



## Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 08:23 PM JST

PDB ID : 8X48  
EMDB ID : EMD-38042  
Title : Cryo-EM structure of Ryanodine receptor 1 (EGTA)  
Authors : Chen, Q.; Hu, H.  
Deposited on : 2023-11-15  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

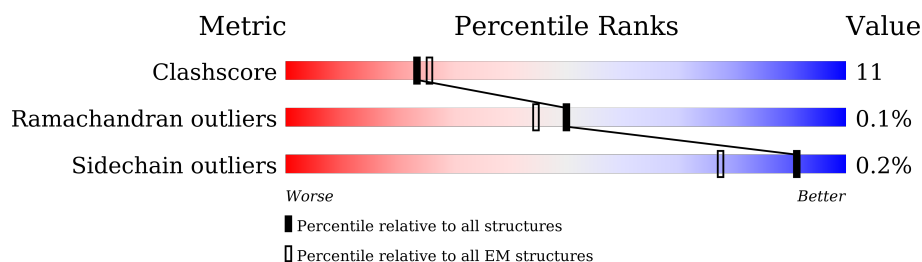
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5037	 51% 14% 35%
1	B	5037	 51% 14% 35%
1	C	5037	 51% 14% 35%
1	D	5037	 51% 14% 35%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 95972 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

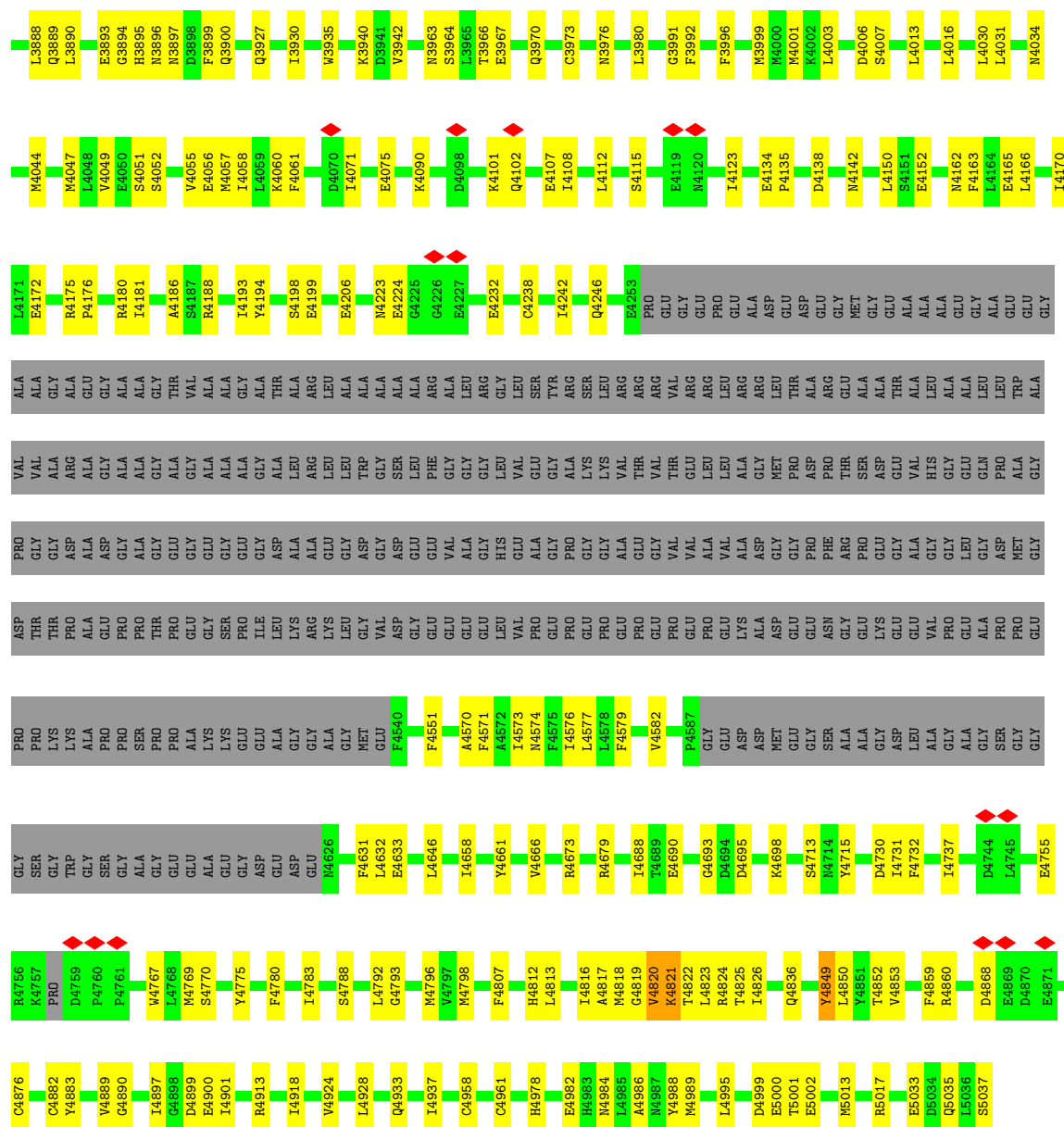
- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3289	Total 23993	C 15289	N 4189	O 4376	S 139	0	0
1	B	3289	Total 23993	C 15289	N 4189	O 4376	S 139	0	0
1	C	3289	Total 23993	C 15289	N 4189	O 4376	S 139	0	0
1	D	3289	Total 23993	C 15289	N 4189	O 4376	S 139	0	0



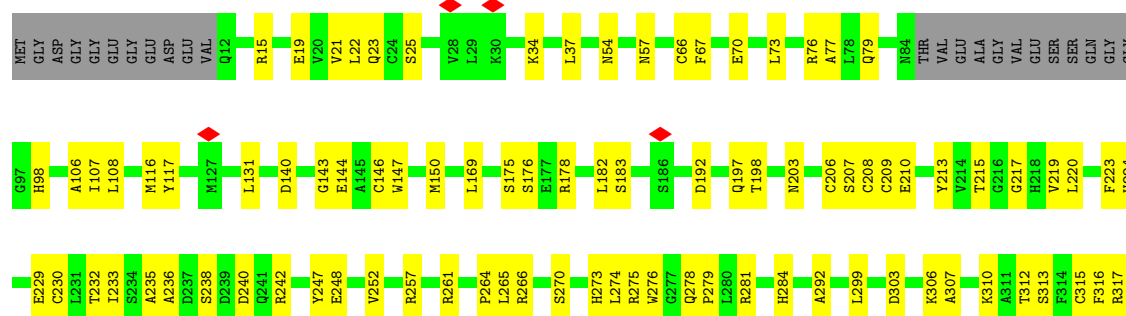
PRO	PRO	GLU	N2414	GLU	A2421	P2438	A2450	L2451	R2452	R2453	R2454	R2455	R2456	D2464	V2467	R2468	R2469	R2470	R2471	L2472	Q2475	L2479	GLY	LYS	ASP	GLY	ALA	LEU	VAL	Q2487	R2513	R2514	R2562	THR	LYS	CYS	A2566	R2567	R2568	R2583	R2584	R2587	R2591	R2604	ASP						
I2281	E2292	L2295	E2296	E2297	V2298	V2299	L2302	D2320	P2325	F2337	F2340	V2341	N2342	V2346	E2347	E2348	V2353	V2354	L2357	I2358	C2363	L2368	R2369	G2370	E2371	G2372	G2373	L2377	I2380	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	ARG	ARG	HIS	PHE	GLY	GLU							
V2149	M2153	L2159	E2296	E2297	V2298	V2299	V2168	N2176	N2184	N2187	N2188	H2194	L2197	E2205	T2206	V2207	R2208	E2209	V2210	R2211	V2212	G2217	G2218	E2219	T2220	K2221	E2222	L2223	M2228	L2254	L2257	L2258	L2263	Q2268	G2269	S2270	T2271	P2272	L2273	D2274	V2275	A2276	A2277	A2278							
E2047	G2048	GLU	GLU	GLU	GLU	PRO	GLU	GLU	L1922	M1929	K1930	L1931	K1936	M1939	L1943	E1944	Y1945	D1948	Q1952	R1953	R1954	Y1955	E1956	E1963	R1964	Y1965	V1966	S1987	A1988	A1989	R1996	S2000	P2001	Q2002	Q2003	E2004	Q2005	I2006	N2007	L2010	H2011	F2012	P2022	L2023	P2024	E2025	D2026	L2027	R2028	Q2029	C2042
L1848	L1849	M1850	M1851	F1854	V1859	T1862	M1865	T1866	E1867	P1868	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU			
P1749	K1753	G1754	G1755	M1756	A1757	H1760	V1765	G1766	T1769	S1770	L1771	R1772	P1773	P1774	H1775	H1776	V1783	A1784	A1785	LEU	ALA	ALA	GLY	VAL	ALA	GLU	ALA	PRO	A1796	R1797	R1808	D1809	K1810	M1814	L1815	G1816	E1817	A1818	V1819	P1829	V1830	G1831	Q1837	L1844	V1845	S1846	T1847				
C1630	M1637	C1647	M1648	D1649	L1650	L1651	E1652	L1653	R1656	L1657	D1658	L1659	F1662	H1665	T1666	L1667	R1668	G1677	N1678	R1679	L1680	L1694	L1698	H1702	L1703	P1704	L1707	R1708	Y1712	D1713	L1714	L1715	I1716	S1717	L1718	H1719	L1720	A1723	R1727	M1730	L1738	T1742	R1743								
ILE	ILE	LEU	ASN	T1430	T1454	D1456	V1495	S1502	PRO	G1504	V1520	S1536	E1543	P1544	N1545	T1546	K1547	L1548	F1564	GLU	LEU	GLY	LYS	GLN	LYS	ASN	ILE	M1573	L1595	Q1598	M1599	L1600	M1601	P1602	V1603	S1604	W1605	V1615	THR	ARG	ALA	GLY	E1622	G1625							
VAL	GLU	GLN	PRO	VAL	ARG	ALA	ASN	GLU	LYS	THR	GLU	LYS	ASN	LYS	LYS	ARG	PHE	PHE	ALA	LYS	ALA	LYS	ALA	MET	MET	THR	GLY	PRO	ALA	PRO	ALA	LEU	ARG	PRO	HIS	VAL	VAL	PRO	ALA	ASP	ASN	THR	PRO	GLY	GLY						
LYS	PRO	ALA	LEU	ASP	LEU	SER	HIS	VAL	ARG	LEU	THR	P979	A980	S1006	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	ALA	ARG	ARG	ASN	PRO	R1020	L1039	C1040	Q1041	R1044	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	GLN	GLU	GLU	VAL	ASN	GLN	SER	ARG	TRP		

[illegible]



• Molecule 1: Ryanodine receptor 1

Chain B: 51% 14% 35%

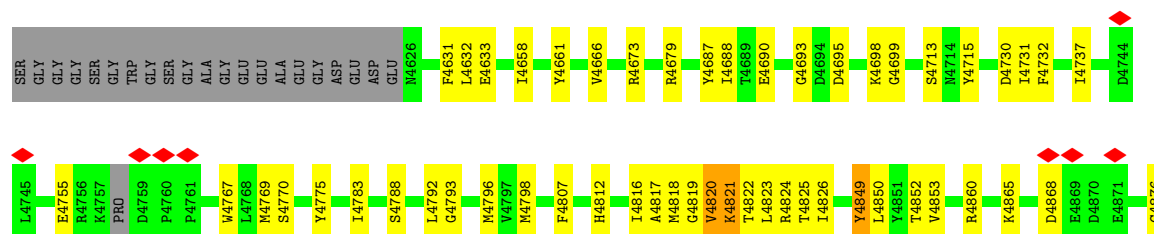












# Molecule 1: Ryanodine receptor 1







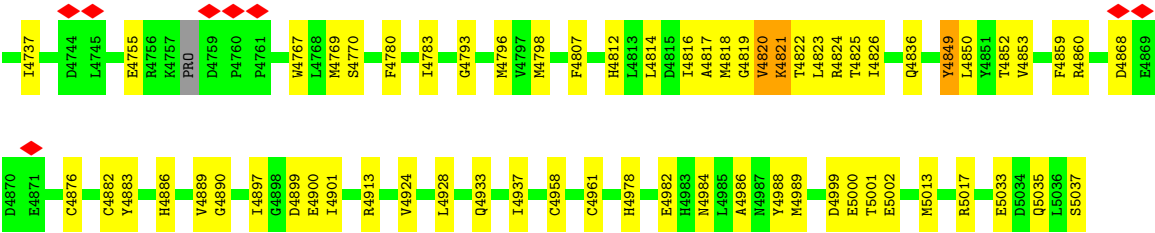












## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60110	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.660	Depositor
Minimum map value	-1.411	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.35	Depositor
Map size ( $\text{\AA}$ )	523.2, 523.2, 523.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.09, 1.09, 1.09	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.28	0/24473	0.51	0/33293
1	B	0.28	0/24473	0.51	0/33293
1	C	0.28	0/24473	0.51	0/33293
1	D	0.28	0/24473	0.51	0/33293
All	All	0.28	0/97892	0.51	0/133172

