A:1778:SER:O	1:A:1885:ARG:NH2	2.34	0.61
3:C:138:GLU:OE2	3:C:141:SER:HB2	2.00	0.61
4:E:1610:LEU:HB3	2:F:400:TRP:CH2	2.35	0.61
3:G:138:GLU:OE2	3:G:141:SER:HB2	2.00	0.61
1:A:1131:CYS:HB2	4:E:1098:THR:HA	1.83	0.61
1:A:1414:MET:HE3	1:A:1492:LEU:HD22	1.83	0.61
1:A:1886:VAL:HG13	1:A:1896:ILE:HG22	1.82	0.61
1:A:1159:PHE:HD2	4:E:1159:PHE:HD2	1.48	0.61
1:A:1932:PHE:O	1:A:1936:ARG:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:933:MET:HE1	4:E:981:ARG:CG	2.30	0.61
4:E:1227:MET:HB3	4:E:1297:ILE:HD11	1.81	0.61
4:E:1250:ARG:NH2	2:F:781:SER:HB3	2.15	0.61
4:E:1667:GLY:N	2:F:347:ARG:O	2.33	0.61
2:B:346:SER:O	2:B:348:ILE:HG12	2.01	0.61
2:B:700:LEU:HD22	2:B:735:MET:HG3	1.83	0.61
4:E:1529:ARG:HA	4:E:1532:TYR:CE2	2.35	0.61
1:A:1401:ARG:HH22	1:A:1516:GLU:HB2	1.65	0.61
4:E:1639:VAL:HG21	2:F:394:PHE:HE1	1.66	0.61
2:F:700:LEU:HD22	2:F:735:MET:HG3	1.83	0.61
1:A:1631:HIS:HD2	1:A:1632:PRO:HD2	1.64	0.61
1:A:1860:LEU:HB3	1:A:1979:MET:CE	2.30	0.61
2:B:341:ARG:HH12	3:C:145:MET:HE2	1.66	0.61
4:E:1132:VAL:O	4:E:1132:VAL:HG12	2.01	0.61
4:E:1886:VAL:HG13	4:E:1896:ILE:HG22	1.82	0.61
4:E:1077:LYS:O	4:E:1081:GLN:CB	2.48	0.60
4:E:1778:SER:O	4:E:1885:ARG:NH2	2.34	0.60
4:E:1953:LEU:HD22	4:E:1980:PHE:CE1	2.35	0.60
1:A:977:HIS:HD2	1:A:982:ILE:HB	1.65	0.60
3:G:75:THR:HG22	3:G:75:THR:O	2.01	0.60
3:C:214:GLY:HA3	3:C:229:ARG:HG3	1.83	0.60
2:B:277:SER:OG	3:C:193:THR:HB	2.01	0.60
3:C:12:TRP:O	3:C:15:GLU:HG3	2.02	0.60
3:C:58:HIS:O	3:C:61:PHE:HB3	2.02	0.60
4:E:1414:MET:HE3	4:E:1492:LEU:HD22	1.83	0.60
4:E:1538:LYS:HG3	4:E:1539:GLN:OE1	2.02	0.60
2:F:113:TYR:HB3	2:F:155:LEU:HD21	1.82	0.60
2:F:348:ILE:HG13	2:F:348:ILE:O	2.01	0.60
4:E:1332:ILE:HG21	4:E:1551:SER:HB2	1.84	0.60
4:E:1655:PRO:HA	4:E:1690:ASN:HD21	1.67	0.60
2:F:539:ARG:O	2:F:543:GLN:HB2	2.01	0.60
3:G:12:TRP:O	3:G:15:GLU:HG3	2.02	0.60
2:B:94:GLU:HB2	2:B:137:ARG:HH12	1.67	0.60
3:G:58:HIS:O	3:G:61:PHE:HB3	2.02	0.60
2:B:172:VAL:O	2:B:176:TYR:HB2	2.02	0.60
2:F:330:LEU:HD11	3:G:137:HIS:CE1	2.36	0.60
2:B:275:GLU:OE1	3:C:190:ALA:HA	2.01	0.60
1:A:1128:ARG:CD	4:E:1051:GLU:HG3	2.28	0.60
1:A:1852:GLY:N	1:A:1892:GLY:O	2.33	0.60
4:E:1522:GLU:OE1	4:E:1522:GLU:N	2.32	0.59
2:F:172:VAL:O	2:F:176:TYR:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1993:ASP:CG	1:A:1994:ILE:HD12	2.27	0.59
4:E:2010:ALA:O	4:E:2014:LYS:N	2.28	0.59
1:A:1128:ARG:NH1	1:A:1130:ALA:HB2	2.17	0.59
1:A:2071:ALA:O	1:A:2075:MET:HG2	2.02	0.59
3:C:123:LEU:HB3	3:C:162:TYR:CZ	2.37	0.59
2:F:452:GLU:HG2	2:F:456:LYS:HE2	1.83	0.59
2:F:751:ARG:O	2:F:755:GLU:HG2	2.02	0.59
2:B:113:TYR:HB3	2:B:155:LEU:HD21	1.82	0.59
2:B:539:ARG:O	2:B:543:GLN:HB2	2.01	0.59
3:G:123:LEU:HB3	3:G:162:TYR:CZ	2.37	0.59
1:A:1655:PRO:HA	1:A:1690:ASN:HD21	1.67	0.59
2:B:452:GLU:HG2	2:B:456:LYS:HE2	1.83	0.59
2:B:751:ARG:O	2:B:755:GLU:HG2	2.02	0.59
2:B:11:GLU:O	2:B:15:GLU:CB	2.50	0.59
2:B:496:LEU:HD23	2:B:499:LYS:HD2	1.85	0.59
4:E:1756:GLU:O	4:E:1759:LYS:HG2	2.03	0.59
1:A:29:UNK:CB	2:B:809:GLN:HE22	2.16	0.59
1:A:1538:LYS:HG3	1:A:1539:GLN:OE1	2.02	0.59
3:C:75:THR:HG22	3:C:75:THR:O	2.01	0.59
1:A:1132:VAL:O	1:A:1132:VAL:HG12	2.01	0.59
1:A:1590:ILE:HG13	1:A:1594:VAL:HG21	1.83	0.59
4:E:1963:ILE:HG12	4:E:1973:HIS:CD2	2.38	0.59
4:E:2071:ALA:O	4:E:2075:MET:HG2	2.02	0.59
1:A:1562:PHE:O	1:A:1563:LYS:HE2	2.03	0.59
1:A:1685:HIS:HE1	1:A:1730:PHE:HD2	1.51	0.59
1:A:1857:GLN:O	1:A:1979:MET:SD	2.61	0.59
1:A:1963:ILE:HG12	1:A:1973:HIS:CD2	2.38	0.59
2:F:341:ARG:HH22	3:G:145:MET:HE2	1.68	0.59
1:A:442:UNK:C	1:A:444:UNK:N	2.65	0.58
1:A:1756:GLU:O	1:A:1759:LYS:HG2	2.02	0.58
1:A:1943:MET:HG3	1:A:2016:PHE:HE1	1.67	0.58
4:E:1953:LEU:HD22	4:E:1980:PHE:HE1	1.65	0.58
1:A:1128:ARG:HA	4:E:1055:LYS:HB3	1.84	0.58
1:A:27:UNK:HA	2:B:821:PHE:HD2	1.68	0.58
1:A:1332:ILE:HG21	1:A:1551:SER:HB2	1.84	0.58
4:E:1277:LEU:HD22	4:E:1616:ASP:OD2	2.03	0.58
4:E:1902:CYS:O	4:E:1903:THR:OG1	2.15	0.58
2:F:319:PHE:HB2	3:G:132:LYS:HE2	1.85	0.58
1:A:1386:PHE:HZ	1:A:1496:LEU:HD23	1.69	0.58
2:B:422:GLU:OE1	2:B:425:ARG:NH2	2.36	0.58
4:E:1014:LEU:HB2	4:E:1057:PHE:HE2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1685:HIS:HE1	4:E:1730:PHE:HD2	1.51	0.58
4:E:1862:LEU:HD11	4:E:1883:PRO:O	2.03	0.58
3:G:186:LEU:HD12	3:G:189:ASN:HB3	1.86	0.58
1:A:1590:ILE:HG13	1:A:1594:VAL:HG23	1.85	0.58
1:A:1651:LEU:CD1	1:A:1686:GLN:HG3	2.33	0.58
4:E:1044:PRO:HD2	4:E:1050:ARG:HG2	1.85	0.58
1:A:1317:VAL:HG11	1:A:1364:VAL:HG11	1.85	0.58
2:F:11:GLU:O	2:F:15:GLU:CB	2.50	0.58
4:E:1360:LEU:HD21	4:E:1375:ARG:CZ	2.33	0.58
4:E:1896:ILE:HD12	4:E:1896:ILE:O	2.04	0.58
2:F:422:GLU:OE1	2:F:425:ARG:NH2	2.36	0.58
1:A:1196:LEU:HD23	1:A:1214:LEU:HD13	1.85	0.58
1:A:1360:LEU:HD21	1:A:1375:ARG:CZ	2.33	0.58
1:A:2006:GLY:HA2	1:A:2010:ALA:HB3	1.86	0.58
4:E:1400:LEU:HD21	4:E:1507:TYR:CD2	2.39	0.58
4:E:1501:GLU:HA	4:E:1504:ILE:HG22	1.86	0.58
4:E:2006:GLY:HA2	4:E:2010:ALA:HB3	1.84	0.58
2:F:346:SER:CB	2:F:355:ARG:NH1	2.43	0.58
1:A:1404:ILE:HD11	1:A:1503:LEU:HB3	1.86	0.58
1:A:1896:ILE:O	1:A:1896:ILE:HD12	2.04	0.58
4:E:1386:PHE:HZ	4:E:1496:LEU:HD23	1.69	0.58
4:E:1404:ILE:HD11	4:E:1503:LEU:HB3	1.86	0.58
4:E:1562:PHE:O	4:E:1563:LYS:HE2	2.03	0.58
4:E:1860:LEU:CD2	4:E:1979:MET:CE	2.40	0.58
1:A:951:MET:HE1	1:A:954:LYS:NZ	2.19	0.57
1:A:1794:PRO:HA	1:A:1804:LEU:H	1.69	0.57
4:E:1141:ALA:O	4:E:1145:LEU:HG	2.04	0.57
3:G:188:TYR:HD1	3:G:195:MET:HE2	1.69	0.57
1:A:1014:LEU:HB2	1:A:1057:PHE:HE2	1.67	0.57
1:A:1258:MET:HE2	1:A:1262:GLN:OE1	2.04	0.57
4:E:951:MET:HE1	4:E:954:LYS:NZ	2.19	0.57
2:F:94:GLU:HB2	2:F:137:ARG:HH12	1.67	0.57
1:A:1862:LEU:HD11	1:A:1883:PRO:O	2.03	0.57
4:E:1370:ILE:HG12	2:F:758:ALA:HB2	1.85	0.57
2:F:247:ARG:NH1	2:F:281:PRO:O	2.38	0.57
2:F:496:LEU:HD23	2:F:499:LYS:HD2	1.85	0.57
1:A:1044:PRO:HD2	1:A:1050:ARG:HG2	1.85	0.57
1:A:1501:GLU:HA	1:A:1504:ILE:HG22	1.86	0.57
2:B:112:ASP:OD2	2:B:115:GLU:HB3	2.05	0.57
3:C:188:TYR:HD1	3:C:195:MET:HE2	1.69	0.57
1:A:939:VAL:HG13	1:A:942:LYS:HZ1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1921:THR:HG23	1:A:1926:ASP:HA	1.87	0.57
2:B:175:CYS:O	2:B:179:ALA:HB2	2.04	0.57
2:B:247:ARG:NH1	2:B:281:PRO:O	2.38	0.57
4:E:1299:ILE:O	4:E:1303:VAL:HG23	2.04	0.57
1:A:1113:TYR:O	1:A:1135:ASP:HB3	2.04	0.57
1:A:1979:MET:HE2	1:A:1980:PHE:CD2	2.40	0.57
4:E:1852:GLY:N	4:E:1892:GLY:O	2.33	0.57
1:A:1277:LEU:HD22	1:A:1616:ASP:OD2	2.03	0.57
1:A:1512:ALA:HB3	1:A:1513:PRO:HD3	1.86	0.57
2:B:389:ALA:O	2:B:399:LEU:HD21	2.05	0.57
2:F:112:ASP:OD2	2:F:115:GLU:HB3	2.05	0.57
1:A:1141:ALA:O	1:A:1145:LEU:HG	2.04	0.57
4:E:1317:VAL:HG11	4:E:1364:VAL:HG11	1.85	0.57
1:A:1299:ILE:O	1:A:1303:VAL:HG23	2.04	0.57
1:A:1683:LEU:HG	1:A:1687:PHE:HE2	1.70	0.57
4:E:1196:LEU:HD23	4:E:1214:LEU:HD13	1.85	0.57
2:F:175:CYS:O	2:F:179:ALA:HB2	2.04	0.57
2:F:402:GLN:NE2	3:G:277:LEU:HD12	2.19	0.57
1:A:1786:ASP:OD1	1:A:1787:ILE:N	2.38	0.56
2:B:491:GLY:O	2:B:495:VAL:HG23	2.05	0.56
4:E:1779:ASN:ND2	4:E:1897:GLU:HG3	2.20	0.56
2:F:487:ALA:O	2:F:493:GLN:NE2	2.33	0.56
1:A:1924:TYR:O	1:A:1931:ALA:CB	2.53	0.56
1:A:1979:MET:HE2	1:A:1980:PHE:CE2	2.40	0.56
2:B:340:ASN:OD1	2:B:340:ASN:O	2.23	0.56
3:C:253:TRP:CH2	3:C:286:LEU:HD22	2.40	0.56
4:E:1258:MET:HE2	4:E:1262:GLN:OE1	2.04	0.56
4:E:1950:LEU:HD22	4:E:1955:ILE:CG2	2.36	0.56
3:G:245:TYR:HA	3:G:248:PHE:HD2	1.70	0.56
1:A:182:UNK:CB	1:A:201:UNK:O	2.53	0.56
1:A:933:MET:HE1	1:A:981:ARG:CG	2.34	0.56
1:A:1590:ILE:HB	1:A:1612:TRP:CE3	2.39	0.56
1:A:1896:ILE:HD13	5:A:2201:E4S:C06	2.35	0.56
3:C:186:LEU:HD12	3:C:189:ASN:HB3	1.86	0.56
4:E:1512:ALA:HB3	4:E:1513:PRO:HD3	1.86	0.56
4:E:1590:ILE:CA	4:E:1612:TRP:CZ3	2.88	0.56
4:E:1786:ASP:OD1	4:E:1787:ILE:N	2.38	0.56
2:F:587:PHE:HD1	2:F:701:HIS:CE1	2.05	0.56
2:B:784:GLU:O	2:B:788:ARG:HG2	2.05	0.56
3:C:245:TYR:HA	3:C:248:PHE:HD2	1.70	0.56
2:F:784:GLU:O	2:F:788:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:PRO:HB3	1:A:1221:MET:HE1	1.86	0.56
4:E:1186:PRO:HB3	4:E:1221:MET:HE1	1.86	0.56
3:G:253:TRP:CH2	3:G:286:LEU:HD22	2.41	0.56
1:A:1192:ALA:HA	1:A:1195:LYS:NZ	2.21	0.56
4:E:976:ASN:HD21	4:E:1013:ILE:HG23	1.71	0.56
2:F:389:ALA:O	2:F:399:LEU:HD21	2.05	0.56
2:F:737:GLY:HA3	2:F:753:TYR:CE1	2.41	0.56
1:A:1779:ASN:ND2	1:A:1897:GLU:HG3	2.20	0.56
4:E:2011:THR:N	4:E:2012:PRO:HD2	2.21	0.56
1:A:1227:MET:HB2	1:A:1297:ILE:HD11	1.87	0.56
2:F:491:GLY:O	2:F:495:VAL:HG23	2.05	0.56
1:A:1580:PRO:HG2	1:A:1608:HIS:NE2	2.21	0.56
1:A:1586:VAL:CG2	1:A:1587:PRO:CD	2.83	0.56
1:A:1979:MET:CE	1:A:1980:PHE:CE2	2.89	0.56
4:E:1946:TYR:HB3	4:E:1973:HIS:CE1	2.41	0.56
1:A:1098:THR:HA	4:E:1131:CYS:HB2	1.87	0.55
2:B:144:ALA:O	2:B:148:LYS:HB2	2.06	0.55
2:B:155:LEU:O	2:B:168:ARG:NH2	2.40	0.55
2:B:271:ARG:HD2	3:C:249:TYR:CD1	2.41	0.55
4:E:1261:GLU:OE2	2:F:488:SER:OG	2.22	0.55
4:E:1921:THR:HG23	4:E:1926:ASP:HA	1.87	0.55
1:A:1400:LEU:HD21	1:A:1507:TYR:HD2	1.72	0.55
1:A:1687:PHE:O	1:A:1691:MET:HG2	2.06	0.55
2:B:107:ASN:HB3	2:B:112:ASP:HB3	1.89	0.55
4:E:1957:ASP:CG	4:E:1957:ASP:O	2.49	0.55
2:F:82:LEU:HD11	2:F:102:ILE:HG22	1.89	0.55
1:A:1522:GLU:OE1	1:A:1522:GLU:N	2.32	0.55
2:B:82:LEU:HD11	2:B:102:ILE:HG22	1.88	0.55
4:E:1586:VAL:HG12	4:E:1613:ALA:CB	2.36	0.55
4:E:1896:ILE:HD13	5:E:2201:E4S:C06	2.37	0.55
2:F:26:ILE:HD13	2:F:29:LEU:HD12	1.87	0.55
1:A:1330:LEU:O	1:A:1330:LEU:HD23	2.07	0.55
4:E:1621:LEU:CD2	4:E:1642:LEU:HD11	2.36	0.55
3:G:237:MET:O	3:G:241:LEU:HG	2.07	0.55
2:B:493:GLN:O	2:B:497:GLN:HG3	2.07	0.55
4:E:1651:LEU:CD1	4:E:1686:GLN:HG3	2.34	0.55
2:F:787:LEU:O	2:F:791:VAL:HG23	2.06	0.55
2:B:26:ILE:HD13	2:B:29:LEU:HD12	1.87	0.55
2:B:104:ALA:HA	2:B:107:ASN:HD22	1.70	0.55
2:B:752:TRP:HA	2:B:755:GLU:CG	2.37	0.55
4:E:976:ASN:ND2	4:E:1013:ILE:HG23	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1227:MET:HB2	4:E:1297:ILE:HD11	1.87	0.55
4:E:1371:ARG:O	4:E:1375:ARG:CB	2.55	0.55
4:E:1860:LEU:CB	4:E:1979:MET:HE1	2.37	0.55
1:A:1030:PRO:O	1:A:1043:VAL:HG22	2.07	0.55
1:A:1647:PRO:O	1:A:1651:LEU:HB2	2.07	0.55
1:A:1759:LYS:O	1:A:1762:LEU:HB3	2.06	0.55
2:B:737:GLY:HA3	2:B:753:TYR:CE1	2.41	0.55
4:E:1580:PRO:HG2	4:E:1608:HIS:NE2	2.21	0.55
4:E:1944:ALA:CA	4:E:2016:PHE:CE1	2.89	0.55
4:E:2024:TYR:CE2	4:E:2070:ALA:HB1	2.42	0.55
2:B:42:ASP:HB2	2:B:91:LEU:HG	1.89	0.55
4:E:1661:LEU:HD21	4:E:1673:ILE:HD12	1.89	0.55
2:B:274:CYS:HB3	3:C:192:LEU:H	1.71	0.55
4:E:1192:ALA:HA	4:E:1195:LYS:NZ	2.21	0.55
4:E:1216:TRP:CH2	4:E:1255:ALA:HA	2.42	0.55
2:F:104:ALA:HA	2:F:107:ASN:HD22	1.70	0.55
2:B:534:ALA:O	2:B:538:VAL:HG23	2.07	0.55
4:E:1683:LEU:HG	4:E:1687:PHE:HE2	1.70	0.55
4:E:1794:PRO:HA	4:E:1804:LEU:H	1.70	0.55
4:E:2045:GLY:C	4:E:2046:LEU:HD12	2.32	0.55
2:F:155:LEU:O	2:F:168:ARG:NH2	2.40	0.55
2:F:707:ILE:HD11	2:F:739:ILE:HG12	1.88	0.55
1:A:1261:GLU:OE2	2:B:489:LEU:HG	2.06	0.54
1:A:1661:LEU:HD21	1:A:1673:ILE:HD12	1.89	0.54
2:B:420:LEU:HD22	2:B:433:ILE:HG23	1.88	0.54
2:B:787:LEU:O	2:B:791:VAL:HG23	2.06	0.54
4:E:1639:VAL:HG21	2:F:394:PHE:CE1	2.43	0.54
3:G:85:CYS:SG	3:G:86:TYR:N	2.81	0.54
4:E:1687:PHE:O	4:E:1691:MET:HG2	2.06	0.54
2:F:493:GLN:O	2:F:497:GLN:HG3	2.07	0.54
2:F:752:TRP:HA	2:F:755:GLU:CG	2.37	0.54
3:G:28:ALA:HA	3:G:71:LEU:HD21	1.89	0.54
1:A:182:UNK:CA	1:A:201:UNK:CB	2.85	0.54
1:A:1114:ASN:OD1	1:A:1117:ASN:N	2.38	0.54
2:B:707:ILE:HD11	2:B:739:ILE:HG12	1.88	0.54
4:E:1621:LEU:HD21	4:E:1642:LEU:HD11	1.88	0.54
4:E:1759:LYS:O	4:E:1762:LEU:HB3	2.07	0.54
2:F:144:ALA:O	2:F:148:LYS:HB2	2.06	0.54
3:G:60:LEU:CD2	3:G:75:THR:HG21	2.37	0.54
1:A:1201:ILE:HD11	1:A:1237:LEU:HA	1.89	0.54
1:A:1216:TRP:CH2	1:A:1255:ALA:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1636:GLN:HG2	2:F:394:PHE:CD1	2.41	0.54
2:F:42:ASP:HB2	2:F:91:LEU:HG	1.89	0.54
2:F:176:TYR:HB3	2:F:225:ALA:HB2	1.90	0.54
1:A:182:UNK:N	1:A:201:UNK:CB	2.70	0.54
1:A:1849:PHE:CD1	1:A:1895:VAL:HG22	2.43	0.54
1:A:2010:ALA:O	1:A:2014:LYS:HG3	2.07	0.54
4:E:1367:ASN:ND2	4:E:1369:THR:HG22	2.22	0.54
4:E:1569:GLY:O	4:E:1573:THR:CB	2.55	0.54
4:E:1952:LEU:O	4:E:2060:ARG:NH1	2.40	0.54
2:F:101:LEU:HD11	2:F:125:LEU:HD21	1.90	0.54
1:A:1154:TYR:O	1:A:1158:ARG:HG2	2.08	0.54
1:A:1621:LEU:HD21	1:A:1642:LEU:HD11	1.88	0.54
2:B:224:ARG:CZ	2:B:228:LEU:HD21	2.38	0.54
2:B:768:GLN:HE21	2:B:800:VAL:HG23	1.73	0.54
3:C:237:MET:O	3:C:241:LEU:HG	2.07	0.54
4:E:1647:PRO:O	4:E:1651:LEU:HB2	2.07	0.54
4:E:1974:ILE:HG21	5:E:2201:E4S:C05	2.37	0.54
2:F:246:LEU:HD21	2:F:261:ILE:CG2	2.38	0.54
1:A:1621:LEU:CD2	1:A:1642:LEU:HD11	2.36	0.54
1:A:1682:LEU:HD11	1:A:1780:PRO:HB3	1.89	0.54
1:A:1877:LEU:HB3	1:A:1879:LEU:HD13	1.89	0.54
2:B:251:THR:HG22	2:B:253:THR:H	1.73	0.54
3:C:135:VAL:HG13	3:C:136:TYR:CD1	2.43	0.54
4:E:1030:PRO:O	4:E:1043:VAL:HG22	2.07	0.54
4:E:1201:ILE:HD11	4:E:1237:LEU:HA	1.89	0.54
4:E:1849:PHE:CD1	4:E:1895:VAL:HG22	2.43	0.54
4:E:968:ALA:O	4:E:972:LEU:HG	2.08	0.54
2:F:242:PHE:HD2	2:F:265:LEU:HD13	1.73	0.54
2:F:515:HIS:CD2	3:G:229:ARG:NH1	2.75	0.54
4:E:1617:PRO:HD3	4:E:1645:PHE:HE2	1.72	0.54
2:F:107:ASN:HB3	2:F:112:ASP:HB3	1.89	0.54
2:F:224:ARG:CZ	2:F:228:LEU:HD21	2.38	0.54
2:F:534:ALA:O	2:F:538:VAL:HG23	2.07	0.54
1:A:1617:PRO:HD3	1:A:1645:PHE:HE2	1.72	0.54
4:E:1330:LEU:HD23	4:E:1330:LEU:O	2.07	0.54
4:E:1951:PHE:HD2	4:E:1952:LEU:HD22	1.74	0.54
1:A:1890:ALA:HB1	1:A:1891:PRO:HD2	1.89	0.53
4:E:1757:ARG:O	4:E:1760:ALA:HB3	2.08	0.53
4:E:1877:LEU:HB3	4:E:1879:LEU:HD13	1.89	0.53
2:F:137:ARG:HG2	2:F:141:ILE:HD12	1.89	0.53
2:F:250:GLU:OE2	2:F:255:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:420:LEU:HD22	2:F:433:ILE:HG23	1.88	0.53
3:G:156:GLY:O	3:G:157:LEU:HD23	2.08	0.53
3:G:211:CYS:O	3:G:266:ARG:NH2	2.37	0.53
1:A:1509:PRO:HG2	1:A:2022:ARG:HE	1.73	0.53
1:A:2011:THR:N	1:A:2012:PRO:HD2	2.22	0.53
2:B:137:ARG:HG2	2:B:141:ILE:HD12	1.89	0.53
2:B:176:TYR:HB3	2:B:225:ALA:HB2	1.90	0.53
3:C:85:CYS:SG	3:C:86:TYR:N	2.80	0.53
4:E:975:PHE:O	4:E:983:ARG:HB2	2.08	0.53
4:E:1682:LEU:HD11	4:E:1780:PRO:HB3	1.89	0.53
4:E:1794:PRO:HA	4:E:1804:LEU:N	2.24	0.53
1:A:1569:GLY:O	1:A:1573:THR:CB	2.55	0.53
1:A:1747:ILE:HD12	1:A:1748:ILE:HG13	1.91	0.53
2:B:487:ALA:O	2:B:493:GLN:NE2	2.33	0.53
3:C:83:ILE:O	3:C:87:LEU:CB	2.50	0.53
3:C:199:SER:O	3:C:203:LEU:HB3	2.09	0.53
4:E:1238:LEU:HD11	4:E:1248:PHE:CD2	2.44	0.53
4:E:1332:ILE:CG2	4:E:1551:SER:HB2	2.38	0.53
4:E:1942:SER:OG	4:E:1971:ILE:HG22	2.08	0.53
3:G:126:THR:HG22	3:G:159:LYS:CB	2.39	0.53
1:A:1411:TRP:CE3	1:A:1525:VAL:HG22	2.43	0.53
1:A:2045:GLY:C	1:A:2046:LEU:HD12	2.33	0.53
2:B:814:ASP:HA	2:B:817:ALA:HB3	1.91	0.53
1:A:1371:ARG:O	1:A:1375:ARG:CB	2.55	0.53
1:A:1905:ARG:HG2	1:A:1961:GLY:H	1.72	0.53
2:B:242:PHE:HD2	2:B:265:LEU:HD13	1.73	0.53
4:E:1508:ASN:N	4:E:1509:PRO:HD3	2.21	0.53
1:A:1091:VAL:HG13	4:E:1225:HIS:HE1	1.73	0.53
1:A:1332:ILE:CG2	1:A:1551:SER:HB2	2.38	0.53
1:A:1568:ILE:HD12	1:A:1569:GLY:N	2.24	0.53
1:A:1794:PRO:HA	1:A:1804:LEU:N	2.23	0.53
1:A:2011:THR:OG1	1:A:2012:PRO:HD3	2.08	0.53
4:E:1154:TYR:O	4:E:1158:ARG:HG2	2.08	0.53
4:E:1569:GLY:O	4:E:1573:THR:HB	2.09	0.53
2:F:119:ILE:HG12	2:F:122:ARG:HH22	1.74	0.53
2:F:251:THR:HG22	2:F:253:THR:H	1.73	0.53
2:F:405:LEU:HB2	3:G:277:LEU:HD13	1.91	0.53
3:G:50:SER:O	3:G:53:LEU:HD13	2.09	0.53
1:A:1569:GLY:O	1:A:1573:THR:HB	2.09	0.53
1:A:1636:GLN:O	1:A:1640:LYS:HG3	2.09	0.53
4:E:1227:MET:HE1	4:E:1298:TRP:HE3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1636:GLN:O	4:E:1640:LYS:HG3	2.09	0.53
2:F:768:GLN:HE21	2:F:800:VAL:HG23	1.73	0.53
1:A:968:ALA:O	1:A:972:LEU:HG	2.08	0.53
1:A:1902:CYS:O	1:A:1903:THR:OG1	2.15	0.53
1:A:1943:MET:HG3	1:A:2016:PHE:CE1	2.43	0.53
1:A:1951:PHE:HD2	1:A:1952:LEU:HD22	1.74	0.53
2:B:101:LEU:HD11	2:B:125:LEU:HD21	1.90	0.53
2:B:120:TYR:HB3	2:B:148:LYS:HE3	1.91	0.53
3:C:28:ALA:HA	3:C:71:LEU:HD21	1.90	0.53
4:E:1193:MET:HG2	4:E:1233:CYS:SG	2.49	0.53
4:E:1857:GLN:O	4:E:1979:MET:SD	2.67	0.53
1:A:1227:MET:HE1	1:A:1298:TRP:HE3	1.74	0.53
1:A:1757:ARG:O	1:A:1760:ALA:HB3	2.09	0.53
2:B:119:ILE:HG12	2:B:122:ARG:HH22	1.74	0.53
2:B:246:LEU:HD21	2:B:261:ILE:CG2	2.38	0.53
2:B:469:LYS:HE2	2:B:473:TYR:HE2	1.74	0.53
3:C:156:GLY:O	3:C:157:LEU:HD23	2.08	0.53
4:E:1890:ALA:HB1	4:E:1891:PRO:HD2	1.89	0.53
4:E:1974:ILE:HG21	5:E:2201:E4S:C07	2.39	0.53
4:E:2032:ASP:O	4:E:2036:SER:CB	2.56	0.53
3:G:135:VAL:HG13	3:G:136:TYR:CD1	2.43	0.53
1:A:1010:MET:HE2	1:A:1061:CYS:HA	1.91	0.52
2:B:544:LEU:HD13	3:C:229:ARG:HH22	1.74	0.52
4:E:1190:THR:HG23	4:E:1194:PHE:HE2	1.74	0.52
4:E:1411:TRP:CE3	4:E:1525:VAL:HG22	2.43	0.52
4:E:1568:ILE:HD12	4:E:1569:GLY:N	2.24	0.52
4:E:1632:PRO:CG	2:F:345:LEU:HD13	2.39	0.52
4:E:1908:LEU:HD13	4:E:1919:TYR:HB2	1.90	0.52
