



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 01:40 PM UTC

PDB ID : 8EWI / pdb_00008ewi
EMDB ID : EMD-28646
Title : Structure of the human UBR5 HECT-type E3 ubiquitin ligase in a tetrameric form
Authors : Wang, F.; He, Q.; Lin, G.; Li, H.
Deposited on : 2022-10-23
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

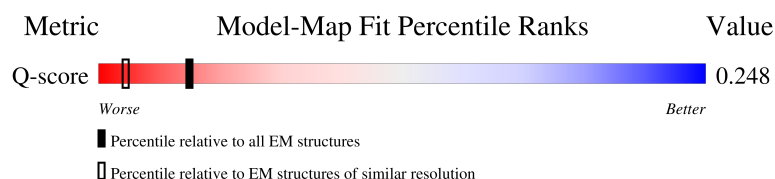
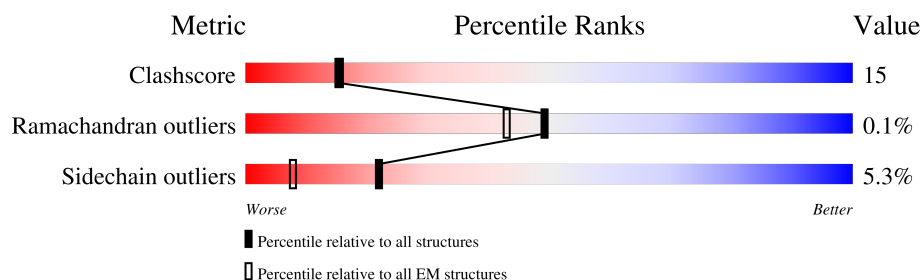
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	2799	9% 41% 21% • 37%
1	B	2799	10% 41% 20% • 37%
1	C	2799	11% 42% 20% • 37%
1	D	2799	11% 40% 21% • 37%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 55708 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 E3 ubiquitin-protein ligase UBR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1775	Total	C	N	O	S	0	0
			13924	8781	2440	2599	104		
1	B	1775	Total	C	N	O	S	0	0
			13924	8781	2440	2599	104		
1	C	1775	Total	C	N	O	S	0	0
			13924	8781	2440	2599	104		
1	D	1775	Total	C	N	O	S	0	0
			13924	8781	2440	2599	104		

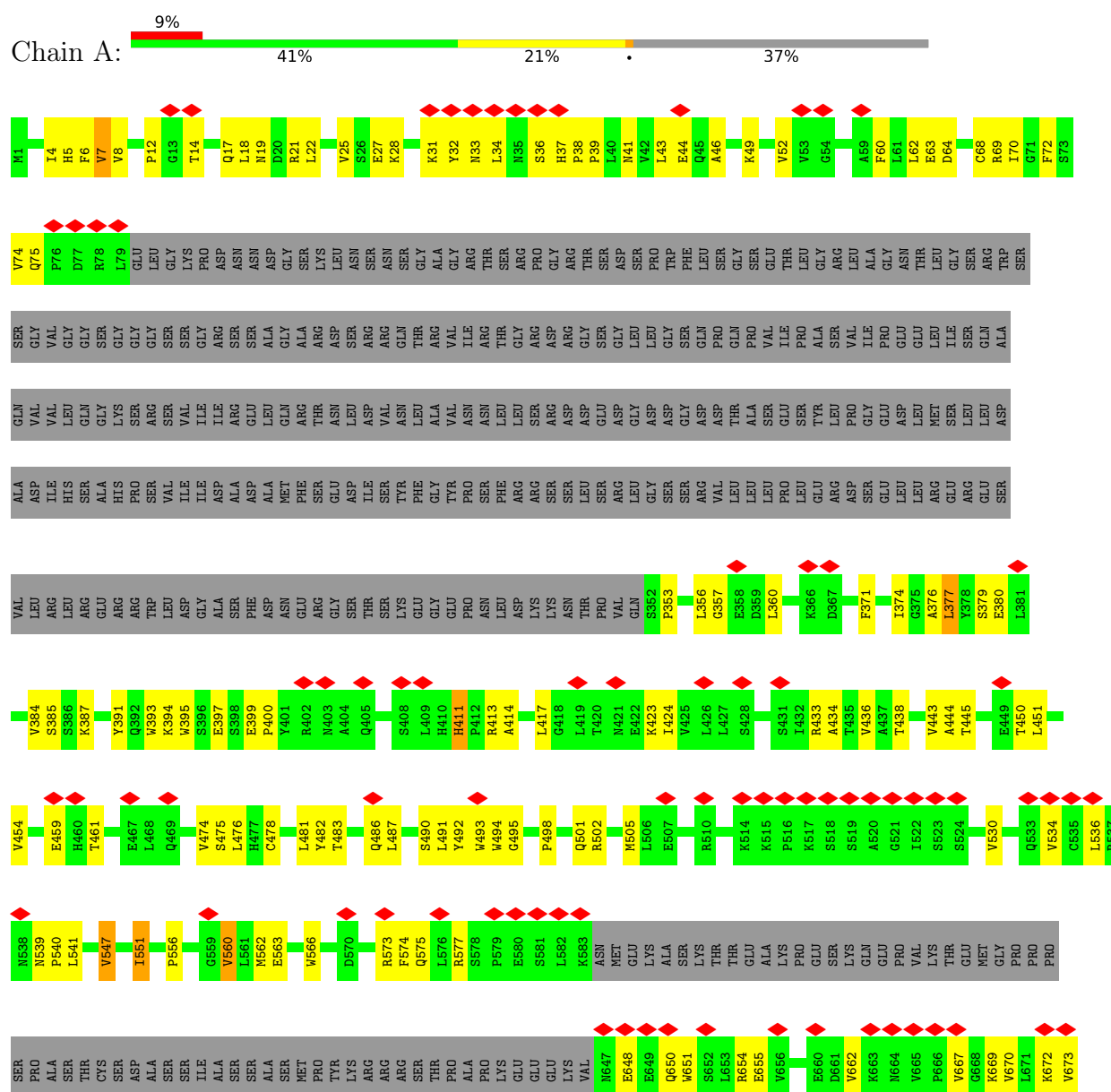
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	3	Total	Zn	0
			3	3	
2	B	3	Total	Zn	0
			3	3	
2	C	3	Total	Zn	0
			3	3	
2	D	3	Total	Zn	0
			3	3	