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23993	0	21998	502	0
1	B	23993	0	21998	497	0
1	C	23993	0	21998	491	0
1	D	23993	0	21998	503	0
All	All	95972	0	87992	1977	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1977) 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:4816:ILE:HG23	1:A:4817:ALA:N	1.93	0.84
1:C:4816:ILE:HG23	1:C:4817:ALA:N	1.93	0.83
1:D:4055:VAL:HA	1:D:4058:ILE:HD12	1.60	0.83
1:C:4055:VAL:HA	1:C:4058:ILE:HD12	1.60	0.83
1:A:4055:VAL:HA	1:A:4058:ILE:HD12	1.60	0.83
1:B:4055:VAL:HA	1:B:4058:ILE:HD12	1.60	0.83
1:D:4816:ILE:HG23	1:D:4817:ALA:N	1.93	0.83
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.62	0.81
1:B:4816:ILE:HG23	1:B:4817:ALA:N	1.93	0.81
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.62	0.80
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.62	0.80
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.62	0.80
1:B:662:TRP:HA	1:B:809:ALA:HB3	1.68	0.76
1:C:662:TRP:HA	1:C:809:ALA:HB3	1.68	0.76
1:A:662:TRP:HA	1:A:809:ALA:HB3	1.68	0.75
1:D:662:TRP:HA	1:D:809:ALA:HB3	1.68	0.75
1:D:4816:ILE:CG2	1:D:4817:ALA:N	2.50	0.75
1:A:4816:ILE:CG2	1:A:4817:ALA:N	2.50	0.74
1:D:303:ASP:H	1:D:306:LYS:HZ2	1.35	0.74
1:B:4816:ILE:CG2	1:B:4817:ALA:N	2.50	0.74
1:D:456:SER:O	1:D:464:LYS:NZ	2.21	0.74
1:C:4816:ILE:CG2	1:C:4817:ALA:N	2.50	0.73
1:B:456:SER:O	1:B:464:LYS:NZ	2.21	0.73
1:A:456:SER:O	1:A:464:LYS:NZ	2.21	0.73
1:C:303:ASP:H	1:C:306:LYS:HZ2	1.36	0.73
1:B:303:ASP:H	1:B:306:LYS:HZ2	1.37	0.72
1:C:456:SER:O	1:C:464:LYS:NZ	2.21	0.72
1:A:303:ASP:H	1:A:306:LYS:HZ2	1.38	0.72
1:B:2022:PRO:HD2	1:B:2028:ARG:HH22	1.55	0.72
1:D:4199:GLU:N	1:D:4199:GLU:OE2	2.23	0.71
1:C:2022:PRO:HD2	1:C:2028:ARG:HH22	1.55	0.71
1:A:2022:PRO:HD2	1:A:2028:ARG:HH22	1.55	0.71
1:A:2194:HIS:HB3	1:A:2197:LEU:HD23	1.72	0.71
1:C:2194:HIS:HB3	1:C:2197:LEU:HD23	1.72	0.71
1:D:2194:HIS:HB3	1:D:2197:LEU:HD23	1.72	0.70
1:C:4199:GLU:OE2	1:C:4199:GLU:N	2.23	0.70
1:B:606:LEU:O	1:B:617:ASN:ND2	2.25	0.70
1:A:606:LEU:O	1:A:617:ASN:ND2	2.25	0.70
1:D:2022:PRO:HD2	1:D:2028:ARG:HH22	1.55	0.70
1:B:2194:HIS:HB3	1:B:2197:LEU:HD23	1.72	0.69
1:B:4199:GLU:N	1:B:4199:GLU:OE2	2.23	0.69
1:A:4199:GLU:N	1:A:4199:GLU:OE2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:793:LEU:HD12	1:C:797:HIS:HB2	1.74	0.69
1:D:793:LEU:HD12	1:D:797:HIS:HB2	1.74	0.69
1:D:606:LEU:O	1:D:617:ASN:ND2	2.25	0.69
1:C:606:LEU:O	1:C:617:ASN:ND2	2.25	0.69
1:C:3935:TRP:HH2	1:D:77:ALA:HB2	1.58	0.69
1:B:1703:LEU:HA	1:B:1708:ARG:HH21	1.58	0.69
1:C:1703:LEU:HA	1:C:1708:ARG:HH21	1.58	0.68
1:A:1703:LEU:HA	1:A:1708:ARG:HH21	1.58	0.68
1:B:4978:HIS:ND1	1:B:4982:GLU:OE1	2.27	0.68
1:A:2438:PRO:HB3	1:A:2450:ALA:HB1	1.76	0.68
1:A:4978:HIS:ND1	1:A:4982:GLU:OE1	2.27	0.68
1:C:2184:ASN:O	1:C:2188:ASN:ND2	2.27	0.68
1:D:2184:ASN:O	1:D:2188:ASN:ND2	2.27	0.68
1:C:2438:PRO:HB3	1:C:2450:ALA:HB1	1.76	0.68
1:B:3935:TRP:HH2	1:C:77:ALA:HB2	1.58	0.67
1:A:77:ALA:HB2	1:D:3935:TRP:HH2	1.58	0.67
1:D:2438:PRO:HB3	1:D:2450:ALA:HB1	1.76	0.67
1:A:708:GLY:H	1:A:713:SER:HB3	1.60	0.67
1:D:4978:HIS:ND1	1:D:4982:GLU:OE1	2.27	0.67
1:A:793:LEU:HD12	1:A:797:HIS:HB2	1.74	0.67
1:A:2271:THR:HG22	1:A:2273:LEU:H	1.59	0.67
1:B:793:LEU:HD12	1:B:797:HIS:HB2	1.74	0.67
1:B:2438:PRO:HB3	1:B:2450:ALA:HB1	1.76	0.67
1:A:533:ASN:ND2	1:A:536:ASN:OD1	2.28	0.67
1:B:2184:ASN:O	1:B:2188:ASN:ND2	2.27	0.67
1:C:792:LEU:HD22	1:C:798:GLY:HA2	1.77	0.67
1:C:1099:GLU:HB3	1:C:1101:ARG:HH22	1.60	0.67
1:C:4978:HIS:ND1	1:C:4982:GLU:OE1	2.27	0.67
1:B:1099:GLU:HB3	1:B:1101:ARG:HH22	1.60	0.67
1:A:2184:ASN:O	1:A:2188:ASN:ND2	2.27	0.67
1:A:3935:TRP:HH2	1:B:77:ALA:HB2	1.58	0.67
1:A:4661:TYR:HH	1:A:4788:SER:HG	1.41	0.67
1:B:792:LEU:HD22	1:B:798:GLY:HA2	1.77	0.67
1:D:533:ASN:ND2	1:D:536:ASN:OD1	2.28	0.67
1:D:1099:GLU:HB3	1:D:1101:ARG:HH22	1.60	0.67
1:C:2271:THR:HG22	1:C:2273:LEU:H	1.59	0.67
1:B:533:ASN:ND2	1:B:536:ASN:OD1	2.28	0.67
1:D:1703:LEU:HA	1:D:1708:ARG:HH21	1.58	0.66
1:B:708:GLY:H	1:B:713:SER:HB3	1.60	0.66
1:B:401:ALA:O	1:B:404:ILE:HG13	1.96	0.66
1:D:708:GLY:H	1:D:713:SER:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2271:THR:HG22	1:B:2273:LEU:H	1.59	0.66
1:D:792:LEU:HD22	1:D:798:GLY:HA2	1.77	0.66
1:D:2271:THR:HG22	1:D:2273:LEU:H	1.59	0.66
1:B:4821:LYS:O	1:B:4822:THR:C	2.34	0.66
1:C:1771:LEU:HD12	1:C:2153:MET:SD	2.36	0.66
1:A:401:ALA:O	1:A:404:ILE:HG13	1.96	0.66
1:C:533:ASN:ND2	1:C:536:ASN:OD1	2.28	0.66
1:A:1099:GLU:HB3	1:A:1101:ARG:HH22	1.60	0.66
1:C:708:GLY:H	1:C:713:SER:HB3	1.60	0.66
1:A:455:PRO:HB2	1:A:464:LYS:HZ3	1.61	0.65
1:A:792:LEU:HD22	1:A:798:GLY:HA2	1.77	0.65
1:D:1771:LEU:HD12	1:D:2153:MET:SD	2.36	0.65
1:A:1152:MET:N	1:A:1152:MET:SD	2.69	0.65
1:B:1771:LEU:HD12	1:B:2153:MET:SD	2.36	0.65
1:B:1152:MET:N	1:B:1152:MET:SD	2.69	0.65
1:B:4661:TYR:HH	1:B:4788:SER:HG	1.44	0.65
1:C:401:ALA:O	1:C:404:ILE:HG13	1.96	0.65
1:A:1771:LEU:HD12	1:A:2153:MET:SD	2.36	0.65
1:C:1152:MET:N	1:C:1152:MET:SD	2.69	0.65
1:A:627:PRO:O	1:A:629:ARG:NH1	2.30	0.65
1:A:2131:LEU:HB3	1:A:3662:ILE:HG21	1.79	0.65
1:D:627:PRO:O	1:D:629:ARG:NH1	2.30	0.65
1:C:627:PRO:O	1:C:629:ARG:NH1	2.30	0.65
1:D:1152:MET:N	1:D:1152:MET:SD	2.69	0.65
1:B:627:PRO:O	1:B:629:ARG:NH1	2.30	0.65
1:C:4821:LYS:O	1:C:4822:THR:C	2.34	0.65
1:D:793:LEU:HB2	1:D:797:HIS:H	1.62	0.65
1:D:2131:LEU:HB3	1:D:3662:ILE:HG21	1.79	0.65
1:D:1770:SER:OG	1:D:1952:GLN:NE2	2.31	0.64
1:B:2131:LEU:HB3	1:B:3662:ILE:HG21	1.79	0.64
1:C:1770:SER:OG	1:C:1952:GLN:NE2	2.31	0.64
1:A:3658:LYS:HD2	1:A:3661:TRP:CZ3	2.33	0.64
1:D:401:ALA:O	1:D:404:ILE:HG13	1.96	0.64
1:C:1996:ARG:O	1:C:1996:ARG:NH1	2.27	0.64
1:A:1072:VAL:HG12	1:A:1195:GLY:HA2	1.80	0.64
1:D:3658:LYS:HD2	1:D:3661:TRP:CZ3	2.33	0.64
1:B:793:LEU:HB2	1:B:797:HIS:H	1.62	0.64
1:A:793:LEU:HB2	1:A:797:HIS:H	1.62	0.64
1:B:1770:SER:OG	1:B:1952:GLN:NE2	2.31	0.64
1:D:1072:VAL:HG12	1:D:1195:GLY:HA2	1.80	0.64
1:A:1770:SER:OG	1:A:1952:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:793:LEU:HB2	1:C:797:HIS:H	1.62	0.64
1:C:2131:LEU:HB3	1:C:3662:ILE:HG21	1.79	0.63
1:D:4821:LYS:O	1:D:4822:THR:C	2.34	0.63
1:B:4817:ALA:C	1:B:4819:GLY:H	2.02	0.63
1:A:4817:ALA:C	1:A:4819:GLY:H	2.02	0.63
1:D:411:TYR:HB3	1:D:486:LEU:HD21	1.79	0.63
1:B:3658:LYS:HD2	1:B:3661:TRP:CZ3	2.33	0.63
1:C:553:ARG:HE	1:C:593:HIS:HE1	1.47	0.63
1:C:3658:LYS:HD2	1:C:3661:TRP:CZ3	2.33	0.63
1:A:411:TYR:HB3	1:A:486:LEU:HD21	1.79	0.63
1:A:4900:GLU:N	1:A:4900:GLU:OE2	2.32	0.63
1:B:411:TYR:HB3	1:B:486:LEU:HD21	1.79	0.63
1:C:411:TYR:HB3	1:C:486:LEU:HD21	1.79	0.63
1:C:4817:ALA:C	1:C:4819:GLY:H	2.02	0.63
1:A:2026:ASP:O	1:A:2029:GLN:NE2	2.29	0.63
1:B:553:ARG:HE	1:B:593:HIS:HE1	1.47	0.63
1:C:1072:VAL:HG12	1:C:1195:GLY:HA2	1.80	0.63
1:A:3658:LYS:HA	1:A:3661:TRP:CE3	2.34	0.63
1:C:210:GLU:HB3	1:C:273:HIS:HE1	1.64	0.62
1:A:4821:LYS:O	1:A:4822:THR:C	2.34	0.62
1:B:1954:ARG:NH1	1:B:2042:CYS:SG	2.72	0.62
1:B:2205:GLU:N	1:B:2205:GLU:OE2	2.32	0.62
1:B:4900:GLU:N	1:B:4900:GLU:OE2	2.32	0.62
1:D:2205:GLU:OE2	1:D:2205:GLU:N	2.32	0.62
1:D:210:GLU:HB3	1:D:273:HIS:HE1	1.64	0.62
1:D:1954:ARG:NH1	1:D:2042:CYS:SG	2.72	0.62
1:D:4817:ALA:C	1:D:4819:GLY:H	2.02	0.62
1:B:1072:VAL:HG12	1:B:1195:GLY:HA2	1.80	0.62
1:B:3658:LYS:HA	1:B:3661:TRP:CE3	2.34	0.62
1:C:4900:GLU:OE2	1:C:4900:GLU:N	2.32	0.62
1:D:4900:GLU:N	1:D:4900:GLU:OE2	2.32	0.62
1:A:210:GLU:HB3	1:A:273:HIS:HE1	1.64	0.62
1:A:1647:CYS:SG	1:A:1648:MET:N	2.73	0.62
1:B:210:GLU:HB3	1:B:273:HIS:HE1	1.64	0.62
1:C:3658:LYS:HA	1:C:3661:TRP:CE3	2.34	0.62
1:C:4817:ALA:O	1:C:4819:GLY:N	2.33	0.62
1:A:2205:GLU:N	1:A:2205:GLU:OE2	2.32	0.62
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.82	0.62
1:B:4666:VAL:HG22	1:B:4783:ILE:HD11	1.82	0.62
1:C:1647:CYS:SG	1:C:1648:MET:N	2.73	0.62
1:D:553:ARG:HE	1:D:593:HIS:HE1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1743:ARG:O	1:D:1964:ARG:NH2	2.33	0.62
1:D:4666:VAL:HG22	1:D:4783:ILE:HD11	1.82	0.62
1:B:1647:CYS:SG	1:B:1648:MET:N	2.73	0.62
1:B:4224:GLU:N	1:B:4224:GLU:OE2	2.33	0.62
1:D:455:PRO:HB2	1:D:464:LYS:HZ3	1.65	0.62
1:A:553:ARG:HE	1:A:593:HIS:HE1	1.47	0.61
1:D:1647:CYS:SG	1:D:1648:MET:N	2.73	0.61
1:A:597:HIS:HB3	1:A:1665:HIS:HD2	1.65	0.61
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.82	0.61
1:D:3658:LYS:HA	1:D:3661:TRP:CE3	2.34	0.61
1:A:4666:VAL:HG22	1:A:4783:ILE:HD11	1.82	0.61
1:B:1743:ARG:O	1:B:1964:ARG:NH2	2.33	0.61
1:B:3935:TRP:CH2	1:C:77:ALA:HB2	2.36	0.61
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.82	0.61
1:C:3897:ASN:H	1:C:3900:GLN:HE21	1.48	0.61
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.82	0.61
1:A:4817:ALA:O	1:A:4819:GLY:N	2.33	0.61
1:B:597:HIS:HB3	1:B:1665:HIS:HD2	1.65	0.61
1:B:720:HIS:HA	1:B:729:PRO:HA	1.82	0.61
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.33	0.61
1:C:1954:ARG:NH1	1:C:2042:CYS:SG	2.72	0.61
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.33	0.61
1:A:1954:ARG:NH1	1:A:2042:CYS:SG	2.72	0.61
1:B:4817:ALA:O	1:B:4819:GLY:N	2.33	0.61
1:C:597:HIS:HB3	1:C:1665:HIS:CD2	2.36	0.61
1:D:597:HIS:HB3	1:D:1665:HIS:CD2	2.36	0.61
1:D:4224:GLU:OE2	1:D:4224:GLU:N	2.33	0.61
1:A:1743:ARG:O	1:A:1964:ARG:NH2	2.33	0.61
1:C:720:HIS:HA	1:C:729:PRO:HA	1.82	0.61
1:C:4666:VAL:HG22	1:C:4783:ILE:HD11	1.82	0.61
1:A:4224:GLU:N	1:A:4224:GLU:OE2	2.33	0.61
1:C:3935:TRP:CH2	1:D:77:ALA:HB2	2.36	0.61
1:D:4820:VAL:O	1:D:4821:LYS:C	2.39	0.61
1:B:2026:ASP:O	1:B:2029:GLN:NE2	2.29	0.61
1:B:2281:ILE:HG23	1:B:2341:VAL:HG11	1.83	0.61
1:C:455:PRO:HB2	1:C:464:LYS:HZ3	1.66	0.61
1:C:2257:LEU:HD11	1:C:2276:ALA:HB2	1.82	0.61
1:C:4224:GLU:N	1:C:4224:GLU:OE2	2.33	0.61
1:D:4817:ALA:O	1:D:4819:GLY:N	2.33	0.61
1:D:597:HIS:HB3	1:D:1665:HIS:HD2	1.65	0.61
1:D:2026:ASP:O	1:D:2029:GLN:NE2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:HIS:HA	1:A:729:PRO:HA	1.82	0.60
1:A:893:TYR:HB2	1:A:907:LEU:HB2	1.83	0.60
1:A:3896:ASN:HD22	1:A:3899:PHE:HB2	1.66	0.60
1:B:15:ARG:NH2	1:B:98:HIS:O	2.34	0.60
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.33	0.60
1:D:2281:ILE:HG23	1:D:2341:VAL:HG11	1.83	0.60
1:C:893:TYR:HB2	1:C:907:LEU:HB2	1.83	0.60
1:C:3896:ASN:HD22	1:C:3899:PHE:HB2	1.66	0.60
1:D:720:HIS:HA	1:D:729:PRO:HA	1.82	0.60
1:A:15:ARG:NH2	1:A:98:HIS:O	2.34	0.60
1:A:77:ALA:HB2	1:D:3935:TRP:CH2	2.36	0.60
1:B:893:TYR:HB2	1:B:907:LEU:HB2	1.83	0.60
1:B:4958:CYS:SG	1:B:4961:CYS:O	2.60	0.60
1:C:597:HIS:HB3	1:C:1665:HIS:HD2	1.65	0.60
1:C:4820:VAL:O	1:C:4821:LYS:C	2.39	0.60
1:D:15:ARG:NH2	1:D:98:HIS:O	2.34	0.60
1:D:19:GLU:HB2	1:D:206:CYS:HB3	1.83	0.60
1:D:4958:CYS:SG	1:D:4961:CYS:O	2.60	0.60
1:C:2281:ILE:HG23	1:C:2341:VAL:HG11	1.83	0.60
1:A:19:GLU:HB2	1:A:206:CYS:HB3	1.83	0.60
1:A:2257:LEU:HD11	1:A:2276:ALA:HB2	1.82	0.60
1:C:1939:MET:N	1:C:1939:MET:SD	2.75	0.60
1:D:3897:ASN:H	1:D:3900:GLN:HE21	1.48	0.60
1:A:4958:CYS:SG	1:A:4961:CYS:O	2.60	0.60
1:B:597:HIS:HB3	1:B:1665:HIS:CD2	2.36	0.60
1:C:15:ARG:NH2	1:C:98:HIS:O	2.34	0.60
1:D:1996:ARG:O	1:D:1996:ARG:NH1	2.27	0.60
1:D:3896:ASN:HD22	1:D:3899:PHE:HB2	1.66	0.60
1:C:4206:GLU:N	1:C:4206:GLU:OE2	2.35	0.60
1:A:1243:PRO:HA	1:A:1601:MET:O	2.02	0.60
1:A:2281:ILE:HG23	1:A:2341:VAL:HG11	1.83	0.60
1:B:2116:LEU:O	1:B:2120:MET:HG3	2.02	0.60
1:C:794:GLY:H	1:C:798:GLY:HA3	1.66	0.60
1:D:456:SER:OG	1:D:457:GLU:N	2.35	0.60
1:A:597:HIS:HB3	1:A:1665:HIS:CD2	2.36	0.60
1:B:19:GLU:HB2	1:B:206:CYS:HB3	1.83	0.60
1:B:2257:LEU:HD11	1:B:2276:ALA:HB2	1.82	0.60
1:B:3897:ASN:H	1:B:3900:GLN:HE21	1.48	0.60
1:C:456:SER:OG	1:C:457:GLU:N	2.35	0.60
1:D:1243:PRO:HA	1:D:1601:MET:O	2.02	0.60
1:D:4206:GLU:N	1:D:4206:GLU:OE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:GLY:H	1:A:798:GLY:HA3	1.66	0.60
1:B:1939:MET:SD	1:B:1939:MET:N	2.75	0.60
1:B:4820:VAL:O	1:B:4821:LYS:C	2.39	0.60
1:C:1743:ARG:O	1:C:1964:ARG:NH2	2.33	0.60
1:C:2149:VAL:O	1:C:2153:MET:HG2	2.02	0.60
1:C:4958:CYS:SG	1:C:4961:CYS:O	2.60	0.60
1:D:893:TYR:HB2	1:D:907:LEU:HB2	1.83	0.60
1:B:1929:MET:SD	1:B:1929:MET:N	2.75	0.59
1:D:1929:MET:N	1:D:1929:MET:SD	2.75	0.59
1:D:4731:ILE:HG23	1:D:4732:PHE:HD1	1.67	0.59
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.33	0.59
1:B:2149:VAL:O	1:B:2153:MET:HG2	2.02	0.59
1:C:1929:MET:N	1:C:1929:MET:SD	2.75	0.59
1:D:2149:VAL:O	1:D:2153:MET:HG2	2.02	0.59
1:A:2116:LEU:O	1:A:2120:MET:HG3	2.02	0.59
1:A:765:GLN:HB2	1:A:1520:VAL:HA	1.85	0.59
1:A:1996:ARG:O	1:A:1996:ARG:NH1	2.27	0.59
1:A:3935:TRP:CH2	1:B:77:ALA:HB2	2.36	0.59
1:D:765:GLN:HB2	1:D:1520:VAL:HA	1.85	0.59
1:D:794:GLY:H	1:D:798:GLY:HA3	1.66	0.59
1:A:4731:ILE:HG23	1:A:4732:PHE:HD1	1.67	0.59
1:B:456:SER:OG	1:B:457:GLU:N	2.35	0.59
1:B:1111:PRO:HD3	1:B:1605:TRP:HE1	1.68	0.59
1:C:765:GLN:HB2	1:C:1520:VAL:HA	1.85	0.59
1:A:4820:VAL:O	1:A:4821:LYS:C	2.39	0.59
1:B:1243:PRO:HA	1:B:1601:MET:O	2.02	0.59
1:B:3896:ASN:HD22	1:B:3899:PHE:HB2	1.66	0.59
1:C:1243:PRO:HA	1:C:1601:MET:O	2.02	0.59
1:D:1939:MET:N	1:D:1939:MET:SD	2.75	0.59
1:A:3897:ASN:H	1:A:3900:GLN:HE21	1.48	0.59
1:B:765:GLN:HB2	1:B:1520:VAL:HA	1.85	0.59
1:B:1996:ARG:O	1:B:1996:ARG:NH1	2.27	0.59
1:C:4731:ILE:HG23	1:C:4732:PHE:HD1	1.67	0.59
1:A:70:GLU:HB2	1:A:108:LEU:HD22	1.85	0.59
1:A:150:MET:HG2	1:A:169:LEU:HD12	1.85	0.59
1:A:1111:PRO:HD3	1:A:1605:TRP:HE1	1.68	0.59
1:B:4206:GLU:N	1:B:4206:GLU:OE2	2.35	0.59
1:D:2116:LEU:O	1:D:2120:MET:HG3	2.02	0.59
1:A:1939:MET:N	1:A:1939:MET:SD	2.75	0.59
1:B:794:GLY:H	1:B:798:GLY:HA3	1.66	0.59
1:C:73:LEU:O	1:C:106:ALA:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1111:PRO:HD3	1:C:1605:TRP:HE1	1.68	0.59
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.85	0.59
1:D:2257:LEU:HD11	1:D:2276:ALA:HB2	1.82	0.59
1:D:2292:GLU:N	1:D:2292:GLU:OE2	2.36	0.59
1:B:4731:ILE:HG23	1:B:4732:PHE:HD1	1.67	0.59
1:C:2116:LEU:O	1:C:2120:MET:HG3	2.02	0.59
1:D:1111:PRO:HD3	1:D:1605:TRP:HE1	1.68	0.59
1:A:4206:GLU:N	1:A:4206:GLU:OE2	2.35	0.58
1:D:70:GLU:HB2	1:D:108:LEU:HD22	1.85	0.58
1:C:19:GLU:HB2	1:C:206:CYS:HB3	1.83	0.58
1:C:2026:ASP:O	1:C:2029:GLN:NE2	2.29	0.58
1:C:2205:GLU:N	1:C:2205:GLU:OE2	2.32	0.58
1:D:3825:GLU:OE1	1:D:3825:GLU:N	2.36	0.58
1:A:315:CYS:SG	1:A:316:PHE:N	2.76	0.58
1:A:456:SER:OG	1:A:457:GLU:N	2.35	0.58
1:A:5033:GLU:HA	1:A:5037:SER:HB2	1.85	0.58
1:B:455:PRO:HB2	1:B:464:LYS:HZ3	1.68	0.58
1:B:2353:VAL:O	1:B:2357:LEU:HG	2.03	0.58
1:D:315:CYS:SG	1:D:316:PHE:N	2.76	0.58
1:A:2149:VAL:O	1:A:2153:MET:HG2	2.02	0.58
1:A:2292:GLU:OE2	1:A:2292:GLU:N	2.36	0.58
1:C:70:GLU:HB2	1:C:108:LEU:HD22	1.85	0.58
1:B:73:LEU:O	1:B:106:ALA:N	2.35	0.58
1:B:4031:LEU:HD23	1:B:4034:ASN:HD21	1.69	0.58
1:C:2292:GLU:N	1:C:2292:GLU:OE2	2.36	0.58
1:D:1085:SER:O	1:D:1088:TRP:NE1	2.37	0.58
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.85	0.58
1:B:2292:GLU:N	1:B:2292:GLU:OE2	2.36	0.58
1:B:3825:GLU:OE1	1:B:3825:GLU:N	2.36	0.58
1:C:150:MET:HG2	1:C:169:LEU:HD12	1.85	0.58
1:C:315:CYS:SG	1:C:316:PHE:N	2.76	0.58
1:C:5033:GLU:HA	1:C:5037:SER:HB2	1.85	0.58
1:D:1196:PRO:O	1:D:1198:GLN:NE2	2.36	0.58
1:B:150:MET:HG2	1:B:169:LEU:HD12	1.85	0.58
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.85	0.58
1:B:70:GLU:HB2	1:B:108:LEU:HD22	1.85	0.58
1:A:1929:MET:N	1:A:1929:MET:SD	2.75	0.58
1:C:2353:VAL:O	1:C:2357:LEU:HG	2.03	0.58
1:D:2353:VAL:O	1:D:2357:LEU:HG	2.03	0.58
1:D:5033:GLU:HA	1:D:5037:SER:HB2	1.85	0.58
1:A:76:ARG:O	1:A:79:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:CYS:SG	1:B:316:PHE:N	2.76	0.57
1:B:5033:GLU:HA	1:B:5037:SER:HB2	1.85	0.57
1:C:1089:TYR:HB2	1:C:1152:MET:HG3	1.86	0.57
1:C:4031:LEU:HD23	1:C:4034:ASN:HD21	1.69	0.57
1:D:150:MET:HG2	1:D:169:LEU:HD12	1.85	0.57
1:D:4031:LEU:HD23	1:D:4034:ASN:HD21	1.69	0.57
1:A:4823:LEU:O	1:A:4824:ARG:C	2.42	0.57
1:C:209:CYS:SG	1:C:210:GLU:N	2.78	0.57
1:A:1936:LYS:HA	1:A:1939:MET:HG2	1.87	0.57
1:D:1680:ARG:NH1	1:D:1797:ARG:H	2.03	0.57
1:A:2353:VAL:O	1:A:2357:LEU:HG	2.03	0.57
1:C:1936:LYS:HA	1:C:1939:MET:HG2	1.87	0.57
1:D:76:ARG:O	1:D:79:GLN:HG3	2.04	0.57
1:A:1085:SER:O	1:A:1088:TRP:NE1	2.37	0.57
1:A:1089:TYR:HB2	1:A:1152:MET:HG3	1.86	0.57
1:A:1680:ARG:NH1	1:A:1797:ARG:H	2.03	0.57
1:B:76:ARG:O	1:B:79:GLN:HG3	2.04	0.57
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.85	0.57
1:A:3825:GLU:OE1	1:A:3825:GLU:N	2.36	0.57
1:B:209:CYS:SG	1:B:210:GLU:N	2.78	0.57
1:C:1680:ARG:NH1	1:C:1797:ARG:H	2.03	0.57
1:D:4823:LEU:O	1:D:4824:ARG:C	2.42	0.57
1:B:2012:PHE:HB3	1:B:2022:PRO:HD3	1.86	0.57
1:A:2012:PHE:HB3	1:A:2022:PRO:HD3	1.86	0.57
1:B:668:VAL:O	1:B:741:GLU:N	2.35	0.57
1:C:4933:GLN:O	1:C:4937:ILE:HG12	2.05	0.57
1:C:116:MET:HE1	1:C:140:ASP:H	1.68	0.57
1:C:786:GLY:N	1:C:1630:CYS:O	2.38	0.57
1:A:209:CYS:SG	1:A:210:GLU:N	2.78	0.56
1:B:1936:LYS:HA	1:B:1939:MET:HG2	1.87	0.56
1:D:209:CYS:SG	1:D:210:GLU:N	2.78	0.56
1:A:217:GLY:O	1:A:261:ARG:NH1	2.38	0.56
1:A:2209:GLU:HA	1:A:2212:VAL:HG12	1.87	0.56
1:B:217:GLY:O	1:B:261:ARG:NH1	2.38	0.56
1:B:4817:ALA:C	1:B:4819:GLY:N	2.57	0.56
1:B:4933:GLN:O	1:B:4937:ILE:HG12	2.05	0.56
1:C:2012:PHE:HB3	1:C:2022:PRO:HD3	1.86	0.56
1:C:3825:GLU:N	1:C:3825:GLU:OE1	2.36	0.56
1:D:786:GLY:N	1:D:1630:CYS:O	2.38	0.56
1:A:317:ARG:NE	1:A:349:GLN:OE1	2.32	0.56
1:B:786:GLY:N	1:B:1630:CYS:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1085:SER:O	1:B:1088:TRP:NE1	2.37	0.56
1:B:1089:TYR:HB2	1:B:1152:MET:HG3	1.86	0.56
1:B:4769:MET:SD	1:B:4769:MET:N	2.73	0.56
1:C:2209:GLU:HA	1:C:2212:VAL:HG12	1.87	0.56
1:D:1936:LYS:HA	1:D:1939:MET:HG2	1.87	0.56
1:D:2209:GLU:HA	1:D:2212:VAL:HG12	1.87	0.56
1:A:4031:LEU:HD23	1:A:4034:ASN:HD21	1.69	0.56
1:B:2209:GLU:HA	1:B:2212:VAL:HG12	1.87	0.56
1:C:76:ARG:O	1:C:79:GLN:HG3	2.04	0.56
1:C:1196:PRO:O	1:C:1198:GLN:NE2	2.36	0.56
1:A:395:GLN:HG3	1:A:397:GLU:HG3	1.88	0.56
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.38	0.56
1:C:4817:ALA:C	1:C:4819:GLY:N	2.57	0.56
1:D:217:GLY:O	1:D:261:ARG:NH1	2.38	0.56
1:D:1089:TYR:HB2	1:D:1152:MET:HG3	1.86	0.56
1:D:3845:ASN:O	1:D:3848:GLU:HG3	2.06	0.56
1:A:4679:ARG:NH1	1:A:4715:TYR:OH	2.39	0.56
1:B:2438:PRO:HG2	1:B:2454:ARG:HB2	1.87	0.56
1:C:4823:LEU:O	1:C:4824:ARG:C	2.42	0.56
1:D:73:LEU:O	1:D:106:ALA:N	2.35	0.56
1:A:3845:ASN:O	1:A:3848:GLU:HG3	2.06	0.56
1:A:4817:ALA:C	1:A:4819:GLY:N	2.57	0.56
1:D:2012:PHE:HB3	1:D:2022:PRO:HD3	1.86	0.56
1:A:786:GLY:N	1:A:1630:CYS:O	2.38	0.56
1:A:2438:PRO:HG2	1:A:2454:ARG:HB2	1.87	0.56
1:B:1680:ARG:NH1	1:B:1797:ARG:H	2.03	0.56
1:C:217:GLY:O	1:C:261:ARG:NH1	2.38	0.56
1:D:4933:GLN:O	1:D:4937:ILE:HG12	2.05	0.56
1:B:219:VAL:HG12	1:B:261:ARG:HB2	1.88	0.56
1:C:4679:ARG:NH1	1:C:4715:TYR:OH	2.39	0.56
1:A:73:LEU:O	1:A:106:ALA:N	2.35	0.56
1:B:1196:PRO:O	1:B:1198:GLN:NE2	2.36	0.56
1:C:320:LYS:HA	1:C:356:TRP:CH2	2.41	0.56
1:A:763:PRO:O	1:A:765:GLN:NE2	2.39	0.55
1:B:379:HIS:HD2	1:B:381:GLU:H	1.54	0.55
1:B:4679:ARG:NH1	1:B:4715:TYR:OH	2.39	0.55
1:C:2438:PRO:HG2	1:C:2454:ARG:HB2	1.87	0.55
1:C:2467:VAL:HA	1:C:2470:ILE:HB	1.88	0.55
1:C:4769:MET:SD	1:C:4769:MET:N	2.73	0.55
1:A:2467:VAL:HA	1:A:2470:ILE:HB	1.88	0.55
1:A:4090:LYS:HE2	1:A:4112:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLN:HG3	1:B:397:GLU:HG3	1.88	0.55
1:B:763:PRO:O	1:B:765:GLN:NE2	2.39	0.55
1:B:3845:ASN:O	1:B:3848:GLU:HG3	2.06	0.55
1:C:763:PRO:O	1:C:765:GLN:NE2	2.39	0.55
1:C:4090:LYS:HE2	1:C:4112:LEU:HD22	1.88	0.55
1:C:4793:GLY:O	1:C:4796:MET:HB3	2.06	0.55
1:D:2467:VAL:HA	1:D:2470:ILE:HB	1.88	0.55
1:B:320:LYS:HA	1:B:356:TRP:CH2	2.41	0.55
1:C:144:GLU:O	1:C:175:SER:OG	2.24	0.55
1:C:534:ARG:HH22	1:C:572:PRO:HD2	1.72	0.55
1:D:320:LYS:HA	1:D:356:TRP:CH2	2.41	0.55
1:D:4817:ALA:C	1:D:4819:GLY:N	2.57	0.55
1:A:379:HIS:HD2	1:A:381:GLU:H	1.54	0.55
1:B:534:ARG:HH22	1:B:572:PRO:HD2	1.72	0.55
1:B:582:HIS:O	1:B:585:SER:OG	2.18	0.55
1:C:710:ASP:OD1	1:C:710:ASP:N	2.40	0.55
1:C:3845:ASN:O	1:C:3848:GLU:HG3	2.06	0.55
1:D:4679:ARG:NH1	1:D:4715:TYR:OH	2.39	0.55
1:D:4793:GLY:O	1:D:4796:MET:HB3	2.06	0.55
1:D:1653:LEU:HA	1:D:1656:ARG:HB2	1.89	0.55
1:A:534:ARG:HH22	1:A:572:PRO:HD2	1.72	0.55
1:A:4933:GLN:O	1:A:4937:ILE:HG12	2.05	0.55
1:B:2467:VAL:HA	1:B:2470:ILE:HB	1.88	0.55
1:B:4793:GLY:O	1:B:4796:MET:HB3	2.06	0.55
1:C:219:VAL:HG12	1:C:261:ARG:HB2	1.88	0.55
1:D:710:ASP:N	1:D:710:ASP:OD1	2.40	0.55
1:A:144:GLU:O	1:A:175:SER:OG	2.24	0.55
1:A:219:VAL:HG12	1:A:261:ARG:HB2	1.88	0.55
1:A:4793:GLY:O	1:A:4796:MET:HB3	2.06	0.55
1:C:312:THR:OG1	1:C:313:SER:N	2.40	0.55
1:D:395:GLN:HG3	1:D:397:GLU:HG3	1.88	0.55
1:D:4090:LYS:HE2	1:D:4112:LEU:HD22	1.88	0.55
1:C:2629:ASP:O	1:C:2633:LEU:N	2.40	0.55
1:D:534:ARG:HH22	1:D:572:PRO:HD2	1.72	0.55
1:D:763:PRO:O	1:D:765:GLN:NE2	2.39	0.55
1:D:2438:PRO:HG2	1:D:2454:ARG:HB2	1.87	0.55
1:B:4090:LYS:HE2	1:B:4112:LEU:HD22	1.88	0.55
1:C:1085:SER:O	1:C:1088:TRP:NE1	2.37	0.55
1:C:4822:THR:O	1:C:4823:LEU:C	2.44	0.55
1:A:320:LYS:HA	1:A:356:TRP:CH2	2.41	0.55
1:A:2629:ASP:O	1:A:2633:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:GLN:HG3	1:C:397:GLU:HG3	1.88	0.55
1:D:4822:THR:O	1:D:4823:LEU:C	2.44	0.55
1:B:710:ASP:OD1	1:B:710:ASP:N	2.40	0.54
1:C:1653:LEU:HA	1:C:1656:ARG:HB2	1.89	0.54
1:D:4052:SER:HA	1:D:4055:VAL:HG22	1.89	0.54
1:A:182:LEU:HB3	1:A:198:THR:HG21	1.90	0.54
1:B:1152:MET:HB3	1:B:1223:PHE:CE2	2.43	0.54
1:C:1152:MET:HB3	1:C:1223:PHE:CE2	2.43	0.54
1:A:1089:TYR:HE1	1:A:1150:GLY:HA3	1.73	0.54
1:B:1859:VAL:HA	1:B:1862:ILE:HG22	1.90	0.54
1:D:144:GLU:O	1:D:175:SER:OG	2.24	0.54
1:A:565:TYR:O	1:A:569:ILE:HG12	2.08	0.54
1:A:706:GLY:HA3	1:A:782:SER:HB2	1.90	0.54
1:A:710:ASP:N	1:A:710:ASP:OD1	2.40	0.54
1:B:21:VAL:HG12	1:B:66:CYS:HA	1.90	0.54
1:B:4823:LEU:O	1:B:4824:ARG:C	2.42	0.54
1:C:292:ALA:HB2	1:C:312:THR:HG22	1.90	0.54
1:C:2354:VAL:O	1:C:2358:ILE:HG22	2.08	0.54
1:D:1859:VAL:HA	1:D:1862:ILE:HG22	1.90	0.54
1:A:312:THR:OG1	1:A:313:SER:N	2.40	0.54
1:A:1859:VAL:HA	1:A:1862:ILE:HG22	1.90	0.54
1:B:706:GLY:HA3	1:B:782:SER:HB2	1.90	0.54
1:B:5002:GLU:OE1	1:B:5002:GLU:N	2.39	0.54
1:C:1859:VAL:HA	1:C:1862:ILE:HG22	1.90	0.54
1:D:206:CYS:SG	1:D:207:SER:N	2.81	0.54
1:D:213:TYR:CD2	1:D:337:PRO:HB2	2.43	0.54
1:D:379:HIS:HD2	1:D:381:GLU:H	1.54	0.54
1:D:920:TYR:O	1:D:923:GLN:HG3	2.08	0.54
1:A:206:CYS:SG	1:A:207:SER:N	2.81	0.54
1:A:1966:VAL:HG21	1:A:3649:ALA:HB1	1.90	0.54
1:A:2348:GLU:OE1	1:A:2348:GLU:N	2.38	0.54
1:A:4822:THR:O	1:A:4823:LEU:C	2.44	0.54
1:B:182:LEU:HB3	1:B:198:THR:HG21	1.90	0.54
1:C:706:GLY:HA3	1:C:782:SER:HB2	1.90	0.54
1:D:299:LEU:HD23	1:D:377:ILE:HD12	1.90	0.54
1:A:21:VAL:HG12	1:A:66:CYS:HA	1.90	0.54
1:A:5002:GLU:OE1	1:A:5002:GLU:N	2.39	0.54
1:B:1089:TYR:HE1	1:B:1150:GLY:HA3	1.73	0.54
1:B:4052:SER:HA	1:B:4055:VAL:HG22	1.89	0.54
1:C:206:CYS:SG	1:C:207:SER:N	2.81	0.54
1:C:213:TYR:CD2	1:C:337:PRO:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4577:LEU:HD21	1:C:4807:PHE:HA	1.90	0.54
1:D:312:THR:OG1	1:D:313:SER:N	2.40	0.54
1:D:706:GLY:HA3	1:D:782:SER:HB2	1.90	0.54
1:A:1653:LEU:HA	1:A:1656:ARG:HB2	1.89	0.54
1:A:2354:VAL:O	1:A:2358:ILE:HG22	2.08	0.54
1:A:4052:SER:HA	1:A:4055:VAL:HG22	1.89	0.54
1:A:4730:ASP:OD2	1:D:4101:LYS:NZ	2.41	0.54
1:B:206:CYS:SG	1:B:207:SER:N	2.81	0.54
1:B:920:TYR:O	1:B:923:GLN:HG3	2.08	0.54
1:B:4816:ILE:CG2	1:B:4817:ALA:H	2.21	0.54
1:C:379:HIS:HD2	1:C:381:GLU:H	1.54	0.54
1:B:908:VAL:HB	1:B:912:SER:HB3	1.90	0.54
1:B:1653:LEU:HA	1:B:1656:ARG:HB2	1.89	0.54
1:B:2354:VAL:O	1:B:2358:ILE:HG22	2.08	0.54
1:C:908:VAL:HB	1:C:912:SER:HB3	1.90	0.54
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.38	0.54
1:D:565:TYR:O	1:D:569:ILE:HG12	2.08	0.54
1:B:144:GLU:O	1:B:175:SER:OG	2.24	0.53
1:B:299:LEU:HD23	1:B:377:ILE:HD12	1.90	0.53
1:B:2380:ILE:HD13	1:B:2469:ILE:HG13	1.90	0.53
1:B:4961:CYS:SG	1:B:4978:HIS:NE2	2.81	0.53
1:C:21:VAL:HG12	1:C:66:CYS:HA	1.90	0.53
1:C:565:TYR:O	1:C:569:ILE:HG12	2.08	0.53
1:C:4052:SER:HA	1:C:4055:VAL:HG22	1.89	0.53
1:D:908:VAL:HB	1:D:912:SER:HB3	1.90	0.53
1:D:4961:CYS:SG	1:D:4978:HIS:NE2	2.81	0.53
1:A:247:TYR:HB2	1:A:374:LYS:HB2	1.90	0.53
1:A:668:VAL:O	1:A:741:GLU:N	2.35	0.53
1:A:1152:MET:HB3	1:A:1223:PHE:CE2	2.43	0.53
1:A:2380:ILE:HD13	1:A:2469:ILE:HG13	1.90	0.53
1:A:3770:LEU:HD22	1:A:3804:ILE:HD11	1.91	0.53
1:A:4101:LYS:NZ	1:B:4730:ASP:OD2	2.41	0.53
1:D:219:VAL:HG12	1:D:261:ARG:HB2	1.88	0.53
1:D:349:GLN:NE2	1:D:354:GLY:O	2.42	0.53
1:D:2354:VAL:O	1:D:2358:ILE:HG22	2.08	0.53
1:D:3770:LEU:HD22	1:D:3804:ILE:HD11	1.91	0.53
1:D:3777:GLU:N	1:D:3777:GLU:OE2	2.41	0.53
1:B:4658:ILE:HG13	1:B:4796:MET:CE	2.39	0.53
1:C:379:HIS:CD2	1:C:382:GLY:H	2.27	0.53
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.25	0.53
1:D:292:ALA:HB2	1:D:312:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1966:VAL:HG21	1:D:3649:ALA:HB1	1.90	0.53
1:A:564:LEU:HD23	1:A:568:LEU:HD13	1.91	0.53
1:A:863:LEU:HD23	1:A:868:GLU:HA	1.91	0.53
1:A:1196:PRO:O	1:A:1198:GLN:NE2	2.36	0.53
1:B:238:SER:OG	1:B:240:ASP:OD1	2.27	0.53
1:B:4823:LEU:O	1:B:4826:ILE:N	2.42	0.53
1:C:116:MET:HE3	1:C:117:TYR:H	1.74	0.53
1:C:1966:VAL:HG21	1:C:3649:ALA:HB1	1.90	0.53
1:D:1152:MET:HB3	1:D:1223:PHE:CE2	2.43	0.53
1:B:1966:VAL:HG21	1:B:3649:ALA:HB1	1.90	0.53
1:B:4577:LEU:HD21	1:B:4807:PHE:HA	1.90	0.53
1:B:4822:THR:O	1:B:4823:LEU:C	2.44	0.53
1:C:281:ARG:NH1	1:C:307:ALA:O	2.42	0.53
1:C:349:GLN:NE2	1:C:354:GLY:O	2.42	0.53
1:C:668:VAL:O	1:C:741:GLU:N	2.35	0.53
1:C:2380:ILE:HD13	1:C:2469:ILE:HG13	1.90	0.53
1:D:247:TYR:HB2	1:D:374:LYS:HB2	1.90	0.53
1:D:379:HIS:CD2	1:D:382:GLY:H	2.27	0.53
1:A:908:VAL:HB	1:A:912:SER:HB3	1.90	0.53
1:B:564:LEU:HD23	1:B:568:LEU:HD13	1.91	0.53
1:C:299:LEU:HD21	1:C:378:LEU:HG	1.91	0.53
1:C:662:TRP:H	1:C:748:LEU:HG	1.74	0.53
1:C:4101:LYS:NZ	1:D:4730:ASP:OD2	2.41	0.53
1:D:182:LEU:HB3	1:D:198:THR:HG21	1.90	0.53
1:D:564:LEU:HD23	1:D:568:LEU:HD13	1.91	0.53
1:D:1089:TYR:HE1	1:D:1150:GLY:HA3	1.73	0.53
1:A:3777:GLU:N	1:A:3777:GLU:OE2	2.41	0.53
1:A:4823:LEU:O	1:A:4826:ILE:N	2.42	0.53
1:B:131:LEU:HD12	1:B:178:ARG:NH2	2.24	0.53
1:B:247:TYR:HB2	1:B:374:LYS:HB2	1.90	0.53
1:B:662:TRP:H	1:B:748:LEU:HG	1.74	0.53
1:B:3777:GLU:N	1:B:3777:GLU:OE2	2.41	0.53
1:B:4816:ILE:HG12	1:B:4823:LEU:HD12	1.91	0.53
1:C:4823:LEU:O	1:C:4826:ILE:N	2.42	0.53
1:D:3731:LYS:O	1:D:3731:LYS:HD3	2.09	0.53
1:D:4577:LEU:HD21	1:D:4807:PHE:HA	1.90	0.53
1:A:661:LYS:HG2	1:A:748:LEU:HB3	1.91	0.53
1:B:379:HIS:CD2	1:B:382:GLY:H	2.27	0.53
1:B:3731:LYS:O	1:B:3731:LYS:HD3	2.09	0.53
1:C:182:LEU:HB3	1:C:198:THR:HG21	1.90	0.53
1:C:317:ARG:NE	1:C:349:GLN:OE1	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1089:TYR:HE1	1:C:1150:GLY:HA3	1.73	0.53
1:C:3731:LYS:O	1:C:3731:LYS:HD3	2.09	0.53
1:D:21:VAL:HG12	1:D:66:CYS:HA	1.90	0.53
1:D:1077:ALA:HA	1:D:1236:THR:HA	1.91	0.53
1:D:2380:ILE:HD13	1:D:2469:ILE:HG13	1.90	0.53
1:D:4823:LEU:O	1:D:4826:ILE:N	2.42	0.53
1:A:281:ARG:NH1	1:A:307:ALA:O	2.42	0.53
1:A:662:TRP:H	1:A:748:LEU:HG	1.74	0.53
1:A:4769:MET:SD	1:A:4769:MET:N	2.73	0.53
1:B:292:ALA:HB2	1:B:312:THR:HG22	1.90	0.53
1:B:565:TYR:O	1:B:569:ILE:HG12	2.08	0.53
1:B:4101:LYS:NZ	1:C:4730:ASP:OD2	2.41	0.53
1:C:615:ARG:NH2	1:C:1677:GLY:O	2.42	0.53
1:C:3770:LEU:HD22	1:C:3804:ILE:HD11	1.91	0.53
1:C:4658:ILE:HG13	1:C:4796:MET:CE	2.39	0.53
1:D:131:LEU:HD12	1:D:178:ARG:NH2	2.24	0.53
1:D:281:ARG:NH1	1:D:307:ALA:O	2.42	0.53
1:D:299:LEU:HD21	1:D:378:LEU:HG	1.91	0.53
1:D:668:VAL:O	1:D:741:GLU:N	2.35	0.53
1:A:920:TYR:O	1:A:923:GLN:HG3	2.08	0.52
1:A:1680:ARG:HH12	1:A:1797:ARG:H	1.56	0.52
1:A:4816:ILE:HG12	1:A:4823:LEU:HD12	1.91	0.52
1:B:213:TYR:CD2	1:B:337:PRO:HB2	2.43	0.52
1:B:281:ARG:NH1	1:B:307:ALA:O	2.42	0.52
1:B:349:GLN:NE2	1:B:354:GLY:O	2.42	0.52
1:B:3770:LEU:HD22	1:B:3804:ILE:HD11	1.91	0.52
1:C:247:TYR:HB2	1:C:374:LYS:HB2	1.90	0.52
1:C:299:LEU:HD23	1:C:377:ILE:HD12	1.90	0.52
1:C:564:LEU:HD23	1:C:568:LEU:HD13	1.91	0.52
1:C:920:TYR:O	1:C:923:GLN:HG3	2.08	0.52
1:C:3777:GLU:N	1:C:3777:GLU:OE2	2.41	0.52
1:D:317:ARG:NE	1:D:349:GLN:OE1	2.32	0.52
1:D:662:TRP:H	1:D:748:LEU:HG	1.74	0.52
1:D:863:LEU:HD23	1:D:868:GLU:HA	1.91	0.52
1:A:379:HIS:CD2	1:A:382:GLY:H	2.27	0.52
1:A:3731:LYS:O	1:A:3731:LYS:HD3	2.09	0.52
1:A:4658:ILE:HG13	1:A:4796:MET:CE	2.39	0.52
1:B:1680:ARG:HH12	1:B:1797:ARG:H	1.56	0.52
1:C:3778:MET:HA	1:C:3781:GLN:HE21	1.75	0.52
1:A:299:LEU:HD21	1:A:378:LEU:HG	1.91	0.52
1:A:1105:ALA:O	1:A:1189:LEU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3778:MET:HA	1:A:3781:GLN:HE21	1.75	0.52
1:A:4577:LEU:HD21	1:A:4807:PHE:HA	1.90	0.52
1:B:615:ARG:NH2	1:B:1677:GLY:O	2.42	0.52
1:C:4690:GLU:N	1:C:4690:GLU:OE2	2.43	0.52
1:C:4816:ILE:CG2	1:C:4817:ALA:H	2.21	0.52
1:D:116:MET:HE3	1:D:117:TYR:H	1.75	0.52
1:D:4198:SER:OG	1:D:4199:GLU:N	2.43	0.52
1:A:4816:ILE:CG2	1:A:4817:ALA:H	2.21	0.52
1:B:2025:GLU:HA	1:B:2028:ARG:HE	1.74	0.52
1:B:4198:SER:OG	1:B:4199:GLU:N	2.43	0.52
1:D:238:SER:OG	1:D:240:ASP:OD1	2.27	0.52
1:D:3778:MET:HA	1:D:3781:GLN:HE21	1.75	0.52
1:A:131:LEU:HD12	1:A:178:ARG:NH2	2.24	0.52
1:A:292:ALA:HB2	1:A:312:THR:HG22	1.90	0.52
1:A:299:LEU:HD23	1:A:377:ILE:HD12	1.90	0.52
1:A:615:ARG:NH2	1:A:1677:GLY:O	2.42	0.52
1:A:4961:CYS:SG	1:A:4978:HIS:NE2	2.81	0.52
1:B:1240:LYS:O	1:B:1603:VAL:HA	2.10	0.52
1:B:4690:GLU:N	1:B:4690:GLU:OE2	2.43	0.52
1:C:863:LEU:HD23	1:C:868:GLU:HA	1.91	0.52
1:C:1077:ALA:HA	1:C:1236:THR:HA	1.91	0.52
1:C:2025:GLU:HA	1:C:2028:ARG:HE	1.74	0.52
1:A:758:ARG:HG3	1:A:763:PRO:HB3	1.91	0.52
1:B:312:THR:OG1	1:B:313:SER:N	2.40	0.52
1:B:1077:ALA:HA	1:B:1236:THR:HA	1.91	0.52
1:C:3940:LYS:NZ	1:C:3942:VAL:O	2.35	0.52
1:D:4690:GLU:N	1:D:4690:GLU:OE2	2.43	0.52
1:A:213:TYR:CD2	1:A:337:PRO:HB2	2.43	0.52
1:B:299:LEU:HD21	1:B:378:LEU:HG	1.91	0.52
1:B:1155:LEU:HD12	1:B:1155:LEU:H	1.75	0.52
1:C:1240:LYS:O	1:C:1603:VAL:HA	2.10	0.52
1:C:1680:ARG:HH12	1:C:1797:ARG:H	1.56	0.52
1:D:661:LYS:HG2	1:D:748:LEU:HB3	1.91	0.52
1:D:1240:LYS:O	1:D:1603:VAL:HA	2.10	0.52
1:A:1077:ALA:HA	1:A:1236:THR:HA	1.91	0.52
1:A:1155:LEU:H	1:A:1155:LEU:HD12	1.75	0.52
1:A:4198:SER:OG	1:A:4199:GLU:N	2.43	0.52
1:A:4690:GLU:N	1:A:4690:GLU:OE2	2.43	0.52
1:B:661:LYS:HG2	1:B:748:LEU:HB3	1.91	0.52
1:C:1259:ARG:NH2	1:C:1595:LEU:O	2.43	0.52
1:C:3726:ALA:HA	1:C:3729:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4658:ILE:HG13	1:D:4796:MET:CE	2.39	0.52
1:B:2629:ASP:O	1:B:2633:LEU:N	2.40	0.52
1:C:1814:MET:O	1:C:1817:GLU:HG3	2.10	0.52
1:D:1680:ARG:HH12	1:D:1797:ARG:H	1.56	0.52
1:A:303:ASP:H	1:A:306:LYS:NZ	2.07	0.52
1:A:4044:MET:HE2	1:A:4044:MET:N	2.25	0.52