4:E:2010:ALA:O	4:E:2014:LYS:HG3	2.08	0.52
1:A:1250:ARG:HD3	2:B:785:LYS:HB2	1.92	0.52
1:A:1292:VAL:HB	1:A:1348:PRO:HG2	1.91	0.52
2:B:703:ALA:O	2:B:707:ILE:HG12	2.09	0.52
3:C:221:ARG:NH1	3:C:258:LYS:HB3	2.25	0.52
1:A:1908:LEU:HD13	1:A:1919:TYR:HB2	1.90	0.52
1:A:2024:TYR:CE2	1:A:2070:ALA:HB1	2.42	0.52
1:A:2032:ASP:O	1:A:2036:SER:CB	2.56	0.52
3:C:60:LEU:CD2	3:C:75:THR:HG21	2.37	0.52
4:E:1683:LEU:HG	4:E:1687:PHE:CE2	2.44	0.52
1:A:1238:LEU:HD11	1:A:1248:PHE:CD2	2.44	0.52
1:A:1486:MET:O	1:A:1489:ARG:HG2	2.10	0.52
1:A:1932:PHE:CE1	1:A:1936:ARG:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2024:TYR:OH	1:A:2061:PHE:O	2.23	0.52
3:C:126:THR:HG22	3:C:159:LYS:CB	2.39	0.52
4:E:1012:ASP:HB3	4:E:1035:PRO:HD2	1.91	0.52
4:E:1014:LEU:HB2	4:E:1057:PHE:CE2	2.44	0.52
4:E:1486:MET:O	4:E:1489:ARG:HG2	2.10	0.52
2:F:131:THR:HA	2:F:308:ARG:NH1	2.24	0.52
3:G:84:TRP:HZ3	3:G:210:ILE:HG22	1.75	0.52
3:G:199:SER:O	3:G:203:LEU:HB3	2.09	0.52
1:A:1012:ASP:HB3	1:A:1035:PRO:HD2	1.91	0.52
1:A:2023:GLY:O	1:A:2027:VAL:HG23	2.10	0.52
4:E:1369:THR:CG2	4:E:1370:ILE:N	2.73	0.52
3:G:221:ARG:NH1	3:G:258:LYS:HB3	2.25	0.52
1:A:1190:THR:HG23	1:A:1194:PHE:HE2	1.74	0.52
1:A:1246:VAL:HG21	1:A:1315:ASP:OD2	2.09	0.52
2:B:563:LYS:HD2	2:B:565:TYR:OH	2.09	0.52
4:E:1671:GLU:OE1	2:F:348:ILE:HD11	2.10	0.52
2:F:814:ASP:HA	2:F:817:ALA:HB3	1.91	0.52
1:A:1942:SER:OG	1:A:1971:ILE:HG22	2.09	0.52
1:A:1950:LEU:CD2	1:A:1955:ILE:HD13	2.18	0.52
1:A:2072:ASN:O	1:A:2076:LYS:CB	2.58	0.52
2:B:142:ALA:HA	2:B:145:TYR:CD2	2.37	0.52
2:B:515:HIS:O	2:B:519:PHE:HB2	2.10	0.52
2:B:750:ARG:HH22	2:B:779:ARG:HH11	1.57	0.52
3:C:50:SER:O	3:C:53:LEU:HD13	2.09	0.52
4:E:1208:PRO:O	4:E:1212:HIS:HB3	2.10	0.52
4:E:1666:MET:HA	2:F:347:ARG:HB3	1.90	0.52
4:E:1978:PHE:CD1	4:E:1982:SER:CB	2.93	0.52
4:E:1886:VAL:CG1	4:E:1896:ILE:HG22	2.40	0.52
2:F:172:VAL:HA	2:F:176:TYR:HD2	1.75	0.52
2:F:469:LYS:HE2	2:F:473:TYR:HE2	1.74	0.52
2:F:548:ASP:HB3	2:F:551:SER:HB2	1.92	0.52
1:A:1193:MET:HG2	1:A:1233:CYS:SG	2.49	0.52
4:E:1246:VAL:HG21	4:E:1315:ASP:OD2	2.09	0.52
2:F:563:LYS:HD2	2:F:565:TYR:OH	2.09	0.52
2:F:703:ALA:O	2:F:707:ILE:HG12	2.09	0.52
3:G:126:THR:HG22	3:G:159:LYS:CA	2.40	0.52
1:A:1683:LEU:HG	1:A:1687:PHE:CE2	2.44	0.52
2:B:250:GLU:OE2	2:B:255:GLN:HG2	2.09	0.52
2:B:274:CYS:CB	3:C:192:LEU:H	2.22	0.52
4:E:973:VAL:O	4:E:976:ASN:OD1	2.28	0.52
4:E:1010:MET:HE2	4:E:1061:CYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:215:TYR:O	3:G:218:GLN:HG3	2.10	0.52
2:B:366:TYR:CE1	2:B:389:ALA:HB2	2.46	0.51
3:C:211:CYS:O	3:C:266:ARG:HD3	2.09	0.51
4:E:1586:VAL:HG12	4:E:1613:ALA:O	2.09	0.51
4:E:1606:LEU:HA	2:F:387:GLU:OE2	2.10	0.51
2:F:120:TYR:HB3	2:F:148:LYS:HE3	1.91	0.51
3:G:82:LEU:HA	3:G:85:CYS:SG	2.50	0.51
1:A:1084:LEU:HD23	4:E:1140:MET:HE2	1.92	0.51
1:A:1131:CYS:CA	4:E:1098:THR:HG23	2.40	0.51
1:A:1952:LEU:O	1:A:2060:ARG:NH1	2.40	0.51
1:A:1958:ARG:O	1:A:1959:HIS:CG	2.63	0.51
1:A:1963:ILE:HD13	1:A:1995:LYS:CD	2.40	0.51
4:E:1114:ASN:OD1	4:E:1117:ASN:N	2.38	0.51
2:F:30:VAL:HG21	2:F:48:LEU:HD21	1.92	0.51
1:A:1122:ALA:H	1:A:1125:LEU:HD21	1.75	0.51
2:B:172:VAL:HA	2:B:176:TYR:HD2	1.75	0.51
3:C:199:SER:O	3:C:203:LEU:CB	2.59	0.51
4:E:1509:PRO:HG2	4:E:2022:ARG:HE	1.73	0.51
1:A:1104:THR:HG22	4:E:1108:LEU:HD21	1.93	0.51
1:A:1208:PRO:O	1:A:1212:HIS:HB3	2.10	0.51
4:E:1747:ILE:HD12	4:E:1748:ILE:HG13	1.91	0.51
2:F:179:ALA:O	2:F:183:ALA:HB2	2.11	0.51
1:A:1072:ALA:HB1	1:A:1075:VAL:HG12	1.93	0.51
1:A:1136:TYR:HB2	4:E:1101:ALA:HB1	1.92	0.51
1:A:1763:SER:O	1:A:1766:SER:HB2	2.11	0.51
2:B:548:ASP:HB3	2:B:551:SER:HB2	1.92	0.51
4:E:1292:VAL:HB	4:E:1348:PRO:HG2	1.91	0.51
4:E:1758:LYS:O	4:E:1761:CYS:HB2	2.10	0.51
2:F:408:MET:HE2	2:F:440:LEU:HD11	1.92	0.51
1:A:1758:LYS:O	1:A:1761:CYS:HB2	2.10	0.51
1:A:1886:VAL:CG1	1:A:1896:ILE:HG22	2.40	0.51
1:A:1898:CYS:HA	5:A:2201:E4S:C11	2.41	0.51
1:A:1932:PHE:O	1:A:1936:ARG:HB3	2.11	0.51
2:B:30:VAL:HG21	2:B:48:LEU:HD21	1.92	0.51
2:B:375:ARG:CZ	3:C:242:THR:HG23	2.41	0.51
4:E:1014:LEU:CD2	4:E:1098:THR:HG22	2.41	0.51
4:E:1370:ILE:HD11	2:F:754:GLU:HB3	1.92	0.51
4:E:2079:GLN:O	4:E:2083:LEU:HG	2.11	0.51
2:F:366:TYR:CE1	2:F:389:ALA:HB2	2.46	0.51
3:G:156:GLY:C	3:G:157:LEU:HD23	2.36	0.51
2:B:515:HIS:O	2:B:519:PHE:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1383:PHE:HE2	4:E:1488:ARG:HE	1.58	0.51
4:E:2072:ASN:O	4:E:2076:LYS:CB	2.58	0.51
1:A:1197:THR:O	1:A:1201:ILE:HG12	2.11	0.51
1:A:1293:THR:O	1:A:1296:TYR:HB3	2.11	0.51
1:A:1538:LYS:HE2	1:A:1539:GLN:NE2	2.26	0.51
1:A:1940:ILE:HG23	1:A:2016:PHE:HD1	1.75	0.51
2:B:173:ILE:HG23	2:B:177:GLU:OE1	2.11	0.51
3:C:84:TRP:HZ3	3:C:210:ILE:HG22	1.75	0.51
3:C:116:LYS:HZ1	3:C:121:LYS:HB2	1.76	0.51
3:C:215:TYR:O	3:C:218:GLN:HG3	2.10	0.51
4:E:1763:SER:O	4:E:1766:SER:HB2	2.10	0.51
4:E:1944:ALA:HB2	4:E:2016:PHE:CD1	2.46	0.51
4:E:1944:ALA:HA	4:E:2016:PHE:CE1	2.46	0.51
4:E:2056:LEU:O	4:E:2060:ARG:HG3	2.11	0.51
2:F:173:ILE:HG23	2:F:177:GLU:OE1	2.11	0.51
2:B:45:GLU:OE1	2:B:81:HIS:ND1	2.44	0.51
2:B:131:THR:HA	2:B:308:ARG:NH1	2.25	0.51
4:E:1197:THR:O	4:E:1201:ILE:HG12	2.11	0.51
2:F:515:HIS:O	2:F:519:PHE:HB2	2.10	0.51
2:F:750:ARG:HH22	2:F:779:ARG:HH11	1.58	0.51
4:E:1072:ALA:HB1	4:E:1075:VAL:HG12	1.93	0.51
4:E:1940:ILE:HG23	4:E:2016:PHE:HD1	1.75	0.51
2:F:258:ARG:HA	2:F:261:ILE:HG22	1.92	0.51
2:F:278:TYR:HE1	2:F:327:GLU:OE1	1.94	0.51
2:F:515:HIS:O	2:F:519:PHE:CB	2.59	0.51
1:A:1014:LEU:CD2	1:A:1098:THR:HG22	2.41	0.50
1:A:1944:ALA:CA	1:A:2016:PHE:HE1	2.24	0.50
1:A:2028:ARG:HH12	1:A:2065:MET:C	2.16	0.50
2:B:495:VAL:HG12	2:B:499:LYS:HE3	1.93	0.50
4:E:328:UNK:O	4:E:331:UNK:N	2.43	0.50
4:E:1954:GLN:HG3	4:E:2060:ARG:CZ	2.38	0.50
2:F:495:VAL:HG12	2:F:499:LYS:HE3	1.93	0.50
1:A:1996:LEU:HD12	1:A:2081:CYS:SG	2.52	0.50
3:C:123:LEU:HB2	3:C:163:SER:HB3	1.93	0.50
3:C:126:THR:HG22	3:C:159:LYS:CA	2.40	0.50
3:C:156:GLY:C	3:C:157:LEU:HD23	2.36	0.50
4:E:934:GLN:O	4:E:938:ALA:CB	2.59	0.50
4:E:1122:ALA:H	4:E:1125:LEU:HD21	1.75	0.50
4:E:2023:GLY:O	4:E:2027:VAL:HG23	2.10	0.50
2:F:403:PHE:O	2:F:406:SER:OG	2.24	0.50
3:G:84:TRP:CZ3	3:G:210:ILE:HG22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:UNK:O	1:A:330:UNK:N	2.45	0.50
1:A:1007:LEU:O	1:A:1011:LEU:HD13	2.12	0.50
1:A:1556:VAL:O	1:A:1559:PRO:HD2	2.11	0.50
1:A:1631:HIS:CD2	1:A:1632:PRO:HD2	2.45	0.50
1:A:1920:PHE:CE2	1:A:1932:PHE:CD1	2.95	0.50
2:B:179:ALA:O	2:B:183:ALA:HB2	2.11	0.50
2:B:403:PHE:O	2:B:406:SER:OG	2.24	0.50
2:B:408:MET:HE2	2:B:440:LEU:HD11	1.92	0.50
4:E:1556:VAL:O	4:E:1559:PRO:HD2	2.10	0.50
4:E:1605:GLU:O	4:E:1606:LEU:HG	2.11	0.50
4:E:1944:ALA:HB2	4:E:2016:PHE:CE1	2.46	0.50
2:F:579:TYR:HA	3:G:175:GLN:HG3	1.93	0.50
3:G:199:SER:O	3:G:203:LEU:CB	2.59	0.50
1:A:1508:ASN:N	1:A:1509:PRO:HD3	2.22	0.50
4:E:1128:ARG:NH1	4:E:1130:ALA:HB3	2.26	0.50
4:E:1849:PHE:HD1	4:E:1895:VAL:HG22	1.76	0.50
2:F:45:GLU:OE1	2:F:81:HIS:ND1	2.44	0.50
2:F:170:GLN:HA	2:F:173:ILE:HD12	1.93	0.50
2:F:478:LEU:HD23	2:F:504:PHE:HZ	1.76	0.50
1:A:1400:LEU:HD13	1:A:1506:TRP:HZ3	1.76	0.50
1:A:1596:TRP:HE1	1:A:1601:ALA:HA	1.77	0.50
1:A:2056:LEU:O	1:A:2060:ARG:HG3	2.11	0.50
3:C:88:ALA:O	3:C:92:SER:OG	2.29	0.50
3:C:178:PHE:CD2	3:C:232:VAL:HA	2.47	0.50
4:E:933:MET:HE1	4:E:981:ARG:CB	2.42	0.50
4:E:1586:VAL:CG1	4:E:1613:ALA:HB1	2.41	0.50
4:E:1860:LEU:HB3	4:E:1979:MET:SD	2.50	0.50
4:E:1908:LEU:H	4:E:1908:LEU:HD23	1.77	0.50
1:A:1014:LEU:HB2	1:A:1057:PHE:CE2	2.44	0.50
1:A:1101:ALA:CB	4:E:1131:CYS:SG	2.96	0.50
1:A:1128:ARG:HD3	4:E:1051:GLU:CD	2.36	0.50
1:A:2031:MET:HG3	1:A:2061:PHE:HD2	1.76	0.50
1:A:2079:GLN:O	1:A:2083:LEU:HG	2.11	0.50
2:B:170:GLN:HA	2:B:173:ILE:HD12	1.93	0.50
2:B:235:LEU:HB2	2:B:291:LEU:C	2.36	0.50
4:E:1137:SER:O	4:E:1141:ALA:CB	2.60	0.50
4:E:1293:THR:O	4:E:1296:TYR:HB3	2.11	0.50
4:E:1400:LEU:HD13	4:E:1506:TRP:HZ3	1.76	0.50
4:E:1538:LYS:HE2	4:E:1539:GLN:NE2	2.26	0.50
4:E:1978:PHE:HB3	4:E:1982:SER:HB3	1.93	0.50
2:F:113:TYR:HB3	2:F:155:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:79:LEU:HD12	3:G:80:PRO:HD3	1.93	0.50
1:A:934:GLN:O	1:A:938:ALA:CB	2.59	0.50
1:A:1590:ILE:HG13	1:A:1612:TRP:HZ3	1.77	0.50
1:A:1908:LEU:HD23	1:A:1908:LEU:H	1.77	0.50
4:E:1848:ILE:CG1	4:E:1896:ILE:HD11	2.42	0.50
4:E:1878:ASP:C	4:E:1879:LEU:HD12	2.37	0.50
2:F:235:LEU:HB2	2:F:291:LEU:C	2.36	0.50
3:G:88:ALA:O	3:G:92:SER:OG	2.29	0.50
1:A:1104:THR:HG22	4:E:1108:LEU:CD2	2.41	0.50
1:A:1130:ALA:HB1	4:E:1096:GLN:HE22	1.76	0.50
1:A:1137:SER:O	1:A:1141:ALA:CB	2.60	0.50
2:B:478:LEU:HD23	2:B:504:PHE:HZ	1.76	0.50
3:C:82:LEU:HA	3:C:85:CYS:SG	2.50	0.50
4:E:1596:TRP:HE1	4:E:1601:ALA:HA	1.77	0.50
1:A:1031:TYR:CE1	1:A:1042:THR:HG22	2.47	0.50
1:A:1081:GLN:HG3	1:A:1143:LEU:HD13	1.94	0.50
1:A:1383:PHE:HE2	1:A:1488:ARG:HE	1.58	0.50
1:A:1586:VAL:HG13	1:A:1613:ALA:HB3	1.94	0.50
2:B:258:ARG:HA	2:B:261:ILE:HG22	1.92	0.50
2:B:273:MET:HA	3:C:193:THR:OG1	2.12	0.50
2:B:326:GLU:OE2	3:C:125:PHE:HB2	2.11	0.50
3:C:84:TRP:CZ3	3:C:210:ILE:HG22	2.47	0.50
3:C:169:ARG:HH11	3:C:170:GLU:H	1.60	0.50
3:C:264:ILE:O	3:C:268:GLN:HG3	2.12	0.50
4:E:1007:LEU:O	4:E:1011:LEU:HD13	2.12	0.50
4:E:1373:VAL:HG11	2:F:758:ALA:O	2.11	0.50
1:A:1848:ILE:CG1	1:A:1896:ILE:HD11	2.42	0.49
1:A:1849:PHE:HD1	1:A:1895:VAL:HG22	1.76	0.49
4:E:1128:ARG:HD2	4:E:1128:ARG:O	2.12	0.49
4:E:1401:ARG:NH2	4:E:1516:GLU:OE1	2.45	0.49
2:F:141:ILE:HG22	2:F:145:TYR:CE2	2.47	0.49
2:F:787:LEU:HD13	2:F:804:LEU:N	2.27	0.49
3:G:123:LEU:HB2	3:G:163:SER:HB3	1.93	0.49
1:A:1590:ILE:HG13	1:A:1612:TRP:CZ3	2.47	0.49
1:A:1605:GLU:O	1:A:1606:LEU:HG	2.11	0.49
1:A:1878:ASP:C	1:A:1879:LEU:HD12	2.37	0.49
1:A:1996:LEU:CD1	1:A:2081:CYS:SG	3.00	0.49
4:E:1114:ASN:O	4:E:1118:THR:OG1	2.20	0.49
4:E:2031:MET:HG3	4:E:2061:PHE:HD2	1.77	0.49
2:F:752:TRP:O	2:F:755:GLU:HB2	2.12	0.49
3:G:274:GLU:HG2	3:G:275:PRO:CD	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:PRO:O	1:A:1212:HIS:CB	2.61	0.49
1:A:1735:PHE:O	1:A:1739:ASN:CB	2.59	0.49
1:A:1862:LEU:HD21	1:A:1885:ARG:HA	1.93	0.49
2:B:752:TRP:O	2:B:755:GLU:HB2	2.12	0.49
3:C:214:GLY:HA3	3:C:229:ARG:CG	2.43	0.49
4:E:1081:GLN:HG3	4:E:1143:LEU:HD13	1.94	0.49
4:E:1259:THR:HG21	4:E:1295:HIS:NE2	2.27	0.49
4:E:1777:PRO:O	4:E:1887:VAL:HG21	2.12	0.49
4:E:1932:PHE:CE2	4:E:1936:ARG:HD3	2.48	0.49
1:A:1114:ASN:CB	1:A:1135:ASP:HB3	2.40	0.49
4:E:1321:SER:O	4:E:1325:GLN:HB3	2.13	0.49
4:E:1944:ALA:N	4:E:2016:PHE:HE1	2.11	0.49
1:A:1741:ILE:HG23	1:A:1803:TYR:OH	2.13	0.49
2:B:141:ILE:HG22	2:B:145:TYR:CE2	2.47	0.49
2:B:408:MET:SD	3:C:273:PRO:HG3	2.52	0.49
4:E:1031:TYR:CE1	4:E:1042:THR:HG22	2.48	0.49
4:E:1119:THR:HG21	4:E:1402:GLU:HA	1.94	0.49
4:E:1503:LEU:O	4:E:1506:TRP:N	2.46	0.49
4:E:1924:TYR:HD1	4:E:1931:ALA:HB1	1.78	0.49
4:E:1948:LEU:O	4:E:1952:LEU:HD23	2.11	0.49
2:F:75:LEU:HD22	2:F:106:LEU:HD13	1.95	0.49
3:G:264:ILE:O	3:G:268:GLN:HG3	2.12	0.49
1:A:1401:ARG:NH2	1:A:1516:GLU:OE1	2.46	0.49
2:B:75:LEU:HD22	2:B:106:LEU:HD13	1.95	0.49
2:B:587:PHE:CE1	2:B:701:HIS:ND1	2.80	0.49
3:C:79:LEU:HD12	3:C:80:PRO:HD3	1.94	0.49
4:E:1741:ILE:HG23	4:E:1803:TYR:OH	2.13	0.49
2:F:281:PRO:HB2	3:G:135:VAL:HG21	1.94	0.49
2:F:548:ASP:OD1	2:F:549:ALA:N	2.46	0.49
3:G:116:LYS:HZ2	3:G:121:LYS:HB2	1.78	0.49
1:A:1978:PHE:HD1	1:A:1982:SER:HB3	1.72	0.49
2:B:469:LYS:HE2	2:B:473:TYR:CE2	2.48	0.49
2:F:128:LEU:HD22	2:F:137:ARG:NH2	2.27	0.49
2:F:240:GLY:O	2:F:244:GLU:HG3	2.13	0.49
3:G:178:PHE:CD2	3:G:232:VAL:HA	2.47	0.49
1:A:1098:THR:HG23	4:E:1131:CYS:CA	2.42	0.49
2:B:113:TYR:HB3	2:B:155:LEU:HD11	1.94	0.49
4:E:1321:SER:O	4:E:1325:GLN:CB	2.61	0.49
4:E:1346:ILE:HD12	4:E:1407:MET:SD	2.53	0.49
4:E:1631:HIS:CD2	4:E:1632:PRO:HD2	2.45	0.49
4:E:1862:LEU:HD21	4:E:1885:ARG:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:HD22	2:B:137:ARG:NH2	2.27	0.49
4:E:1208:PRO:O	4:E:1212:HIS:CB	2.61	0.49
4:E:1573:THR:O	4:E:1577:ARG:HB2	2.13	0.49
4:E:1860:LEU:HB3	4:E:1979:MET:CE	2.43	0.49
4:E:1877:LEU:HB3	4:E:1879:LEU:CD1	2.43	0.49
4:E:2006:GLY:HA2	4:E:2010:ALA:CB	2.42	0.49
4:E:2024:TYR:OH	4:E:2061:PHE:O	2.23	0.49
3:G:237:MET:CA	3:G:240:MET:HG2	2.40	0.49
3:G:245:TYR:HA	3:G:248:PHE:CD2	2.48	0.49
1:A:1321:SER:O	1:A:1325:GLN:CB	2.61	0.49
1:A:1559:PRO:HB3	1:A:1568:ILE:HD13	1.95	0.49
1:A:1699:GLU:CB	1:A:1702:HIS:CD2	2.86	0.49
1:A:1882:PHE:HE2	1:A:1899:ILE:HG12	1.78	0.49
1:A:1940:ILE:HG23	1:A:2016:PHE:CD1	2.48	0.49
1:A:2017:MET:O	1:A:2021:VAL:HG22	2.13	0.49
2:B:576:LEU:HD13	2:B:586:LEU:HD23	1.95	0.49
2:B:787:LEU:HD13	2:B:804:LEU:N	2.27	0.49
4:E:1381:THR:O	4:E:1384:ASP:HB3	2.12	0.49
4:E:1685:HIS:CE1	4:E:1731:TYR:HB3	2.47	0.49
4:E:1940:ILE:HG23	4:E:2016:PHE:CD1	2.48	0.49
2:F:601:GLU:HA	2:F:604:LEU:HD12	1.95	0.49
3:G:169:ARG:HH11	3:G:170:GLU:H	1.60	0.49
1:A:1507:TYR:O	1:A:1509:PRO:HD3	2.13	0.48
4:E:1590:ILE:O	4:E:1593:LEU:N	2.46	0.48
4:E:1954:GLN:OE1	4:E:1954:GLN:HA	2.12	0.48
3:G:54:GLU:HA	3:G:101:ILE:HD11	1.95	0.48
3:G:221:ARG:HH12	3:G:258:LYS:HD3	1.78	0.48
1:A:1119:THR:HG21	1:A:1402:GLU:HA	1.95	0.48
1:A:1259:THR:HG21	1:A:1295:HIS:NE2	2.27	0.48
1:A:1346:ILE:HD12	1:A:1407:MET:SD	2.53	0.48
1:A:1777:PRO:O	1:A:1887:VAL:HG21	2.12	0.48
4:E:1944:ALA:HA	4:E:2016:PHE:CZ	2.48	0.48
2:F:139:ARG:HB2	2:F:186:TYR:CE1	2.48	0.48
2:F:576:LEU:HD13	2:F:586:LEU:HD23	1.95	0.48
1:A:1996:LEU:HA	1:A:2000:MET:HE3	1.95	0.48
2:B:218:LEU:O	2:B:222:LEU:HD13	2.14	0.48
2:B:548:ASP:OD1	2:B:549:ALA:N	2.46	0.48
2:B:601:GLU:HA	2:B:604:LEU:HD12	1.96	0.48
3:C:245:TYR:HA	3:C:248:PHE:CD2	2.48	0.48
3:C:274:GLU:HG2	3:C:275:PRO:CD	2.37	0.48
4:E:27:UNK:HA	2:F:821:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1231:LEU:HD22	4:E:1301:PHE:CD1	2.48	0.48
4:E:1631:HIS:CE1	4:E:1633:LEU:HD12	2.49	0.48
1:A:1381:THR:O	1:A:1384:ASP:HB3	2.12	0.48
1:A:1685:HIS:CE1	1:A:1731:TYR:HB3	2.48	0.48
2:B:220:THR:O	2:B:224:ARG:HB3	2.13	0.48
4:E:1214:LEU:HG	4:E:1234:TRP:HE1	1.78	0.48
4:E:1878:ASP:O	4:E:1941:ARG:HG3	2.14	0.48
4:E:2011:THR:OG1	4:E:2012:PRO:HD3	2.13	0.48
2:F:218:LEU:O	2:F:222:LEU:HD13	2.14	0.48
1:A:1321:SER:O	1:A:1325:GLN:HB3	2.12	0.48
1:A:1731:TYR:HA	1:A:1734:GLU:HB3	1.96	0.48
2:B:178:LYS:HE2	2:B:306:LEU:HD21	1.96	0.48
2:B:227:VAL:HG12	2:B:231:LYS:HE3	1.94	0.48
2:B:592:LEU:HD23	2:B:595:LEU:HD12	1.96	0.48
4:E:1981:GLU:HA	4:E:1981:GLU:OE1	2.14	0.48
2:F:51:SER:O	2:F:55:GLN:CB	2.61	0.48
2:F:227:VAL:HG12	2:F:231:LYS:HE3	1.94	0.48
2:F:519:PHE:CE1	2:F:551:SER:HA	2.48	0.48
1:A:1503:LEU:O	1:A:1506:TRP:N	2.46	0.48
2:B:240:GLY:O	2:B:244:GLU:HG3	2.13	0.48
3:C:86:TYR:O	3:C:90:SER:CB	2.61	0.48
4:E:1031:TYR:HA	4:E:1041:ILE:O	2.14	0.48
4:E:1586:VAL:CG2	4:E:1587:PRO:CD	2.89	0.48
4:E:1670:ARG:NH1	2:F:349:PRO:HB2	2.28	0.48
4:E:1735:PHE:O	4:E:1739:ASN:CB	2.59	0.48
2:F:178:LYS:HE2	2:F:306:LEU:HD21	1.96	0.48
2:F:227:VAL:O	2:F:231:LYS:HG3	2.14	0.48
2:B:113:TYR:CB	2:B:155:LEU:HD21	2.43	0.48
2:B:179:ALA:O	2:B:183:ALA:CB	2.61	0.48
4:E:1349:ARG:NE	4:E:1385:TYR:HB2	2.29	0.48
4:E:1692:LYS:HA	4:E:1695:ILE:CD1	2.44	0.48
2:F:179:ALA:O	2:F:183:ALA:CB	2.61	0.48
2:F:469:LYS:HE2	2:F:473:TYR:CE2	2.48	0.48
1:A:1214:LEU:HG	1:A:1234:TRP:HE1	1.78	0.48
1:A:1231:LEU:HD22	1:A:1301:PHE:CD1	2.48	0.48
1:A:1692:LYS:HA	1:A:1695:ILE:CD1	2.44	0.48
2:B:139:ARG:HB2	2:B:186:TYR:CE1	2.48	0.48
4:E:1391:LYS:C	4:E:1502:ARG:HH22	2.22	0.48
4:E:1731:TYR:HA	4:E:1734:GLU:HB3	1.96	0.48
4:E:1978:PHE:HD1	4:E:1982:SER:CB	2.27	0.48
2:F:92:LYS:HB2	2:F:95:PHE:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:341:ARG:NH2	3:G:145:MET:HE2	2.29	0.48
3:G:83:ILE:O	3:G:87:LEU:CB	2.50	0.48
1:A:1031:TYR:HA	1:A:1041:ILE:O	2.14	0.48
2:B:227:VAL:O	2:B:231:LYS:HG3	2.14	0.48
2:B:584:ILE:HA	2:B:587:PHE:HD2	1.79	0.48
3:C:265:TYR:CZ	3:C:269:LEU:HD11	2.49	0.48
4:E:1994:ILE:CG2	4:E:1995:LYS:H	2.26	0.48
2:F:142:ALA:HA	2:F:145:TYR:CD2	2.37	0.48
2:F:178:LYS:HG2	2:F:306:LEU:HD21	1.96	0.48
2:F:220:THR:O	2:F:224:ARG:HB3	2.13	0.48
2:F:587:PHE:CE1	2:F:701:HIS:ND1	2.80	0.48
3:G:86:TYR:O	3:G:90:SER:CB	2.61	0.48
3:G:265:TYR:CZ	3:G:269:LEU:HD11	2.49	0.48
1:A:1351:LYS:O	1:A:1354:THR:HB	2.14	0.48
1:A:1590:ILE:HG23	1:A:1591:LYS:N	2.29	0.48
4:E:2028:ARG:HH12	4:E:2065:MET:C	2.16	0.48
2:F:584:ILE:HA	2:F:587:PHE:HD2	1.79	0.48
1:A:939:VAL:HG13	1:A:942:LYS:NZ	2.29	0.47
1:A:1068:ALA:O	1:A:1076:THR:OG1	2.31	0.47
1:A:1853:ASP:OD1	1:A:1854:ASP:N	2.47	0.47
2:B:519:PHE:CE1	2:B:551:SER:HA	2.48	0.47
3:C:221:ARG:HH12	3:C:258:LYS:HD3	1.78	0.47
4:E:1227:MET:HE1	4:E:1298:TRP:CE3	2.49	0.47
4:E:1559:PRO:HB3	4:E:1568:ILE:HD13	1.95	0.47
2:F:113:TYR:CB	2:F:155:LEU:HD21	2.44	0.47
1:A:947:PHE:CE1	1:A:951:MET:HE3	2.49	0.47
1:A:1128:ARG:HB3	4:E:1051:GLU:HG3	1.96	0.47