3 Residue-property plots

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

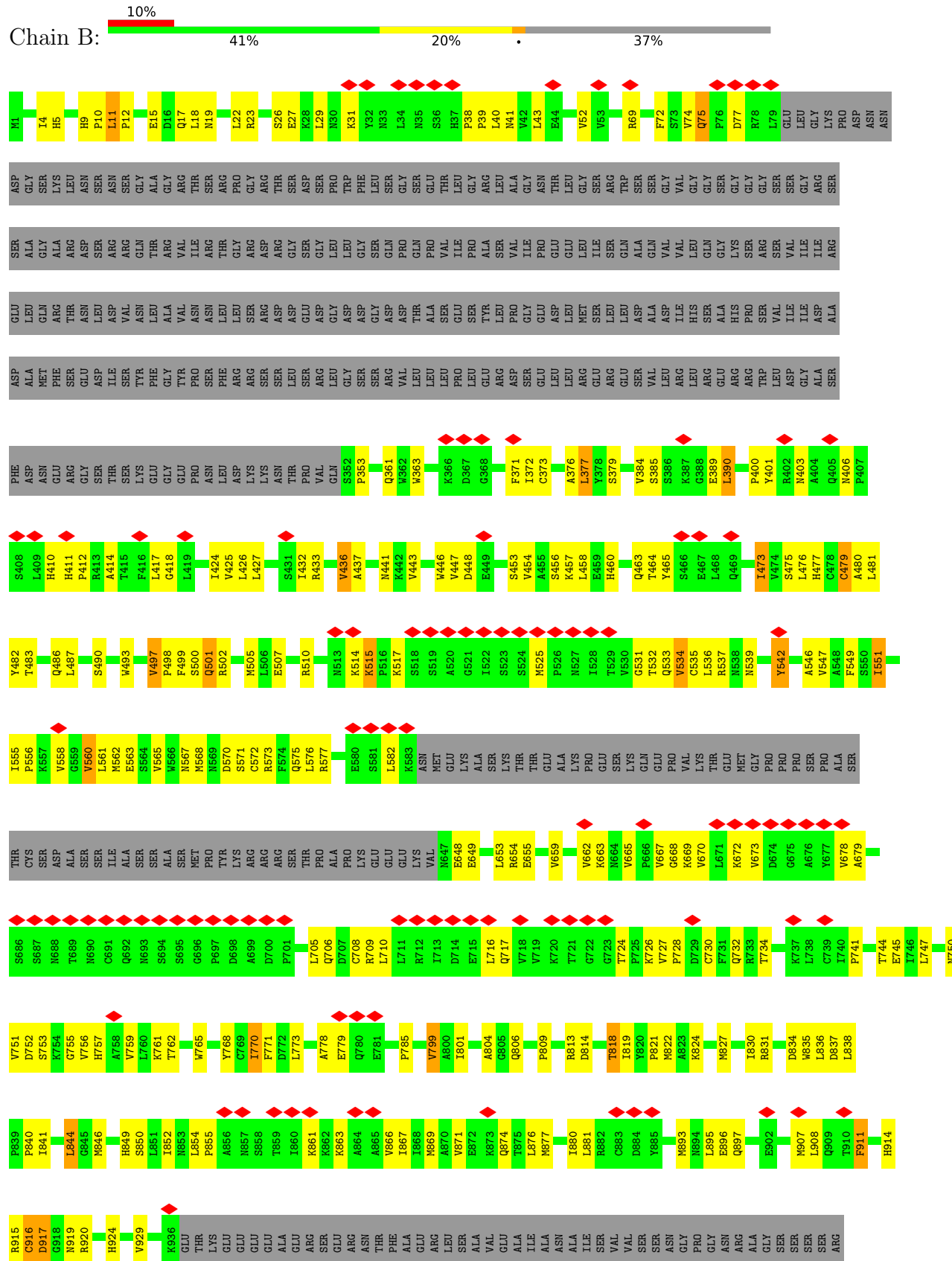
• Molecule 1: E3 ubiquitin-protein ligase UBR5