1:B:577:ILE:O	1:B:579:GLN:NE2	2.39	0.52
1:B:3778:MET:HA	1:B:3781:GLN:HE21	1.75	0.52
1:C:2207:VAL:HA	1:C:2210:VAL:HG12	1.92	0.52
1:D:582:HIS:O	1:D:585:SER:OG	2.18	0.52
1:D:2025:GLU:HA	1:D:2028:ARG:HE	1.74	0.52
1:A:2025:GLU:HA	1:A:2028:ARG:HE	1.74	0.51
1:B:1965:TYR:OH	1:B:2027:ILE:O	2.22	0.51
1:D:758:ARG:HG3	1:D:763:PRO:HB3	1.91	0.51
1:A:349:GLN:NE2	1:A:354:GLY:O	2.42	0.51
1:B:1105:ALA:O	1:B:1189:LEU:N	2.43	0.51
1:D:303:ASP:H	1:D:306:LYS:NZ	2.07	0.51
1:B:863:LEU:HD23	1:B:868:GLU:HA	1.91	0.51
1:B:1814:MET:O	1:B:1817:GLU:HG3	2.10	0.51
1:B:3726:ALA:HA	1:B:3729:MET:HE3	1.92	0.51
1:C:661:LYS:HG2	1:C:748:LEU:HB3	1.91	0.51
1:D:615:ARG:NH2	1:D:1677:GLY:O	2.42	0.51
1:D:747:CYS:SG	1:D:756:SER:N	2.84	0.51
1:D:1259:ARG:NH2	1:D:1595:LEU:O	2.43	0.51
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.38	0.51
1:B:758:ARG:HG3	1:B:763:PRO:HB3	1.91	0.51
1:B:4688:ILE:HD12	1:B:4737:ILE:HD12	1.92	0.51
1:C:4661:TYR:HH	1:C:4788:SER:HG	1.37	0.51
1:C:5002:GLU:OE1	1:C:5002:GLU:N	2.39	0.51
1:D:2629:ASP:O	1:D:2633:LEU:N	2.40	0.51
1:D:4769:MET:SD	1:D:4769:MET:N	2.73	0.51
1:D:4816:ILE:HG12	1:D:4823:LEU:HD12	1.91	0.51
1:A:1240:LYS:O	1:A:1603:VAL:HA	2.10	0.51
1:A:2206:THR:HA	1:A:2209:GLU:OE2	2.11	0.51
1:B:3658:LYS:HD2	1:B:3661:TRP:CE3	2.46	0.51
1:C:747:CYS:SG	1:C:756:SER:N	2.84	0.51
1:C:758:ARG:HG3	1:C:763:PRO:HB3	1.91	0.51
1:C:1749:PRO:HB3	1:C:1760:HIS:HA	1.93	0.51
1:C:3658:LYS:HD2	1:C:3661:TRP:CE3	2.46	0.51
1:C:4798:MET:HB3	1:C:4812:HIS:CE1	2.46	0.51
1:A:116:MET:HE3	1:A:117:TYR:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4688:ILE:HD12	1:A:4737:ILE:HD12	1.92	0.51
1:B:257:ARG:O	1:B:284:HIS:NE2	2.44	0.51
1:C:131:LEU:HD12	1:C:178:ARG:NH2	2.24	0.51
1:C:2206:THR:HA	1:C:2209:GLU:OE2	2.11	0.51
1:C:4897:ILE:HG13	1:C:4901:ILE:HD11	1.93	0.51
1:D:3726:ALA:HA	1:D:3729:MET:HE3	1.92	0.51
1:A:747:CYS:SG	1:A:756:SER:N	2.84	0.51
1:B:197:GLN:OE1	1:B:197:GLN:N	2.44	0.51
1:B:2206:THR:HA	1:B:2209:GLU:OE2	2.11	0.51
1:B:3680:ALA:HB3	1:B:3697:PRO:HG2	1.92	0.51
1:B:4798:MET:HB3	1:B:4812:HIS:CE1	2.46	0.51
1:C:4688:ILE:HD12	1:C:4737:ILE:HD12	1.92	0.51
1:C:4816:ILE:HG12	1:C:4823:LEU:HD12	1.91	0.51
1:D:197:GLN:N	1:D:197:GLN:OE1	2.44	0.51
1:D:4819:GLY:O	1:D:4820:VAL:C	2.49	0.51
1:A:207:SER:OG	1:A:208:CYS:N	2.44	0.51
1:A:238:SER:OG	1:A:240:ASP:OD1	2.27	0.51
1:A:3658:LYS:HD2	1:A:3661:TRP:CE3	2.46	0.51
1:B:1259:ARG:NH2	1:B:1595:LEU:O	2.43	0.51
1:C:238:SER:OG	1:C:240:ASP:OD1	2.27	0.51
1:C:2024:PRO:O	1:C:2028:ARG:NH2	2.30	0.51
1:D:2207:VAL:HA	1:D:2210:VAL:HG12	1.92	0.51
1:D:3680:ALA:HB3	1:D:3697:PRO:HG2	1.92	0.51
1:D:4897:ILE:HG13	1:D:4901:ILE:HD11	1.93	0.51
1:B:3973:CYS:SG	1:B:3976:ASN:ND2	2.83	0.51
1:C:197:GLN:OE1	1:C:197:GLN:N	2.44	0.51
1:C:1155:LEU:H	1:C:1155:LEU:HD12	1.75	0.51
1:D:116:MET:HE1	1:D:140:ASP:H	1.75	0.51
1:D:1155:LEU:H	1:D:1155:LEU:HD12	1.75	0.51
1:D:1749:PRO:HB3	1:D:1760:HIS:HA	1.93	0.51
1:D:5002:GLU:N	1:D:5002:GLU:OE1	2.39	0.51
1:A:116:MET:HE1	1:A:140:ASP:H	1.75	0.51
1:A:3726:ALA:HA	1:A:3729:MET:HE3	1.92	0.51
1:B:143:GLY:HA2	1:B:146:CYS:SG	2.51	0.51
1:C:303:ASP:H	1:C:306:LYS:NZ	2.07	0.51
1:C:4186:ALA:H	1:C:4188:ARG:HH22	1.59	0.51
1:B:317:ARG:NE	1:B:349:GLN:OE1	2.32	0.50
1:B:747:CYS:SG	1:B:756:SER:N	2.84	0.50
1:A:2207:VAL:HA	1:A:2210:VAL:HG12	1.92	0.50
1:A:2302:LEU:HD23	1:A:2363:CYS:HB2	1.93	0.50
1:A:4798:MET:HB3	1:A:4812:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ASP:H	1:B:306:LYS:NZ	2.07	0.50
1:D:4186:ALA:H	1:D:4188:ARG:HH22	1.59	0.50
1:A:257:ARG:O	1:A:284:HIS:NE2	2.44	0.50
1:A:3680:ALA:HB3	1:A:3697:PRO:HG2	1.92	0.50
1:A:4897:ILE:HG13	1:A:4901:ILE:HD11	1.93	0.50
1:B:886:ARG:HB3	1:B:891:TRP:HB2	1.94	0.50
1:B:1703:LEU:HB3	1:B:1708:ARG:HE	1.77	0.50
1:B:4186:ALA:H	1:B:4188:ARG:HH22	1.59	0.50
1:D:1703:LEU:HB3	1:D:1708:ARG:HE	1.77	0.50
1:D:1814:MET:O	1:D:1817:GLU:HG3	2.10	0.50
1:D:4688:ILE:HD12	1:D:4737:ILE:HD12	1.92	0.50
1:A:4658:ILE:HG13	1:A:4796:MET:HE2	1.92	0.50
1:B:1749:PRO:HB3	1:B:1760:HIS:HA	1.93	0.50
1:C:530:ILE:HD11	1:C:537:CYS:HA	1.93	0.50
1:C:4003:LEU:HB2	1:C:4013:LEU:HD13	1.94	0.50
1:C:4198:SER:OG	1:C:4199:GLU:N	2.43	0.50
1:D:143:GLY:HA2	1:D:146:CYS:SG	2.51	0.50
1:D:2206:THR:HA	1:D:2209:GLU:OE2	2.11	0.50
1:D:4816:ILE:CG2	1:D:4817:ALA:H	2.21	0.50
1:A:197:GLN:N	1:A:197:GLN:OE1	2.44	0.50
1:A:223:PHE:CD1	1:A:230:CYS:HB3	2.46	0.50
1:B:207:SER:OG	1:B:208:CYS:N	2.44	0.50
1:B:2302:LEU:HD23	1:B:2363:CYS:HB2	1.93	0.50
1:C:223:PHE:HD1	1:C:230:CYS:HB3	1.76	0.50
1:C:1164:LEU:O	1:C:1167:GLU:HG3	2.12	0.50
1:D:4798:MET:HB3	1:D:4812:HIS:CE1	2.46	0.50
1:A:577:ILE:O	1:A:579:GLN:NE2	2.39	0.50
1:A:886:ARG:HB3	1:A:891:TRP:HB2	1.94	0.50
1:A:1164:LEU:O	1:A:1167:GLU:HG3	2.12	0.50
1:A:4573:ILE:HA	1:A:4576:ILE:HG22	1.94	0.50
1:B:929:LEU:HD23	1:B:932:LEU:HD21	1.93	0.50
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.45	0.50
1:C:1703:LEU:HB3	1:C:1708:ARG:HE	1.77	0.50
1:D:207:SER:OG	1:D:208:CYS:N	2.44	0.50
1:D:1164:LEU:O	1:D:1167:GLU:HG3	2.12	0.50
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.45	0.50
1:D:2348:GLU:OE1	1:D:2348:GLU:N	2.38	0.50
1:D:4573:ILE:HA	1:D:4576:ILE:HG22	1.94	0.50
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.45	0.50
1:A:4186:ALA:H	1:A:4188:ARG:HH22	1.59	0.50
1:B:2207:VAL:HA	1:B:2210:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3734:HIS:O	1:B:3738:GLY:N	2.43	0.50
1:B:4897:ILE:HG13	1:B:4901:ILE:HD11	1.93	0.50
1:C:143:GLY:HA2	1:C:146:CYS:SG	2.51	0.50
1:C:229:GLU:HA	1:C:248:GLU:O	2.12	0.50
1:C:929:LEU:HD23	1:C:932:LEU:HD21	1.93	0.50
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.45	0.50
1:C:3680:ALA:HB3	1:C:3697:PRO:HG2	1.92	0.50
1:D:223:PHE:CD1	1:D:230:CYS:HB3	2.46	0.50
1:D:530:ILE:HD11	1:D:537:CYS:HA	1.93	0.50
1:A:1814:MET:O	1:A:1817:GLU:HG3	2.10	0.50
1:B:229:GLU:HA	1:B:248:GLU:O	2.12	0.50
1:C:1105:ALA:O	1:C:1189:LEU:N	2.43	0.50
1:C:2302:LEU:HD23	1:C:2363:CYS:HB2	1.93	0.50
1:D:229:GLU:HA	1:D:248:GLU:O	2.12	0.50
1:D:3658:LYS:HD2	1:D:3661:TRP:CE3	2.46	0.50
1:A:3734:HIS:O	1:A:3738:GLY:N	2.43	0.50
1:B:4044:MET:N	1:B:4044:MET:HE2	2.27	0.50
1:C:207:SER:OG	1:C:208:CYS:N	2.44	0.50
1:C:223:PHE:CD1	1:C:230:CYS:HB3	2.46	0.50
1:D:4003:LEU:HB2	1:D:4013:LEU:HD13	1.94	0.50
1:A:1749:PRO:HB3	1:A:1760:HIS:HA	1.93	0.49
1:A:4819:GLY:O	1:A:4820:VAL:C	2.49	0.49
1:B:223:PHE:CD1	1:B:230:CYS:HB3	2.46	0.49
1:C:4961:CYS:SG	1:C:4978:HIS:NE2	2.81	0.49
1:D:929:LEU:HD23	1:D:932:LEU:HD21	1.93	0.49
1:D:2302:LEU:HD23	1:D:2363:CYS:HB2	1.93	0.49
1:A:1259:ARG:NH2	1:A:1595:LEU:O	2.43	0.49
1:A:1703:LEU:HB3	1:A:1708:ARG:HE	1.77	0.49
1:A:4172:GLU:OE2	1:A:4175:ARG:NH1	2.46	0.49
1:B:530:ILE:HD11	1:B:537:CYS:HA	1.93	0.49
1:B:1164:LEU:O	1:B:1167:GLU:HG3	2.12	0.49
1:B:4006:ASP:OD1	1:B:4007:SER:N	2.45	0.49
1:C:4006:ASP:OD1	1:C:4007:SER:N	2.45	0.49
1:D:1105:ALA:O	1:D:1189:LEU:N	2.43	0.49
1:D:4044:MET:N	1:D:4044:MET:HE2	2.27	0.49
1:D:4056:GLU:HB2	1:D:4166:LEU:HD13	1.94	0.49
1:A:229:GLU:HA	1:A:248:GLU:O	2.12	0.49
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.31	0.49
1:B:3999:MET:HG3	1:B:4016:LEU:HD22	1.95	0.49
1:B:4003:LEU:HB2	1:B:4013:LEU:HD13	1.94	0.49
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:SER:HB2	1:A:34:LYS:HZ2	1.77	0.49
1:A:670:GLU:H	1:A:740:PRO:HB3	1.78	0.49
1:A:891:TRP:CE3	1:A:904:HIS:HB2	2.48	0.49
1:B:670:GLU:H	1:B:740:PRO:HB3	1.78	0.49
1:C:1243:PRO:HB2	1:C:1600:LEU:HD12	1.95	0.49
1:D:223:PHE:HD1	1:D:230:CYS:HB3	1.76	0.49
1:D:1243:PRO:HB2	1:D:1600:LEU:HD12	1.95	0.49
1:D:3734:HIS:O	1:D:3738:GLY:N	2.43	0.49
1:A:143:GLY:HA2	1:A:146:CYS:SG	2.51	0.49
1:A:223:PHE:HD1	1:A:230:CYS:HB3	1.76	0.49
1:A:1243:PRO:HB2	1:A:1600:LEU:HD12	1.95	0.49
1:A:3999:MET:HG3	1:A:4016:LEU:HD22	1.95	0.49
1:B:223:PHE:HD1	1:B:230:CYS:HB3	1.76	0.49
1:B:4172:GLU:OE2	1:B:4175:ARG:NH1	2.46	0.49
1:D:891:TRP:CE3	1:D:904:HIS:HB2	2.48	0.49
1:D:3999:MET:HG3	1:D:4016:LEU:HD22	1.95	0.49
1:D:4006:ASP:OD1	1:D:4007:SER:N	2.45	0.49
1:D:4632:LEU:HD12	1:D:4633:GLU:H	1.78	0.49
1:A:929:LEU:HD23	1:A:932:LEU:HD21	1.93	0.49
1:A:4006:ASP:OD1	1:A:4007:SER:N	2.45	0.49
1:A:4056:GLU:HB2	1:A:4166:LEU:HD13	1.94	0.49
1:B:4573:ILE:HA	1:B:4576:ILE:HG22	1.94	0.49
1:C:54:ASN:HD21	1:C:57:ASN:HD22	1.60	0.49
1:C:886:ARG:HB3	1:C:891:TRP:HB2	1.94	0.49
1:D:886:ARG:HB3	1:D:891:TRP:HB2	1.94	0.49
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.25	0.49
1:A:66:CYS:SG	1:A:67:PHE:N	2.86	0.49
1:A:3940:LYS:NZ	1:A:3942:VAL:O	2.35	0.49
1:B:116:MET:HE3	1:B:117:TYR:H	1.76	0.49
1:B:1774:PRO:HG2	1:B:1776:HIS:NE2	2.28	0.49
1:B:1829:PRO:HB3	1:B:1837:GLN:HG3	1.95	0.49
1:C:3676:ASP:OD1	1:C:3676:ASP:N	2.46	0.49
1:C:3999:MET:HG3	1:C:4016:LEU:HD22	1.95	0.49
1:A:468:LEU:O	1:A:472:ARG:HG3	2.13	0.49
1:A:1829:PRO:HB3	1:A:1837:GLN:HG3	1.95	0.49
1:A:3762:ARG:NH2	1:A:4755:GLU:O	2.46	0.49
1:C:4056:GLU:HB2	1:C:4166:LEU:HD13	1.94	0.49
1:C:4573:ILE:HA	1:C:4576:ILE:HG22	1.94	0.49
1:D:54:ASN:HD21	1:D:57:ASN:HD22	1.60	0.49
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.95	0.49
1:D:3676:ASP:OD1	1:D:3676:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4001:MET:HE1	1:D:4061:PHE:HB2	1.95	0.49
1:A:3670:GLU:OE1	1:A:3670:GLU:N	2.46	0.49
1:B:3670:GLU:OE1	1:B:3670:GLU:N	2.46	0.49
1:B:4632:LEU:HD12	1:B:4633:GLU:H	1.78	0.49
1:C:248:GLU:OE1	1:C:373:LYS:NZ	2.46	0.49
1:C:670:GLU:H	1:C:740:PRO:HB3	1.78	0.49
1:C:3973:CYS:SG	1:C:3976:ASN:ND2	2.83	0.49
1:D:4107:GLU:OE1	1:D:4107:GLU:N	2.41	0.49
1:A:530:ILE:HD11	1:A:537:CYS:HA	1.93	0.49
1:A:4003:LEU:HB2	1:A:4013:LEU:HD13	1.94	0.49
1:B:891:TRP:CE3	1:B:904:HIS:HB2	2.48	0.49
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.95	0.49
1:B:4001:MET:HE1	1:B:4061:PHE:HB2	1.95	0.49
1:B:468:LEU:O	1:B:472:ARG:HG3	2.13	0.48
1:B:1243:PRO:HB2	1:B:1600:LEU:HD12	1.95	0.48
1:C:582:HIS:O	1:C:585:SER:OG	2.18	0.48
1:C:891:TRP:CE3	1:C:904:HIS:HB2	2.48	0.48
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.31	0.48
1:C:2004:GLU:HA	1:C:2007:ASN:ND2	2.28	0.48
1:C:2587:TYR:O	1:C:2591:ARG:N	2.45	0.48
1:D:3670:GLU:OE1	1:D:3670:GLU:N	2.46	0.48
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.31	0.48
1:A:1194:LEU:HG	1:A:1198:GLN:HB2	1.95	0.48
1:A:1965:TYR:OH	1:A:2027:ILE:O	2.22	0.48
1:B:54:ASN:HD21	1:B:57:ASN:HD22	1.60	0.48
1:B:66:CYS:SG	1:B:67:PHE:N	2.86	0.48
1:C:1774:PRO:HG2	1:C:1776:HIS:NE2	2.28	0.48
1:C:1965:TYR:OH	1:C:2027:ILE:O	2.22	0.48
1:C:4172:GLU:OE2	1:C:4175:ARG:NH1	2.46	0.48
1:C:4632:LEU:HD12	1:C:4633:GLU:H	1.78	0.48
1:D:670:GLU:H	1:D:740:PRO:HB3	1.78	0.48
1:D:1006:SER:O	1:D:1020:ARG:N	2.46	0.48
1:A:3973:CYS:SG	1:A:3976:ASN:ND2	2.83	0.48
1:A:4001:MET:HE1	1:A:4061:PHE:HB2	1.95	0.48
1:A:4632:LEU:HD12	1:A:4633:GLU:H	1.78	0.48
1:A:4852:THR:HG21	1:A:4883:TYR:HB2	1.95	0.48
1:A:4901:ILE:HD12	1:A:4913:ARG:NH2	2.28	0.48
1:C:257:ARG:O	1:C:284:HIS:NE2	2.44	0.48
1:C:3734:HIS:O	1:C:3738:GLY:N	2.43	0.48
1:C:4044:MET:HE2	1:C:4044:MET:N	2.28	0.48
1:D:66:CYS:SG	1:D:67:PHE:N	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:O	1:D:284:HIS:NE2	2.44	0.48
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.31	0.48
1:D:4901:ILE:HD12	1:D:4913:ARG:NH2	2.28	0.48
1:A:5013:MET:O	1:A:5017:ARG:N	2.47	0.48
1:B:4852:THR:HG21	1:B:4883:TYR:HB2	1.95	0.48
1:C:66:CYS:SG	1:C:67:PHE:N	2.86	0.48
1:C:468:LEU:O	1:C:472:ARG:HG3	2.13	0.48
1:C:1194:LEU:HG	1:C:1198:GLN:HB2	1.95	0.48
1:D:4172:GLU:OE2	1:D:4175:ARG:NH1	2.46	0.48
1:B:3762:ARG:NH2	1:B:4755:GLU:O	2.46	0.48
1:B:3940:LYS:NZ	1:B:3942:VAL:O	2.35	0.48
1:B:4056:GLU:HB2	1:B:4166:LEU:HD13	1.94	0.48
1:B:4819:GLY:O	1:B:4820:VAL:C	2.49	0.48
1:B:5013:MET:O	1:B:5017:ARG:N	2.47	0.48
1:C:4958:CYS:SG	1:C:4961:CYS:N	2.87	0.48
1:C:5013:MET:O	1:C:5017:ARG:N	2.47	0.48
1:D:1829:PRO:HB3	1:D:1837:GLN:HG3	1.95	0.48
1:D:2004:GLU:HA	1:D:2007:ASN:ND2	2.28	0.48
1:D:4108:ILE:O	1:D:4112:LEU:HG	2.14	0.48
1:A:1774:PRO:HG2	1:A:1776:HIS:NE2	2.28	0.48
1:C:577:ILE:O	1:C:579:GLN:NE2	2.39	0.48
1:C:3762:ARG:NH2	1:C:4755:GLU:O	2.46	0.48
1:A:1220:GLN:CD	1:A:1220:GLN:H	2.17	0.48
1:B:1006:SER:O	1:B:1020:ARG:N	2.46	0.48
1:C:1829:PRO:HB3	1:C:1837:GLN:HG3	1.95	0.48
1:C:3670:GLU:N	1:C:3670:GLU:OE1	2.46	0.48
1:D:1194:LEU:HG	1:D:1198:GLN:HB2	1.95	0.48
1:D:1220:GLN:CD	1:D:1220:GLN:H	2.17	0.48
1:B:2004:GLU:HA	1:B:2007:ASN:ND2	2.28	0.48
1:B:4958:CYS:SG	1:B:4961:CYS:N	2.87	0.48
1:C:25:SER:HB2	1:C:34:LYS:HZ2	1.78	0.48
1:D:1774:PRO:HG2	1:D:1776:HIS:NE2	2.28	0.48
1:A:721:LEU:N	1:A:728:ARG:O	2.47	0.48
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.95	0.48
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.47	0.48
1:B:1194:LEU:HG	1:B:1198:GLN:HB2	1.95	0.48
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.47	0.48
1:C:1006:SER:O	1:C:1020:ARG:N	2.46	0.48
1:C:3647:HIS:O	1:C:3651:ASN:ND2	2.47	0.48
1:C:4901:ILE:HD12	1:C:4913:ARG:NH2	2.28	0.48
1:D:468:LEU:O	1:D:472:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4958:CYS:SG	1:D:4961:CYS:N	2.87	0.48
1:B:116:MET:HE1	1:B:140:ASP:H	1.79	0.48
1:B:213:TYR:HD2	1:B:337:PRO:HB2	1.79	0.48
1:B:1220:GLN:CD	1:B:1220:GLN:H	2.17	0.48
1:B:2348:GLU:OE1	1:B:2348:GLU:N	2.38	0.48
1:C:213:TYR:HD2	1:C:337:PRO:HB2	1.79	0.48
1:C:721:LEU:N	1:C:728:ARG:O	2.47	0.48
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.47	0.48
1:D:213:TYR:HD2	1:D:337:PRO:HB2	1.79	0.48
1:D:3762:ARG:NH2	1:D:4755:GLU:O	2.46	0.48
1:A:54:ASN:HD21	1:A:57:ASN:HD22	1.60	0.47
1:A:2228:MET:SD	1:A:2228:MET:N	2.86	0.47
1:A:4108:ILE:O	1:A:4112:LEU:HG	2.14	0.47
1:B:3897:ASN:H	1:B:3900:GLN:NE2	2.12	0.47
1:C:4852:THR:HG21	1:C:4883:TYR:HB2	1.95	0.47
1:D:273:HIS:CE1	1:D:337:PRO:HB3	2.49	0.47
1:D:5013:MET:O	1:D:5017:ARG:N	2.47	0.47
1:A:497:TYR:HA	1:A:503:PHE:CD2	2.50	0.47
1:A:1006:SER:O	1:A:1020:ARG:N	2.46	0.47
1:A:4057:MET:HA	1:A:4060:LYS:HG2	1.97	0.47
1:B:310:LYS:O	1:B:310:LYS:NZ	2.45	0.47
1:B:4658:ILE:HG13	1:B:4796:MET:HE2	1.95	0.47
1:B:5001:THR:OG1	1:B:5002:GLU:OE1	2.27	0.47
1:C:4108:ILE:O	1:C:4112:LEU:HG	2.14	0.47
1:D:2469:ILE:H	1:D:2469:ILE:HD12	1.80	0.47
1:D:3889:GLN:HB2	1:D:3964:SER:HA	1.97	0.47
1:A:273:HIS:CE1	1:A:337:PRO:HB3	2.49	0.47
1:B:526:LEU:O	1:B:530:ILE:HG22	2.15	0.47
1:B:2587:TYR:O	1:B:2591:ARG:N	2.45	0.47
1:C:4057:MET:HA	1:C:4060:LYS:HG2	1.97	0.47
1:C:4819:GLY:O	1:C:4820:VAL:C	2.49	0.47
1:D:4679:ARG:HH21	1:D:5017:ARG:NH1	2.12	0.47
1:A:213:TYR:HD2	1:A:337:PRO:HB2	1.79	0.47
1:A:310:LYS:O	1:A:310:LYS:NZ	2.45	0.47
1:A:3647:HIS:O	1:A:3651:ASN:ND2	2.47	0.47
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.25	0.47
1:B:716:PHE:HE1	1:B:730:VAL:HG21	1.79	0.47
1:B:2228:MET:N	1:B:2228:MET:SD	2.86	0.47
1:B:3647:HIS:O	1:B:3651:ASN:ND2	2.47	0.47
1:B:4679:ARG:HH21	1:B:5017:ARG:NH1	2.12	0.47
1:C:1220:GLN:H	1:C:1220:GLN:CD	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:LEU:N	1:D:728:ARG:O	2.47	0.47
1:D:2587:TYR:O	1:D:2591:ARG:N	2.45	0.47
1:D:4057:MET:HA	1:D:4060:LYS:HG2	1.97	0.47
1:A:3897:ASN:H	1:A:3900:GLN:NE2	2.12	0.47
1:B:497:TYR:HA	1:B:503:PHE:CD2	2.50	0.47
1:B:721:LEU:N	1:B:728:ARG:O	2.47	0.47
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.48	0.47
1:B:4901:ILE:HD12	1:B:4913:ARG:NH2	2.28	0.47
1:D:1637:MET:HG3	1:D:1650:ILE:HG21	1.97	0.47
1:D:2228:MET:N	1:D:2228:MET:SD	2.86	0.47
1:D:3647:HIS:O	1:D:3651:ASN:ND2	2.47	0.47
1:A:526:LEU:O	1:A:530:ILE:HG22	2.15	0.47
1:A:3889:GLN:HB2	1:A:3964:SER:HA	1.97	0.47
1:A:4679:ARG:HH21	1:A:5017:ARG:NH1	2.12	0.47
1:A:4958:CYS:SG	1:A:4961:CYS:N	2.87	0.47
1:B:1704:PRO:HG2	1:B:1707:LEU:HB3	1.97	0.47
1:C:313:SER:HB2	1:C:350:HIS:CE1	2.50	0.47
1:C:2113:SER:O	1:C:2113:SER:OG	2.33	0.47
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.48	0.47
1:D:497:TYR:HA	1:D:503:PHE:CD2	2.50	0.47
1:A:248:GLU:OE1	1:A:373:LYS:NZ	2.46	0.47
1:A:582:HIS:O	1:A:585:SER:OG	2.18	0.47
1:A:716:PHE:HE1	1:A:730:VAL:HG21	1.79	0.47
1:A:1087:ARG:HB3	1:A:1223:PHE:CD2	2.50	0.47
1:A:1704:PRO:HG2	1:A:1707:LEU:HB3	1.97	0.47
1:B:232:THR:OG1	1:B:233:ILE:N	2.48	0.47
1:B:2113:SER:O	1:B:2113:SER:OG	2.33	0.47
1:B:4057:MET:HA	1:B:4060:LYS:HG2	1.97	0.47
1:B:4108:ILE:O	1:B:4112:LEU:HG	2.14	0.47
1:C:265:LEU:HD12	1:C:279:PRO:HB2	1.97	0.47
1:C:1637:MET:HG3	1:C:1650:ILE:HG21	1.97	0.47
1:C:4001:MET:HE1	1:C:4061:PHE:HB2	1.96	0.47
1:C:4582:VAL:HG11	1:D:4860:ARG:HD2	1.97	0.47
1:C:4679:ARG:HH21	1:C:5017:ARG:NH1	2.12	0.47
1:D:248:GLU:OE1	1:D:373:LYS:NZ	2.46	0.47
1:D:313:SER:HB2	1:D:350:HIS:CE1	2.50	0.47
1:D:716:PHE:HE1	1:D:730:VAL:HG21	1.79	0.47
1:D:5001:THR:OG1	1:D:5002:GLU:OE1	2.27	0.47
1:A:313:SER:HB2	1:A:350:HIS:CE1	2.50	0.47
1:A:551:LEU:HG	1:A:553:ARG:HD2	1.97	0.47
1:A:1211:LEU:HB3	1:A:1214:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LEU:HG	1:B:553:ARG:HD2	1.97	0.47
1:B:1087:ARG:HB3	1:B:1223:PHE:CD2	2.50	0.47
1:B:4242:ILE:O	1:B:4246:GLN:HG2	2.15	0.47
1:C:497:TYR:HA	1:C:503:PHE:CD2	2.50	0.47
1:D:551:LEU:HG	1:D:553:ARG:HD2	1.97	0.47
1:D:4852:THR:HG21	1:D:4883:TYR:HB2	1.95	0.47
1:A:3752:SER:N	1:A:3755:GLU:OE2	2.44	0.47
1:A:4162:ASN:O	1:A:4166:LEU:HG	2.15	0.47
1:A:4242:ILE:O	1:A:4246:GLN:HG2	2.15	0.47
1:B:265:LEU:HD12	1:B:279:PRO:HB2	1.97	0.47
1:B:313:SER:HB2	1:B:350:HIS:CE1	2.50	0.47
1:B:1287:LEU:CB	1:B:1598:GLN:H	2.28	0.47
1:B:4107:GLU:OE1	1:B:4107:GLU:N	2.41	0.47
1:B:4162:ASN:O	1:B:4166:LEU:HG	2.15	0.47
1:C:2176:ASN:OD1	1:C:2176:ASN:N	2.48	0.47
1:D:1087:ARG:HB3	1:D:1223:PHE:CD2	2.50	0.47
1:D:1704:PRO:HG2	1:D:1707:LEU:HB3	1.97	0.47
1:D:4112:LEU:O	1:D:4115:SER:OG	2.32	0.47
1:A:1287:LEU:CB	1:A:1598:GLN:H	2.28	0.47
1:C:716:PHE:HE1	1:C:730:VAL:HG21	1.79	0.47
1:C:3752:SER:N	1:C:3755:GLU:OE2	2.44	0.47
1:A:1637:MET:HG3	1:A:1650:ILE:HG21	1.97	0.46
1:A:1707:LEU:HD23	1:A:1708:ARG:HG3	1.96	0.46
1:A:1939:MET:O	1:A:1943:LEU:HG	2.16	0.46
1:A:2004:GLU:HA	1:A:2007:ASN:ND2	2.28	0.46
1:B:276:TRP:CD2	1:B:318:VAL:HG22	2.51	0.46
1:C:276:TRP:CD2	1:C:318:VAL:HG22	2.51	0.46
1:C:526:LEU:O	1:C:530:ILE:HG22	2.15	0.46
1:C:1087:ARG:HB3	1:C:1223:PHE:CD2	2.50	0.46
1:C:4112:LEU:O	1:C:4115:SER:OG	2.32	0.46
1:D:192:ASP:OD1	1:D:192:ASP:N	2.48	0.46
1:D:526:LEU:O	1:D:530:ILE:HG22	2.15	0.46
1:D:1190:PRO:HD3	1:D:1226:PHE:CZ	2.51	0.46
1:D:1211:LEU:HB3	1:D:1214:PHE:HB2	1.97	0.46
1:D:2024:PRO:O	1:D:2028:ARG:NH2	2.30	0.46
1:A:626:LEU:HD11	1:A:630:GLU:H	1.80	0.46
1:B:626:LEU:HD11	1:B:630:GLU:H	1.80	0.46
1:B:1190:PRO:HD3	1:B:1226:PHE:CZ	2.51	0.46
1:B:1707:LEU:HD23	1:B:1708:ARG:HG3	1.96	0.46
1:C:743:VAL:HB	1:C:760:ASN:HD21	1.80	0.46
1:C:1211:LEU:HB3	1:C:1214:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1707:LEU:HD23	1:C:1708:ARG:HG3	1.96	0.46
1:C:1939:MET:O	1:C:1943:LEU:HG	2.16	0.46
1:D:1939:MET:O	1:D:1943:LEU:HG	2.16	0.46
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.47	0.46
1:A:460:GLN:N	1:A:463:GLU:OE1	2.49	0.46
1:A:1190:PRO:HD3	1:A:1226:PHE:CZ	2.51	0.46
1:A:2469:ILE:H	1:A:2469:ILE:HD12	1.80	0.46
1:A:3653:PHE:HA	1:A:3656:SER:OG	2.16	0.46
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.48	0.46
1:B:1211:LEU:HB3	1:B:1214:PHE:HB2	1.97	0.46
1:B:1939:MET:O	1:B:1943:LEU:HG	2.16	0.46
1:C:2228:MET:SD	1:C:2228:MET:N	2.86	0.46
1:C:2348:GLU:OE1	1:C:2348:GLU:N	2.38	0.46
1:C:2469:ILE:H	1:C:2469:ILE:HD12	1.80	0.46
1:C:5001:THR:OG1	1:C:5002:GLU:OE1	2.27	0.46
1:D:232:THR:OG1	1:D:233:ILE:N	2.48	0.46
1:D:3963:ASN:O	1:D:3966:THR:OG1	2.30	0.46
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.48	0.46
1:A:275:ARG:HD3	1:A:336:PRO:HD2	1.97	0.46
1:A:4071:ILE:HD11	1:A:4102:GLN:HE21	1.81	0.46
1:A:4860:ARG:HD2	1:D:4582:VAL:HG11	1.97	0.46
1:B:235:ALA:HA	1:B:257:ARG:HD3	1.98	0.46
1:C:235:ALA:HA	1:C:257:ARG:HD3	1.98	0.46
1:C:551:LEU:HG	1:C:553:ARG:HD2	1.97	0.46
1:C:1190:PRO:HD3	1:C:1226:PHE:CZ	2.51	0.46
1:D:460:GLN:N	1:D:463:GLU:OE1	2.49	0.46
1:D:1287:LEU:CB	1:D:1598:GLN:H	2.28	0.46
1:A:2587:TYR:O	1:A:2591:ARG:N	2.45	0.46
1:B:2469:ILE:HD12	1:B:2469:ILE:H	1.80	0.46
1:B:3653:PHE:HA	1:B:3656:SER:OG	2.16	0.46
1:B:3889:GLN:HB2	1:B:3964:SER:HA	1.97	0.46
1:C:236:ALA:HA	1:C:242:ARG:HD2	1.98	0.46
1:C:460:GLN:N	1:C:463:GLU:OE1	2.49	0.46
1:C:626:LEU:HD11	1:C:630:GLU:H	1.80	0.46
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.49	0.46
1:D:343:GLU:OE1	1:D:343:GLU:N	2.49	0.46
1:D:708:GLY:HA3	1:D:722:TRP:HB3	1.98	0.46
1:A:236:ALA:HA	1:A:242:ARG:HD2	1.98	0.46
1:A:1702:HIS:O	1:A:1708:ARG:NH2	2.49	0.46
1:B:708:GLY:HA3	1:B:722:TRP:HB3	1.98	0.46
1:B:1637:MET:HG3	1:B:1650:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3752:SER:N	1:B:3755:GLU:OE2	2.44	0.46
1:C:273:HIS:CE1	1:C:337:PRO:HB3	2.49	0.46
1:D:236:ALA:HA	1:D:242:ARG:HD2	1.98	0.46
1:D:278:GLN:N	1:D:315:CYS:SG	2.89	0.46
1:D:1707:LEU:HD23	1:D:1708:ARG:HG3	1.96	0.46
1:D:2113:SER:OG	1:D:2113:SER:O	2.33	0.46
1:D:3897:ASN:H	1:D:3900:GLN:NE2	2.12	0.46
1:D:4999:ASP:OD1	1:D:5000:GLU:N	2.49	0.46
1:A:2024:PRO:O	1:A:2028:ARG:NH2	2.30	0.46
1:B:236:ALA:HA	1:B:242:ARG:HD2	1.98	0.46
1:B:278:GLN:N	1:B:315:CYS:SG	2.89	0.46
1:B:343:GLU:OE1	1:B:343:GLU:N	2.49	0.46
1:C:2337:PHE:HA	1:C:2340:PHE:HB2	1.98	0.46
1:D:265:LEU:HD12	1:D:279:PRO:HB2	1.97	0.46
1:D:743:VAL:HB	1:D:760:ASN:HD21	1.80	0.46
1:D:1124:PHE:HE2	1:D:1143:TRP:HE1	1.63	0.46
1:D:3973:CYS:SG	1:D:3976:ASN:ND2	2.83	0.46
1:D:4579:PHE:HB2	1:D:4631:PHE:HE1	1.81	0.46
1:A:562:GLU:OE1	1:A:598:LYS:NZ	2.41	0.46
1:B:224:HIS:HB3	1:B:229:GLU:HB3	1.98	0.46
1:C:232:THR:OG1	1:C:233:ILE:N	2.48	0.46
1:C:1665:HIS:HA	1:C:1668:ARG:HG2	1.98	0.46
1:C:1704:PRO:HG2	1:C:1707:LEU:HB3	1.97	0.46
1:C:3889:GLN:HB2	1:C:3964:SER:HA	1.97	0.46
1:C:4999:ASP:OD1	1:C:5000:GLU:N	2.49	0.46
1:D:577:ILE:O	1:D:579:GLN:NE2	2.39	0.46
1:D:1665:HIS:HA	1:D:1668:ARG:HG2	1.98	0.46
1:D:2176:ASN:OD1	1:D:2176:ASN:N	2.48	0.46
1:A:192:ASP:OD1	1:A:192:ASP:N	2.48	0.46
1:A:708:GLY:HA3	1:A:722:TRP:HB3	1.98	0.46
1:A:2113:SER:O	1:A:2113:SER:OG	2.33	0.46
1:A:4582:VAL:HG11	1:B:4860:ARG:HD2	1.97	0.46
1:B:192:ASP:N	1:B:192:ASP:OD1	2.48	0.46
1:B:273:HIS:CE1	1:B:337:PRO:HB3	2.49	0.46
1:B:2337:PHE:HA	1:B:2340:PHE:HB2	1.98	0.46
1:C:275:ARG:HD3	1:C:336:PRO:HD2	1.97	0.46
1:C:4162:ASN:O	1:C:4166:LEU:HG	2.15	0.46
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.77	0.46
1:A:343:GLU:OE1	1:A:343:GLU:N	2.49	0.46
1:A:1124:PHE:HE2	1:A:1143:TRP:HE1	1.63	0.46
1:A:2176:ASN:OD1	1:A:2176:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4071:ILE:HD11	1:B:4102:GLN:HE21	1.81	0.46
1:C:278:GLN:N	1:C:315:CYS:SG	2.89	0.46
1:C:4044:MET:O	1:C:4047:MET:HG3	2.16	0.46
1:C:4579:PHE:HB2	1:C:4631:PHE:HE1	1.81	0.46
1:D:276:TRP:CD2	1:D:318:VAL:HG22	2.51	0.46
1:D:626:LEU:HD11	1:D:630:GLU:H	1.80	0.46
1:D:3653:PHE:HA	1:D:3656:SER:OG	2.16	0.46
1:D:4044:MET:O	1:D:4047:MET:HG3	2.16	0.46
1:A:224:HIS:HB3	1:A:229:GLU:HB3	1.98	0.45
1:A:265:LEU:HD12	1:A:279:PRO:HB2	1.97	0.45
1:A:4999:ASP:OD1	1:A:5000:GLU:N	2.49	0.45
1:B:460:GLN:N	1:B:463:GLU:OE1	2.49	0.45
1:B:794:GLY:N	1:B:798:GLY:HA3	2.30	0.45
1:B:1665:HIS:HA	1:B:1668:ARG:HG2	1.98	0.45
1:B:4582:VAL:HG11	1:C:4860:ARG:HD2	1.97	0.45
1:B:4999:ASP:OD1	1:B:5000:GLU:N	2.49	0.45
1:C:1132:TRP:NE1	1:C:1136:SER:OG	2.49	0.45
1:D:1126:GLY:HA3	1:D:1143:TRP:CE2	2.51	0.45
1:D:1702:HIS:O	1:D:1708:ARG:NH2	2.49	0.45
1:D:2337:PHE:HA	1:D:2340:PHE:HB2	1.98	0.45
1:D:3663:LEU:HD23	1:D:3663:LEU:H	1.80	0.45
1:D:4242:ILE:O	1:D:4246:GLN:HG2	2.15	0.45
1:A:1132:TRP:NE1	1:A:1136:SER:OG	2.49	0.45
1:A:3676:ASP:N	1:A:3676:ASP:OD1	2.46	0.45
1:A:3888:LEU:HD23	1:A:3888:LEU:HA	1.82	0.45
1:A:4112:LEU:O	1:A:4115:SER:OG	2.32	0.45
1:A:4579:PHE:HB2	1:A:4631:PHE:HE1	1.81	0.45
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.49	0.45
1:C:794:GLY:N	1:C:798:GLY:HA3	2.30	0.45
1:C:1287:LEU:CB	1:C:1598:GLN:H	2.28	0.45
1:C:1653:LEU:HD11	1:C:1659:LEU:HB2	1.99	0.45
1:C:4876:CYS:HA	1:C:4882:CYS:HB2	1.98	0.45
1:D:4868:ASP:N	1:D:4868:ASP:OD1	2.49	0.45
1:D:4876:CYS:HA	1:D:4882:CYS:HB2	1.98	0.45
1:A:232:THR:OG1	1:A:233:ILE:N	2.48	0.45
1:A:743:VAL:HB	1:A:760:ASN:HD21	1.80	0.45
1:A:1665:HIS:HA	1:A:1668:ARG:HG2	1.98	0.45
1:B:743:VAL:HB	1:B:760:ASN:HD21	1.80	0.45
1:B:1132:TRP:NE1	1:B:1136:SER:OG	2.49	0.45
1:B:4868:ASP:OD1	1:B:4868:ASP:N	2.49	0.45
1:C:192:ASP:N	1:C:192:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:GLU:OE1	1:C:343:GLU:N	2.49	0.45
1:C:708:GLY:HA3	1:C:722:TRP:HB3	1.98	0.45
1:C:1124:PHE:HE2	1:C:1143:TRP:HE1	1.63	0.45
1:C:4658:ILE:HG13	1:C:4796:MET:HE2	1.98	0.45
1:D:215:THR:HG22	1:D:273:HIS:HA	1.98	0.45
1:D:235:ALA:HA	1:D:257:ARG:HD3	1.98	0.45
1:D:1653:LEU:HD11	1:D:1659:LEU:HB2	1.99	0.45
1:D:4071:ILE:HD11	1:D:4102:GLN:HE21	1.81	0.45
1:D:4162:ASN:O	1:D:4166:LEU:HG	2.15	0.45
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.49	0.45
1:A:235:ALA:HA	1:A:257:ARG:HD3	1.98	0.45
1:B:182:LEU:H	1:B:198:THR:HG21	1.82	0.45
1:B:2452:ARG:O	1:B:2456:ILE:HG12	2.17	0.45
1:C:2452:ARG:O	1:C:2456:ILE:HG12	2.17	0.45
1:C:3653:PHE:HA	1:C:3656:SER:OG	2.16	0.45
1:D:1132:TRP:NE1	1:D:1136:SER:OG	2.49	0.45
1:A:182:LEU:H	1:A:198:THR:HG21	1.82	0.45
1:A:745:SER:OG	1:A:758:ARG:HB3	2.16	0.45
1:A:1126:GLY:HA3	1:A:1143:TRP:CE2	2.51	0.45
1:A:2010:LEU:HD21	1:A:3657:TYR:HD1	1.81	0.45
1:A:3963:ASN:O	1:A:3966:THR:OG1	2.30	0.45
1:A:4044:MET:O	1:A:4047:MET:HG3	2.16	0.45
1:A:4876:CYS:HA	1:A:4882:CYS:HB2	1.98	0.45
1:A:4890:GLY:HA2	1:A:4897:ILE:HD13	1.99	0.45
1:A:5001:THR:OG1	1:A:5002:GLU:OE1	2.27	0.45
1:B:1702:HIS:O	1:B:1708:ARG:NH2	2.49	0.45
1:B:3663:LEU:HD23	1:B:3663:LEU:H	1.80	0.45
1:D:275:ARG:HD3	1:D:336:PRO:HD2	1.97	0.45
1:A:278:GLN:N	1:A:315:CYS:SG	2.89	0.45
1:A:2000:SER:O	1:A:2005:GLN:HB2	2.16	0.45
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.50	0.45
1:B:745:SER:OG	1:B:758:ARG:HB3	2.16	0.45
1:B:864:PRO:O	1:B:868:GLU:N	2.41	0.45
1:B:1126:GLY:HA3	1:B:1143:TRP:CE2	2.51	0.45
1:B:3676:ASP:OD1	1:B:3676:ASP:N	2.46	0.45
1:B:3845:ASN:O	1:B:3849:ARG:HG2	2.17	0.45
1:B:3890:LEU:HD23	1:B:3890:LEU:HA	1.83	0.45
1:B:4876:CYS:HA	1:B:4882:CYS:HB2	1.98	0.45
1:C:350:HIS:CE1	1:C:352:ALA:HB3	2.52	0.45
1:C:1126:GLY:HA3	1:C:1143:TRP:CE2	2.51	0.45
1:C:4242:ILE:O	1:C:4246:GLN:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:ASP:HB3	1:D:725:HIS:CE1	2.52	0.45
1:A:2452:ARG:O	1:A:2456:ILE:HG12	2.17	0.45
1:A:3663:LEU:HD23	1:A:3663:LEU:H	1.80	0.45
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.49	0.45
1:B:350:HIS:CE1	1:B:352:ALA:HB3	2.52	0.45
1:B:464:LYS:HE2	1:B:464:LYS:HB2	1.71	0.45
1:C:182:LEU:H	1:C:198:THR:HG21	1.82	0.45
1:C:358:THR:HG21	1:C:382:GLY:HA3	1.99	0.45
1:C:2010:LEU:HD21	1:C:3657:TYR:HD1	1.81	0.45
1:C:3996:PHE:CD1	1:C:4016:LEU:HD11	2.52	0.45
1:C:4071:ILE:HD11	1:C:4102:GLN:HE21	1.81	0.45
1:D:794:GLY:N	1:D:798:GLY:HA3	2.30	0.45
1:A:709:ASP:HB3	1:A:725:HIS:CE1	2.52	0.45
1:A:1650:ILE:HD12	1:A:1653:LEU:HD23	1.99	0.45
1:B:215:THR:HG22	1:B:273:HIS:HA	1.98	0.45
1:B:636:ASN:HB3	1:B:702:TRP:HZ3	1.82	0.45
1:B:2024:PRO:O	1:B:2028:ARG:NH2	2.30	0.45
1:B:2277:ALA:HB1	1:B:2337:PHE:HD2	1.82	0.45
1:B:4044:MET:O	1:B:4047:MET:HG3	2.16	0.45
1:C:4051:SER:O	1:C:4055:VAL:HG13	2.17	0.45
1:D:1090:PHE:CE1	1:D:1151:CYS:HB2	2.52	0.45
1:A:794:GLY:N	1:A:798:GLY:HA3	2.30	0.45
1:A:1653:LEU:HD11	1:A:1659:LEU:HB2	1.99	0.45
1:A:3996:PHE:CD1	1:A:4016:LEU:HD11	2.52	0.45
1:A:5035:GLN:OE1	1:A:5035:GLN:N	2.47	0.45
1:B:3927:GLN:HB2	1:B:3992:PHE:CE2	2.52	0.45
1:B:4579:PHE:HB2	1:B:4631:PHE:HE1	1.81	0.45
1:C:709:ASP:HB3	1:C:725:HIS:CE1	2.52	0.45
1:C:1161:ILE:HG23	1:C:1177:THR:HG21	1.99	0.45
1:C:2277:ALA:HB1	1:C:2337:PHE:HD2	1.82	0.45
1:C:3663:LEU:H	1:C:3663:LEU:HD23	1.80	0.45
1:C:4027:LEU:HA	1:C:4027:LEU:HD23	1.73	0.45
1:D:894:GLY:HA3	1:D:903:LEU:HD11	1.99	0.45
1:D:3996:PHE:CD1	1:D:4016:LEU:HD11	2.52	0.45
1:A:215:THR:HG22	1:A:273:HIS:HA	1.98	0.45
1:A:2207:VAL:O	1:A:2210:VAL:HG12	2.17	0.45
1:A:2337:PHE:HA	1:A:2340:PHE:HB2	1.98	0.45
1:A:3927:GLN:HB2	1:A:3992:PHE:CE2	2.52	0.45
1:B:1124:PHE:HE2	1:B:1143:TRP:HE1	1.63	0.45
1:B:1844:LEU:O	1:B:1847:THR:HG22	2.18	0.45
1:B:4731:ILE:HG23	1:B:4732:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:HIS:HB3	1:C:229:GLU:HB3	1.98	0.45
1:C:2000:SER:O	1:C:2005:GLN:HB2	2.16	0.45
1:C:3963:ASN:O	1:C:3966:THR:OG1	2.30	0.45
1:C:4731:ILE:HG23	1:C:4732:PHE:CD1	2.51	0.45
1:D:350:HIS:CE1	1:D:352:ALA:HB3	2.52	0.45
1:D:1819:VAL:HG11	1:D:1865:MET:SD	2.57	0.45
1:D:2000:SER:O	1:D:2005:GLN:HB2	2.16	0.45
1:D:4672:LYS:HE3	1:D:4672:LYS:HB2	1.80	0.45
1:A:276:TRP:CD2	1:A:318:VAL:HG22	2.51	0.44
1:A:636:ASN:HB3	1:A:702:TRP:HZ3	1.82	0.44
1:A:894:GLY:HA3	1:A:903:LEU:HD11	1.99	0.44
1:A:1090:PHE:CE1	1:A:1151:CYS:HB2	2.52	0.44
1:A:3790:THR:O	1:A:3790:THR:OG1	2.33	0.44
1:B:709:ASP:HB3	1:B:725:HIS:CE1	2.52	0.44
1:B:1770:SER:OG	1:B:1956:GLU:OE2	2.34	0.44
1:B:1819:VAL:HG11	1:B:1865:MET:SD	2.57	0.44
1:B:3963:ASN:O	1:B:3966:THR:OG1	2.30	0.44
1:B:4051:SER:O	1:B:4055:VAL:HG13	2.17	0.44
1:C:215:THR:HG22	1:C:273:HIS:HA	1.98	0.44
1:C:1702:HIS:O	1:C:1708:ARG:NH2	2.49	0.44
1:D:2277:ALA:HB1	1:D:2337:PHE:HD2	1.82	0.44
1:D:2452:ARG:O	1:D:2456:ILE:HG12	2.17	0.44
1:D:4056:GLU:O	1:D:4060:LYS:HG2	2.18	0.44
1:A:1819:VAL:HG11	1:A:1865:MET:SD	2.57	0.44
1:A:3845:ASN:O	1:A:3849:ARG:HG2	2.17	0.44
1:B:275:ARG:HD3	1:B:336:PRO:HD2	1.97	0.44
1:B:1650:ILE:HD12	1:B:1653:LEU:HD23	1.99	0.44
1:B:1662:PHE:O	1:B:1666:THR:HG22	2.18	0.44
1:B:2207:VAL:O	1:B:2210:VAL:HG12	2.17	0.44
1:B:2296:GLU:HA	1:B:2299:VAL:HG22	1.99	0.44
1:C:894:GLY:HA3	1:C:903:LEU:HD11	1.99	0.44
1:C:4051:SER:O	1:C:4051:SER:OG	2.33	0.44
1:D:22:LEU:HD12	1:D:37:LEU:HD23	2.00	0.44
1:D:224:HIS:HB3	1:D:229:GLU:HB3	1.98	0.44
1:D:3790:THR:O	1:D:3790:THR:OG1	2.33	0.44
1:D:3940:LYS:NZ	1:D:3942:VAL:O	2.35	0.44
1:A:4056:GLU:O	1:A:4060:LYS:HG2	2.18	0.44
1:B:1161:ILE:HG23	1:B:1177:THR:HG21	1.99	0.44
1:B:1653:LEU:HD11	1:B:1659:LEU:HB2	1.99	0.44
1:B:2010:LEU:HD21	1:B:3657:TYR:HD1	1.81	0.44
1:C:745:SER:OG	1:C:758:ARG:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1749:PRO:HB2	1:C:1755:GLY:HA3	2.00	0.44
1:C:1848:LEU:HD23	1:C:1848:LEU:HA	1.83	0.44
1:C:3845:ASN:O	1:C:3849:ARG:HG2	2.17	0.44
1:C:4890:GLY:HA2	1:C:4897:ILE:HD13	1.99	0.44
1:D:745:SER:OG	1:D:758:ARG:HB3	2.16	0.44
1:D:1931:LEU:O	1:D:1936:LYS:HE3	2.18	0.44
1:D:2010:LEU:HD21	1:D:3657:TYR:HD1	1.81	0.44
1:D:2296:GLU:HA	1:D:2299:VAL:HG22	1.99	0.44
1:D:4658:ILE:HG13	1:D:4796:MET:HE2	1.99	0.44
1:A:350:HIS:CE1	1:A:352:ALA:HB3	2.52	0.44
1:A:2277:ALA:HB1	1:A:2337:PHE:HD2	1.82	0.44
1:A:2296:GLU:HA	1:A:2299:VAL:HG22	1.99	0.44