1:A:1573:THR:O	1:A:1577:ARG:HB2	2.13	0.47
2:B:173:ILE:HG23	2:B:177:GLU:CD	2.39	0.47
4:E:2017:MET:O	4:E:2021:VAL:HG22	2.13	0.47
2:F:592:LEU:HD23	2:F:595:LEU:HD12	1.96	0.47
1:A:1570:ASN:O	1:A:1574:ARG:HB2	2.14	0.47
3:C:260:LEU:HD13	3:C:282:ILE:HG21	1.96	0.47
4:E:1569:GLY:O	4:E:1573:THR:OG1	2.31	0.47
4:E:1570:ASN:O	4:E:1574:ARG:HB2	2.14	0.47
2:F:325:THR:OG1	2:F:376:ARG:NH2	2.47	0.47
2:F:519:PHE:CZ	2:F:550:ASN:HB3	2.49	0.47
1:A:1090:TRP:CZ2	4:E:1144:ASN:HB3	2.50	0.47
1:A:1349:ARG:NE	1:A:1385:TYR:HB2	2.29	0.47
1:A:1938:ASN:HA	1:A:1941:ARG:HG2	1.95	0.47
2:B:92:LYS:HB2	2:B:95:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:690:HIS:CG	2:B:691:PRO:HD3	2.49	0.47
3:C:54:GLU:HA	3:C:101:ILE:HD11	1.95	0.47
4:E:947:PHE:CE1	4:E:951:MET:HE3	2.49	0.47
4:E:1351:LYS:O	4:E:1354:THR:HB	2.14	0.47
2:F:173:ILE:HG23	2:F:177:GLU:CD	2.39	0.47
2:F:224:ARG:NE	2:F:228:LEU:HD11	2.29	0.47
1:A:1051:GLU:O	1:A:1055:LYS:HG2	2.15	0.47
2:B:371:ILE:HD11	3:C:282:ILE:CD1	2.45	0.47
2:B:519:PHE:CZ	2:B:550:ASN:HB3	2.49	0.47
2:B:752:TRP:HA	2:B:755:GLU:HG3	1.96	0.47
4:E:939:VAL:HG13	4:E:942:LYS:NZ	2.29	0.47
1:A:1317:VAL:HG11	1:A:1364:VAL:CG1	2.45	0.47
1:A:1391:LYS:C	1:A:1502:ARG:HH22	2.22	0.47
1:A:1529:ARG:O	1:A:1533:ILE:HG13	2.15	0.47
1:A:1590:ILE:HB	1:A:1612:TRP:CZ3	2.50	0.47
2:B:51:SER:O	2:B:55:GLN:CB	2.61	0.47
3:C:237:MET:CA	3:C:240:MET:HG2	2.40	0.47
4:E:1507:TYR:O	4:E:1509:PRO:HD3	2.12	0.47
1:A:1101:ALA:CB	4:E:1136:TYR:HB2	2.39	0.47
1:A:1137:SER:O	1:A:1141:ALA:HB2	2.15	0.47
1:A:1266:LEU:H	1:A:1295:HIS:CE1	2.33	0.47
1:A:1404:ILE:O	1:A:1408:ILE:HG13	2.15	0.47
1:A:1877:LEU:HB3	1:A:1879:LEU:CD1	2.43	0.47
1:A:1904:SER:HB2	1:A:1907:GLN:CG	2.42	0.47
3:C:252:GLU:OE1	3:C:255:LEU:HD12	2.15	0.47
4:E:1051:GLU:O	4:E:1055:LYS:HG2	2.15	0.47
4:E:1266:LEU:H	4:E:1295:HIS:CE1	2.33	0.47
4:E:1317:VAL:HG11	4:E:1364:VAL:CG1	2.45	0.47
4:E:1737:PHE:CE2	4:E:1741:ILE:HD11	2.50	0.47
4:E:1853:ASP:OD1	4:E:1854:ASP:N	2.47	0.47
2:F:83:THR:O	2:F:87:ASP:CB	2.61	0.47
2:F:688:PRO:HG2	2:F:691:PRO:HG2	1.97	0.47
3:G:221:ARG:NH1	3:G:258:LYS:HD3	2.30	0.47
3:G:252:GLU:OE1	3:G:255:LEU:HD12	2.15	0.47
1:A:1631:HIS:CE1	1:A:1633:LEU:HD12	2.48	0.47
1:A:1951:PHE:HE1	1:A:2077:VAL:HG11	1.79	0.47
1:A:2006:GLY:HA2	1:A:2010:ALA:CB	2.45	0.47
2:B:178:LYS:HG2	2:B:306:LEU:HD21	1.96	0.47
2:B:325:THR:OG1	2:B:376:ARG:NH2	2.47	0.47
3:C:178:PHE:CE1	3:C:181:LEU:HD11	2.49	0.47
4:E:206:UNK:O	4:E:210:UNK:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1404:ILE:O	4:E:1408:ILE:HG13	2.15	0.47
1:A:1737:PHE:CE2	1:A:1741:ILE:HD11	2.50	0.47
2:B:224:ARG:NE	2:B:228:LEU:HD11	2.29	0.47
2:B:434:PRO:HG2	2:B:458:VAL:HG22	1.97	0.47
3:C:139:PRO:O	3:C:142:ILE:HG22	2.15	0.47
3:C:159:LYS:HD2	3:C:160:VAL:N	2.30	0.47
4:E:1529:ARG:O	4:E:1533:ILE:HG13	2.15	0.47
4:E:1597:HIS:ND1	4:E:1602:ASP:OD2	2.45	0.47
4:E:1712:LEU:O	4:E:1716:VAL:HG23	2.15	0.47
1:A:1010:MET:HG3	1:A:1064:ILE:HD11	1.96	0.47
1:A:1015:GLN:NE2	1:A:1099:GLY:H	2.13	0.47
1:A:1250:ARG:NE	2:B:785:LYS:HB2	2.30	0.47
1:A:1768:VAL:HG23	1:A:1769:LYS:H	1.80	0.47
3:C:274:GLU:CG	3:C:275:PRO:HD3	2.40	0.47
4:E:1658:VAL:O	4:E:1661:LEU:HB2	2.15	0.47
4:E:1768:VAL:HG23	4:E:1769:LYS:H	1.80	0.47
3:G:260:LEU:HD13	3:G:282:ILE:HG21	1.96	0.47
1:A:939:VAL:HA	1:A:942:LYS:HZ3	1.79	0.46
1:A:1093:GLY:O	4:E:1137:SER:OG	2.29	0.46
1:A:1493:LEU:HB3	1:A:1528:TRP:NE1	2.31	0.46
1:A:1544:VAL:HG22	1:A:1558:LEU:CD2	2.45	0.46
1:A:1875:VAL:HG21	1:A:2026:ALA:HB1	1.98	0.46
2:B:8:SER:OG	2:B:9:ARG:N	2.48	0.46
4:E:1015:GLN:NE2	4:E:1099:GLY:H	2.13	0.46
4:E:1276:PRO:HG2	4:E:1277:LEU:HD12	1.97	0.46
4:E:1538:LYS:HG3	4:E:1539:GLN:CD	2.40	0.46
4:E:1544:VAL:HG22	4:E:1558:LEU:CD2	2.45	0.46
4:E:1731:TYR:HB2	4:E:1735:PHE:CE1	2.50	0.46
4:E:2034:VAL:CG1	4:E:2057:LEU:HD21	2.43	0.46
2:F:346:SER:HB2	2:F:355:ARG:HH12	1.72	0.46
3:G:204:CYS:O	3:G:208:SER:HB2	2.15	0.46
1:A:1114:ASN:O	1:A:1118:THR:OG1	2.20	0.46
1:A:1993:ASP:CG	1:A:1994:ILE:CD1	2.88	0.46
2:B:576:LEU:HD21	2:B:585:LEU:HB2	1.97	0.46
3:C:204:CYS:O	3:C:208:SER:HB2	2.15	0.46
4:E:1761:CYS:O	4:E:1764:ALA:HB3	2.16	0.46
4:E:1951:PHE:HE1	4:E:2077:VAL:HG11	1.79	0.46
2:F:436:LEU:HD23	3:G:271:LEU:HD23	1.98	0.46
2:F:690:HIS:CG	2:F:691:PRO:HD3	2.50	0.46
3:G:172:LEU:HD21	3:G:177:ARG:CB	2.45	0.46
1:A:1238:LEU:HD22	1:A:1305:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:PRO:O	1:A:1636:GLN:HG3	2.16	0.46
1:A:1944:ALA:N	1:A:2016:PHE:HE1	2.13	0.46
2:B:515:HIS:H	3:C:229:ARG:HH12	1.62	0.46
2:B:832:PRO:HB3	2:B:836:PHE:CZ	2.51	0.46
4:E:1068:ALA:O	4:E:1076:THR:OG1	2.32	0.46
4:E:1010:MET:HG3	4:E:1064:ILE:HD11	1.96	0.46
2:F:340:ASN:OD1	2:F:340:ASN:O	2.34	0.46
2:F:576:LEU:HD21	2:F:585:LEU:HB2	1.97	0.46
1:A:1647:PRO:HB3	1:A:1683:LEU:HD22	1.96	0.46
1:A:1658:VAL:O	1:A:1661:LEU:HB2	2.15	0.46
3:C:218:GLN:O	3:C:222:LYS:N	2.43	0.46
4:E:2035:VAL:HG13	4:E:2054:ILE:HG23	1.97	0.46
1:A:2061:PHE:O	1:A:2062:SER:OG	2.32	0.46
2:B:688:PRO:HG2	2:B:691:PRO:HG2	1.97	0.46
4:E:1137:SER:O	4:E:1141:ALA:HB2	2.15	0.46
4:E:1924:TYR:OH	4:E:1968:LYS:N	2.48	0.46
3:G:139:PRO:O	3:G:142:ILE:HG22	2.15	0.46
2:B:220:THR:O	2:B:224:ARG:CB	2.64	0.46
3:C:260:LEU:CD1	3:C:282:ILE:HG21	2.46	0.46
4:E:1011:LEU:HD21	4:E:1103:ALA:HB2	1.97	0.46
4:E:1498:THR:O	4:E:1501:GLU:HG2	2.15	0.46
4:E:1950:LEU:HD12	4:E:1994:ILE:HG23	1.96	0.46
2:F:8:SER:OG	2:F:9:ARG:N	2.48	0.46
2:F:449:GLU:HG2	2:F:453:LYS:HZ2	1.81	0.46
2:F:519:PHE:HE1	2:F:551:SER:HA	1.80	0.46
3:G:124:SER:HB2	3:G:159:LYS:HD3	1.97	0.46
3:G:159:LYS:HD2	3:G:160:VAL:N	2.30	0.46
1:A:1096:GLN:NE2	4:E:1130:ALA:O	2.47	0.46
1:A:1731:TYR:HB2	1:A:1735:PHE:CE1	2.50	0.46
1:A:1924:TYR:OH	1:A:1968:LYS:N	2.48	0.46
1:A:1958:ARG:O	1:A:1959:HIS:CD2	2.69	0.46
1:A:2018:GLU:OE2	1:A:2022:ARG:NH1	2.49	0.46
2:B:20:GLU:OE1	2:B:22:GLN:NE2	2.49	0.46
2:B:712:PRO:HB3	2:B:742:LEU:HD23	1.97	0.46
3:C:124:SER:HB2	3:C:159:LYS:HD3	1.97	0.46
4:E:1128:ARG:HH11	4:E:1130:ALA:HB3	1.80	0.46
4:E:1400:LEU:HD21	4:E:1507:TYR:HD2	1.77	0.46
4:E:1647:PRO:HB3	4:E:1683:LEU:HD22	1.96	0.46
4:E:1724:SER:HA	4:E:1728:LYS:HB2	1.98	0.46
2:F:20:GLU:OE1	2:F:22:GLN:NE2	2.49	0.46
3:G:260:LEU:CD1	3:G:282:ILE:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:THR:CG2	4:E:1108:LEU:HD21	2.45	0.46
1:A:1498:THR:O	1:A:1501:GLU:HG2	2.15	0.46
1:A:1712:LEU:O	1:A:1716:VAL:HG23	2.15	0.46
3:C:221:ARG:NH1	3:C:258:LYS:HD3	2.30	0.46
4:E:1529:ARG:HD2	4:E:1533:ILE:CD1	2.46	0.46
2:F:220:THR:O	2:F:224:ARG:CB	2.64	0.46
2:F:344:VAL:HG11	2:F:351:HIS:CE1	2.50	0.46
2:F:545:GLN:NE2	3:G:229:ARG:O	2.49	0.46
1:A:1227:MET:HE1	1:A:1298:TRP:CE3	2.49	0.46
1:A:1232:ALA:HB2	4:E:1094:LEU:HD21	1.96	0.46
1:A:1861:ALA:HB2	1:A:1979:MET:HE3	1.98	0.46
1:A:2035:VAL:HG13	1:A:2054:ILE:HG23	1.97	0.46
1:A:2036:SER:O	1:A:2039:THR:HG22	2.16	0.46
2:B:271:ARG:HD2	3:C:249:TYR:CD2	2.51	0.46
2:F:423:CYS:HB3	2:F:433:ILE:HD13	1.98	0.46
1:A:1098:THR:HG23	4:E:1131:CYS:N	2.31	0.45
1:A:1108:LEU:HD21	4:E:1104:THR:HG22	1.98	0.45
1:A:1569:GLY:O	1:A:1573:THR:OG1	2.31	0.45
2:B:167:ASP:OD2	2:B:169:GLU:HB3	2.16	0.45
4:E:1238:LEU:HD22	4:E:1305:ARG:CZ	2.46	0.45
4:E:1529:ARG:HD2	4:E:1533:ILE:HD11	1.98	0.45
3:G:108:VAL:O	3:G:112:GLU:HG2	2.16	0.45
1:A:185:UNK:CB	1:A:205:UNK:CB	2.94	0.45
1:A:1276:PRO:HG2	1:A:1277:LEU:HD12	1.97	0.45
1:A:1510:LEU:CD2	1:A:2017:MET:HB3	2.46	0.45
1:A:1529:ARG:HD2	1:A:1533:ILE:CD1	2.46	0.45
1:A:1538:LYS:HG3	1:A:1539:GLN:CD	2.40	0.45
1:A:1724:SER:HA	1:A:1728:LYS:HB2	1.98	0.45
4:E:1950:LEU:CD2	4:E:1955:ILE:HG21	2.45	0.45
2:F:434:PRO:HG2	2:F:458:VAL:HG22	1.97	0.45
1:A:1306:PHE:HA	1:A:1320:PHE:HE2	1.81	0.45
3:C:172:LEU:HD21	3:C:177:ARG:CB	2.45	0.45
4:E:1848:ILE:HD11	4:E:1896:ILE:HD11	1.98	0.45
4:E:1875:VAL:HG21	4:E:2026:ALA:HB1	1.97	0.45
4:E:2018:GLU:OE2	4:E:2022:ARG:NH1	2.49	0.45
2:F:242:PHE:CD2	2:F:265:LEU:HD13	2.51	0.45
2:F:832:PRO:HB3	2:F:836:PHE:CZ	2.51	0.45
3:G:45:ILE:O	3:G:45:ILE:HG22	2.17	0.45
3:G:64:TYR:CZ	3:G:108:VAL:HG13	2.51	0.45
1:A:1051:GLU:HG3	4:E:1128:ARG:HB3	1.97	0.45
1:A:1211:LEU:HD11	1:A:1248:PHE:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1932:PHE:CZ	1:A:1936:ARG:HD2	2.40	0.45
2:B:327:GLU:O	2:B:331:LEU:HG	2.16	0.45
2:B:423:CYS:HB3	2:B:433:ILE:HD13	1.98	0.45
4:E:1493:LEU:HB3	4:E:1528:TRP:NE1	2.31	0.45
4:E:1510:LEU:CD2	4:E:2017:MET:HB3	2.46	0.45
4:E:1632:PRO:O	4:E:1636:GLN:HG3	2.16	0.45
1:A:1134:LYS:CG	1:A:1136:TYR:CE2	2.92	0.45
1:A:1137:SER:N	4:E:1101:ALA:HB2	2.31	0.45
1:A:1234:TRP:O	1:A:1238:LEU:HD13	2.17	0.45
1:A:1298:TRP:O	1:A:1301:PHE:N	2.49	0.45
1:A:1639:VAL:HG21	2:B:394:PHE:HE1	1.82	0.45
1:A:2011:THR:OG1	1:A:2012:PRO:CD	2.64	0.45
2:B:613:TRP:CE3	2:B:695:LEU:HD13	2.52	0.45
2:B:711:LYS:HB3	2:B:714:GLU:OE1	2.17	0.45
3:C:108:VAL:O	3:C:112:GLU:HG2	2.16	0.45
2:F:535:LEU:O	2:F:539:ARG:HG2	2.17	0.45
2:F:586:LEU:HD13	2:F:609:MET:HG2	1.98	0.45
2:F:752:TRP:HA	2:F:755:GLU:HG3	1.96	0.45
1:A:1411:TRP:O	1:A:1415:PHE:HB2	2.17	0.45
1:A:1761:CYS:O	1:A:1764:ALA:HB3	2.16	0.45
2:B:185:LEU:O	2:B:189:GLU:CB	2.63	0.45
2:B:435:LEU:HG	3:C:271:LEU:HD21	1.99	0.45
2:B:693:MET:O	2:B:697:GLN:HG2	2.16	0.45
3:C:79:LEU:N	3:C:80:PRO:HD2	2.32	0.45
4:E:1904:SER:HB2	4:E:1907:GLN:CG	2.42	0.45
2:F:712:PRO:HB3	2:F:742:LEU:HD23	1.97	0.45
3:G:79:LEU:N	3:G:80:PRO:HD2	2.32	0.45
1:A:1131:CYS:HB2	4:E:1098:THR:CG2	2.34	0.45
1:A:1637:TYR:O	1:A:1641:VAL:HG23	2.16	0.45
1:A:1699:GLU:HG2	1:A:1702:HIS:NE2	2.32	0.45
1:A:2010:ALA:O	1:A:2014:LYS:N	2.30	0.45
1:A:2072:ASN:HA	1:A:2075:MET:HG2	1.99	0.45
2:B:271:ARG:HB2	3:C:249:TYR:CD2	2.52	0.45
2:B:519:PHE:HE1	2:B:551:SER:HA	1.80	0.45
4:E:1196:LEU:HD11	4:E:1210:LEU:HD22	1.99	0.45
4:E:1400:LEU:HD13	4:E:1506:TRP:CZ3	2.52	0.45
2:F:693:MET:O	2:F:697:GLN:HG2	2.16	0.45
3:G:274:GLU:CG	3:G:275:PRO:HD3	2.40	0.45
1:A:1011:LEU:HD21	1:A:1103:ALA:HB2	1.97	0.45
2:B:83:THR:O	2:B:87:ASP:CB	2.61	0.45
2:B:418:LYS:O	2:B:421:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:535:LEU:O	2:B:539:ARG:HG2	2.17	0.45
4:E:414:UNK:C	4:E:416:UNK:N	2.80	0.45
4:E:1298:TRP:O	4:E:1301:PHE:N	2.50	0.45
4:E:1329:SER:HA	4:E:1377:LYS:NZ	2.32	0.45
4:E:1637:TYR:O	4:E:1641:VAL:HG23	2.16	0.45
4:E:1958:ARG:C	4:E:1959:HIS:CG	2.95	0.45
2:F:247:ARG:NH2	2:F:282:LEU:HD23	2.32	0.45
2:F:449:GLU:HG2	2:F:453:LYS:NZ	2.32	0.45
1:A:1066:GLN:HA	1:A:1110:PHE:CZ	2.52	0.45
1:A:1590:ILE:CG1	1:A:1594:VAL:HG21	2.46	0.45
2:B:247:ARG:HB3	2:B:312:VAL:HG13	1.98	0.45
2:F:167:ASP:OD2	2:F:169:GLU:HB3	2.16	0.45
3:G:11:GLU:HA	3:G:14:SER:OG	2.17	0.45
3:G:211:CYS:O	3:G:266:ARG:HD3	2.15	0.45
1:A:1225:HIS:HE1	4:E:1091:VAL:HG13	1.82	0.45
1:A:1306:PHE:HD1	1:A:1320:PHE:HD2	1.64	0.45
1:A:1963:ILE:CD1	1:A:1995:LYS:CD	2.89	0.45
3:C:64:TYR:CZ	3:C:108:VAL:HG13	2.51	0.45
3:C:200:LEU:O	3:C:204:CYS:HB2	2.16	0.45
4:E:1211:LEU:HD11	4:E:1248:PHE:HD1	1.82	0.45
1:A:1590:ILE:CG1	1:A:1612:TRP:HZ3	2.28	0.44
1:A:1657:ILE:O	1:A:1660:ALA:HB3	2.18	0.44
4:E:1501:GLU:HA	4:E:1504:ILE:CG2	2.47	0.44
2:F:435:LEU:HG	3:G:271:LEU:HD21	1.98	0.44
2:F:613:TRP:CE3	2:F:695:LEU:HD13	2.52	0.44
1:A:1277:LEU:HD21	1:A:2033:ALA:HB2	1.99	0.44
1:A:1329:SER:HA	1:A:1377:LYS:NZ	2.32	0.44
1:A:2006:GLY:HA3	1:A:2013:PHE:HB2	1.98	0.44
1:A:2034:VAL:CG1	1:A:2057:LEU:HD21	2.43	0.44
2:B:247:ARG:NH2	2:B:282:LEU:HD23	2.32	0.44
2:B:452:GLU:O	2:B:456:LYS:HG3	2.17	0.44
2:B:489:LEU:O	2:B:493:GLN:HG3	2.17	0.44
3:C:110:ASN:OD1	3:C:168:GLN:HB2	2.18	0.44
4:E:1379:TYR:OH	4:E:1417:ASP:OD2	2.33	0.44
4:E:1667:GLY:H	2:F:347:ARG:HA	1.82	0.44
4:E:2006:GLY:HA3	4:E:2013:PHE:HB2	1.98	0.44
4:E:2036:SER:O	4:E:2039:THR:HG22	2.16	0.44
2:F:452:GLU:O	2:F:456:LYS:HG3	2.17	0.44
2:F:738:GLN:HE22	2:F:769:ARG:HG3	1.83	0.44
2:F:768:GLN:CD	2:F:799:GLU:HB2	2.42	0.44
1:A:1196:LEU:HD11	1:A:1210:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1929:THR:O	1:A:1933:GLN:CG	2.53	0.44
1:A:1943:MET:CB	1:A:1971:ILE:HG21	2.40	0.44
3:C:86:TYR:HH	3:C:100:CYS:N	2.16	0.44
4:E:1369:THR:HG23	4:E:1370:ILE:HG13	1.98	0.44
4:E:1411:TRP:O	4:E:1415:PHE:HB2	2.17	0.44
2:F:108:TYR:CZ	2:F:150:LEU:HB3	2.53	0.44
3:G:110:ASN:OD1	3:G:168:GLN:HB2	2.18	0.44
3:G:200:LEU:O	3:G:204:CYS:HB2	2.16	0.44
3:G:237:MET:HA	3:G:240:MET:CG	2.43	0.44
1:A:934:GLN:O	1:A:938:ALA:HB2	2.18	0.44
1:A:1051:GLU:HG3	4:E:1128:ARG:HG2	2.00	0.44
1:A:1246:VAL:HG13	1:A:1247:PRO:HD3	1.99	0.44
1:A:1260:VAL:HG22	1:A:1267:PHE:CE2	2.53	0.44
1:A:1404:ILE:HD13	1:A:1507:TYR:CE2	2.35	0.44
1:A:1905:ARG:HD3	1:A:1963:ILE:O	2.18	0.44
2:B:108:TYR:CZ	2:B:150:LEU:HB3	2.53	0.44
2:B:768:GLN:CD	2:B:799:GLU:HB2	2.42	0.44
3:C:11:GLU:HA	3:C:14:SER:OG	2.17	0.44
4:E:1066:GLN:HA	4:E:1110:PHE:CZ	2.52	0.44
4:E:1400:LEU:CD2	4:E:1507:TYR:HD2	2.26	0.44
1:A:1995:LYS:HG2	1:A:2000:MET:HE1	2.00	0.44
2:B:449:GLU:HG2	2:B:453:LYS:HZ3	1.83	0.44
2:B:715:ALA:O	2:B:719:THR:HG22	2.18	0.44
2:B:738:GLN:HE22	2:B:769:ARG:HG3	1.83	0.44
4:E:1306:PHE:HA	4:E:1320:PHE:HE2	1.81	0.44
2:F:715:ALA:O	2:F:719:THR:HG22	2.18	0.44
3:G:109:TYR:CE1	3:G:183:PHE:HB2	2.50	0.44
1:A:1242:ASP:OD1	1:A:1243:GLY:N	2.50	0.44
1:A:1260:VAL:HG22	1:A:1267:PHE:CZ	2.53	0.44
1:A:1359:LEU:HD23	1:A:1359:LEU:O	2.18	0.44
1:A:1848:ILE:HD11	1:A:1896:ILE:HD11	1.98	0.44
1:A:1930:LEU:HD12	1:A:1930:LEU:HA	1.75	0.44
2:B:246:LEU:HA	2:B:246:LEU:HD23	1.83	0.44
2:B:300:ASN:OD1	2:B:301:THR:N	2.50	0.44
2:B:405:LEU:HB3	3:C:277:LEU:HB2	1.99	0.44
2:B:586:LEU:HD13	2:B:609:MET:HG2	1.98	0.44
4:E:1246:VAL:HG13	4:E:1247:PRO:HD3	1.99	0.44
4:E:1260:VAL:HG22	4:E:1267:PHE:CE2	2.53	0.44
4:E:1260:VAL:HG22	4:E:1267:PHE:CZ	2.53	0.44
2:F:246:LEU:HD23	2:F:246:LEU:HA	1.83	0.44
1:A:1529:ARG:HD2	1:A:1533:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1861:ALA:CB	1:A:1979:MET:HB2	2.41	0.44
1:A:1947:SER:OG	1:A:1994:ILE:HG21	2.18	0.44
1:A:2075:MET:HA	1:A:2078:ILE:CG2	2.46	0.44
2:B:242:PHE:CD2	2:B:265:LEU:HD13	2.51	0.44
2:B:341:ARG:HH12	3:C:145:MET:CE	2.30	0.44
2:B:589:LYS:HE2	2:B:593:GLN:NE2	2.33	0.44
3:C:45:ILE:HG22	3:C:45:ILE:O	2.17	0.44
4:E:1154:TYR:CE2	4:E:1158:ARG:HD3	2.53	0.44
4:E:1242:ASP:OD1	4:E:1243:GLY:N	2.50	0.44
4:E:1733:ARG:O	4:E:1737:PHE:HB2	2.18	0.44
4:E:1905:ARG:HD3	4:E:1963:ILE:O	2.18	0.44
4:E:2072:ASN:HA	4:E:2075:MET:HG2	1.99	0.44
2:F:338:MET:HE3	2:F:342:ASP:OD1	2.18	0.44
2:F:418:LYS:O	2:F:421:LYS:HB2	2.17	0.44
2:F:711:LYS:HB3	2:F:714:GLU:OE1	2.17	0.44
3:G:75:THR:CG2	3:G:75:THR:O	2.66	0.44
3:G:79:LEU:O	3:G:83:ILE:HG13	2.18	0.44
3:G:218:GLN:O	3:G:222:LYS:N	2.43	0.44
1:A:1140:MET:HE2	4:E:1084:LEU:HD23	2.00	0.44
1:A:1594:VAL:O	1:A:1594:VAL:HG12	2.18	0.44
2:B:150:LEU:O	2:B:154:LYS:HG2	2.18	0.44
3:C:79:LEU:O	3:C:83:ILE:HG13	2.18	0.44
4:E:1142:SER:O	4:E:1146:ARG:HG3	2.18	0.44
3:G:214:GLY:HA3	3:G:229:ARG:HB3	2.00	0.44
1:A:1010:MET:SD	1:A:1064:ILE:HD11	2.58	0.44
1:A:1400:LEU:HD13	1:A:1506:TRP:CZ3	2.52	0.44
2:B:329:LEU:O	2:B:333:LEU:HG	2.18	0.44
4:E:970:PHE:CE2	4:E:974:ASN:ND2	2.86	0.44
4:E:1234:TRP:O	4:E:1238:LEU:HD13	2.17	0.44
4:E:1306:PHE:HD1	4:E:1320:PHE:HD2	1.64	0.44
4:E:1957:ASP:OD1	4:E:1993:ASP:O	2.36	0.44
4:E:2075:MET:HA	4:E:2078:ILE:CG2	2.46	0.44
2:F:175:CYS:O	2:F:179:ALA:CB	2.66	0.44
2:F:247:ARG:HB3	2:F:312:VAL:HG13	1.98	0.44
1:A:1055:LYS:NZ	4:E:1127:GLU:HB3	2.33	0.43
1:A:1147:ASN:ND2	4:E:1144:ASN:OD1	2.51	0.43
3:C:75:THR:CG2	3:C:75:THR:O	2.66	0.43
4:E:1010:MET:SD	4:E:1064:ILE:HD11	2.58	0.43
4:E:1359:LEU:O	4:E:1359:LEU:HD23	2.18	0.43
3:G:56:VAL:O	3:G:59:GLN:HB3	2.18	0.43
3:G:86:TYR:O	3:G:90:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:LEU:O	1:A:1019:LEU:HD23	2.19	0.43
1:A:1996:LEU:CA	1:A:2000:MET:CE	2.95	0.43
2:B:449:GLU:HG2	2:B:453:LYS:NZ	2.32	0.43
3:C:86:TYR:O	3:C:90:SER:HB2	2.18	0.43
4:E:1924:TYR:CD1	4:E:1931:ALA:HB1	2.53	0.43
4:E:1957:ASP:CB	4:E:1993:ASP:O	2.66	0.43
2:F:68:PRO:HB3	2:F:111:GLY:HA3	2.00	0.43
2:F:613:TRP:CH2	2:F:695:LEU:HD22	2.53	0.43
1:A:1594:VAL:HG22	1:A:1609:VAL:HG11	2.01	0.43
1:A:1663:TYR:OH	1:A:2043:ASP:OD2	2.36	0.43
2:B:408:MET:HG2	3:C:273:PRO:CG	2.49	0.43
2:B:581:GLU:N	3:C:175:GLN:HE22	2.16	0.43
3:C:56:VAL:O	3:C:59:GLN:HB3	2.18	0.43
2:F:489:LEU:O	2:F:493:GLN:HG3	2.17	0.43
2:F:589:LYS:HE2	2:F:593:GLN:NE2	2.33	0.43
1:A:1142:SER:O	1:A:1146:ARG:HG3	2.18	0.43
1:A:1154:TYR:CE2	1:A:1158:ARG:HD3	2.53	0.43
1:A:1482:HIS:O	1:A:1486:MET:HB2	2.18	0.43
1:A:1733:ARG:O	1:A:1737:PHE:HB2	2.18	0.43
2:B:613:TRP:CH2	2:B:695:LEU:HD22	2.53	0.43
3:C:29:THR:HA	3:C:34:LYS:HG3	2.00	0.43
3:C:77:GLN:HG3	3:C:78:PHE:CE2	2.54	0.43
4:E:2036:SER:HA	4:E:2039:THR:HG22	2.00	0.43
2:F:329:LEU:O	2:F:333:LEU:HG	2.18	0.43
2:F:341:ARG:HH12	3:G:145:MET:HG3	1.82	0.43
2:F:438:ALA:O	2:F:442:MET:HG2	2.19	0.43
1:A:1097:HIS:CE1	1:A:1100:LEU:HB2	2.53	0.43
2:B:68:PRO:HB3	2:B:111:GLY:HA3	2.00	0.43
3:C:182:THR:HG22	3:C:183:PHE:CD1	2.54	0.43
4:E:443:UNK:O	4:E:444:UNK:C	2.62	0.43
4:E:1277:LEU:HD21	4:E:2033:ALA:HB2	1.99	0.43
4:E:1482:HIS:O	4:E:1486:MET:HB2	2.18	0.43
4:E:1663:TYR:OH	4:E:2043:ASP:OD2	2.36	0.43
4:E:1850:LYS:HB3	4:E:1850:LYS:HE3	1.74	0.43
4:E:1868:PHE:HD2	4:E:1949:LEU:HG	1.83	0.43
4:E:1944:ALA:N	4:E:2016:PHE:CE1	2.87	0.43
1:A:1597:HIS:ND1	1:A:1602:ASP:OD2	2.45	0.43
2:B:769:ARG:NH1	2:B:772:LEU:HD13	2.34	0.43
4:E:1097:HIS:CE1	4:E:1100:LEU:HB2	2.53	0.43
4:E:1115:LYS:NZ	4:E:1116:GLN:HE21	2.17	0.43
4:E:1908:LEU:CD1	4:E:1919:TYR:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:300:ASN:OD1	2:F:301:THR:N	2.50	0.43
1:A:1137:SER:OG	4:E:1093:GLY:O	2.31	0.43
1:A:1190:THR:HG23	1:A:1194:PHE:CE2	2.53	0.43
1:A:1656:GLN:HB3	1:A:2040:LEU:CD1	2.49	0.43
1:A:2036:SER:HA	1:A:2039:THR:HG22	2.00	0.43
2:B:175:CYS:O	2:B:179:ALA:CB	2.65	0.43
4:E:1594:VAL:HG22	4:E:1609:VAL:HG11	2.01	0.43
4:E:1658:VAL:HG23	4:E:1659:GLN:OE1	2.19	0.43
4:E:1899:ILE:CD1	4:E:1972:ILE:HG21	2.49	0.43
4:E:2061:PHE:O	4:E:2062:SER:OG	2.32	0.43
3:G:182:THR:HG22	3:G:183:PHE:CD1	2.53	0.43
1:A:1586:VAL:HG13	1:A:1613:ALA:CB	2.45	0.43
1:A:1656:GLN:HB3	1:A:2040:LEU:HD13	2.01	0.43
1:A:1699:GLU:CG	1:A:1700:GLU:H	2.10	0.43
4:E:1122:ALA:O	4:E:1125:LEU:HG	2.19	0.43
4:E:1266:LEU:CD2	4:E:1339:MET:HE3	2.45	0.43
3:G:61:PHE:O	3:G:65:ARG:N	2.52	0.43
1:A:1122:ALA:HB3	1:A:1125:LEU:CD2	2.40	0.43
1:A:1401:ARG:NH2	1:A:1516:GLU:HB2	2.33	0.43
2:B:338:MET:HE3	2:B:342:ASP:OD1	2.18	0.43
2:B:438:ALA:O	2:B:442:MET:HG2	2.19	0.43
2:B:501:LEU:O	2:B:505:GLN:HG3	2.19	0.43
4:E:1080:LEU:O	4:E:1083:TYR:N	2.52	0.43
4:E:1369:THR:HG21	2:F:755:GLU:CD	2.44	0.43
4:E:1656:GLN:HB3	4:E:2040:LEU:HD13	2.01	0.43
4:E:2026:ALA:O	4:E:2029:PRO:HD2	2.19	0.43
2:F:150:LEU:O	2:F:154:LYS:HG2	2.18	0.43
1:A:979:HIS:O	1:A:983:ARG:HG2	2.18	0.43
1:A:1250:ARG:CD	2:B:785:LYS:HB2	2.48	0.43
1:A:1899:ILE:CD1	1:A:1972:ILE:HG21	2.49	0.43
2:B:467:GLU:OE2	3:C:216:PRO:HG2	2.19	0.43
2:B:750:ARG:HB2	2:B:773:ILE:HG21	2.01	0.43
4:E:1586:VAL:HG23	4:E:1587:PRO:N	2.34	0.43
3:G:29:THR:HA	3:G:34:LYS:HG3	2.00	0.43
3:G:77:GLN:HG3	3:G:78:PHE:CE2	2.54	0.43
1:A:950:MET:HG2	1:A:954:LYS:HE3	2.01	0.42
1:A:1115:LYS:NZ	1:A:1116:GLN:HE21	2.17	0.42
1:A:1577:ARG:NH2	1:A:1596:TRP:O	2.52	0.42
1:A:1658:VAL:HG23	1:A:1659:GLN:OE1	2.19	0.42
2:B:699:TRP:CE3	2:B:721:GLU:HB2	2.54	0.42
4:E:934:GLN:O	4:E:938:ALA:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1577:ARG:NH2	4:E:1596:TRP:O	2.52	0.42
1:A:1055:LYS:CB	4:E:1128:ARG:HA	2.44	0.42
1:A:1659:GLN:NE2	1:A:2041:MET:HG2	2.34	0.42
2:B:344:VAL:O	2:B:347:ARG:HG3	2.18	0.42
3:C:221:ARG:CZ	3:C:258:LYS:HB3	2.50	0.42
4:E:1010:MET:CE	4:E:1061:CYS:HA	2.49	0.42
4:E:1190:THR:HG23	4:E:1194:PHE:CE2	2.53	0.42
2:F:223:GLN:O	2:F:227:VAL:HG23	2.19	0.42
1:A:1501:GLU:HA	1:A:1504:ILE:CG2	2.47	0.42
1:A:1946:TYR:CB	1:A:1973:HIS:CE1	3.00	0.42
2:B:26:ILE:HB	2:B:27:PRO:HD3	2.02	0.42
2:B:223:GLN:O	2:B:227:VAL:HG23	2.19	0.42
2:B:711:LYS:HE2	2:B:714:GLU:CD	2.45	0.42
3:C:12:TRP:CG	3:C:37:LEU:HD11	2.54	0.42
3:C:178:PHE:O	3:C:182:THR:OG1	2.34	0.42
4:E:1019:LEU:HD23	4:E:1019:LEU:O	2.19	0.42
4:E:1259:THR:CG2	4:E:1295:HIS:NE2	2.83	0.42
4:E:1659:GLN:NE2	4:E:2041:MET:HG2	2.34	0.42
4:E:1780:PRO:HD3	4:E:1885:ARG:HH22	1.84	0.42
2:F:43:MET:HG3	2:F:47:LEU:CD1	2.50	0.42
2:F:338:MET:HE3	2:F:342:ASP:CG	2.44	0.42
2:F:711:LYS:HE2	2:F:714:GLU:CD	2.45	0.42
1:A:1586:VAL:HG23	1:A:1587:PRO:N	2.35	0.42
1:A:1957:ASP:OD1	1:A:1993:ASP:N	2.52	0.42
2:B:242:PHE:HA	2:B:261:ILE:HD11	2.01	0.42
2:B:700:LEU:HD11	2:B:732:VAL:HG22	2.01	0.42
4:E:950:MET:HG2	4:E:954:LYS:HE3	2.01	0.42
4:E:1081:GLN:HE21	4:E:1143:LEU:N	2.18	0.42
4:E:1657:ILE:O	4:E:1660:ALA:HB3	2.18	0.42
4:E:1882:PHE:HE2	4:E:1899:ILE:HG12	1.78	0.42
2:F:769:ARG:NH1	2:F:772:LEU:HD13	2.34	0.42
3:G:64:TYR:OH	3:G:112:GLU:HG2	2.19	0.42
3:G:79:LEU:O	3:G:82:LEU:HG	2.20	0.42
3:G:102:GLU:HB3	3:G:172:LEU:HB3	2.00	0.42
3:G:244:ILE:HG22	3:G:248:PHE:CE2	2.55	0.42
1:A:1341:ARG:HG3	1:A:1385:TYR:HA	2.01	0.42
1:A:1850:LYS:HE3	1:A:1850:LYS:HB3	1.74	0.42
2:B:187:LEU:HB3	2:B:251:THR:HG21	2.00	0.42
3:C:60:LEU:HD23	3:C:75:THR:HG21	2.02	0.42
3:C:61:PHE:O	3:C:65:ARG:N	2.52	0.42
3:C:80:PRO:HA	3:C:83:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:GLU:HB3	3:C:172:LEU:HB3	2.01	0.42
3:C:178:PHE:HE1	3:C:181:LEU:CD1	2.29	0.42
3:C:196:PRO:O	3:C:199:SER:OG	2.34	0.42
4:E:328:UNK:O	4:E:329:UNK:C	2.67	0.42
4:E:1375:ARG:O	4:E:1379:TYR:HD2	2.03	0.42
2:F:699:TRP:CE3	2:F:721:GLU:HB2	2.54	0.42
1:A:228:UNK:O	1:A:232:UNK:CB	2.68	0.42
1:A:1010:MET:CE	1:A:1061:CYS:HA	2.49	0.42
1:A:1920:PHE:CE2	1:A:1932:PHE:HD1	2.36	0.42
2:B:404:ALA:HB2	2:B:419:VAL:HG12	2.02	0.42
2:B:465:THR:HG23	2:B:467:GLU:N	2.32	0.42
3:C:40:SER:O	3:C:44:VAL:HB	2.20	0.42
4:E:27:UNK:HA	2:F:821:PHE:HD2	1.83	0.42
4:E:1590:ILE:O	4:E:1591:LYS:C	2.62	0.42
4:E:1656:GLN:HB3	4:E:2040:LEU:CD1	2.49	0.42
4:E:1787:ILE:HD12	4:E:1807:PHE:CE1	2.55	0.42
4:E:1865:ILE:HG23	4:E:1949:LEU:CD2	2.49	0.42
3:G:12:TRP:CG	3:G:37:LEU:HD11	2.54	0.42
1:A:1787:ILE:HD12	1:A:1807:PHE:CE1	2.55	0.42
1:A:2026:ALA:O	1:A:2029:PRO:HD2	2.19	0.42
2:B:757:LEU:HD23	2:B:757:LEU:HA	1.90	0.42
3:C:192:LEU:HD12	3:C:246:PHE:CG	2.54	0.42
4:E:1149:TYR:O	4:E:1153:VAL:HG23	2.20	0.42
2:F:26:ILE:HB	2:F:27:PRO:HD3	2.02	0.42
2:F:187:LEU:HB3	2:F:251:THR:HG21	2.00	0.42
2:F:332:LEU:HA	2:F:335:SER:HB2	2.02	0.42
2:F:700:LEU:HD11	2:F:732:VAL:HG22	2.01	0.42
1:A:398:UNK:O	1:A:402:UNK:CB	2.68	0.42
1:A:1232:ALA:HB2	4:E:1094:LEU:CD2	2.50	0.42
1:A:1259:THR:CG2	1:A:1295:HIS:NE2	2.83	0.42
1:A:1780:PRO:HD3	1:A:1885:ARG:HH22	1.84	0.42
1:A:1847:ALA:HA	1:A:1898:CYS:H	1.85	0.42
3:C:237:MET:HE1	3:C:270:GLU:OE1	2.19	0.42
4:E:399:UNK:O	4:E:403:UNK:CB	2.68	0.42
4:E:1956:LYS:CG	4:E:1982:SER:OG	2.66	0.42
2:F:404:ALA:HB2	2:F:419:VAL:HG12	2.02	0.42
3:G:63:PHE:CD1	3:G:71:LEU:HD13	2.55	0.42
1:A:1080:LEU:O	1:A:1083:TYR:N	2.52	0.42
1:A:1081:GLN:HE21	1:A:1143:LEU:N	2.18	0.42
1:A:1098:THR:CA	4:E:1131:CYS:HB2	2.50	0.42
1:A:1128:ARG:HH11	1:A:1130:ALA:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1375:ARG:O	1:A:1379:TYR:HD2	2.03	0.42
4:E:1066:GLN:O	4:E:1070:LYS:HG2	2.19	0.42
4:E:1594:VAL:O	4:E:1594:VAL:HG12	2.18	0.42
2:F:371:ILE:CG2	2:F:375:ARG:HH21	2.33	0.42
2:F:386:LEU:HD23	2:F:386:LEU:HA	1.85	0.42
1:A:413:UNK:C	1:A:415:UNK:N	2.81	0.42
1:A:951:MET:HE1	1:A:954:LYS:HZ1	1.85	0.42
1:A:976:ASN:CG	1:A:1017:LEU:HD11	2.44	0.42
1:A:984:ARG:O	1:A:987:ASP:HB3	2.20	0.42
1:A:1149:TYR:O	1:A:1153:VAL:HG23	2.20	0.42
1:A:1266:LEU:CD2	1:A:1339:MET:HE3	2.45	0.42
2:B:371:ILE:CG2	2:B:375:ARG:HH21	2.33	0.42
4:E:1388:CYS:SG	4:E:1389:PRO:HD2	2.60	0.42
4:E:1903:THR:HB	4:E:1965:LEU:O	2.20	0.42
2:F:27:PRO:O	2:F:31:LYS:HB2	2.20	0.42
2:F:242:PHE:HA	2:F:261:ILE:HD11	2.01	0.42
2:F:692:TRP:HE3	2:F:725:LEU:HD22	1.85	0.42
1:A:1046:THR:HG22	1:A:1048:GLU:H	1.86	0.41
1:A:1128:ARG:HB3	4:E:1051:GLU:CG	2.50	0.41
1:A:1379:TYR:OH	1:A:1417:ASP:OD2	2.33	0.41
2:B:386:LEU:HA	2:B:386:LEU:HD23	1.85	0.41
3:C:64:TYR:OH	3:C:112:GLU:HG2	2.19	0.41
3:C:132:LYS:HG2	3:C:133:PRO:O	2.20	0.41
4:E:1950:LEU:CB	4:E:1994:ILE:CD1	2.83	0.41
2:F:501:LEU:O	2:F:505:GLN:HG3	2.19	0.41
2:F:787:LEU:HD23	2:F:787:LEU:HA	1.81	0.41
3:G:79:LEU:HD12	3:G:80:PRO:CD	2.49	0.41
1:A:950:MET:O	1:A:954:LYS:HG3	2.20	0.41
1:A:972:LEU:HD22	1:A:1010:MET:SD	2.60	0.41
1:A:1277:LEU:HD23	1:A:1618:PRO:CG	2.37	0.41
1:A:1940:ILE:O	1:A:1944:ALA:HB2	2.20	0.41
2:B:43:MET:HG3	2:B:47:LEU:CD1	2.50	0.41
3:C:278:VAL:O	3:C:282:ILE:HG12	2.20	0.41
4:E:1696:TYR:CG	4:E:1701:GLY:CA	2.93	0.41
2:F:286:PRO:HG2	2:F:289:SER:HB3	2.02	0.41
1:A:1084:LEU:CD2	4:E:1140:MET:HE2	2.50	0.41
1:A:1277:LEU:HD11	1:A:2030:TYR:CD1	2.55	0.41
1:A:1590:ILE:HB	1:A:1612:TRP:HE3	1.83	0.41
1:A:1748:ILE:HG12	1:A:1758:LYS:CB	2.48	0.41
1:A:1860:LEU:HB3	1:A:1979:MET:SD	2.60	0.41
4:E:1585:ASP:O	4:E:1589:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1847:ALA:HA	4:E:1898:CYS:H	1.85	0.41
4:E:2024:TYR:HH	4:E:2062:SER:HG	1.67	0.41
2:F:695:LEU:HD23	2:F:725:LEU:HD11	2.02	0.41
3:G:40:SER:O	3:G:44:VAL:HB	2.20	0.41
1:A:1122:ALA:O	1:A:1125:LEU:HG	2.19	0.41
1:A:2043:ASP:O	1:A:2044:THR:OG1	2.35	0.41
2:B:338:MET:HE3	2:B:342:ASP:CG	2.44	0.41
2:B:346:SER:HB3	2:B:355:ARG:NH1	2.18	0.41
2:B:487:ALA:HB3	2:B:493:GLN:HG2	2.01	0.41
3:C:79:LEU:O	3:C:82:LEU:HG	2.20	0.41
3:C:237:MET:HA	3:C:240:MET:CG	2.43	0.41
4:E:950:MET:O	4:E:954:LYS:HG3	2.20	0.41
4:E:952:ALA:HB2	4:E:996:LYS:HE3	2.02	0.41
4:E:1085:ASN:HA	4:E:1090:TRP:HZ2	1.85	0.41
4:E:1343:VAL:HG11	4:E:1393:PRO:HG3	2.03	0.41
4:E:1529:ARG:CD	4:E:1533:ILE:HD11	2.51	0.41
4:E:1857:GLN:NE2	4:E:1977:GLY:O	2.54	0.41
2:F:93:SER:O	2:F:97:GLN:HG3	2.21	0.41
3:G:237:MET:HE1	3:G:270:GLU:OE1	2.19	0.41
3:G:278:VAL:O	3:G:282:ILE:HG12	2.20	0.41
1:A:32:UNK:HA	1:A:48:UNK:CB	2.50	0.41
1:A:1066:GLN:O	1:A:1070:LYS:HG2	2.19	0.41
1:A:1388:CYS:SG	1:A:1389:PRO:HD2	2.60	0.41
1:A:1590:ILE:CG1	1:A:1594:VAL:CG2	2.97	0.41
2:B:695:LEU:HD23	2:B:725:LEU:HD11	2.02	0.41
3:C:79:LEU:HD12	3:C:80:PRO:CD	2.50	0.41
2:F:128:LEU:HA	2:F:129:PRO:HD3	1.93	0.41
2:F:259:MET:HB2	2:F:338:MET:HG2	2.02	0.41
2:F:390:MET:SD	2:F:399:LEU:HG	2.61	0.41
3:G:192:LEU:HD12	3:G:246:PHE:CG	2.54	0.41
3:G:200:LEU:HD13	3:G:247:ALA:HA	2.01	0.41
1:A:1085:ASN:HA	1:A:1090:TRP:HZ2	1.86	0.41
2:B:27:PRO:O	2:B:31:LYS:HB2	2.20	0.41
2:B:332:LEU:HA	2:B:335:SER:HB2	2.02	0.41
3:C:57:CYS:O	3:C:60:LEU:HB2	2.21	0.41
3:C:63:PHE:CD1	3:C:71:LEU:HD13	2.55	0.41
4:E:1090:TRP:C	4:E:1093:GLY:H	2.27	0.41
4:E:1277:LEU:HD11	4:E:2030:TYR:CD1	2.55	0.41
4:E:1305:ARG:HD3	4:E:1305:ARG:HA	1.81	0.41
3:G:221:ARG:CZ	3:G:258:LYS:HB3	2.50	0.41
1:A:933:MET:HE2	1:A:981:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1529:ARG:CD	1:A:1533:ILE:HD11	2.51	0.41
2:B:259:MET:HB2	2:B:338:MET:HG2	2.02	0.41
2:B:515:HIS:CE1	2:B:516:GLN:HG3	2.56	0.41
3:C:79:LEU:HD12	3:C:80:PRO:N	2.36	0.41
3:C:244:ILE:HG22	3:C:248:PHE:CE2	2.55	0.41
4:E:1953:LEU:HD23	4:E:1953:LEU:N	2.32	0.41
2:F:803:GLY:O	2:F:807:VAL:HG23	2.20	0.41
1:A:1032:TYR:HE2	1:A:1043:VAL:HG21	1.86	0.41
1:A:1343:VAL:HG11	1:A:1393:PRO:HG3	2.03	0.41
1:A:1617:PRO:HD3	1:A:1645:PHE:CE2	2.54	0.41
1:A:1908:LEU:CD1	1:A:1919:TYR:HB2	2.49	0.41
2:B:695:LEU:HG	2:B:699:TRP:CD1	2.56	0.41
3:C:200:LEU:HD13	3:C:247:ALA:HA	2.01	0.41
4:E:933:MET:HE1	4:E:981:ARG:HB2	2.03	0.41
4:E:1032:TYR:HE2	4:E:1043:VAL:HG21	1.86	0.41
4:E:1341:ARG:HG3	4:E:1385:TYR:HA	2.01	0.41
4:E:1367:ASN:ND2	4:E:1369:THR:CG2	2.83	0.41
4:E:1605:GLU:C	4:E:1606:LEU:HG	2.46	0.41
4:E:1720:THR:HG23	4:E:1731:TYR:OH	2.20	0.41
4:E:1740:LYS:O	4:E:1744:VAL:HG23	2.21	0.41
4:E:1996:LEU:HA	4:E:2000:MET:CE	2.50	0.41
2:F:139:ARG:HD3	2:F:186:TYR:OH	2.21	0.41
2:F:185:LEU:O	2:F:189:GLU:CB	2.63	0.41
2:F:408:MET:HE2	2:F:440:LEU:CD1	2.51	0.41
2:F:750:ARG:HB2	2:F:773:ILE:HG21	2.01	0.41
2:F:787:LEU:HD13	2:F:804:LEU:CA	2.51	0.41
1:A:976:ASN:ND2	1:A:1013:ILE:CG2	2.83	0.41
1:A:1026:HIS:HE1	4:E:2015:TRP:CE3	2.39	0.41
1:A:1185:HIS:CD2	1:A:1186:PRO:HD2	2.46	0.41
1:A:1586:VAL:N	1:A:1587:PRO:HD2	2.36	0.41
1:A:1740:LYS:O	1:A:1744:VAL:HG23	2.21	0.41
1:A:1785:LEU:HD12	1:A:1786:ASP:HB2	2.03	0.41
1:A:1901:ASP:HB3	1:A:1966:ASP:HB2	2.03	0.41
1:A:1951:PHE:CE1	1:A:2077:VAL:HG11	2.55	0.41
2:B:544:LEU:HB3	3:C:229:ARG:HH21	1.85	0.41
2:B:787:LEU:HD13	2:B:804:LEU:CA	2.51	0.41
3:C:159:LYS:HE2	3:C:159:LYS:HB3	1.95	0.41
4:E:972:LEU:HD22	4:E:1010:MET:SD	2.60	0.41
4:E:1641:VAL:O	4:E:1644:SER:OG	2.30	0.41
2:F:134:PRO:HA	2:F:135:PRO:HD3	1.96	0.41
2:F:394:PHE:CD2	2:F:395:GLU:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:531:ILE:HG21	2:F:562:GLN:HG3	2.03	0.41
2:F:576:LEU:CD1	2:F:586:LEU:HD23	2.51	0.41
3:G:211:CYS:C	3:G:266:ARG:HH21	2.24	0.41
1:A:1499:GLU:OE1	1:A:1502:ARG:HD3	2.21	0.41
1:A:1943:MET:HB3	1:A:1971:ILE:CG2	2.43	0.41
2:B:139:ARG:HD3	2:B:186:TYR:OH	2.21	0.41
2:B:576:LEU:CD1	2:B:586:LEU:HD23	2.51	0.41
3:C:29:THR:HA	3:C:34:LYS:HE3	2.03	0.41
4:E:229:UNK:O	4:E:233:UNK:CB	2.68	0.41
4:E:1401:ARG:NH2	4:E:1516:GLU:HB2	2.33	0.41
4:E:1632:PRO:HG2	2:F:345:LEU:HD13	2.03	0.41
4:E:1632:PRO:HG3	2:F:345:LEU:HD13	2.02	0.41
4:E:1896:ILE:HD12	4:E:1896:ILE:C	2.46	0.41
4:E:1950:LEU:C	4:E:1994:ILE:HD11	2.45	0.41
4:E:1951:PHE:CE1	4:E:2077:VAL:HG11	2.55	0.41
2:F:350:GLU:HG2	2:F:350:GLU:O	2.21	0.41
2:F:569:LEU:CD2	2:F:597:ARG:HE	2.34	0.41
1:A:952:ALA:HB2	1:A:996:LYS:HE3	2.02	0.40
1:A:1857:GLN:NE2	1:A:1977:GLY:O	2.54	0.40
3:C:109:TYR:CE1	3:C:183:PHE:HB2	2.50	0.40
4:E:984:ARG:O	4:E:987:ASP:HB3	2.20	0.40
4:E:1122:ALA:HB3	4:E:1125:LEU:CD2	2.40	0.40
4:E:1191:GLN:HG2	4:E:1195:LYS:CE	2.44	0.40
4:E:1367:ASN:CG	4:E:1369:THR:HG22	2.45	0.40
4:E:1624:PHE:O	4:E:1663:TYR:HB2	2.21	0.40
4:E:1642:LEU:O	4:E:1672:TYR:OH	2.39	0.40
2:F:172:VAL:HA	2:F:176:TYR:CD2	2.55	0.40
3:G:80:PRO:HA	3:G:83:ILE:HD12	2.02	0.40
1:A:932:MET:HG3	1:A:934:GLN:H	1.86	0.40
1:A:1148:ARG:HD2	4:E:1087:HIS:NE2	2.35	0.40
1:A:1610:LEU:HB3	2:B:400:TRP:HH2	1.86	0.40
1:A:1896:ILE:HD12	1:A:1896:ILE:C	2.46	0.40
2:B:93:SER:O	2:B:97:GLN:HG3	2.21	0.40
2:B:390:MET:SD	2:B:399:LEU:HG	2.61	0.40
2:B:403:PHE:CE2	2:B:407:LEU:HD11	2.57	0.40
2:B:514:ASP:HA	3:C:229:ARG:HH12	1.86	0.40
4:E:32:UNK:HA	4:E:48:UNK:CB	2.51	0.40
4:E:2008:MET:CE	4:E:2083:LEU:HD21	2.51	0.40
4:E:2011:THR:OG1	4:E:2012:PRO:CD	2.69	0.40
2:F:515:HIS:CE1	2:F:516:GLN:HG3	2.56	0.40
2:F:748:GLU:HA	2:F:751:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:57:CYS:O	3:G:60:LEU:HB2	2.21	0.40
3:G:79:LEU:HD12	3:G:80:PRO:N	2.36	0.40
3:G:132:LYS:HG2	3:G:133:PRO:O	2.20	0.40
1:A:1055:LYS:CB	4:E:1129:PRO:HD2	2.52	0.40
1:A:1134:LYS:HB2	1:A:1136:TYR:CD2	2.56	0.40
1:A:1563:LYS:O	1:A:1565:THR:N	2.53	0.40
1:A:1570:ASN:O	1:A:1574:ARG:CB	2.69	0.40
1:A:1616:ASP:OD1	1:A:1616:ASP:N	2.54	0.40
1:A:1903:THR:HB	1:A:1965:LEU:O	2.20	0.40
1:A:1924:TYR:CB	1:A:1931:ALA:HB1	2.45	0.40
4:E:400:UNK:O	4:E:404:UNK:CB	2.70	0.40
4:E:1237:LEU:CD1	4:E:1238:LEU:HD12	2.52	0.40
4:E:1570:ASN:O	4:E:1574:ARG:CB	2.69	0.40
2:F:487:ALA:HB3	2:F:493:GLN:HG2	2.01	0.40
3:G:60:LEU:HD23	3:G:75:THR:HG21	2.01	0.40
1:A:1191:GLN:HG2	1:A:1195:LYS:CE	2.44	0.40
1:A:1201:ILE:O	1:A:1203:SER:N	2.55	0.40
1:A:1636:GLN:HG2	2:B:394:PHE:HD1	1.86	0.40
2:B:692:TRP:HE3	2:B:725:LEU:HD22	1.85	0.40
2:B:803:GLY:O	2:B:807:VAL:HG23	2.20	0.40
4:E:971:LEU:HD23	4:E:971:LEU:HA	1.91	0.40
4:E:1625:SER:HB3	4:E:2040:LEU:HD21	2.04	0.40
1:A:399:UNK:O	1:A:403:UNK:CB	2.70	0.40
1:A:1011:LEU:CD2	1:A:1103:ALA:HB2	2.52	0.40
1:A:1938:ASN:HB3	1:A:1970:HIS:HD2	1.84	0.40
1:A:1979:MET:HE3	1:A:1980:PHE:CE2	2.56	0.40
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.86	0.40
2:B:396:GLU:O	2:B:400:TRP:HD1	2.04	0.40
2:B:495:VAL:CG1	2:B:499:LYS:HE3	2.52	0.40
2:B:589:LYS:HE2	2:B:593:GLN:HE22	1.86	0.40
3:C:41:LEU:HG	3:C:45:ILE:HB	2.04	0.40
3:C:264:ILE:HG23	3:C:276:LEU:CD1	2.52	0.40
4:E:230:UNK:O	4:E:234:UNK:CB	2.70	0.40
4:E:933:MET:CE	4:E:981:ARG:HB2	2.51	0.40
4:E:1132:VAL:O	4:E:1134:LYS:HG2	2.22	0.40
4:E:1486:MET:HE1	4:E:1489:ARG:HH21	1.87	0.40
4:E:1499:GLU:OE1	4:E:1502:ARG:HD3	2.21	0.40
2:F:368:LEU:HD23	2:F:368:LEU:HA	1.86	0.40
2:F:396:GLU:O	2:F:400:TRP:HD1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1019/1647 (62%)	949 (93%)	70 (7%)	0	100	100
2	B	714/863 (83%)	691 (97%)	23 (3%)	0	100	100
2	F	714/863 (83%)	692 (97%)	22 (3%)	0	100	100
3	C	254/292 (87%)	242 (95%)	12 (5%)	0	100	100
3	G	254/292 (87%)	242 (95%)	12 (5%)	0	100	100
4	E	1019/1648 (62%)	951 (93%)	68 (7%)	0	100	100
All	All	3974/5605 (71%)	3767 (95%)	207 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	901/1022 (88%)	900 (100%)	1 (0%)	88	87
2	B	616/727 (85%)	616 (100%)	0	100	100
2	F	616/727 (85%)	616 (100%)	0	100	100
3	C	236/260 (91%)	236 (100%)	0	100	100
3	G	236/260 (91%)	235 (100%)	1 (0%)	84	81
4	E	901/1022 (88%)	899 (100%)	2 (0%)	87	85
All	All	3506/4018 (87%)	3502 (100%)	4 (0%)	87	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1994	ILE
4	E	1929	THR
4	E	1955	ILE
3	G	182	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	977	HIS
1	A	979	HIS
1	A	1015	GLN
1	A	1026	HIS
1	A	1081	GLN
1	A	1116	GLN
1	A	1213	HIS
1	A	1527	ASN
1	A	1557	GLN
1	A	1631	HIS
1	A	1659	GLN
1	A	1681	GLN
1	A	1685	HIS
1	A	1779	ASN
1	A	1796	GLN
1	A	1973	HIS
1	A	2072	ASN
2	B	22	GLN
2	B	60	HIS
2	B	107	ASN
2	B	234	ASN
2	B	340	ASN
2	B	351	HIS
2	B	446	HIS
2	B	508	HIS
2	B	515	HIS
2	B	540	GLN
2	B	562	GLN
2	B	570	ASN
2	B	701	HIS
2	B	738	GLN
2	B	809	GLN
3	C	73	GLN