1:A:4868:ASP:N	1:A:4868:ASP:OD1	2.49	0.44
1:B:248:GLU:OE1	1:B:373:LYS:NZ	2.46	0.44
1:B:1090:PHE:CE1	1:B:1151:CYS:HB2	2.52	0.44
1:B:2000:SER:O	1:B:2005:GLN:HB2	2.16	0.44
1:B:3996:PHE:CD1	1:B:4016:LEU:HD11	2.52	0.44
1:B:4056:GLU:O	1:B:4060:LYS:HG2	2.18	0.44
1:C:1819:VAL:HG11	1:C:1865:MET:SD	2.57	0.44
1:C:2022:PRO:HB2	1:C:2024:PRO:HD2	2.00	0.44
1:C:2207:VAL:O	1:C:2210:VAL:HG12	2.17	0.44
1:C:4056:GLU:O	1:C:4060:LYS:HG2	2.18	0.44
1:D:182:LEU:H	1:D:198:THR:HG21	1.82	0.44
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.90	0.44
1:D:629:ARG:HB3	1:D:634:GLN:CD	2.38	0.44
1:D:1092:PHE:CE2	1:D:1094:ALA:HB2	2.53	0.44
1:D:5035:GLN:OE1	1:D:5035:GLN:N	2.47	0.44
1:B:894:GLY:HA3	1:B:903:LEU:HD11	1.99	0.44
1:C:107:ILE:HD12	1:C:107:ILE:HA	1.87	0.44
1:C:460:GLN:H	1:C:460:GLN:CD	2.21	0.44
1:C:1090:PHE:CE1	1:C:1151:CYS:HB2	2.52	0.44
1:C:1774:PRO:HG2	1:C:1776:HIS:CE1	2.53	0.44
1:D:1774:PRO:HG2	1:D:1776:HIS:CE1	2.53	0.44
1:D:2022:PRO:HB2	1:D:2024:PRO:HD2	2.00	0.44
1:D:2207:VAL:O	1:D:2210:VAL:HG12	2.17	0.44
1:D:3752:SER:N	1:D:3755:GLU:OE2	2.44	0.44
1:D:4890:GLY:HA2	1:D:4897:ILE:HD13	1.99	0.44
1:A:22:LEU:HD12	1:A:37:LEU:HD23	2.00	0.44
1:A:526:LEU:HD12	1:A:526:LEU:HA	1.82	0.44
1:A:2002:PRO:HA	1:A:2005:GLN:HB3	2.00	0.44
1:A:4850:LEU:O	1:A:4853:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:GLN:H	1:B:460:GLN:CD	2.21	0.44
1:B:1749:PRO:HB2	1:B:1755:GLY:HA3	2.00	0.44
1:B:1931:LEU:O	1:B:1936:LYS:HE3	2.18	0.44
1:B:4890:GLY:HA2	1:B:4897:ILE:HD13	1.99	0.44
1:C:1770:SER:OG	1:C:1956:GLU:OE2	2.34	0.44
1:C:4868:ASP:OD1	1:C:4868:ASP:N	2.49	0.44
1:D:358:THR:HG21	1:D:382:GLY:HA3	1.99	0.44
1:D:1844:LEU:O	1:D:1847:THR:HG22	2.18	0.44
1:D:3845:ASN:O	1:D:3849:ARG:HG2	2.17	0.44
1:A:358:THR:HG21	1:A:382:GLY:HA3	1.99	0.44
1:A:1092:PHE:CE2	1:A:1094:ALA:HB2	2.53	0.44
1:A:1161:ILE:HG23	1:A:1177:THR:HG21	1.99	0.44
1:A:2022:PRO:HB2	1:A:2024:PRO:HD2	2.00	0.44
1:A:4051:SER:O	1:A:4055:VAL:HG13	2.17	0.44
1:B:377:ILE:HD12	1:B:377:ILE:HA	1.84	0.44
1:B:1765:VAL:HG12	1:B:1766:GLY:H	1.83	0.44
1:B:4112:LEU:O	1:B:4115:SER:OG	2.32	0.44
1:C:629:ARG:HB3	1:C:634:GLN:CD	2.38	0.44
1:C:2377:LEU:HD13	1:C:2380:ILE:HD11	1.99	0.44
1:C:3897:ASN:H	1:C:3900:GLN:NE2	2.12	0.44
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.48	0.44
1:A:108:LEU:HD12	1:A:147:TRP:CZ2	2.53	0.44
1:A:683:ARG:NE	1:A:707:VAL:O	2.49	0.44
1:A:1662:PHE:O	1:A:1666:THR:HG22	2.18	0.44
1:A:1844:LEU:O	1:A:1847:THR:HG22	2.18	0.44
1:A:4049:VAL:HA	1:A:4163:PHE:HZ	1.83	0.44
1:A:4984:ASN:C	1:A:4986:ALA:H	2.21	0.44
1:B:884:LEU:O	1:B:888:GLU:HG2	2.18	0.44
1:B:887:ILE:HD13	1:B:907:LEU:HD11	2.00	0.44
1:C:108:LEU:HD12	1:C:147:TRP:CZ2	2.53	0.44
1:C:560:ILE:H	1:C:560:ILE:HD12	1.82	0.44
1:C:1650:ILE:HD12	1:C:1653:LEU:HD23	1.99	0.44
1:C:4134:GLU:HB2	1:C:4135:PRO:HD3	2.00	0.44
1:D:377:ILE:HD12	1:D:377:ILE:HA	1.84	0.44
1:D:1770:SER:OG	1:D:1956:GLU:OE2	2.34	0.44
1:A:1774:PRO:HG2	1:A:1776:HIS:CE1	2.53	0.44
1:A:1931:LEU:O	1:A:1936:LYS:HE3	2.18	0.44
1:A:3890:LEU:HD23	1:A:3890:LEU:HA	1.83	0.44
1:B:2002:PRO:HA	1:B:2005:GLN:HB3	2.00	0.44
1:C:1662:PHE:O	1:C:1666:THR:HG22	2.18	0.44
1:C:1765:VAL:HG12	1:C:1766:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:LYS:HB2	1:D:464:LYS:HE2	1.71	0.44
1:A:116:MET:HE2	1:A:116:MET:HB3	1.88	0.43
1:A:1765:VAL:HG12	1:A:1766:GLY:H	1.83	0.43
1:B:107:ILE:HD12	1:B:107:ILE:HA	1.87	0.43
1:B:358:THR:HG21	1:B:382:GLY:HA3	1.99	0.43
1:B:4223:ASN:HB2	1:B:4224:GLU:OE2	2.18	0.43
1:B:4850:LEU:O	1:B:4853:VAL:HG22	2.17	0.43
1:C:22:LEU:HD12	1:C:37:LEU:HD23	2.00	0.43
1:C:884:LEU:O	1:C:888:GLU:HG2	2.18	0.43
1:C:1844:LEU:O	1:C:1847:THR:HG22	2.18	0.43
1:C:2342:ASN:OD1	1:C:2342:ASN:N	2.51	0.43
1:C:4107:GLU:OE1	1:C:4107:GLU:N	2.41	0.43
1:D:25:SER:HB2	1:D:34:LYS:HZ2	1.83	0.43
1:D:176:SER:OG	1:D:178:ARG:HD3	2.18	0.43
1:D:3927:GLN:HB2	1:D:3992:PHE:CE2	2.52	0.43
1:A:2377:LEU:HD13	1:A:2380:ILE:HD11	1.99	0.43
1:B:4984:ASN:C	1:B:4986:ALA:H	2.21	0.43
1:C:4223:ASN:HB2	1:C:4224:GLU:OE2	2.18	0.43
1:D:636:ASN:HB3	1:D:702:TRP:HZ3	1.82	0.43
1:D:4223:ASN:HB2	1:D:4224:GLU:OE2	2.18	0.43
1:D:4850:LEU:O	1:D:4853:VAL:HG22	2.17	0.43
1:B:108:LEU:HD12	1:B:147:TRP:CZ2	2.53	0.43
1:D:310:LYS:O	1:D:310:LYS:NZ	2.45	0.43
1:D:2377:LEU:HD13	1:D:2380:ILE:HD11	1.99	0.43
1:A:210:GLU:HB3	1:A:273:HIS:CE1	2.50	0.43
1:A:560:ILE:HD12	1:A:560:ILE:H	1.82	0.43
1:A:2025:GLU:HA	1:A:2028:ARG:NE	2.34	0.43
1:A:4223:ASN:HB2	1:A:4224:GLU:OE2	2.18	0.43
1:B:176:SER:OG	1:B:178:ARG:HD3	2.18	0.43
1:B:1847:THR:O	1:B:1850:VAL:HB	2.19	0.43
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.25	0.43
1:C:116:MET:HE3	1:C:117:TYR:N	2.33	0.43
1:C:3927:GLN:HB2	1:C:3992:PHE:CE2	2.52	0.43
1:D:1650:ILE:HD12	1:D:1653:LEU:HD23	1.99	0.43
1:D:1723:ALA:HA	1:D:1775:HIS:HD2	1.84	0.43
1:D:4049:VAL:HA	1:D:4163:PHE:HZ	1.83	0.43
1:D:4819:GLY:C	1:D:4820:VAL:HG23	2.39	0.43
1:A:2342:ASN:OD1	1:A:2342:ASN:N	2.51	0.43
1:A:3895:HIS:HE1	1:A:3970:GLN:HB3	1.84	0.43
1:B:526:LEU:HD12	1:B:526:LEU:HA	1.82	0.43
1:B:1723:ALA:HA	1:B:1775:HIS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2377:LEU:HD13	1:B:2380:ILE:HD11	1.99	0.43
1:B:4134:GLU:HB2	1:B:4135:PRO:HD3	2.00	0.43
1:C:210:GLU:HB3	1:C:273:HIS:CE1	2.50	0.43
1:C:1723:ALA:HA	1:C:1775:HIS:HD2	1.84	0.43
1:D:1765:VAL:HG12	1:D:1766:GLY:H	1.83	0.43
1:D:4051:SER:O	1:D:4055:VAL:HG13	2.17	0.43
1:D:4181:ILE:HG22	1:D:4193:ILE:HB	2.01	0.43
1:D:4731:ILE:HG23	1:D:4732:PHE:CD1	2.51	0.43
1:A:629:ARG:HB3	1:A:634:GLN:CD	2.38	0.43
1:A:672:VAL:HG11	1:A:675:LEU:HD23	2.00	0.43
1:A:884:LEU:O	1:A:888:GLU:HG2	2.18	0.43
1:B:2342:ASN:OD1	1:B:2342:ASN:N	2.51	0.43
1:C:176:SER:OG	1:C:178:ARG:HD3	2.18	0.43
1:C:310:LYS:O	1:C:310:LYS:NZ	2.45	0.43
1:C:636:ASN:HB3	1:C:702:TRP:HZ3	1.82	0.43
1:C:2159:LEU:HA	1:C:2162:ILE:HG22	2.01	0.43
1:C:2296:GLU:HA	1:C:2299:VAL:HG22	1.99	0.43
1:D:460:GLN:H	1:D:460:GLN:CD	2.21	0.43
1:D:1749:PRO:HB2	1:D:1755:GLY:HA3	2.00	0.43
1:A:176:SER:OG	1:A:178:ARG:HD3	2.18	0.43
1:A:413:GLN:OE1	1:A:437:PRO:HG3	2.19	0.43
1:A:460:GLN:CD	1:A:460:GLN:H	2.21	0.43
1:A:1723:ALA:HA	1:A:1775:HIS:HD2	1.84	0.43
1:A:1808:ARG:HG3	1:A:1854:PHE:CE1	2.54	0.43
1:A:1847:THR:O	1:A:1850:VAL:HB	2.19	0.43
1:A:2220:THR:HA	1:A:2223:ILE:HD11	2.00	0.43
1:A:4713:SER:OG	1:A:4775:TYR:OH	2.30	0.43
1:C:455:PRO:HB2	1:C:464:LYS:NZ	2.32	0.43
1:C:1092:PHE:CE2	1:C:1094:ALA:HB2	2.53	0.43
1:C:1713:ASP:O	1:C:1716:ILE:HG22	2.19	0.43
1:C:1723:ALA:HB1	1:C:1851:MET:HG2	2.00	0.43
1:C:2002:PRO:HA	1:C:2005:GLN:HB3	2.00	0.43
1:C:4984:ASN:C	1:C:4986:ALA:H	2.21	0.43
1:D:108:LEU:HD12	1:D:147:TRP:CZ2	2.53	0.43
1:D:455:PRO:HB2	1:D:464:LYS:NZ	2.32	0.43
1:D:560:ILE:H	1:D:560:ILE:HD12	1.82	0.43
1:D:1161:ILE:HG23	1:D:1177:THR:HG21	1.99	0.43
1:D:1713:ASP:O	1:D:1716:ILE:HG22	2.19	0.43
1:D:2159:LEU:HA	1:D:2162:ILE:HG22	2.01	0.43
1:A:455:PRO:HB2	1:A:464:LYS:NZ	2.32	0.43
1:A:1749:PRO:HB2	1:A:1755:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2159:LEU:HA	1:A:2162:ILE:HG22	2.01	0.43
1:B:22:LEU:HD12	1:B:37:LEU:HD23	2.00	0.43
1:B:683:ARG:HG2	1:B:717:ASP:CB	2.49	0.43
1:B:1092:PHE:CE2	1:B:1094:ALA:HB2	2.53	0.43
1:B:1774:PRO:HG2	1:B:1776:HIS:CE1	2.53	0.43
1:C:683:ARG:HG2	1:C:717:ASP:CB	2.49	0.43
1:C:2025:GLU:HA	1:C:2028:ARG:NE	2.34	0.43
1:C:4850:LEU:O	1:C:4853:VAL:HG22	2.17	0.43
1:D:180:LEU:O	1:D:200:TRP:NE1	2.32	0.43
1:D:413:GLN:OE1	1:D:437:PRO:HG3	2.19	0.43
1:D:884:LEU:O	1:D:888:GLU:HG2	2.18	0.43
1:D:1130:GLN:HG2	1:D:1138:PRO:HA	2.00	0.43
1:D:1963:GLU:HA	1:D:3650:CYS:SG	2.59	0.43
1:D:2025:GLU:HA	1:D:2028:ARG:NE	2.34	0.43
1:A:737:LEU:HD13	1:A:737:LEU:HA	1.90	0.43
1:A:4134:GLU:HB2	1:A:4135:PRO:HD3	2.00	0.43
1:A:4819:GLY:C	1:A:4820:VAL:HG23	2.39	0.43
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.77	0.43
1:B:459:LEU:HD12	1:B:464:LYS:HZ3	1.83	0.43
1:B:629:ARG:HB3	1:B:634:GLN:CD	2.38	0.43
1:B:1727:ARG:NH1	1:B:1772:ARG:HB3	2.34	0.43
1:B:3980:LEU:HD23	1:B:3980:LEU:HA	1.81	0.43
1:B:4049:VAL:HA	1:B:4163:PHE:HZ	1.83	0.43
1:B:4693:GLY:C	1:B:4695:ASP:H	2.22	0.43
1:C:864:PRO:O	1:C:868:GLU:N	2.41	0.43
1:C:1931:LEU:O	1:C:1936:LYS:HE3	2.18	0.43
1:D:683:ARG:HG2	1:D:717:ASP:CB	2.49	0.43
1:D:1847:THR:O	1:D:1850:VAL:HB	2.19	0.43
1:A:683:ARG:HG2	1:A:717:ASP:CB	2.49	0.43
1:A:1727:ARG:NH1	1:A:1772:ARG:HB3	2.34	0.43
1:A:3980:LEU:HD23	1:A:3980:LEU:HA	1.81	0.43
1:A:4101:LYS:O	1:A:4102:GLN:HG2	2.19	0.43
1:B:1808:ARG:HG3	1:B:1854:PHE:CE1	2.54	0.43
1:B:2022:PRO:HB2	1:B:2024:PRO:HD2	2.00	0.43
1:B:2159:LEU:HA	1:B:2162:ILE:HG22	2.01	0.43
1:B:4027:LEU:HD23	1:B:4027:LEU:HA	1.73	0.43
1:B:4865:LYS:HA	1:B:4865:LYS:HD2	1.84	0.43
1:C:887:ILE:HD13	1:C:907:LEU:HD11	2.00	0.43
1:C:1130:GLN:HG2	1:C:1138:PRO:HA	2.00	0.43
1:C:1495:VAL:HA	1:C:1536:SER:HA	2.01	0.43
1:C:4693:GLY:C	1:C:4695:ASP:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1662:PHE:O	1:D:1666:THR:HG22	2.18	0.43
1:D:1945:TYR:HA	1:D:1948:ASP:OD2	2.19	0.43
1:D:4984:ASN:C	1:D:4986:ALA:H	2.21	0.43
1:A:232:THR:HG21	1:A:252:VAL:HG11	2.01	0.42
1:A:377:ILE:HD12	1:A:377:ILE:HA	1.84	0.42
1:A:1495:VAL:HA	1:A:1536:SER:HA	2.01	0.42
1:A:3658:LYS:HD2	1:A:3661:TRP:HZ3	1.82	0.42
1:A:3893:GLU:OE1	1:A:3894:GLY:N	2.52	0.42
1:A:3927:GLN:HA	1:A:3930:ILE:HG22	2.01	0.42
1:B:560:ILE:H	1:B:560:ILE:HD12	1.82	0.42
1:B:1945:TYR:HA	1:B:1948:ASP:OD2	2.19	0.42
1:B:2176:ASN:OD1	1:B:2176:ASN:N	2.48	0.42
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.48	0.42
1:C:629:ARG:HD3	1:C:634:GLN:HG2	2.01	0.42
1:C:672:VAL:HG11	1:C:675:LEU:HD23	2.00	0.42
1:C:3895:HIS:HE1	1:C:3970:GLN:HB3	1.84	0.42
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.50	0.42
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.37	0.42
1:D:424:LYS:HE3	1:D:424:LYS:HB3	1.91	0.42
1:D:459:LEU:HD12	1:D:464:LYS:NZ	2.34	0.42
1:D:629:ARG:HD3	1:D:634:GLN:HG2	2.01	0.42
1:D:1008:SER:H	1:D:1020:ARG:N	2.17	0.42
1:D:1723:ALA:HB1	1:D:1851:MET:HG2	2.00	0.42
1:D:1965:TYR:OH	1:D:2027:ILE:O	2.22	0.42
1:D:2002:PRO:HA	1:D:2005:GLN:HB3	2.00	0.42
1:D:4181:ILE:HD11	1:D:4988:TYR:CD2	2.54	0.42
1:A:274:LEU:HB3	1:A:339:ILE:HD12	2.01	0.42
1:A:1723:ALA:HB1	1:A:1851:MET:HG2	2.00	0.42
1:A:4731:ILE:HG23	1:A:4732:PHE:CD1	2.51	0.42
1:B:672:VAL:HG11	1:B:675:LEU:HD23	2.00	0.42
1:B:1723:ALA:HB1	1:B:1851:MET:CG	2.49	0.42
1:B:2220:THR:HA	1:B:2223:ILE:HD11	2.00	0.42
1:C:459:LEU:HD12	1:C:464:LYS:NZ	2.34	0.42
1:C:615:ARG:CZ	1:C:2168:VAL:HG21	2.50	0.42
1:C:1008:SER:H	1:C:1020:ARG:N	2.17	0.42
1:C:1963:GLU:HA	1:C:3650:CYS:SG	2.59	0.42
1:D:34:LYS:HA	1:D:34:LYS:HD2	1.83	0.42
1:D:142:THR:OG1	1:D:144:GLU:OE2	2.22	0.42
1:D:224:HIS:CG	1:D:247:TYR:HE2	2.38	0.42
1:D:672:VAL:HG11	1:D:675:LEU:HD23	2.00	0.42
1:D:3893:GLU:OE1	1:D:3894:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4189:ARG:HE	1:D:4189:ARG:HB2	1.66	0.42
1:A:459:LEU:HD12	1:A:464:LYS:NZ	2.34	0.42
1:A:887:ILE:HD13	1:A:907:LEU:HD11	2.00	0.42
1:A:1770:SER:OG	1:A:1956:GLU:OE2	2.34	0.42
1:A:1943:LEU:HD13	1:A:2098:VAL:HG12	2.01	0.42
1:B:224:HIS:CG	1:B:247:TYR:HE2	2.38	0.42
1:B:3927:GLN:HA	1:B:3930:ILE:HG22	2.01	0.42
1:B:4071:ILE:HD11	1:B:4102:GLN:NE2	2.35	0.42
1:B:4075:GLU:OE1	1:B:4075:GLU:HA	2.19	0.42
1:B:4181:ILE:HD11	1:B:4988:TYR:CD2	2.54	0.42
1:C:4181:ILE:HG22	1:C:4193:ILE:HB	2.01	0.42
1:D:1808:ARG:HG3	1:D:1854:PHE:CE1	2.54	0.42
1:D:2342:ASN:OD1	1:D:2342:ASN:N	2.51	0.42
1:D:4134:GLU:HB2	1:D:4135:PRO:HD3	2.00	0.42
1:A:1713:ASP:O	1:A:1716:ILE:HG22	2.19	0.42
1:A:4071:ILE:HD11	1:A:4102:GLN:NE2	2.35	0.42
1:A:4107:GLU:OE1	1:A:4107:GLU:N	2.41	0.42
1:B:413:GLN:OE1	1:B:437:PRO:HG3	2.19	0.42
1:B:1130:GLN:HG2	1:B:1138:PRO:HA	2.00	0.42
1:B:1713:ASP:O	1:B:1716:ILE:HG22	2.19	0.42
1:B:1943:LEU:HD13	1:B:2098:VAL:HG12	2.01	0.42
1:B:3847:PHE:O	1:B:3850:GLN:HG3	2.19	0.42
1:B:3893:GLU:OE1	1:B:3894:GLY:N	2.52	0.42
1:B:4661:TYR:OH	1:B:4788:SER:OG	2.16	0.42
1:B:4995:LEU:HD23	1:B:4995:LEU:HA	1.86	0.42
1:C:1808:ARG:HG3	1:C:1854:PHE:CE1	2.54	0.42
1:C:1847:THR:O	1:C:1850:VAL:HB	2.19	0.42
1:C:1945:TYR:HA	1:C:1948:ASP:OD2	2.19	0.42
1:C:2220:THR:HA	1:C:2223:ILE:HD11	2.00	0.42
1:C:4672:LYS:HE3	1:C:4672:LYS:HB2	1.80	0.42
1:D:210:GLU:HB3	1:D:273:HIS:CE1	2.50	0.42
1:D:2142:TYR:CE2	1:D:2197:LEU:HD21	2.55	0.42
1:D:2220:THR:HA	1:D:2223:ILE:HD11	2.00	0.42
1:D:4101:LYS:O	1:D:4102:GLN:HG2	2.19	0.42
1:A:1130:GLN:HG2	1:A:1138:PRO:HA	2.00	0.42
1:A:4115:SER:HB2	1:A:4123:ILE:HD12	2.02	0.42
1:B:3895:HIS:HE1	1:B:3970:GLN:HB3	1.84	0.42
1:C:1142:PRO:O	1:C:1144:GLN:NE2	2.53	0.42
1:C:3893:GLU:OE1	1:C:3894:GLY:N	2.52	0.42
1:C:4049:VAL:HA	1:C:4163:PHE:HZ	1.83	0.42
1:C:4819:GLY:C	1:C:4820:VAL:HG23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:ARG:NE	1:D:707:VAL:O	2.49	0.42
1:D:1723:ALA:HB1	1:D:1851:MET:CG	2.49	0.42
1:D:4693:GLY:C	1:D:4695:ASP:H	2.22	0.42
1:A:3789:GLU:CD	1:A:3791:GLY:H	2.22	0.42
1:A:3847:PHE:O	1:A:3850:GLN:HG3	2.19	0.42
1:A:4181:ILE:HD11	1:A:4988:TYR:CD2	2.54	0.42
1:B:25:SER:HB2	1:B:34:LYS:HZ2	1.84	0.42
1:B:266:ARG:NH2	1:B:331:VAL:O	2.53	0.42
1:B:459:LEU:HD12	1:B:464:LYS:NZ	2.34	0.42
1:B:1495:VAL:HA	1:B:1536:SER:HA	2.01	0.42
1:B:1963:GLU:HA	1:B:3650:CYS:SG	2.59	0.42
1:B:4175:ARG:N	1:B:4176:PRO:HD2	2.35	0.42
1:B:4819:GLY:C	1:B:4820:VAL:HG23	2.39	0.42
1:C:21:VAL:HG22	1:C:203:ASN:HB2	2.02	0.42
1:C:62:LEU:HD12	1:C:62:LEU:HA	1.90	0.42
1:C:182:LEU:H	1:C:198:THR:CG2	2.33	0.42
1:C:264:PRO:HG2	1:C:270:SER:HB2	2.02	0.42
1:C:273:HIS:CD2	1:C:334:MET:HG3	2.55	0.42
1:C:1742:THR:HG23	1:C:1769:THR:HG21	2.02	0.42
1:C:4075:GLU:OE1	1:C:4075:GLU:HA	2.19	0.42
1:C:4814:LEU:HD23	1:C:4814:LEU:HA	1.86	0.42
1:D:615:ARG:CZ	1:D:2168:VAL:HG21	2.50	0.42
1:D:1943:LEU:HD13	1:D:2098:VAL:HG12	2.01	0.42
1:D:3665:GLU:OE2	1:D:3666:ASP:N	2.53	0.42
1:A:224:HIS:CG	1:A:247:TYR:HE2	2.38	0.42
1:A:646:PRO:HG3	1:A:791:PHE:HE2	1.85	0.42
1:A:1945:TYR:HA	1:A:1948:ASP:OD2	2.19	0.42
1:A:1963:GLU:HA	1:A:3650:CYS:SG	2.59	0.42
1:A:4995:LEU:HD23	1:A:4995:LEU:HA	1.86	0.42
1:B:232:THR:HG21	1:B:252:VAL:HG11	2.01	0.42
1:B:3888:LEU:HD23	1:B:3888:LEU:HA	1.82	0.42
1:C:4071:ILE:HD11	1:C:4102:GLN:NE2	2.35	0.42
1:D:232:THR:HG21	1:D:252:VAL:HG11	2.01	0.42
1:D:266:ARG:NH2	1:D:331:VAL:O	2.53	0.42
1:D:273:HIS:CD2	1:D:334:MET:HG3	2.55	0.42
1:A:21:VAL:HG22	1:A:203:ASN:HB2	2.02	0.42
1:A:1008:SER:H	1:A:1020:ARG:N	2.17	0.42
1:A:1079:LYS:NZ	1:A:1107:PRO:O	2.53	0.42
1:A:2029:GLN:H	1:A:2029:GLN:HG3	1.62	0.42
1:A:4181:ILE:HG22	1:A:4193:ILE:HB	2.01	0.42
1:B:615:ARG:CZ	1:B:2168:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2025:GLU:HA	1:B:2028:ARG:NE	2.34	0.42
1:B:4673:ARG:NH2	1:B:4698:LYS:HG3	2.35	0.42
1:B:4924:VAL:HA	1:B:4928:LEU:HB2	2.02	0.42
1:C:2142:TYR:CE2	1:C:2197:LEU:HD21	2.55	0.42
1:D:21:VAL:HG22	1:D:203:ASN:HB2	2.02	0.42
1:D:1727:ARG:NH1	1:D:1772:ARG:HB3	2.34	0.42
1:D:3789:GLU:CD	1:D:3791:GLY:H	2.22	0.42
1:D:3895:HIS:HE1	1:D:3970:GLN:HB3	1.84	0.42
1:D:4030:LEU:HD23	1:D:4030:LEU:HA	1.85	0.42
1:A:273:HIS:CD2	1:A:334:MET:HG3	2.55	0.42
1:A:792:LEU:HD23	1:A:792:LEU:HA	1.87	0.42
1:A:1703:LEU:O	1:A:1831:GLY:HA2	2.20	0.42
1:A:4899:ASP:HB2	1:A:4900:GLU:OE2	2.20	0.42
1:B:264:PRO:HG2	1:B:270:SER:HB2	2.02	0.42
1:B:273:HIS:CD2	1:B:334:MET:HG3	2.55	0.42
1:B:562:GLU:OE1	1:B:598:LYS:NZ	2.41	0.42
1:B:683:ARG:NE	1:B:707:VAL:O	2.49	0.42
1:B:1651:LEU:HD22	1:B:1702:HIS:CE1	2.55	0.42
1:B:1703:LEU:O	1:B:1831:GLY:HA2	2.20	0.42
1:B:1723:ALA:HB1	1:B:1851:MET:HG2	2.00	0.42
1:B:1742:THR:HG23	1:B:1769:THR:HG21	2.02	0.42
1:B:1867:GLU:N	1:B:1868:PRO:HD2	2.35	0.42
1:B:3789:GLU:CD	1:B:3791:GLY:H	2.22	0.42
1:C:34:LYS:HA	1:C:34:LYS:HD2	1.83	0.42
1:C:224:HIS:CG	1:C:247:TYR:HE2	2.38	0.42
1:C:274:LEU:HB3	1:C:339:ILE:HD12	2.01	0.42
1:C:1723:ALA:HB1	1:C:1851:MET:CG	2.49	0.42
1:C:2254:LEU:O	1:C:2258:LEU:HG	2.20	0.42
1:C:3847:PHE:O	1:C:3850:GLN:HG3	2.19	0.42
1:C:4181:ILE:HD11	1:C:4988:TYR:CD2	2.54	0.42
1:D:182:LEU:H	1:D:198:THR:CG2	2.33	0.42
1:D:359:TYR:HA	1:D:376:ALA:HA	2.02	0.42
1:D:1495:VAL:HA	1:D:1536:SER:HA	2.01	0.42
1:D:3927:GLN:HA	1:D:3930:ILE:HG22	2.01	0.42
1:D:4115:SER:HB2	1:D:4123:ILE:HD12	2.02	0.42
1:D:4170:ILE:HD12	1:D:4170:ILE:HA	1.90	0.42
1:A:1723:ALA:HB1	1:A:1851:MET:CG	2.49	0.42
1:A:2142:TYR:CE2	1:A:2197:LEU:HD21	2.55	0.42
1:A:4673:ARG:NH2	1:A:4698:LYS:HG3	2.35	0.42
1:B:3665:GLU:OE2	1:B:3666:ASP:N	2.53	0.42
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:HD12	1:C:551:LEU:HA	1.86	0.42
1:D:646:PRO:HG3	1:D:791:PHE:HE2	1.85	0.42
1:D:793:LEU:HD21	1:D:1625:GLY:HA2	2.02	0.42
1:D:887:ILE:HD13	1:D:907:LEU:HD11	2.00	0.42
1:D:1651:LEU:HD22	1:D:1702:HIS:CE1	2.55	0.42
1:D:3847:PHE:O	1:D:3850:GLN:HG3	2.19	0.42
1:D:3980:LEU:HD23	1:D:3980:LEU:HA	1.81	0.42
1:D:4162:ASN:HA	1:D:4165:GLU:OE2	2.20	0.42
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.48	0.41
1:A:1651:LEU:HD22	1:A:1702:HIS:CE1	2.55	0.41
1:A:4986:ALA:O	1:A:4989:MET:HB2	2.20	0.41
1:B:359:TYR:HA	1:B:376:ALA:HA	2.02	0.41
1:B:629:ARG:HD3	1:B:634:GLN:HG2	2.01	0.41
1:B:3661:TRP:HB3	1:B:3662:ILE:H	1.66	0.41
1:B:4115:SER:HB2	1:B:4123:ILE:HD12	2.02	0.41
1:B:4162:ASN:HA	1:B:4165:GLU:OE2	2.20	0.41
1:B:4181:ILE:HG22	1:B:4193:ILE:HB	2.01	0.41
1:C:793:LEU:HD21	1:C:1625:GLY:HA2	2.02	0.41
1:C:3789:GLU:CD	1:C:3791:GLY:H	2.22	0.41
1:C:4899:ASP:HB2	1:C:4900:GLU:OE2	2.20	0.41
1:D:264:PRO:HG2	1:D:270:SER:HB2	2.02	0.41
1:D:1742:THR:HG23	1:D:1769:THR:HG21	2.02	0.41
1:D:3661:TRP:HB3	1:D:3662:ILE:H	1.66	0.41
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.37	0.41
1:A:615:ARG:CZ	1:A:2168:VAL:HG21	2.50	0.41
1:A:1867:GLU:N	1:A:1868:PRO:HD2	2.35	0.41
1:A:4051:SER:O	1:A:4051:SER:OG	2.33	0.41
1:A:4792:LEU:HD23	1:A:4792:LEU:HA	1.91	0.41
1:B:116:MET:HE2	1:B:116:MET:HB3	1.83	0.41
1:B:1718:ILE:HG13	1:B:1719:HIS:CD2	2.55	0.41
1:C:232:THR:HG21	1:C:252:VAL:HG11	2.01	0.41
1:C:266:ARG:NH2	1:C:331:VAL:O	2.53	0.41
1:D:463:GLU:OE2	1:D:463:GLU:N	2.40	0.41
1:D:1142:PRO:O	1:D:1144:GLN:NE2	2.53	0.41
1:D:1867:GLU:N	1:D:1868:PRO:HD2	2.35	0.41
1:D:3658:LYS:HD2	1:D:3661:TRP:HZ3	1.82	0.41
1:D:3888:LEU:HA	1:D:3888:LEU:HD23	1.82	0.41
1:D:4767:TRP:CE2	1:D:4770:SER:HB3	2.56	0.41
1:D:4849:TYR:O	1:D:4853:VAL:HG13	2.20	0.41
1:D:4899:ASP:HB2	1:D:4900:GLU:OE2	2.20	0.41
1:A:1657:LEU:HD12	1:A:1657:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2254:LEU:O	1:A:2258:LEU:HG	2.20	0.41
1:A:2325:PRO:HB2	1:A:2421:ALA:HB1	2.02	0.41
1:B:21:VAL:HG22	1:B:203:ASN:HB2	2.02	0.41
1:B:882:TRP:HE1	1:B:886:ARG:CZ	2.34	0.41
1:B:1698:LEU:HG	1:B:1712:TYR:CZ	2.55	0.41
1:B:2142:TYR:CE2	1:B:2197:LEU:HD21	2.55	0.41
1:B:2255:SER:HA	1:B:2258:LEU:HD12	2.03	0.41
1:B:3927:GLN:NE2	1:B:3991:GLY:HA3	2.36	0.41
1:B:4101:LYS:O	1:B:4102:GLN:HG2	2.19	0.41
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.50	0.41
1:C:2029:GLN:H	1:C:2029:GLN:HG3	1.62	0.41
1:C:3895:HIS:CE1	1:C:3970:GLN:HB3	2.56	0.41
1:C:4175:ARG:N	1:C:4176:PRO:HD2	2.35	0.41
1:D:274:LEU:HB3	1:D:339:ILE:HD12	2.01	0.41
1:D:1079:LYS:NZ	1:D:1107:PRO:O	2.53	0.41
1:D:1718:ILE:HG13	1:D:1719:HIS:CD2	2.55	0.41
1:D:4071:ILE:HD11	1:D:4102:GLN:NE2	2.35	0.41
1:D:4075:GLU:OE1	1:D:4075:GLU:HA	2.19	0.41
1:A:794:GLY:HA3	1:A:811:CYS:SG	2.61	0.41
1:A:891:TRP:HE3	1:A:904:HIS:HB2	1.85	0.41
1:A:4030:LEU:HD23	1:A:4030:LEU:HA	1.85	0.41
1:A:4693:GLY:C	1:A:4695:ASP:H	2.22	0.41
1:B:223:PHE:HD1	1:B:223:PHE:HA	1.74	0.41
1:B:1142:PRO:O	1:B:1144:GLN:NE2	2.53	0.41
1:B:4792:LEU:HD23	1:B:4792:LEU:HA	1.91	0.41
1:C:464:LYS:HE2	1:C:464:LYS:HB2	1.71	0.41
1:C:497:TYR:CE1	1:C:504:ALA:HA	2.56	0.41
1:C:1703:LEU:HA	1:C:1708:ARG:NH2	2.32	0.41
1:C:2187:ASN:OD1	1:C:2187:ASN:N	2.54	0.41
1:C:3927:GLN:HA	1:C:3930:ILE:HG22	2.01	0.41
1:D:864:PRO:O	1:D:868:GLU:N	2.41	0.41
1:D:4889:VAL:HG11	1:D:4900:GLU:HG2	2.03	0.41
1:A:266:ARG:NH2	1:A:331:VAL:O	2.53	0.41
1:A:497:TYR:CE1	1:A:504:ALA:HA	2.56	0.41
1:A:3716:LEU:HD12	1:A:3716:LEU:HA	1.89	0.41
1:A:4075:GLU:OE1	1:A:4075:GLU:HA	2.19	0.41
1:A:4780:PHE:HD1	1:A:4780:PHE:HA	1.78	0.41
1:B:274:LEU:HB3	1:B:339:ILE:HD12	2.01	0.41
1:B:497:TYR:HA	1:B:503:PHE:HD2	1.86	0.41
1:B:793:LEU:HD21	1:B:1625:GLY:HA2	2.02	0.41
1:B:1008:SER:H	1:B:1020:ARG:N	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2278:ALA:HA	1:B:2281:ILE:HD11	2.02	0.41
1:C:1703:LEU:O	1:C:1831:GLY:HA2	2.20	0.41
1:C:1727:ARG:NH1	1:C:1772:ARG:HB3	2.34	0.41
1:C:4101:LYS:O	1:C:4102:GLN:HG2	2.19	0.41
1:C:4115:SER:HB2	1:C:4123:ILE:HD12	2.02	0.41
1:C:4924:VAL:HA	1:C:4928:LEU:HB2	2.02	0.41
1:D:1703:LEU:O	1:D:1831:GLY:HA2	2.20	0.41
1:A:1142:PRO:O	1:A:1144:GLN:NE2	2.53	0.41
1:A:1698:LEU:HG	1:A:1712:TYR:CZ	2.55	0.41
1:A:1848:LEU:HD23	1:A:1848:LEU:HA	1.83	0.41
1:A:3844:LEU:HD12	1:A:3844:LEU:HA	1.93	0.41
1:A:4730:ASP:OD1	1:A:4730:ASP:N	2.54	0.41
1:A:4813:LEU:HD12	1:A:4813:LEU:HA	1.87	0.41
1:B:646:PRO:HG3	1:B:791:PHE:HE2	1.85	0.41
1:C:497:TYR:HA	1:C:503:PHE:HD2	1.86	0.41
1:C:1943:LEU:HD13	1:C:2098:VAL:HG12	2.01	0.41
1:C:4767:TRP:CE2	1:C:4770:SER:HB3	2.56	0.41
1:C:4849:TYR:O	1:C:4853:VAL:HG13	2.20	0.41
1:D:2325:PRO:HB2	1:D:2421:ALA:HB1	2.02	0.41
1:D:4160:LEU:HD12	1:D:4160:LEU:HA	1.86	0.41
1:D:4175:ARG:N	1:D:4176:PRO:HD2	2.35	0.41
1:A:264:PRO:HG2	1:A:270:SER:HB2	2.02	0.41
1:A:629:ARG:HD3	1:A:634:GLN:HG2	2.01	0.41
1:A:882:TRP:HE1	1:A:886:ARG:CZ	2.34	0.41
1:A:1716:ILE:O	1:A:1720:LEU:HD23	2.21	0.41
1:A:1742:THR:HG23	1:A:1769:THR:HG21	2.02	0.41
1:A:4859:PHE:HE2	1:A:4913:ARG:HB2	1.86	0.41
1:A:4889:VAL:HG11	1:A:4900:GLU:HG2	2.03	0.41
1:B:1079:LYS:NZ	1:B:1107:PRO:O	2.53	0.41
1:B:4918:ILE:HD13	1:B:4918:ILE:HA	1.94	0.41
1:B:4986:ALA:O	1:B:4989:MET:HB2	2.20	0.41
1:C:3665:GLU:OE2	1:C:3666:ASP:N	2.53	0.41
1:C:4986:ALA:O	1:C:4989:MET:HB2	2.20	0.41
1:D:610:ASN:OD1	1:D:610:ASN:N	2.54	0.41
1:D:1720:LEU:O	1:D:1724:CYS:N	2.44	0.41
1:D:1968:LYS:HA	1:D:1968:LYS:HD3	1.92	0.41
1:D:2255:SER:HA	1:D:2258:LEU:HD12	2.03	0.41
1:D:4836:GLN:H	1:D:4836:GLN:HG2	1.75	0.41
1:D:4859:PHE:HE2	1:D:4913:ARG:HB2	1.86	0.41
1:D:4986:ALA:O	1:D:4989:MET:HB2	2.20	0.41
1:A:3665:GLU:OE2	1:A:3666:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4175:ARG:N	1:A:4176:PRO:HD2	2.35	0.41
1:A:4924:VAL:HA	1:A:4928:LEU:HB2	2.02	0.41
1:B:792:LEU:HD23	1:B:792:LEU:HA	1.87	0.41
1:B:794:GLY:HA3	1:B:811:CYS:SG	2.61	0.41
1:B:1694:LEU:HD23	1:B:1715:LEU:HB2	2.03	0.41
1:B:4051:SER:O	1:B:4051:SER:OG	2.33	0.41
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.37	0.41
1:B:4713:SER:OG	1:B:4775:TYR:OH	2.30	0.41
1:B:4767:TRP:CE2	1:B:4770:SER:HB3	2.56	0.41
1:B:4823:LEU:O	1:B:4825:THR:N	2.54	0.41
1:C:646:PRO:HG3	1:C:791:PHE:HE2	1.85	0.41
1:C:889:GLN:HB2	1:C:891:TRP:CD1	2.56	0.41
1:C:1867:GLU:N	1:C:1868:PRO:HD2	2.35	0.41
1:C:2278:ALA:HA	1:C:2281:ILE:HD11	2.02	0.41
1:C:2295:LEU:O	1:C:2298:VAL:HG22	2.21	0.41
1:C:4162:ASN:HA	1:C:4165:GLU:OE2	2.20	0.41
1:C:4823:LEU:O	1:C:4825:THR:N	2.54	0.41
1:C:4889:VAL:HG11	1:C:4900:GLU:HG2	2.03	0.41
1:D:274:LEU:HD12	1:D:274:LEU:HA	1.77	0.41
1:D:3713:LYS:HE3	1:D:3713:LYS:HB2	1.88	0.41
1:D:4238:CYS:O	1:D:4242:ILE:HG12	2.21	0.41
1:A:183:SER:HB3	1:A:192:ASP:OD1	2.21	0.41
1:A:220:LEU:HB2	1:A:391:THR:O	2.21	0.41
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.90	0.41
1:A:1243:PRO:HG3	1:A:1502:SER:H	1.86	0.41
1:A:1810:LYS:HE3	1:A:1810:LYS:HB2	1.91	0.41
1:A:2187:ASN:OD1	1:A:2187:ASN:N	2.54	0.41
1:A:2268:GLN:HG2	1:A:2269:GLY:N	2.36	0.41
1:A:2278:ALA:HA	1:A:2281:ILE:HD11	2.02	0.41
1:A:3895:HIS:CE1	1:A:3970:GLN:HB3	2.56	0.41
1:A:3927:GLN:NE2	1:A:3991:GLY:HA3	2.36	0.41
1:A:4162:ASN:HA	1:A:4165:GLU:OE2	2.20	0.41
1:A:4767:TRP:CE2	1:A:4770:SER:HB3	2.56	0.41
1:A:4823:LEU:O	1:A:4825:THR:N	2.54	0.41
1:A:4849:TYR:O	1:A:4853:VAL:HG13	2.20	0.41
1:B:183:SER:HB3	1:B:192:ASP:OD1	2.21	0.41
1:B:455:PRO:HB2	1:B:464:LYS:NZ	2.32	0.41
1:B:497:TYR:CE1	1:B:504:ALA:HA	2.56	0.41
1:B:1075:PHE:HB2	1:B:1192:CYS:SG	2.61	0.41
1:B:1243:PRO:HG3	1:B:1502:SER:H	1.86	0.41
1:B:2254:LEU:O	1:B:2258:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4849:TYR:O	1:B:4853:VAL:HG13	2.20	0.41
1:B:4899:ASP:HB2	1:B:4900:GLU:OE2	2.20	0.41
1:C:1075:PHE:HB2	1:C:1192:CYS:SG	2.61	0.41
1:C:1079:LYS:NZ	1:C:1107:PRO:O	2.53	0.41
1:C:1590:GLN:HG2	1:C:1592:PRO:HD3	2.03	0.41
1:C:1694:LEU:HD23	1:C:1715:LEU:HB2	2.03	0.41
1:C:1716:ILE:O	1:C:1720:LEU:HD23	2.21	0.41
1:C:1718:ILE:HG13	1:C:1719:HIS:CD2	2.55	0.41
1:C:2325:PRO:HB2	1:C:2421:ALA:HB1	2.02	0.41
1:C:2453:ILE:O	1:C:2457:LEU:HG	2.21	0.41
1:C:3927:GLN:NE2	1:C:3991:GLY:HA3	2.36	0.41
1:C:4238:CYS:O	1:C:4242:ILE:HG12	2.21	0.41
1:C:4673:ARG:NH2	1:C:4698:LYS:HG3	2.35	0.41
1:D:223:PHE:HD1	1:D:223:PHE:HA	1.74	0.41
1:D:497:TYR:HA	1:D:503:PHE:HD2	1.86	0.41
1:D:497:TYR:CE1	1:D:504:ALA:HA	2.56	0.41
1:D:889:GLN:HB2	1:D:891:TRP:CD1	2.56	0.41
1:D:1075:PHE:HB2	1:D:1192:CYS:SG	2.61	0.41
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.27	0.41
1:D:1698:LEU:HG	1:D:1712:TYR:CZ	2.55	0.41
1:D:1716:ILE:O	1:D:1720:LEU:HD23	2.21	0.41
1:D:2029:GLN:H	1:D:2029:GLN:HG3	1.62	0.41
1:D:2254:LEU:O	1:D:2258:LEU:HG	2.20	0.41
1:D:2278:ALA:HA	1:D:2281:ILE:HD11	2.02	0.41
1:D:3895:HIS:CE1	1:D:3970:GLN:HB3	2.56	0.41
1:D:4823:LEU:O	1:D:4825:THR:N	2.54	0.41
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.92	0.41
1:A:1694:LEU:HD23	1:A:1715:LEU:HB2	2.03	0.41
1:A:4150:LEU:HD12	1:A:4150:LEU:HA	1.89	0.41
1:A:4180:ARG:HE	1:A:4180:ARG:HB2	1.70	0.41
1:A:4646:LEU:HD23	1:A:4646:LEU:HA	1.85	0.41
1:A:4918:ILE:HD13	1:A:4918:ILE:HA	1.94	0.41
1:B:220:LEU:HB2	1:B:391:THR:O	2.21	0.41
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.48	0.41
1:B:1716:ILE:O	1:B:1720:LEU:HD23	2.21	0.41
1:B:2182:ILE:HD13	1:B:2182:ILE:HA	1.89	0.41
1:C:180:LEU:O	1:C:200:TRP:NE1	2.32	0.41
1:C:3711:THR:HG22	1:C:3713:LYS:HE2	2.03	0.41
1:C:4816:ILE:HG12	1:C:4823:LEU:CD1	2.51	0.41
1:D:882:TRP:HE1	1:D:886:ARG:CZ	2.34	0.41
1:D:1849:LEU:HD12	1:D:1854:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2187:ASN:OD1	1:D:2187:ASN:N	2.54	0.41
1:D:4027:LEU:HD23	1:D:4027:LEU:HA	1.73	0.41
1:D:4658:ILE:HG13	1:D:4796:MET:HE3	2.03	0.41
1:D:4698:LYS:HE3	1:D:4698:LYS:HB2	1.89	0.41
1:A:2295:LEU:O	1:A:2298:VAL:HG22	2.21	0.40
1:A:4698:LYS:HE3	1:A:4698:LYS:HB2	1.89	0.40
1:B:182:LEU:H	1:B:198:THR:CG2	2.33	0.40
1:B:323:LEU:HG	1:B:325:THR:H	1.87	0.40
1:B:1830:VAL:HB	1:B:1837:GLN:OE1	2.21	0.40
1:B:2030:ASP:N	1:B:2030:ASP:OD1	2.54	0.40
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	2.02	0.40
1:C:359:TYR:HA	1:C:376:ALA:HA	2.02	0.40
1:C:891:TRP:HE3	1:C:904:HIS:HB2	1.85	0.40
1:C:1698:LEU:HG	1:C:1712:TYR:CZ	2.55	0.40
1:C:1849:LEU:HD12	1:C:1854:PHE:HD2	1.86	0.40
1:D:183:SER:HB3	1:D:192:ASP:OD1	2.21	0.40
1:D:794:GLY:HA3	1:D:811:CYS:SG	2.61	0.40
1:D:2295:LEU:O	1:D:2298:VAL:HG22	2.21	0.40
1:D:2453:ILE:O	1:D:2457:LEU:HG	2.21	0.40
1:D:4780:PHE:HD1	1:D:4780:PHE:HA	1.78	0.40
1:A:4170:ILE:HD12	1:A:4170:ILE:HA	1.90	0.40
1:B:610:ASN:OD1	1:B:610:ASN:N	2.54	0.40
1:B:686:TRP:CE3	1:B:777:PHE:HB3	2.57	0.40
1:B:1110:ARG:HH22	1:B:1112:ASP:HB2	1.87	0.40
1:B:2295:LEU:O	1:B:2298:VAL:HG22	2.21	0.40
1:C:794:GLY:HA3	1:C:811:CYS:SG	2.61	0.40
1:C:882:TRP:HE1	1:C:886:ARG:CZ	2.34	0.40
1:C:2030:ASP:N	1:C:2030:ASP:OD1	2.54	0.40
1:C:2255:SER:HA	1:C:2258:LEU:HD12	2.03	0.40
1:C:4030:LEU:HD23	1:C:4030:LEU:HA	1.85	0.40
1:D:2030:ASP:N	1:D:2030:ASP:OD1	2.54	0.40
1:D:4673:ARG:NH2	1:D:4698:LYS:HG3	2.35	0.40
1:D:4886:HIS:CE1	1:D:4897:ILE:HG12	2.57	0.40
1:A:322:LYS:HA	1:A:322:LYS:HD2	1.85	0.40
1:A:1849:LEU:HD12	1:A:1854:PHE:HD2	1.86	0.40
1:A:4238:CYS:O	1:A:4242:ILE:HG12	2.21	0.40
1:B:322:LYS:HA	1:B:322:LYS:HD2	1.85	0.40
1:B:2453:ILE:O	1:B:2457:LEU:HG	2.21	0.40
1:B:4816:ILE:HG12	1:B:4823:LEU:CD1	2.51	0.40
1:B:4886:HIS:CE1	1:B:4897:ILE:HG12	2.57	0.40
1:C:115:ARG:HE	1:C:115:ARG:HB3	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:GLN:OE1	1:C:437:PRO:HG3	2.19	0.40
1:C:459:LEU:HD12	1:C:464:LYS:HZ3	1.86	0.40
1:C:568:LEU:HD23	1:C:606:LEU:HD13	2.03	0.40
1:C:4995:LEU:HD23	1:C:4995:LEU:HA	1.86	0.40
1:D:1133:HIS:CE1	1:D:1134:LEU:HD12	2.57	0.40
1:D:1639:LEU:HD12	1:D:1639:LEU:HA	1.93	0.40
1:A:182:LEU:H	1:A:198:THR:CG2	2.33	0.40
1:A:647:ASN:OD1	1:A:647:ASN:N	2.55	0.40
1:A:889:GLN:HB2	1:A:891:TRP:CD1	2.56	0.40
1:A:1718:ILE:HG13	1:A:1719:HIS:CD2	2.55	0.40
1:A:2271:THR:N	1:A:2274:ASP:OD2	2.55	0.40
1:A:4850:LEU:HD23	1:A:4850:LEU:HA	1.94	0.40
1:B:1720:LEU:O	1:B:1724:CYS:N	2.44	0.40
1:B:1936:LYS:HG2	1:B:2105:TRP:CZ2	2.57	0.40
1:B:3842:LEU:HD23	1:B:3842:LEU:HA	1.87	0.40
1:C:183:SER:HB3	1:C:192:ASP:OD1	2.21	0.40
1:C:360:ALA:N	1:C:375:LYS:O	2.37	0.40
1:C:803:LEU:HA	1:C:804:PRO:HD3	1.95	0.40
1:C:1964:ARG:O	1:C:1968:LYS:HG2	2.21	0.40
1:D:220:LEU:HB2	1:D:391:THR:O	2.21	0.40
1:D:647:ASN:OD1	1:D:647:ASN:N	2.55	0.40
1:D:1243:PRO:HG3	1:D:1502:SER:H	1.86	0.40
1:D:3949:ARG:HH22	1:D:3953:LYS:HD3	1.87	0.40
1:D:4814:LEU:HD23	1:D:4814:LEU:HA	1.86	0.40
1:D:4816:ILE:HG12	1:D:4823:LEU:CD1	2.51	0.40
1:D:4924:VAL:HA	1:D:4928:LEU:HB2	2.02	0.40
1:A:299:LEU:HD23	1:A:377:ILE:HA	2.04	0.40
1:A:793:LEU:HD21	1:A:1625:GLY:HA2	2.02	0.40
1:A:864:PRO:O	1:A:868:GLU:N	2.41	0.40
1:A:1936:LYS:HG2	1:A:2105:TRP:CZ2	2.57	0.40
1:A:4816:ILE:HG12	1:A:4823:LEU:CD1	2.51	0.40
1:A:4836:GLN:H	1:A:4836:GLN:HG2	1.75	0.40
1:B:23:GLN:HG2	1:B:34:LYS:HE3	2.03	0.40
1:B:889:GLN:HB2	1:B:891:TRP:CD1	2.56	0.40
1:B:1712:TYR:CG	1:B:1840:PRO:HB3	2.57	0.40
1:B:1849:LEU:HD12	1:B:1854:PHE:HD2	1.86	0.40
1:B:3650:CYS:O	1:B:3654:LEU:HG	2.22	0.40
1:B:3895:HIS:CE1	1:B:3970:GLN:HB3	2.56	0.40
1:B:4889:VAL:HG11	1:B:4900:GLU:HG2	2.03	0.40
1:C:377:ILE:HD12	1:C:377:ILE:HA	1.84	0.40
1:C:445:LEU:O	1:C:449:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1243:PRO:HG3	1:C:1502:SER:H	1.86	0.40
1:C:1749:PRO:HA	1:C:1750:PRO:HD3	1.98	0.40
1:C:3949:ARG:HH22	1:C:3953:LYS:HD3	1.87	0.40
1:D:23:GLN:HG2	1:D:34:LYS:HE3	2.03	0.40
1:D:323:LEU:HG	1:D:325:THR:H	1.87	0.40
1:D:686:TRP:CE3	1:D:777:PHE:HB3	2.57	0.40
1:D:3927:GLN:NE2	1:D:3991:GLY:HA3	2.36	0.40
1:D:4816:ILE:O	1:D:4817:ALA:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3235/5037 (64%)	2954 (91%)	279 (9%)	2 (0%)	48	81
1	B	3235/5037 (64%)	2954 (91%)	279 (9%)	2 (0%)	48	81
1	C	3235/5037 (64%)	2954 (91%)	279 (9%)	2 (0%)	48	81
1	D	3235/5037 (64%)	2954 (91%)	279 (9%)	2 (0%)	48	81
All	All	12940/20148 (64%)	11816 (91%)	1116 (9%)	8 (0%)	50	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4821	LYS
1	B	4821	LYS
1	C	4821	LYS
1	D	4821	LYS
1	A	4818	MET
1	B	4818	MET
1	C	4818	MET