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Mol	Chain	Res	Type
4	E	1015	GLN
4	E	1026	HIS
4	E	1081	GLN
4	E	1096	GLN
4	E	1116	GLN
4	E	1213	HIS
4	E	1527	ASN
4	E	1557	GLN
4	E	1681	GLN
4	E	1685	HIS
4	E	1779	ASN
4	E	1796	GLN
4	E	1857	GLN
4	E	1870	ASN
4	E	1907	GLN
4	E	1959	HIS
4	E	1973	HIS
4	E	2072	ASN
2	F	22	GLN
2	F	60	HIS
2	F	107	ASN
2	F	351	HIS
2	F	402	GLN
2	F	446	HIS
2	F	508	HIS
2	F	515	HIS
2	F	540	GLN
2	F	562	GLN
2	F	570	ASN
2	F	701	HIS
2	F	738	GLN
3	G	137	HIS
3	G	175	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	E4S	A	2201	-	45,46,46	4.46	27 (60%)	64,67,67	3.00	23 (35%)
5	E4S	E	2201	-	45,46,46	4.67	28 (62%)	64,67,67	3.06	25 (39%)

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
5	E4S	A	2201	-	-	10/25/33/33	0/6/6/6
5	E4S	E	2201	-	-	9/25/33/33	0/6/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2201	E4S	C24-C29	11.36	1.52	1.39
5	A	2201	E4S	C24-C29	11.15	1.52	1.39
5	E	2201	E4S	C04-C03	-8.83	1.24	1.39
5	A	2201	E4S	C27-C28	8.38	1.53	1.38
5	E	2201	E4S	C27-C28	8.34	1.53	1.38
5	E	2201	E4S	C06-N01	8.32	1.51	1.34
5	A	2201	E4S	C26-C25	8.03	1.52	1.38
5	E	2201	E4S	C16-C15	8.01	1.51	1.38
5	E	2201	E4S	C26-C25	7.97	1.52	1.38
5	A	2201	E4S	C16-C15	7.60	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2201	E4S	C19-C14	7.45	1.53	1.39
5	E	2201	E4S	C09-N04	-7.15	1.29	1.40
5	A	2201	E4S	C09-N04	-7.12	1.29	1.40
5	A	2201	E4S	C18-C17	6.99	1.52	1.39
5	A	2201	E4S	C19-C14	6.90	1.52	1.39
5	A	2201	E4S	C04-C03	-6.88	1.28	1.39
5	E	2201	E4S	C13-N03	6.71	1.46	1.34
5	A	2201	E4S	C13-N03	6.70	1.45	1.34
5	E	2201	E4S	C18-C17	6.64	1.51	1.39
5	A	2201	E4S	C06-N01	6.58	1.47	1.34
5	A	2201	E4S	C04-C05	6.08	1.50	1.39
5	E	2201	E4S	C04-C05	6.04	1.50	1.39
5	E	2201	E4S	C13-N04	-5.68	1.29	1.39
5	E	2201	E4S	C19-C18	-5.66	1.29	1.38
5	E	2201	E4S	C25-C24	-5.52	1.30	1.39
5	A	2201	E4S	C25-C24	-5.31	1.31	1.39
5	A	2201	E4S	C19-C18	-5.30	1.30	1.38
5	E	2201	E4S	S01-N06	5.16	1.71	1.63
5	A	2201	E4S	C13-N04	-5.13	1.30	1.39
5	A	2201	E4S	C10-N02	4.99	1.49	1.39
5	A	2201	E4S	S01-N06	4.70	1.71	1.63
5	E	2201	E4S	C16-C17	-4.60	1.30	1.39
5	E	2201	E4S	C10-N02	4.57	1.49	1.39
5	A	2201	E4S	C16-C17	-4.49	1.30	1.39
5	A	2201	E4S	C06-C05	-4.24	1.31	1.39
5	A	2201	E4S	C15-C14	-4.05	1.31	1.39
5	E	2201	E4S	C06-C05	-3.96	1.32	1.39
5	E	2201	E4S	C15-C14	-3.73	1.32	1.39
5	E	2201	E4S	C08-C09	-3.09	1.34	1.39
5	E	2201	E4S	C27-C26	-2.97	1.31	1.38
5	A	2201	E4S	C27-C26	-2.96	1.31	1.38
5	E	2201	E4S	C28-C29	-2.92	1.32	1.37
5	A	2201	E4S	C28-C29	-2.90	1.32	1.37
5	E	2201	E4S	O03-S01	2.80	1.46	1.43
5	A	2201	E4S	C11-C10	-2.78	1.35	1.40
5	E	2201	E4S	O04-S01	2.72	1.46	1.43
5	A	2201	E4S	O01-C02	2.71	1.39	1.35
5	A	2201	E4S	O04-S01	2.68	1.46	1.43
5	E	2201	E4S	O01-C02	2.61	1.39	1.35
5	A	2201	E4S	O03-S01	2.46	1.46	1.43
5	A	2201	E4S	C02-N01	-2.40	1.27	1.32
5	A	2201	E4S	C03-S01	2.36	1.80	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2201	E4S	C03-S01	2.13	1.80	1.77
5	E	2201	E4S	C02-N01	-2.11	1.28	1.32
5	E	2201	E4S	C11-C10	-2.06	1.36	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2201	E4S	O04-S01-O03	-14.56	101.83	119.52
5	A	2201	E4S	O04-S01-O03	-13.93	102.60	119.52
5	E	2201	E4S	N03-C13-N04	8.44	132.16	122.10
5	A	2201	E4S	N03-C13-N04	7.87	131.48	122.10
5	A	2201	E4S	C10-C09-N04	-6.51	100.42	105.25
5	A	2201	E4S	N04-C13-N02	-6.23	107.63	112.86
5	E	2201	E4S	N04-C13-N02	-6.01	107.82	112.86
5	E	2201	E4S	N03-C13-N02	-5.48	120.03	124.78
5	A	2201	E4S	C14-N04-C13	-4.69	119.75	126.93
5	E	2201	E4S	C14-N04-C13	-4.51	120.02	126.93
5	A	2201	E4S	N03-C13-N02	-4.49	120.89	124.78
5	A	2201	E4S	C10-N02-C13	-4.24	102.36	105.20
5	E	2201	E4S	C25-C24-C29	4.08	121.68	117.23
5	E	2201	E4S	C23-N05-C20	4.02	120.60	111.57
5	A	2201	E4S	O01-C02-C03	3.90	123.59	117.48
5	E	2201	E4S	C03-S01-N06	3.84	111.82	107.30
5	E	2201	E4S	C28-C29-C24	-3.75	118.98	123.18
5	A	2201	E4S	C25-C24-C29	3.67	121.24	117.23
5	E	2201	E4S	C05-C06-N01	-3.58	118.59	124.28
5	A	2201	E4S	C23-N05-C20	3.53	119.52	111.57
5	A	2201	E4S	C28-C29-C24	-3.51	119.25	123.18
5	E	2201	E4S	C24-N06-S01	-3.35	112.62	123.34
5	E	2201	E4S	C12-C07-C05	3.24	126.85	121.25
5	A	2201	E4S	O01-C02-N01	-3.21	116.52	120.23
5	A	2201	E4S	C01-O01-C02	-3.18	114.23	117.20
5	E	2201	E4S	O03-S01-C03	3.09	112.78	107.68
5	A	2201	E4S	C08-C09-N04	3.02	136.59	130.89
5	A	2201	E4S	C18-C17-N05	-2.88	117.39	121.39
5	E	2201	E4S	C18-C17-N05	-2.87	117.41	121.39
5	E	2201	E4S	C09-C10-N02	-2.84	106.58	110.19
5	E	2201	E4S	C08-C07-C05	-2.80	116.15	120.84
5	E	2201	E4S	C04-C03-S01	-2.76	113.53	118.59
5	A	2201	E4S	C24-N06-S01	-2.71	114.65	123.34
5	E	2201	E4S	C22-C23-N05	-2.63	104.95	109.93
5	A	2201	E4S	C14-N04-C09	-2.60	119.97	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2201	E4S	O03-S01-N06	2.58	113.03	106.74
5	E	2201	E4S	C08-C09-N04	2.54	135.70	130.89
5	E	2201	E4S	C15-C14-N04	2.48	122.58	119.72
5	A	2201	E4S	C03-S01-N06	2.48	110.22	107.30
5	A	2201	E4S	C05-C06-N01	-2.32	120.59	124.28
5	E	2201	E4S	C10-C09-N04	-2.29	103.55	105.25
5	A	2201	E4S	C08-C07-C05	-2.27	117.03	120.84
5	E	2201	E4S	O03-S01-N06	2.26	112.24	106.74
5	E	2201	E4S	C01-O01-C02	-2.25	115.10	117.20
5	A	2201	E4S	C19-C18-C17	-2.24	117.46	120.30
5	A	2201	E4S	C04-C05-C06	2.18	119.44	117.10
5	E	2201	E4S	C06-N01-C02	2.03	121.41	116.51
5	E	2201	E4S	C19-C18-C17	-2.00	117.76	120.30

There are no chirality outliers.

All (19) torsion outliers are listed below:

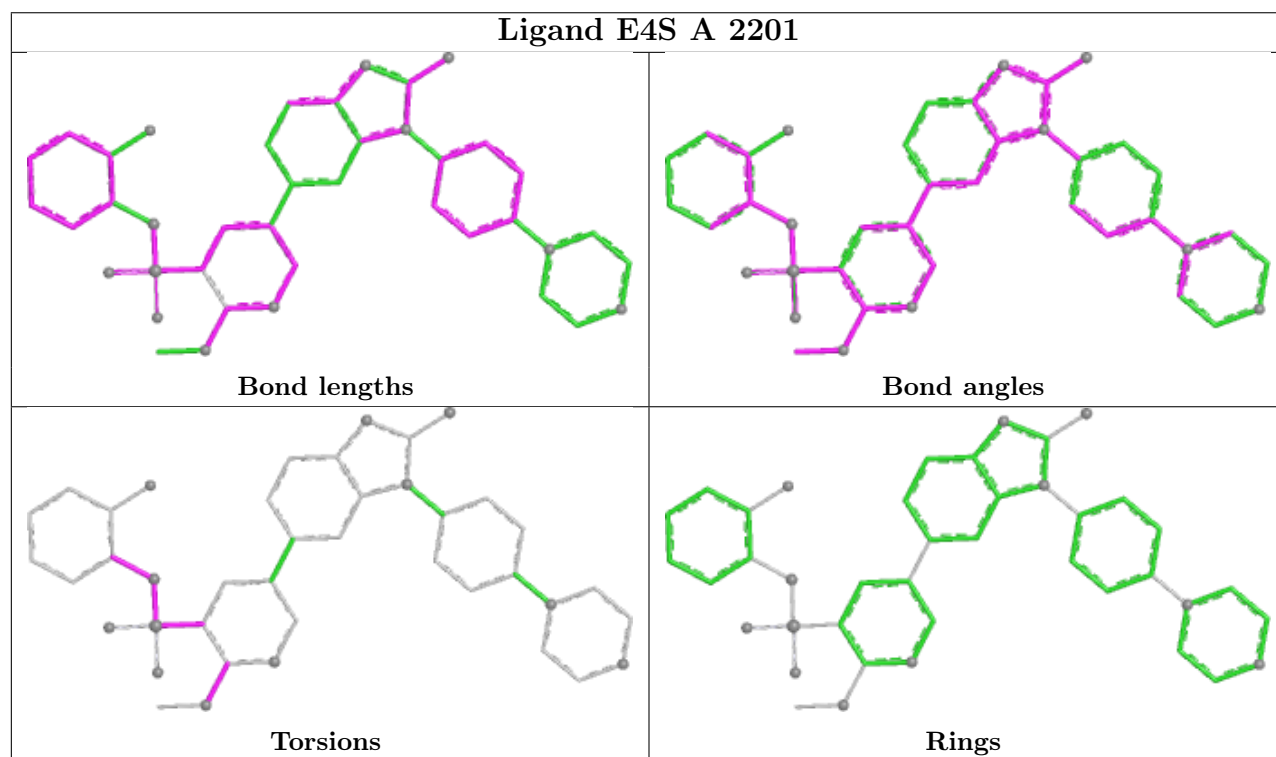
Mol	Chain	Res	Type	Atoms
5	A	2201	E4S	C03-C02-O01-C01
5	A	2201	E4S	N01-C02-O01-C01
5	A	2201	E4S	C02-C03-S01-N06
5	A	2201	E4S	C24-N06-S01-C03
5	E	2201	E4S	C03-C02-O01-C01
5	E	2201	E4S	N01-C02-O01-C01
5	E	2201	E4S	C02-C03-S01-N06
5	E	2201	E4S	C02-C03-S01-O03
5	E	2201	E4S	C02-C03-S01-O04
5	E	2201	E4S	C24-N06-S01-C03
5	A	2201	E4S	C04-C03-S01-N06
5	E	2201	E4S	C04-C03-S01-O03
5	E	2201	E4S	C04-C03-S01-N06
5	A	2201	E4S	C24-N06-S01-O04
5	A	2201	E4S	C02-C03-S01-O03
5	A	2201	E4S	C04-C03-S01-O03
5	E	2201	E4S	C15-C14-N04-C09
5	A	2201	E4S	C02-C03-S01-O04
5	A	2201	E4S	C25-C24-N06-S01