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Mol	Chain	Res	Type
1	D	4818	MET

### 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	2230/4276 (52%)	2225 (100%)	5 (0%)	92	93
1	B	2230/4276 (52%)	2225 (100%)	5 (0%)	92	93
1	C	2230/4276 (52%)	2225 (100%)	5 (0%)	92	93
1	D	2230/4276 (52%)	2225 (100%)	5 (0%)	92	93
All	All	8920/17104 (52%)	8900 (100%)	20 (0%)	91	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1226	PHE
1	A	4551	PHE
1	A	4571	PHE
1	A	4820	VAL
1	A	4849	TYR
1	B	1226	PHE
1	B	4551	PHE
1	B	4571	PHE
1	B	4820	VAL
1	B	4849	TYR
1	C	1226	PHE
1	C	4551	PHE
1	C	4571	PHE
1	C	4820	VAL
1	C	4849	TYR
1	D	1226	PHE
1	D	4551	PHE
1	D	4571	PHE
1	D	4820	VAL
1	D	4849	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	71	GLN
1	A	111	HIS
1	A	151	HIS
1	A	273	HIS
1	A	379	HIS
1	A	461	HIS
1	A	465	GLN
1	A	495	ASN
1	A	533	ASN
1	A	593	HIS
1	A	597	HIS
1	A	735	GLN
1	A	760	ASN
1	A	1084	GLN
1	A	1665	HIS
1	A	1683	HIS
1	A	1696	HIS
1	A	1702	HIS
1	A	1775	HIS
1	A	1949	GLN
1	A	1952	GLN
1	A	3643	ASN
1	A	3651	ASN
1	A	3771	HIS
1	A	3781	GLN
1	A	3814	GLN
1	A	3895	HIS
1	A	3896	ASN
1	A	3897	ASN
1	A	3900	GLN
1	A	3960	GLN
1	A	3976	ASN
1	A	3994	HIS
1	A	3998	HIS
1	A	4020	GLN
1	A	4120	ASN
1	A	4133	GLN
1	A	4153	HIS
1	A	4650	HIS
1	A	4776	GLN