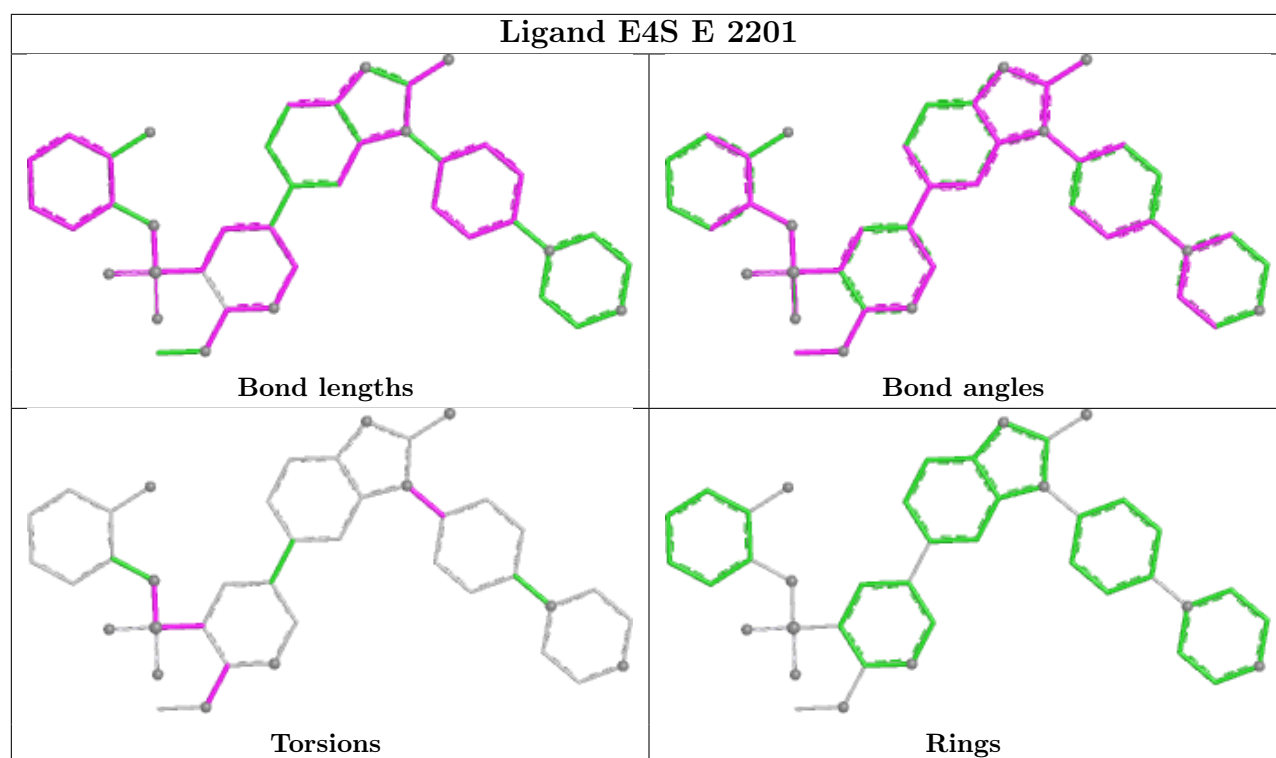
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2201	E4S	3	0
5	E	2201	E4S	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	27
1	A	27

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	194:UNK	C	195:UNK	N	33.07
1	A	175:UNK	C	176:UNK	N	30.98
1	E	175:UNK	C	176:UNK	N	30.98
1	A	437:UNK	C	438:UNK	N	29.73
1	E	438:UNK	C	439:UNK	N	29.73
1	A	52:UNK	C	53:UNK	N	29.41
1	E	52:UNK	C	53:UNK	N	29.40
1	A	194:UNK	C	195:UNK	N	28.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	139:UNK	C	140:UNK	N	27.98
1	E	139:UNK	C	140:UNK	N	27.98
1	E	33:UNK	C	34:UNK	N	25.84
1	A	307:UNK	C	308:UNK	N	25.79
1	E	309:UNK	C	310:UNK	N	25.78
1	A	33:UNK	C	34:UNK	N	25.75
1	E	120:UNK	C	121:UNK	N	25.68
1	A	120:UNK	C	121:UNK	N	25.67
1	A	17:UNK	C	18:UNK	N	22.92
1	E	17:UNK	C	18:UNK	N	22.91
1	A	69:UNK	C	70:UNK	N	19.19
1	E	69:UNK	C	70:UNK	N	19.17
1	A	288:UNK	C	289:UNK	N	17.30
1	E	290:UNK	C	291:UNK	N	17.30
1	A	155:UNK	C	156:UNK	N	14.99
1	E	155:UNK	C	156:UNK	N	14.99
1	E	210:UNK	C	211:UNK	N	14.50
1	A	269:UNK	C	270:UNK	N	13.05
1	E	422:UNK	C	423:UNK	N	13.02
1	A	421:UNK	C	422:UNK	N	13.01
1	E	271:UNK	C	272:UNK	N	12.93
1	A	237:UNK	C	238:UNK	N	12.26
1	E	255:UNK	C	256:UNK	N	12.00
1	A	253:UNK	C	254:UNK	N	11.99
1	E	103:UNK	C	104:UNK	N	11.96
1	A	209:UNK	C	210:UNK	N	11.95
1	A	103:UNK	C	104:UNK	N	11.94
1	A	342:UNK	C	343:UNK	N	11.91
1	E	343:UNK	C	344:UNK	N	11.91
1	A	324:UNK	C	325:UNK	N	11.51
1	A	89:UNK	C	90:UNK	N	10.36
1	E	396:UNK	C	397:UNK	N	10.36
1	A	395:UNK	C	396:UNK	N	10.35
1	E	89:UNK	C	90:UNK	N	10.35
1	A	379:UNK	C	380:UNK	N	10.03
1	E	380:UNK	C	381:UNK	N	10.03
1	E	238:UNK	C	239:UNK	N	9.90
1	A	407:UNK	C	408:UNK	N	8.93
1	E	408:UNK	C	409:UNK	N	8.92
1	A	361:UNK	C	362:UNK	N	8.65
1	E	362:UNK	C	363:UNK	N	8.65
1	E	326:UNK	C	327:UNK	N	8.10

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	476:UNK	C	932:MET	N	7.70
1	E	477:UNK	C	932:MET	N	7.20
1	A	224:UNK	C	225:UNK	N	6.17
1	E	225:UNK	C	226:UNK	N	6.15

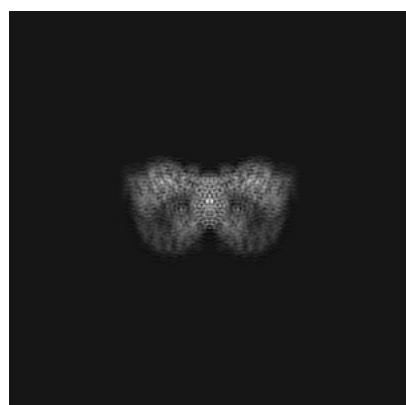
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7129. These allow visual inspection of the internal detail of the map and identification of artifacts.

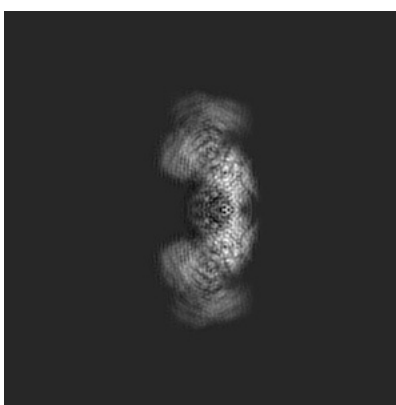
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

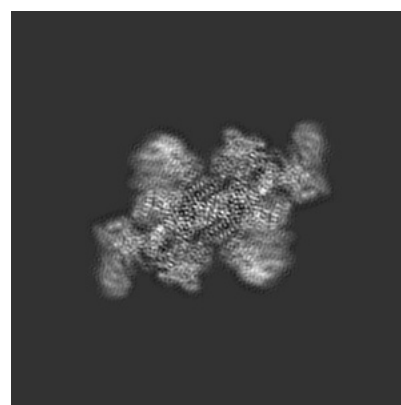
6.1.1 Primary map



X



Y



Z

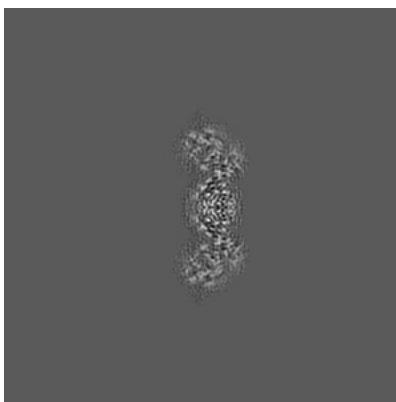
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

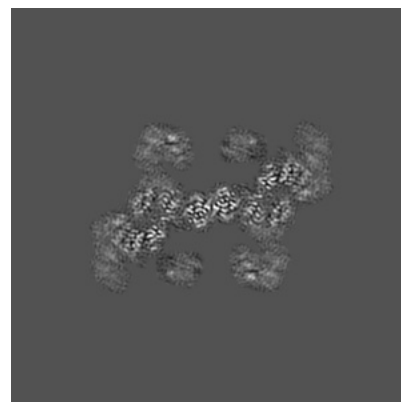
6.2.1 Primary map



X Index: 160



Y Index: 160

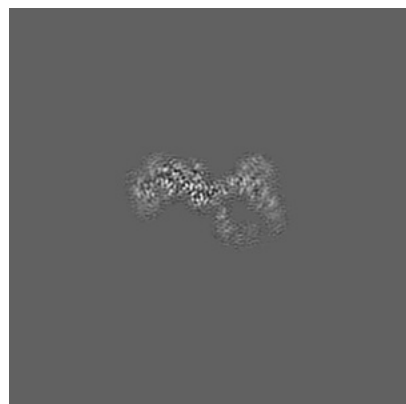


Z Index: 160

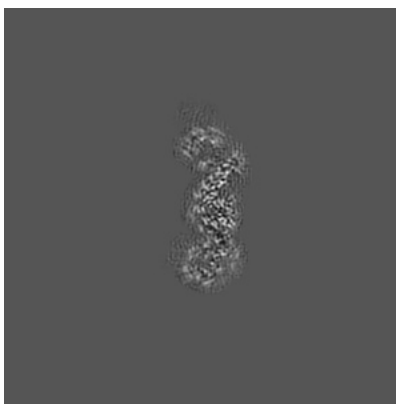
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

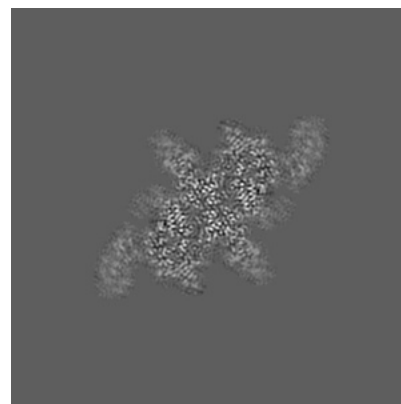
6.3.1 Primary map



X Index: 136



Y Index: 163

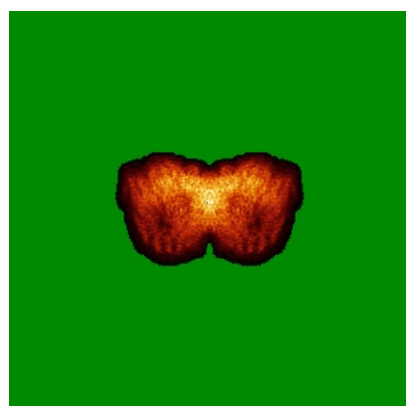


Z Index: 178

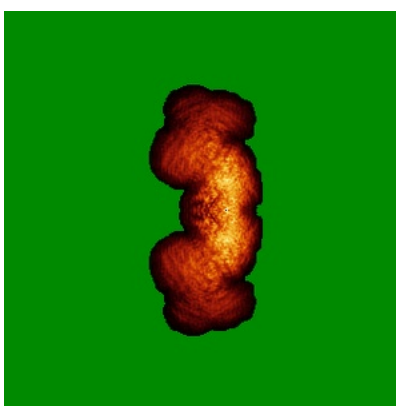
The images above show the largest variance slices of the map in three orthogonal directions.

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

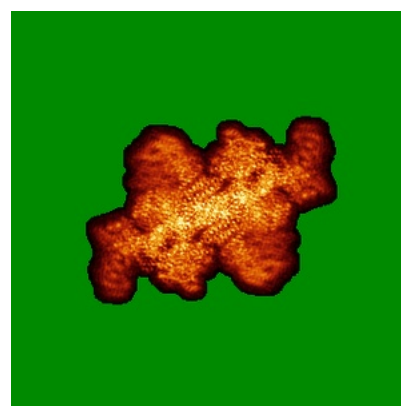
6.4.1 Primary map



X



Y

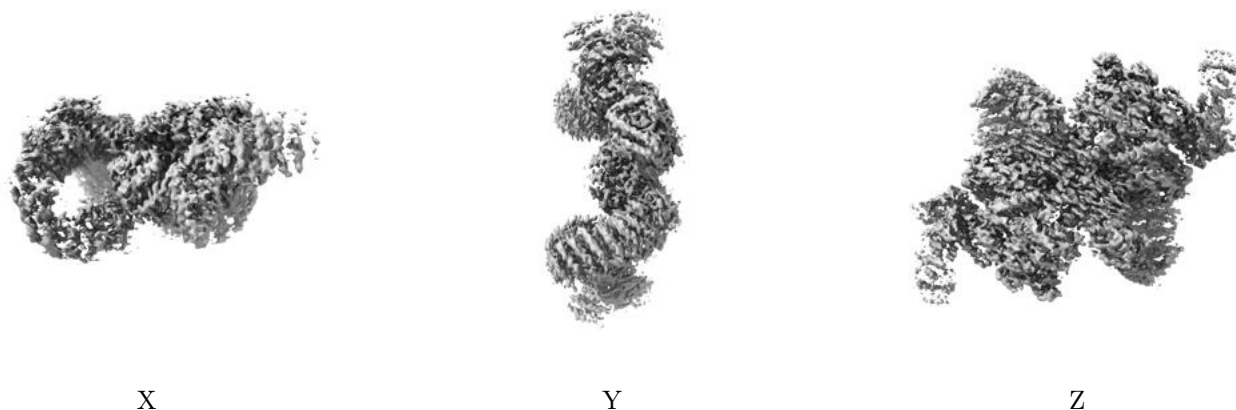


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

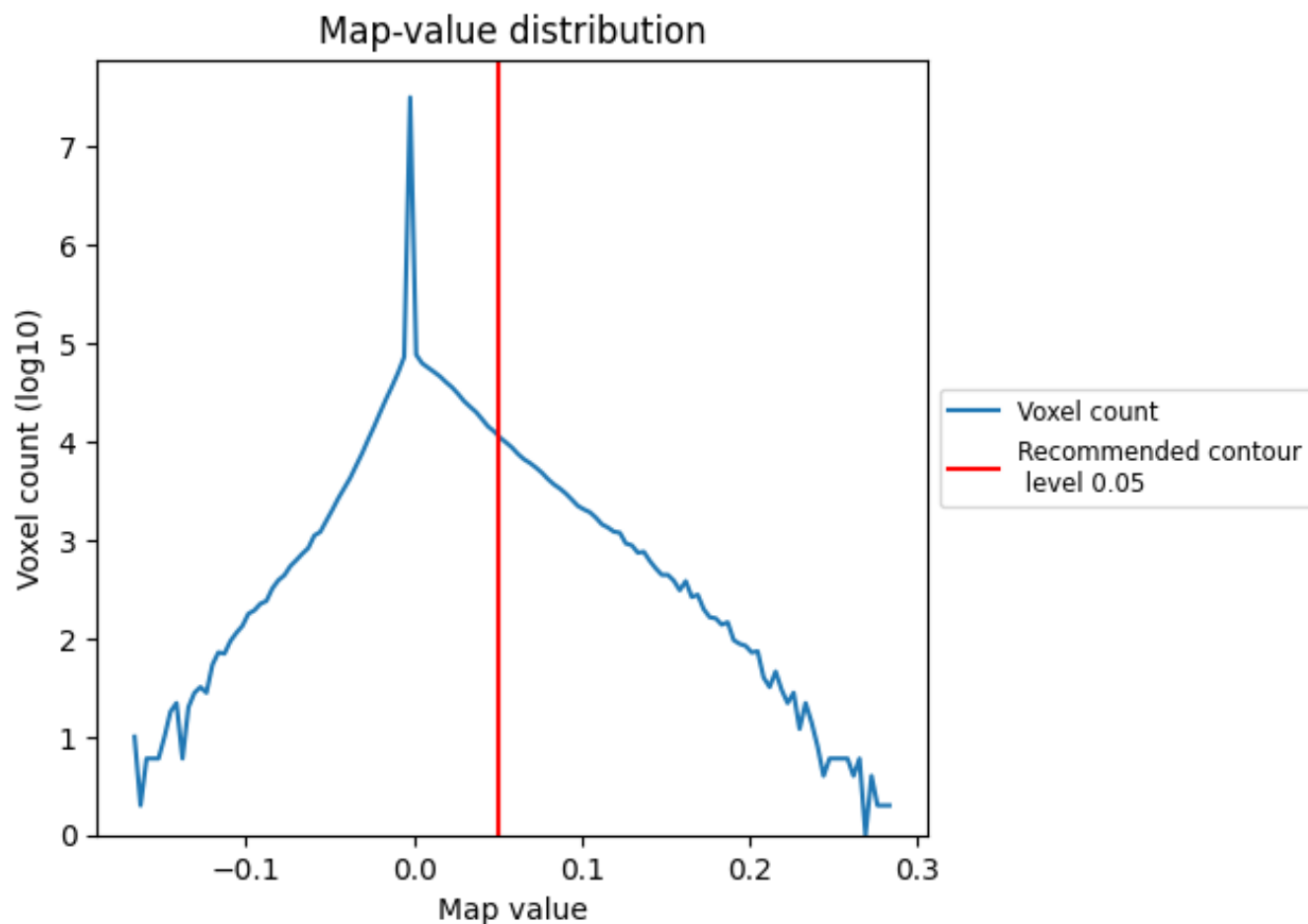
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

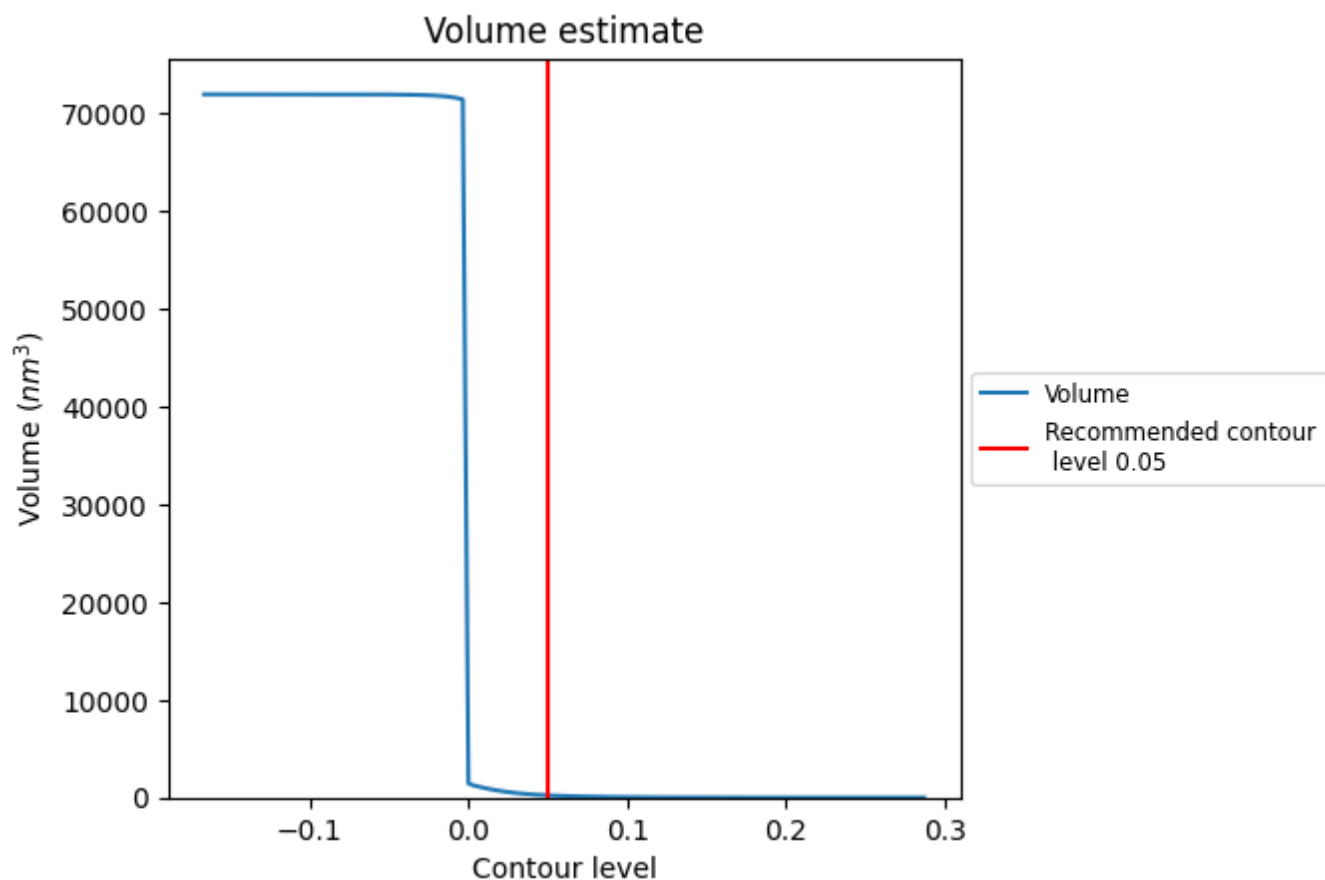
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

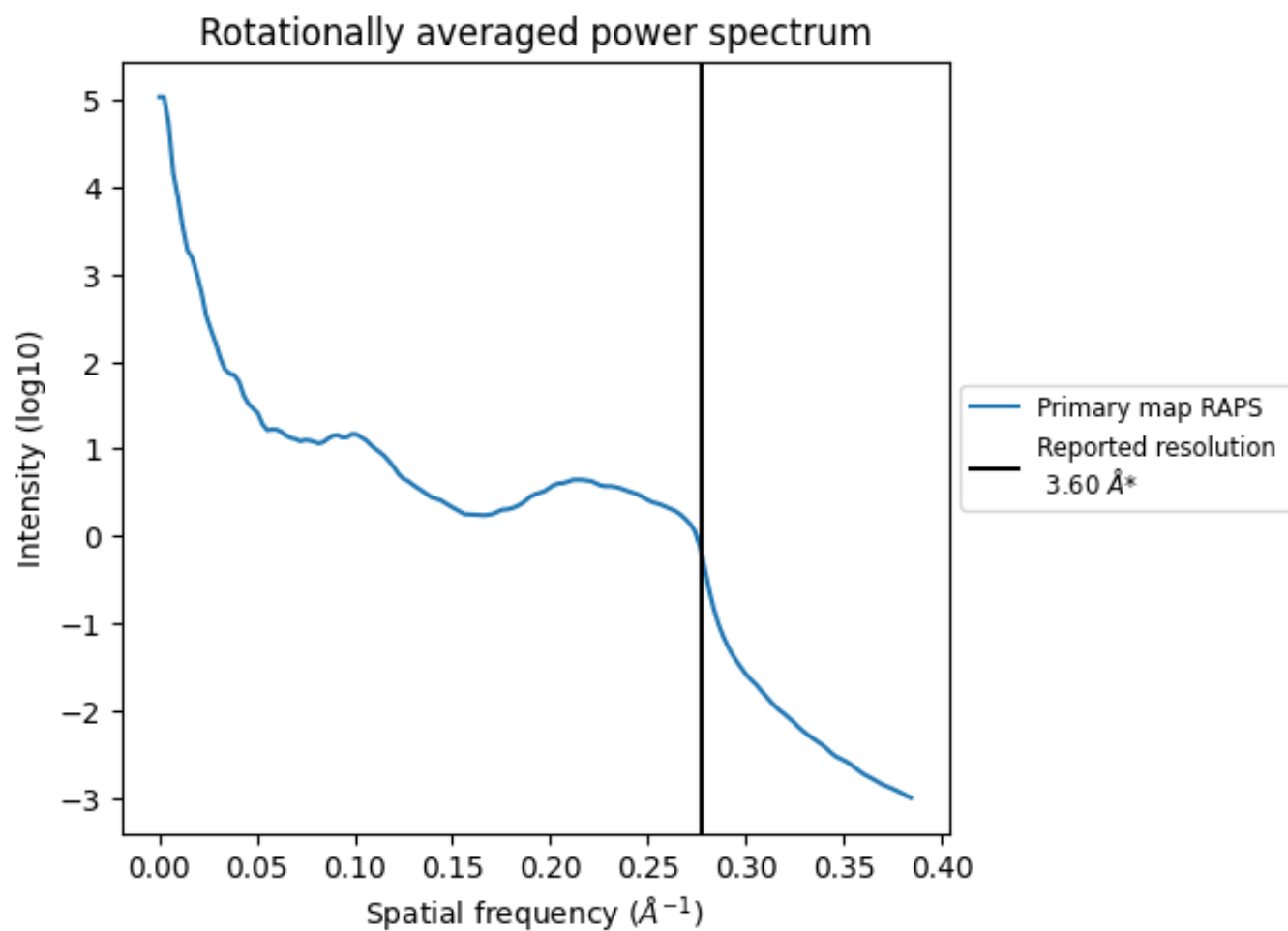
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm^3 ; this corresponds to an approximate mass of 205 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 ⓘ

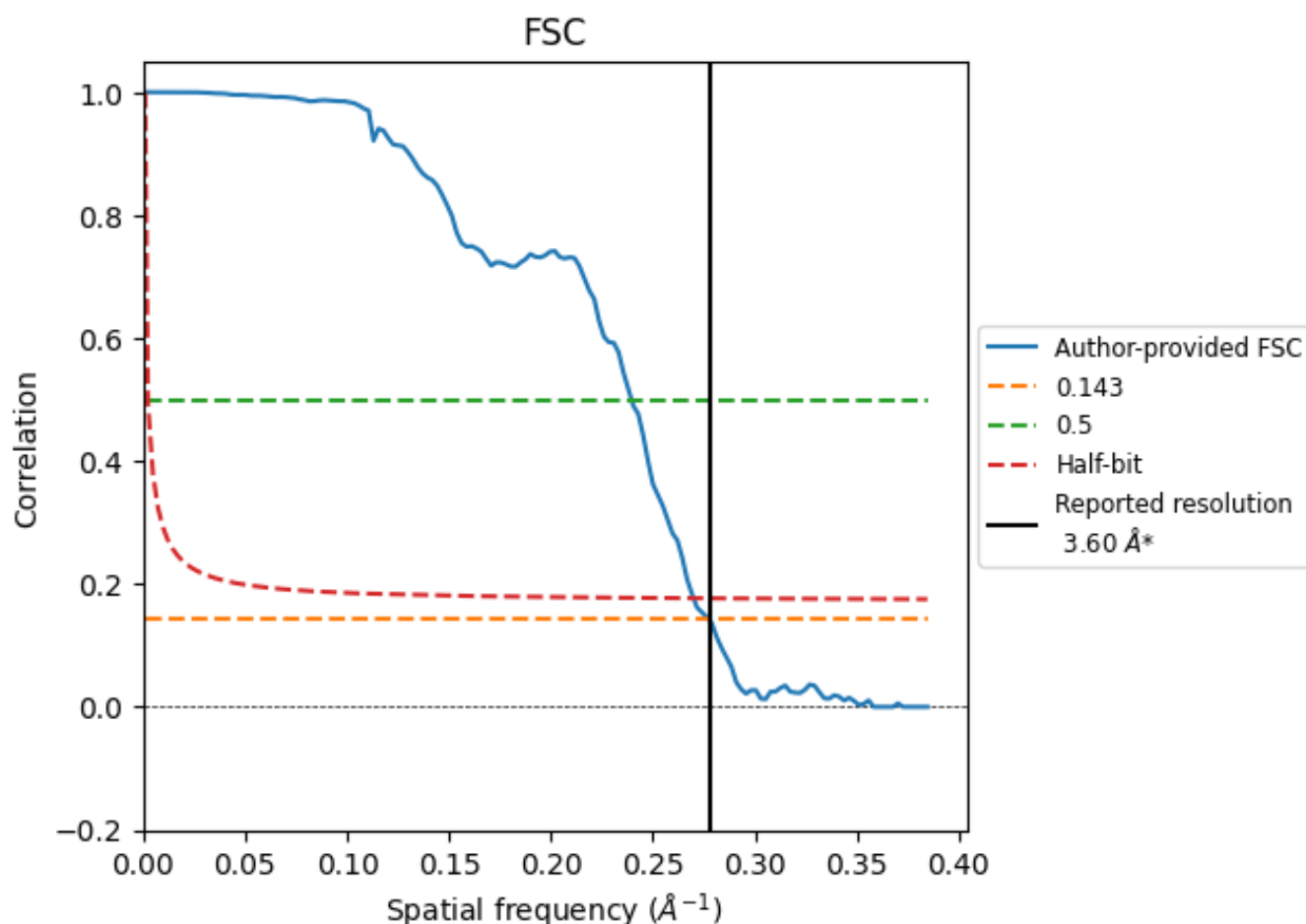


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

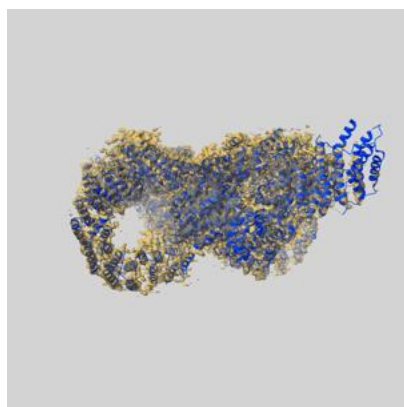
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.18	3.70
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

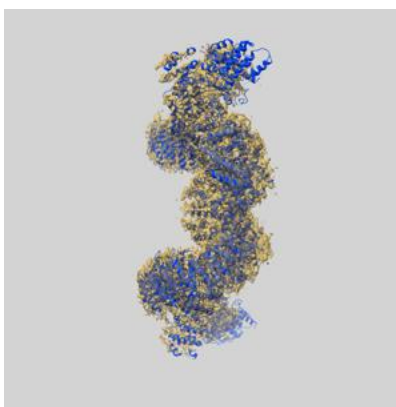
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7129 and PDB model 6BQ1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

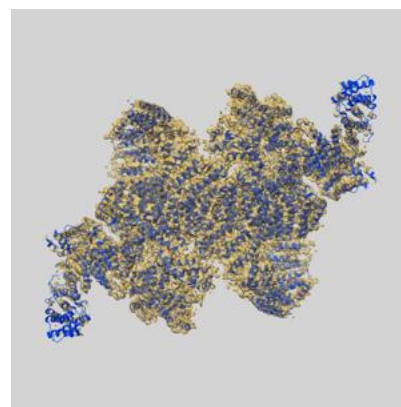
9.1 Map-model overlay [i](#)



X



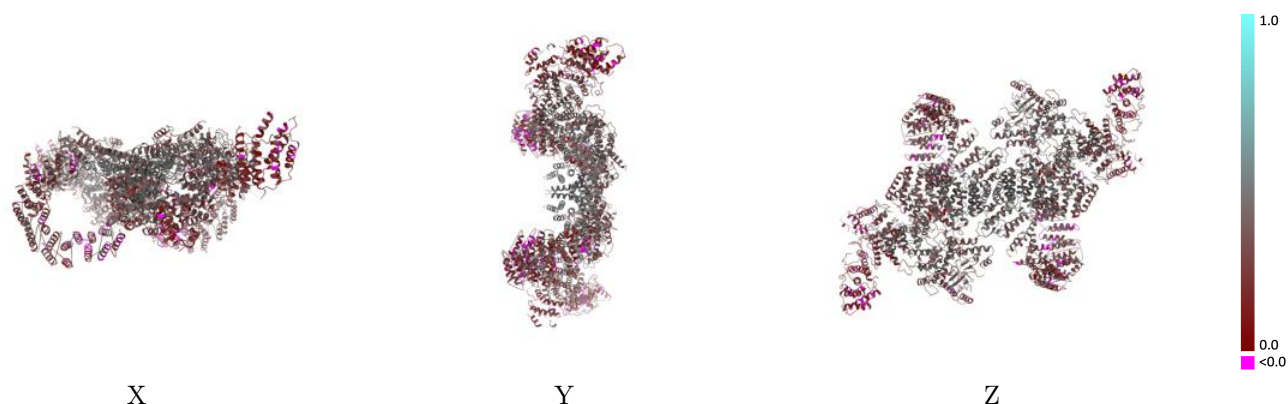
Y



Z

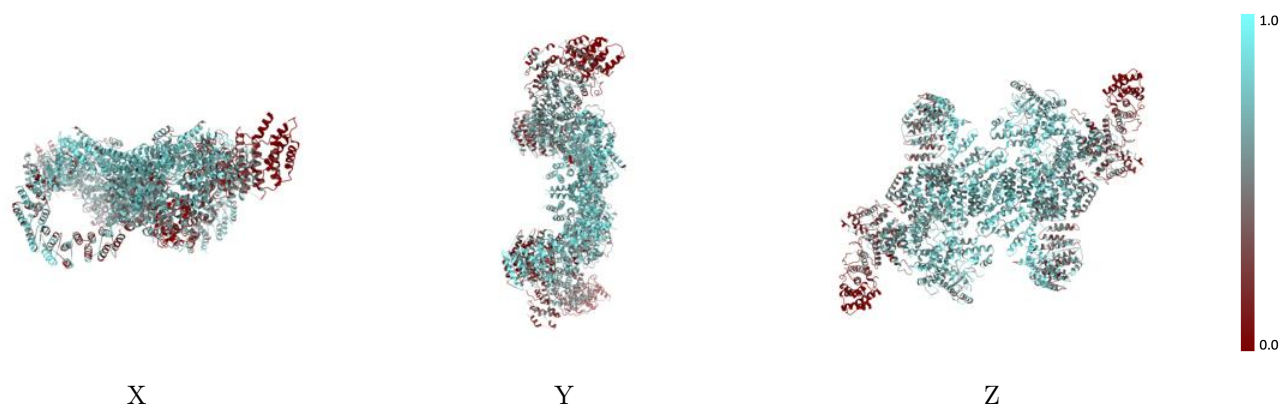
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



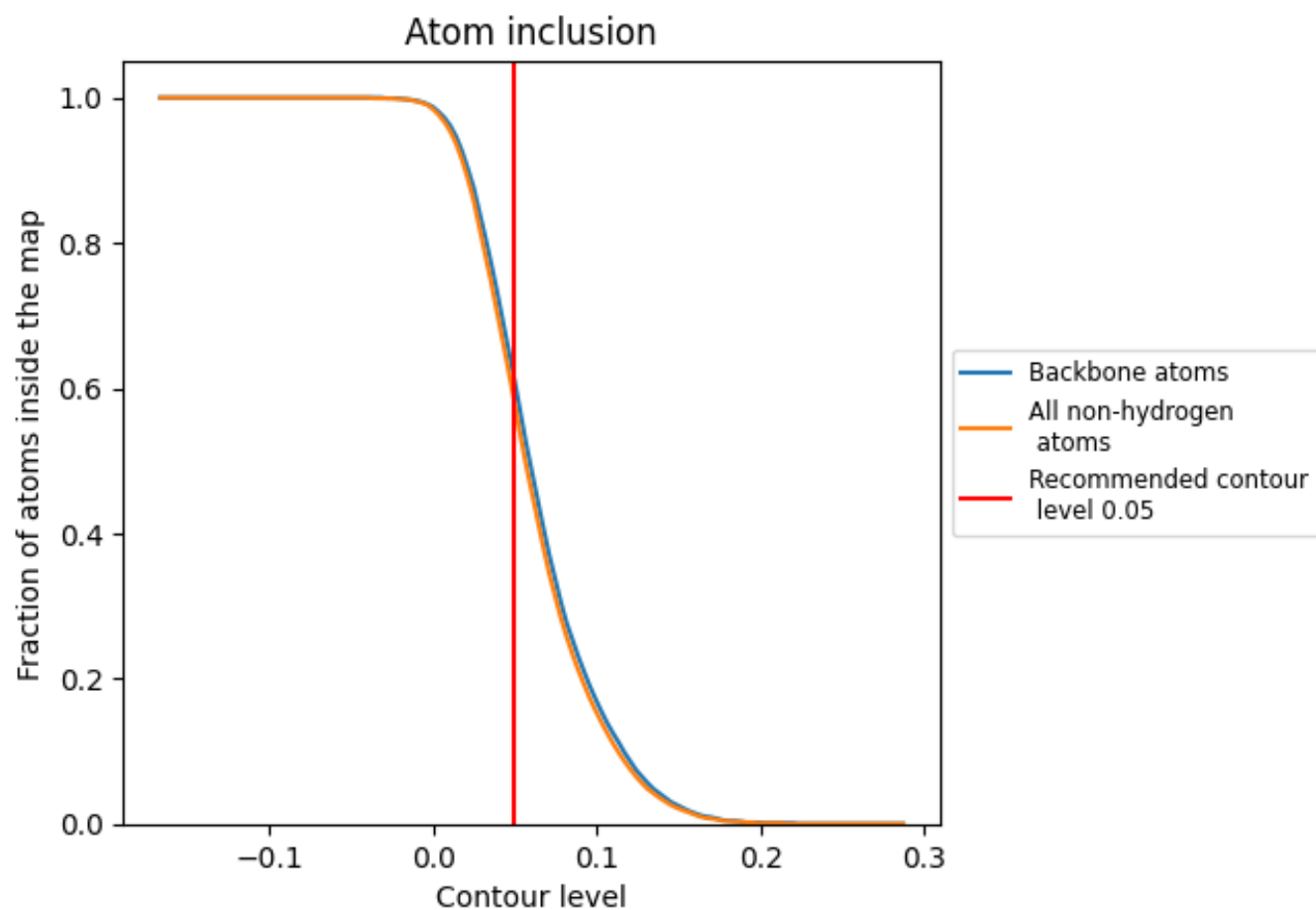
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 58% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5780	0.3410
A	0.6900	0.3680
B	0.4340	0.2940
C	0.3910	0.2800
E	0.7020	0.3820
F	0.4370	0.3040
G	0.3970	0.2830