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Mol	Chain	Res	Type
1	A	4803	HIS
1	A	4886	HIS
1	A	4947	GLN
1	B	57	ASN
1	B	71	GLN
1	B	111	HIS
1	B	151	HIS
1	B	273	HIS
1	B	379	HIS
1	B	461	HIS
1	B	465	GLN
1	B	495	ASN
1	B	593	HIS
1	B	597	HIS
1	B	735	GLN
1	B	760	ASN
1	B	1084	GLN
1	B	1665	HIS
1	B	1683	HIS
1	B	1696	HIS
1	B	1702	HIS
1	B	1775	HIS
1	B	1949	GLN
1	B	1952	GLN
1	B	3643	ASN
1	B	3651	ASN
1	B	3771	HIS
1	B	3781	GLN
1	B	3814	GLN
1	B	3895	HIS
1	B	3896	ASN
1	B	3897	ASN
1	B	3900	GLN
1	B	3960	GLN
1	B	3976	ASN
1	B	3994	HIS
1	B	3998	HIS
1	B	4020	GLN
1	B	4120	ASN
1	B	4133	GLN
1	B	4153	HIS
1	B	4650	HIS

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Mol	Chain	Res	Type
1	B	4776	GLN
1	B	4803	HIS
1	B	4886	HIS
1	B	4947	GLN
1	C	57	ASN
1	C	71	GLN
1	C	111	HIS
1	C	151	HIS
1	C	273	HIS
1	C	379	HIS
1	C	461	HIS
1	C	465	GLN
1	C	495	ASN
1	C	593	HIS
1	C	597	HIS
1	C	735	GLN
1	C	760	ASN
1	C	765	GLN
1	C	1084	GLN
1	C	1665	HIS
1	C	1683	HIS
1	C	1696	HIS
1	C	1702	HIS
1	C	1775	HIS
1	C	1949	GLN
1	C	1952	GLN
1	C	3643	ASN
1	C	3651	ASN
1	C	3771	HIS
1	C	3781	GLN
1	C	3814	GLN
1	C	3895	HIS
1	C	3896	ASN
1	C	3897	ASN
1	C	3900	GLN
1	C	3960	GLN
1	C	3976	ASN
1	C	3994	HIS
1	C	3998	HIS
1	C	4020	GLN
1	C	4120	ASN
1	C	4133	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	C	4153	HIS
1	C	4650	HIS
1	C	4776	GLN
1	C	4803	HIS
1	C	4886	HIS
1	C	4947	GLN
1	D	57	ASN
1	D	71	GLN
1	D	111	HIS
1	D	151	HIS
1	D	273	HIS
1	D	379	HIS
1	D	461	HIS
1	D	465	GLN
1	D	495	ASN
1	D	593	HIS
1	D	597	HIS
1	D	735	GLN
1	D	760	ASN
1	D	1084	GLN
1	D	1665	HIS
1	D	1683	HIS
1	D	1696	HIS
1	D	1702	HIS
1	D	1775	HIS
1	D	1949	GLN
1	D	1952	GLN
1	D	3643	ASN
1	D	3651	ASN
1	D	3771	HIS
1	D	3781	GLN
1	D	3814	GLN
1	D	3895	HIS
1	D	3896	ASN
1	D	3897	ASN
1	D	3900	GLN
1	D	3960	GLN
1	D	3976	ASN
1	D	3994	HIS
1	D	3998	HIS
1	D	4020	GLN
1	D	4120	ASN

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*Continued from previous page...*

Mol	Chain	Res	Type
1	D	4133	GLN
1	D	4153	HIS
1	D	4650	HIS
1	D	4776	GLN
1	D	4803	HIS
1	D	4886	HIS
1	D	4947	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

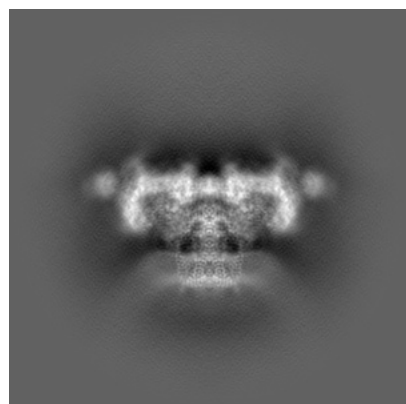
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38042. These allow visual inspection of the internal detail of the map and identification of artifacts.

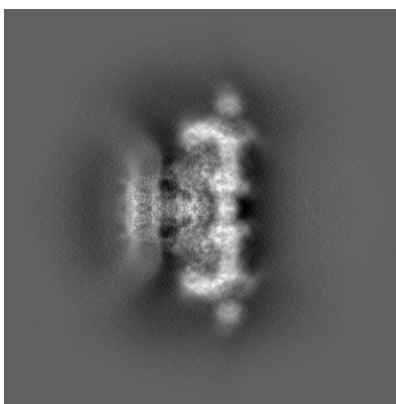
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

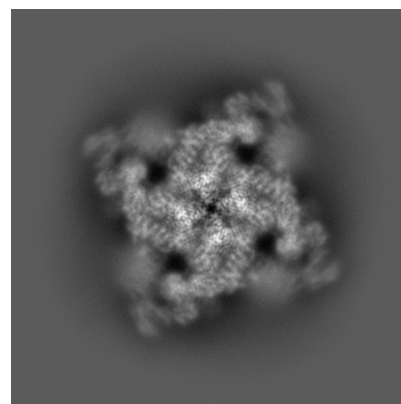
#### 6.1.1 Primary map



X

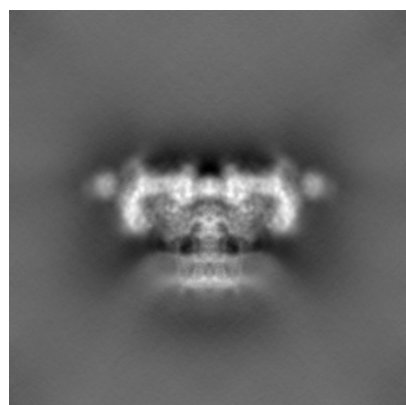


Y

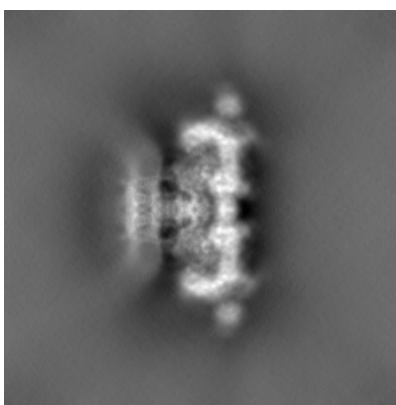


Z

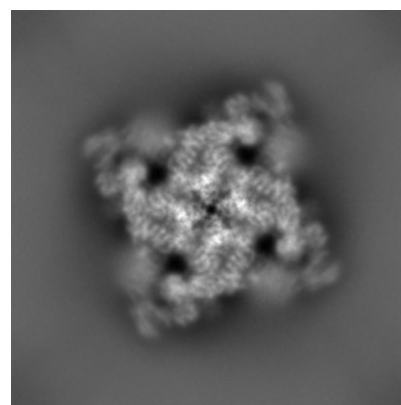
#### 6.1.2 Raw map



X



Y

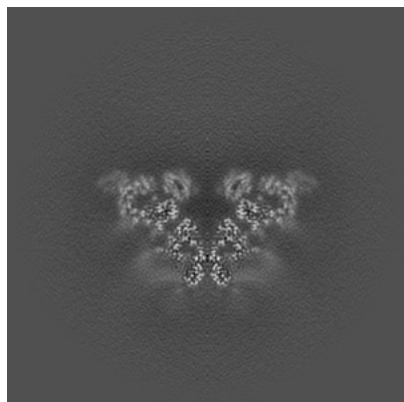


Z

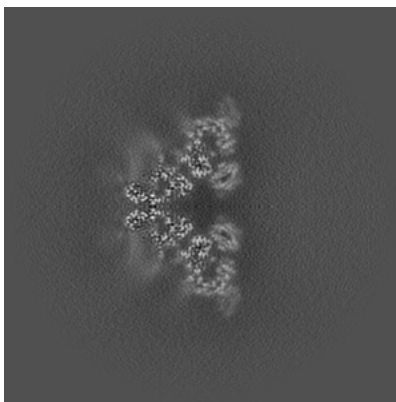
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

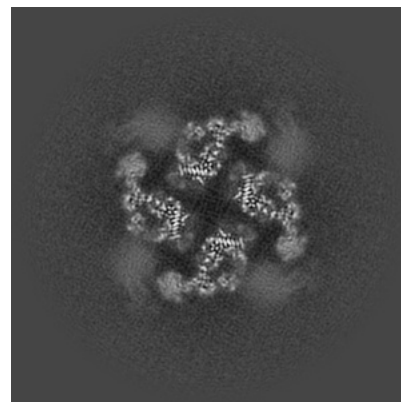
### 6.2.1 Primary map



X Index: 240

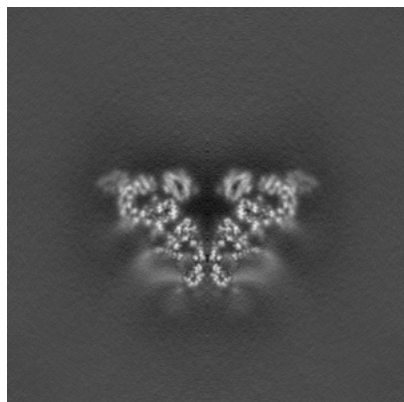


Y Index: 240

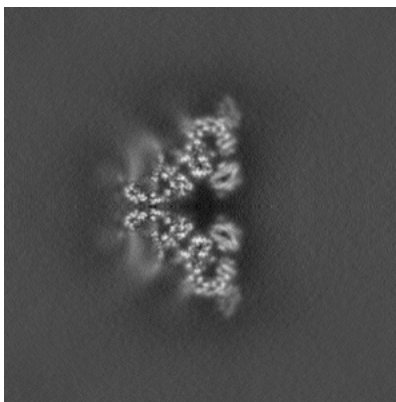


Z Index: 240

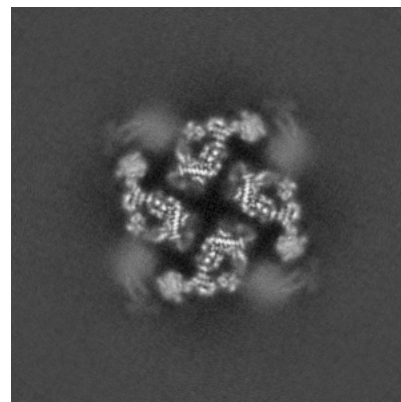
### 6.2.2 Raw map



X Index: 240



Y Index: 240

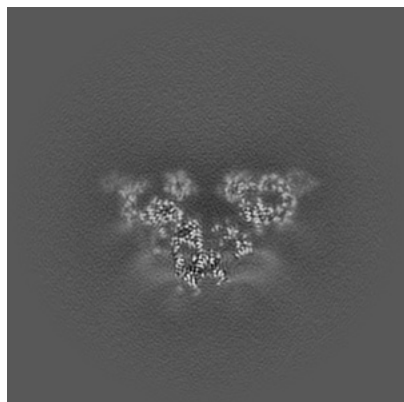


Z Index: 240

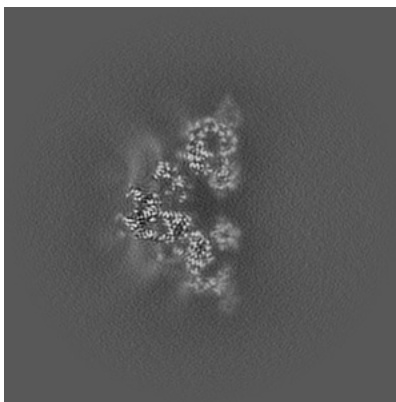
The images above show central slices of the map in three orthogonal directions.

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

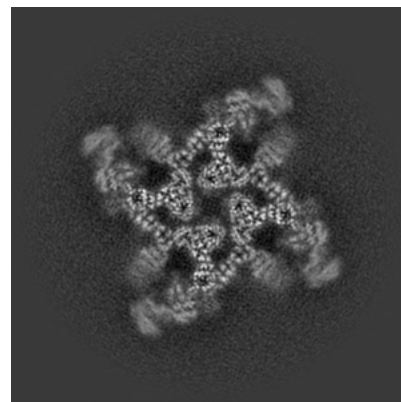
### 6.3.1 Primary map



X Index: 244

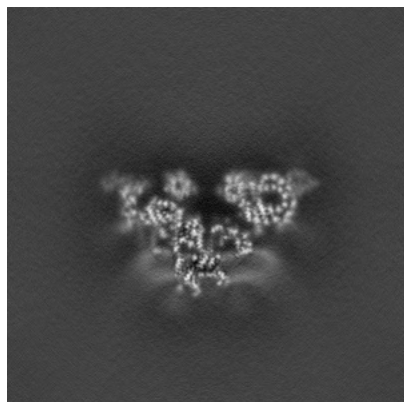


Y Index: 236

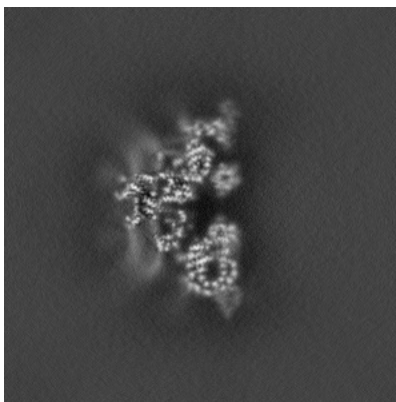


Z Index: 264

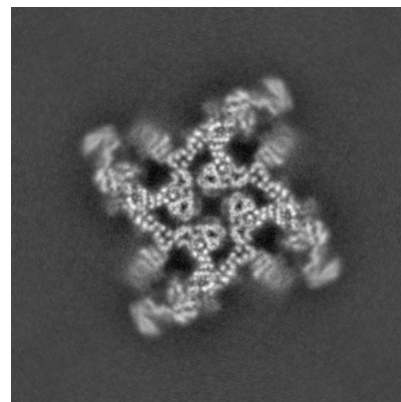
### 6.3.2 Raw map



X Index: 245



Y Index: 245

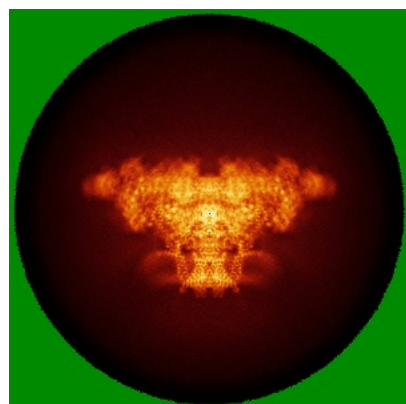


Z Index: 263

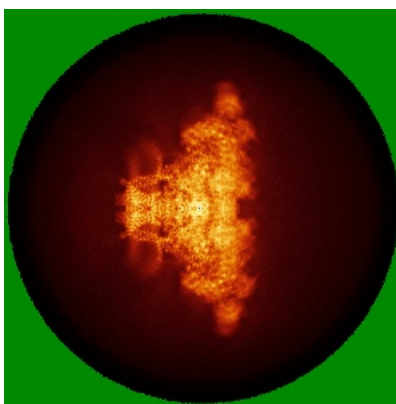
The images above show the largest variance slices of the map in three orthogonal directions.

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

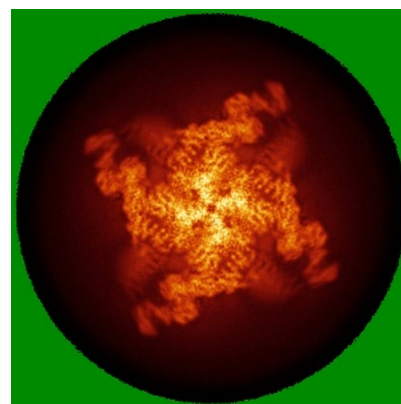
### 6.4.1 Primary map



X

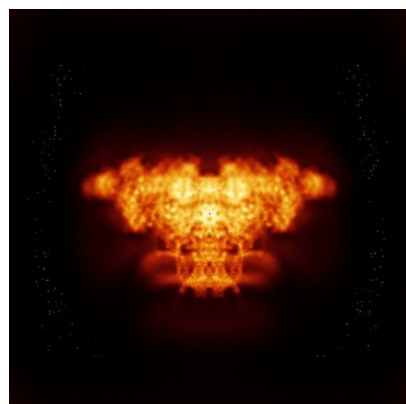


Y

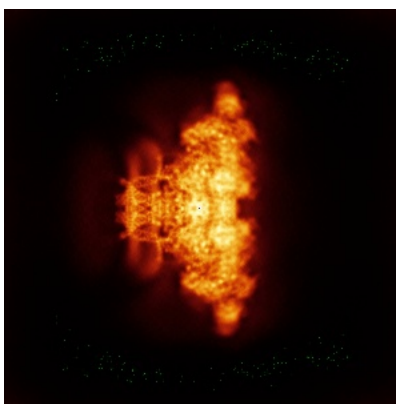


Z

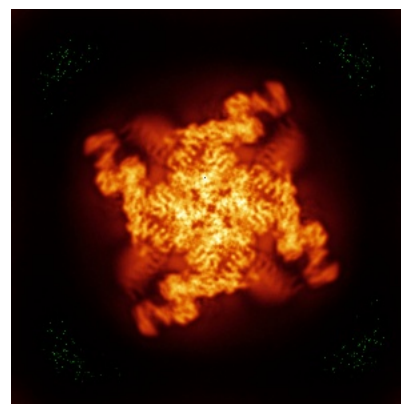
### 6.4.2 Raw map



X



Y



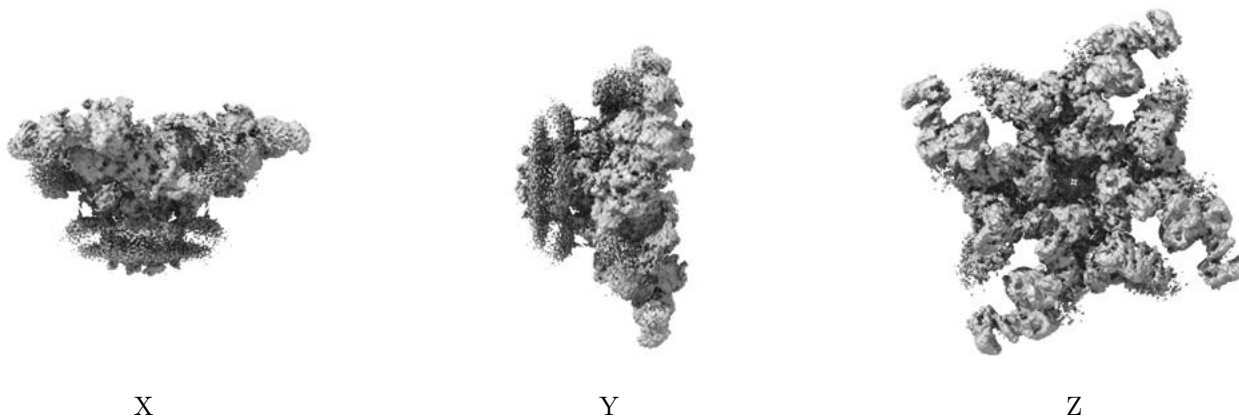
Z

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



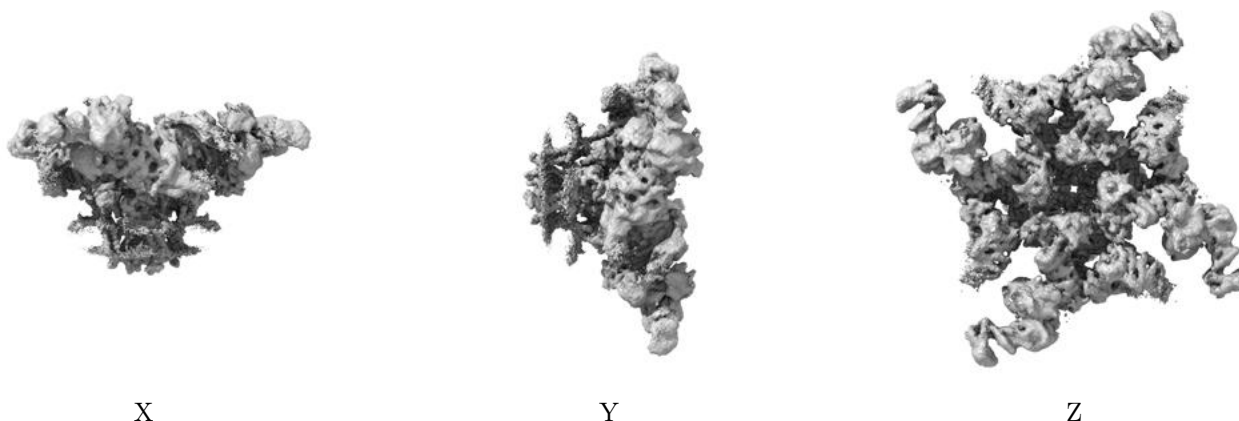
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

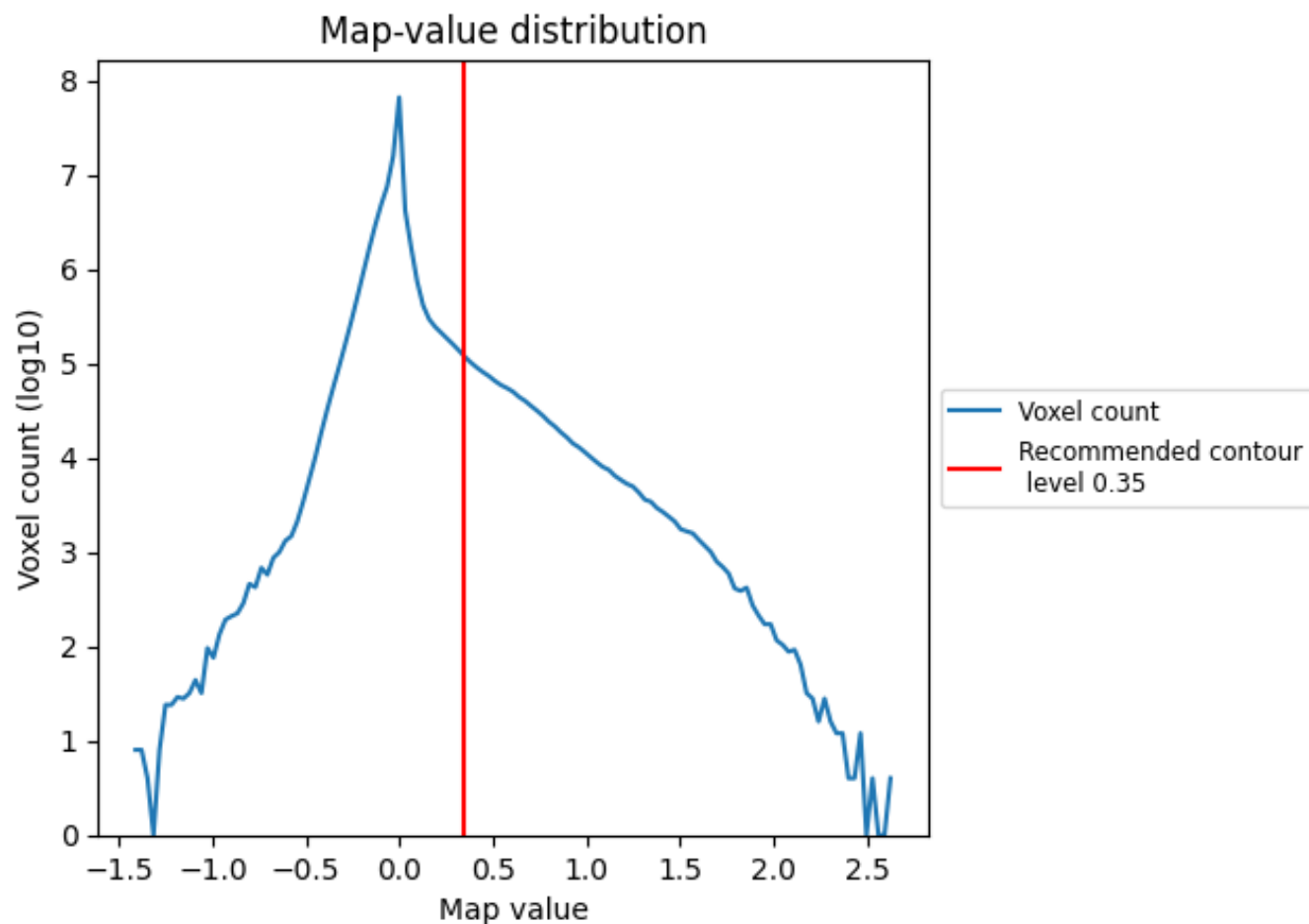
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

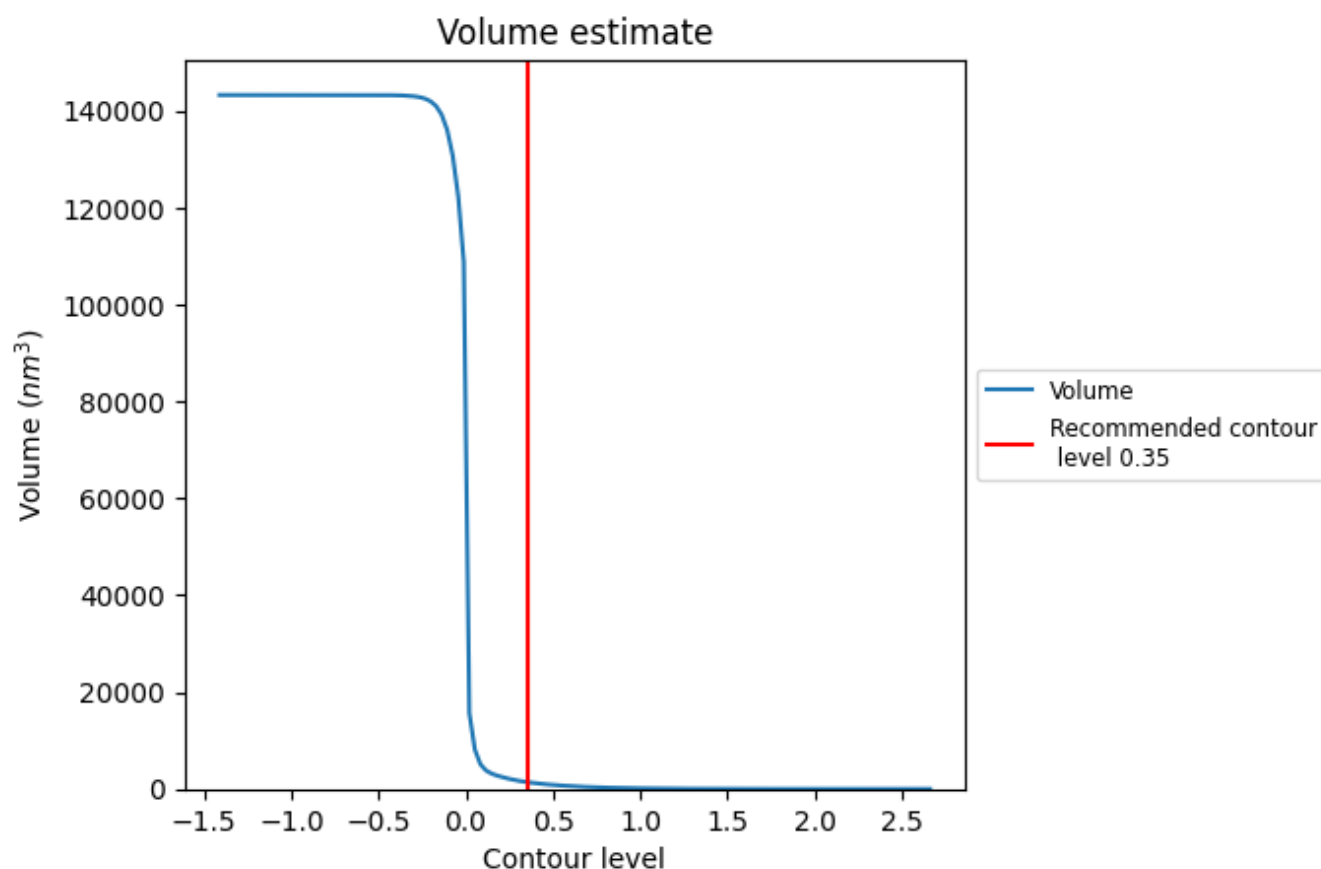
This section contains the results of statistical analysis of the map.

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



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

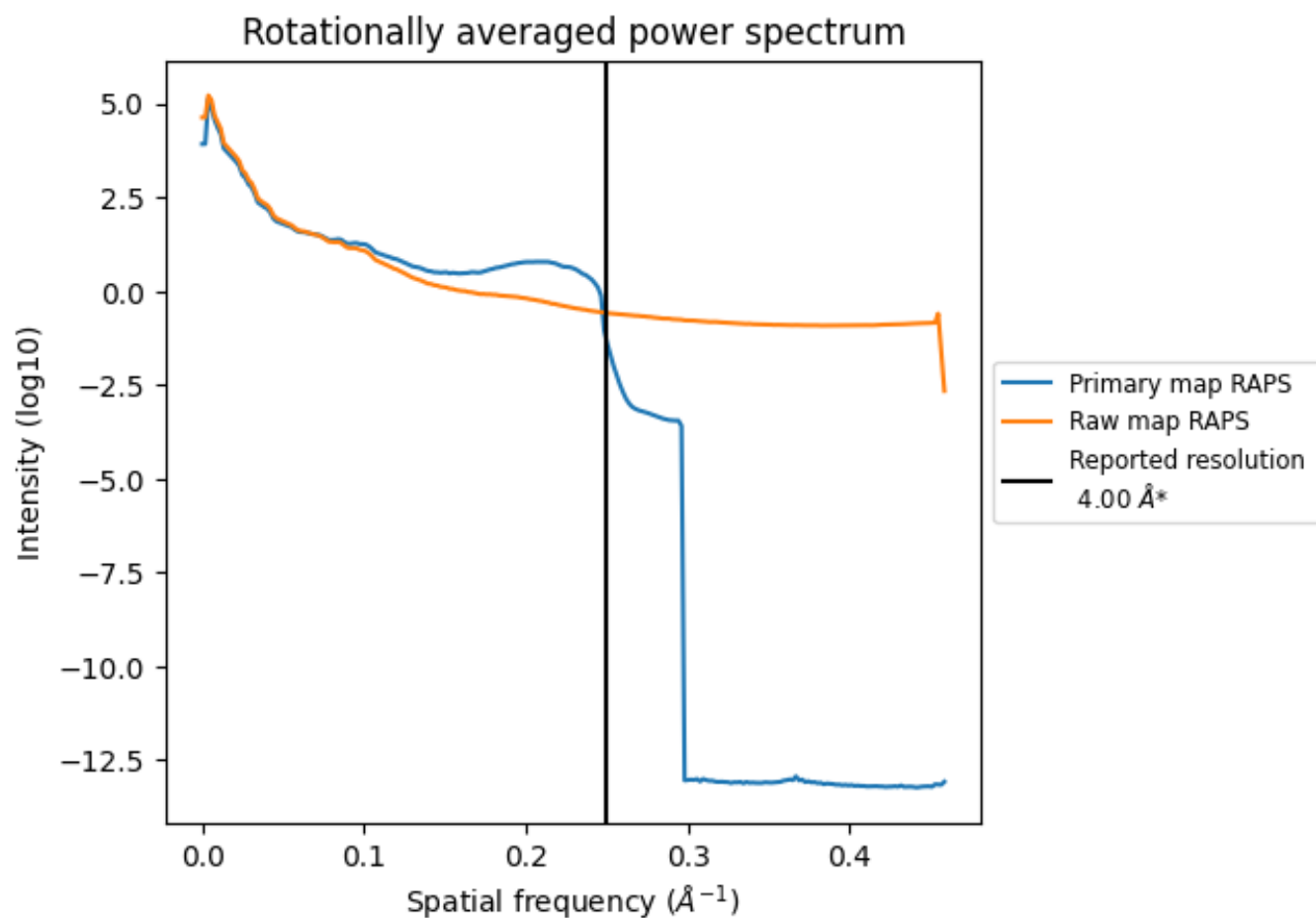
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1415 nm<sup>3</sup>; this corresponds to an approximate mass of 1278 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 ⓘ

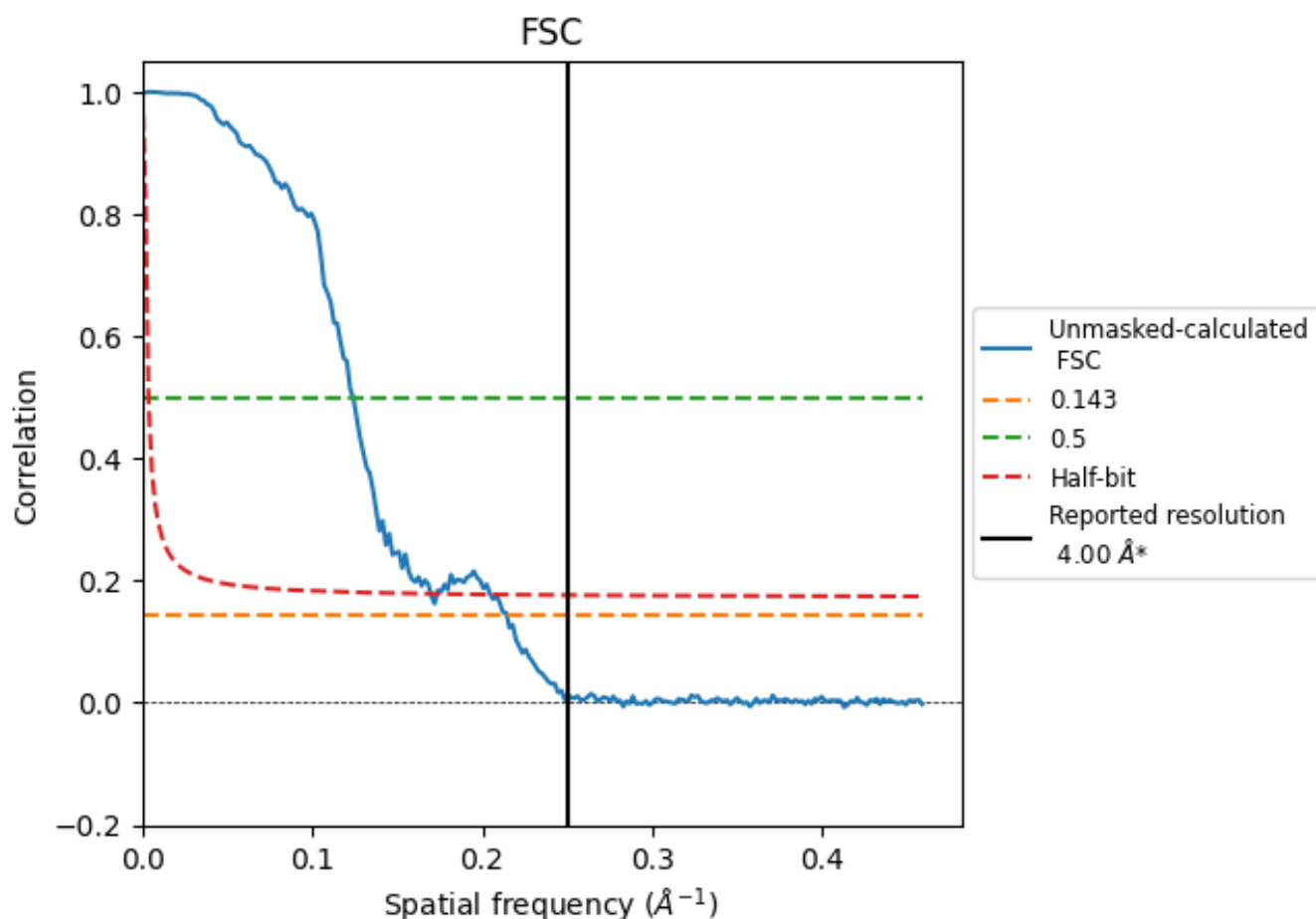


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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 0.250  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

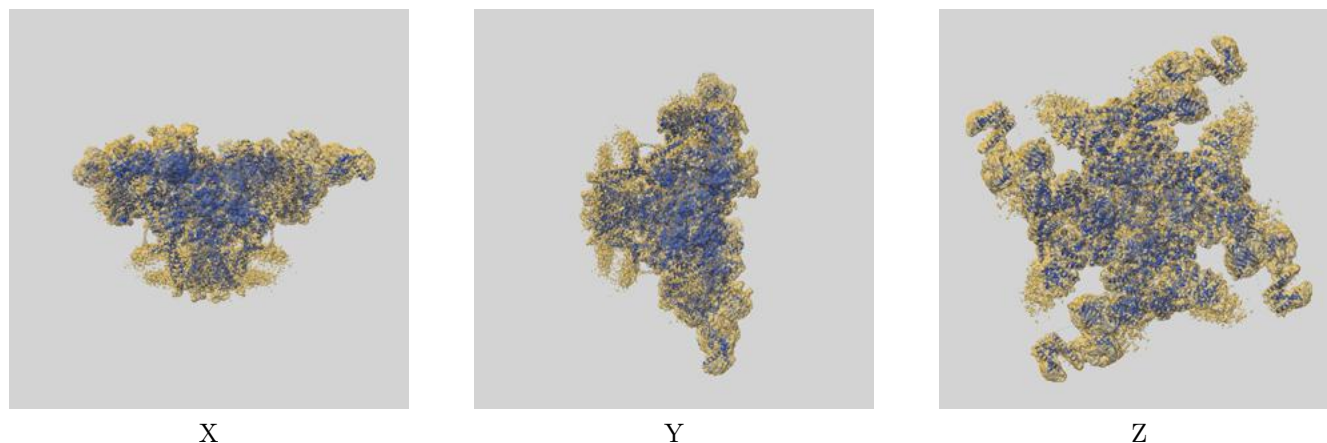
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.66	8.06	5.89

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.66 differs from the reported value 4.0 by more than 10 %

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

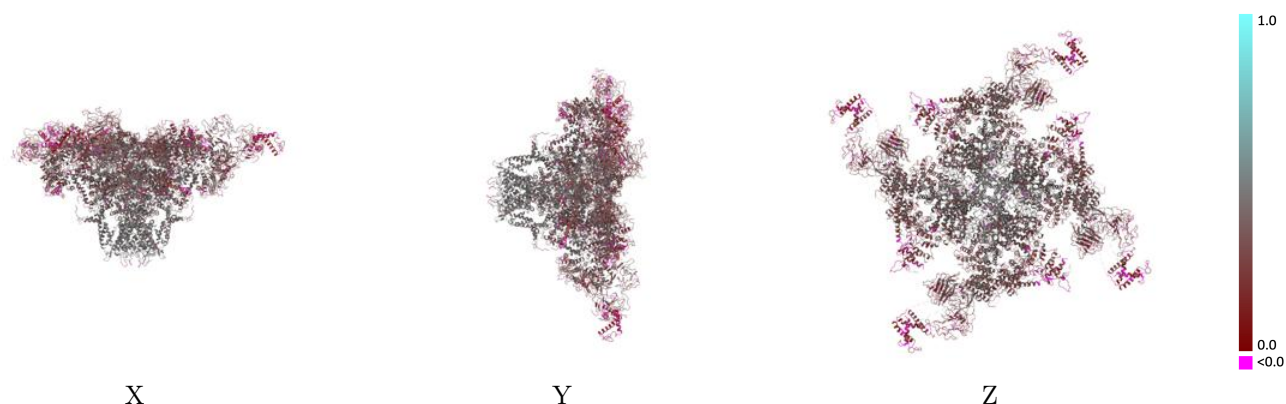
This section contains information regarding the fit between EMDB map EMD-38042 and PDB model 8X48. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



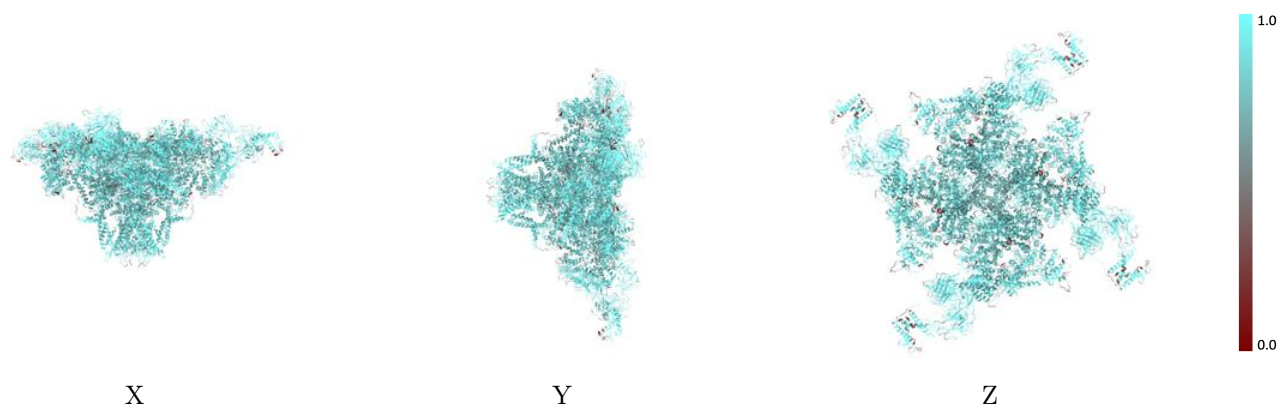
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



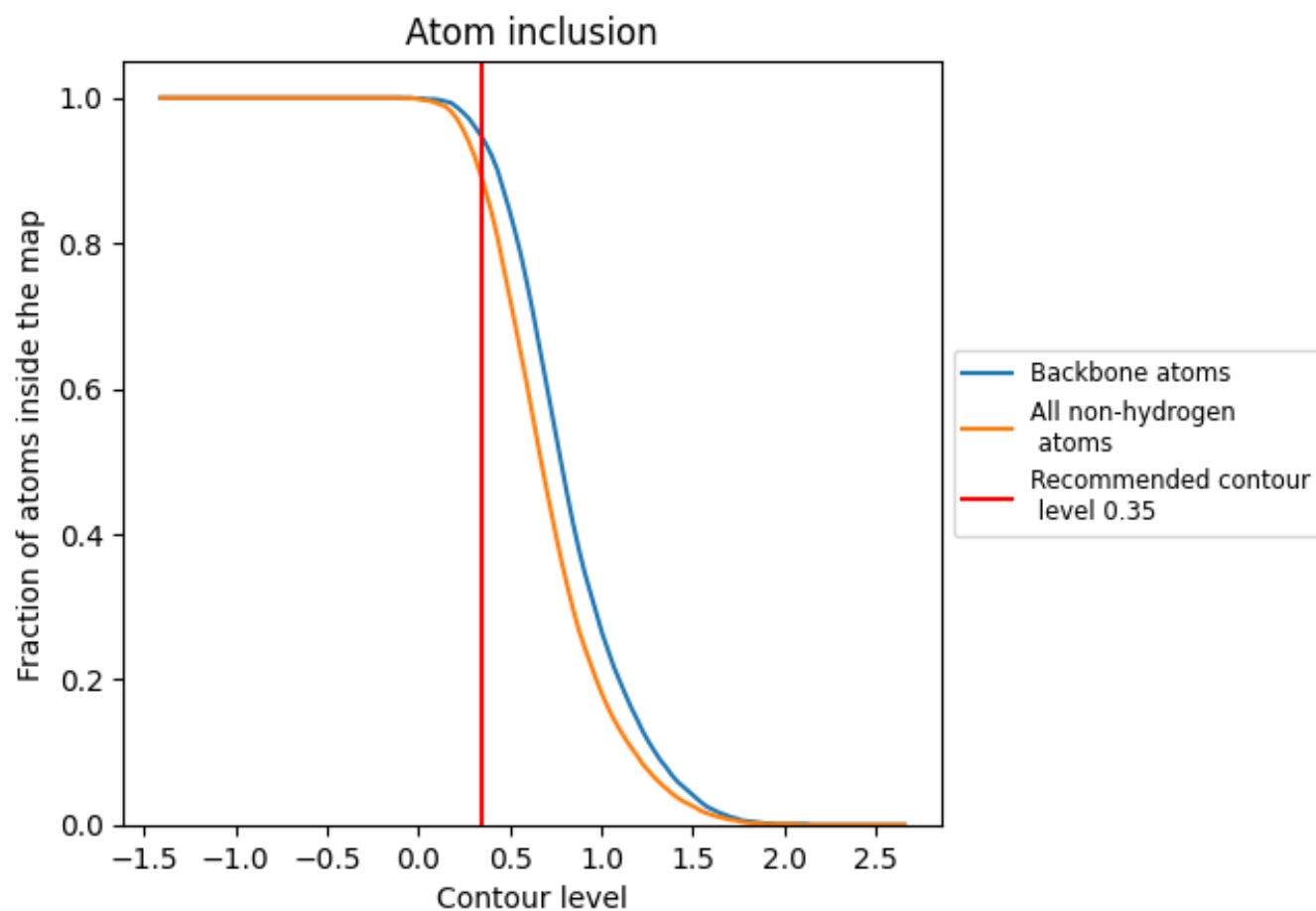
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8870	<div></div> 0.3390
A	<div></div> 0.8860	<div></div> 0.3390
B	<div></div> 0.8870	<div></div> 0.3380
C	<div></div> 0.8860	<div></div> 0.3390
D	<div></div> 0.8870	<div></div> 0.3390