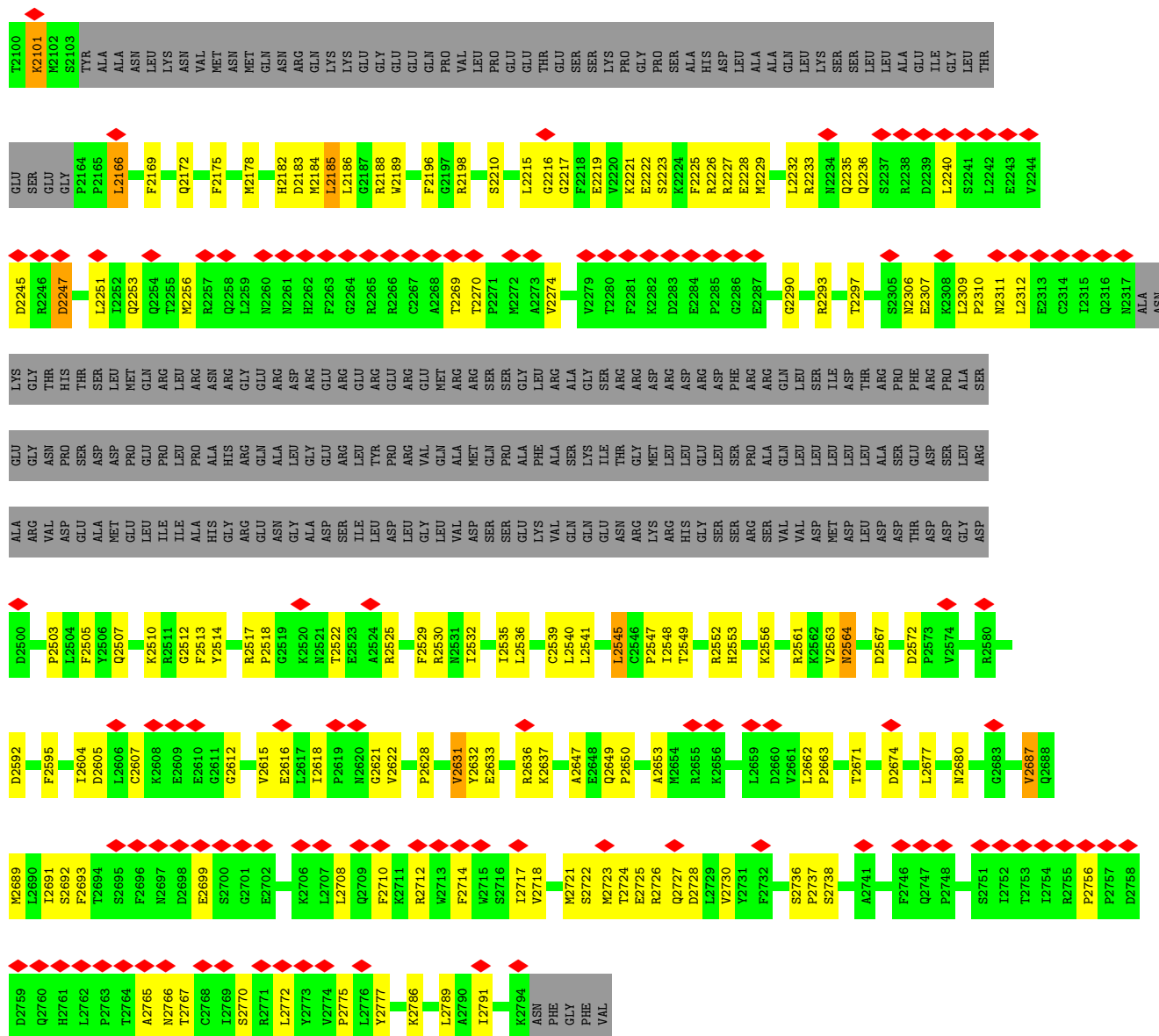




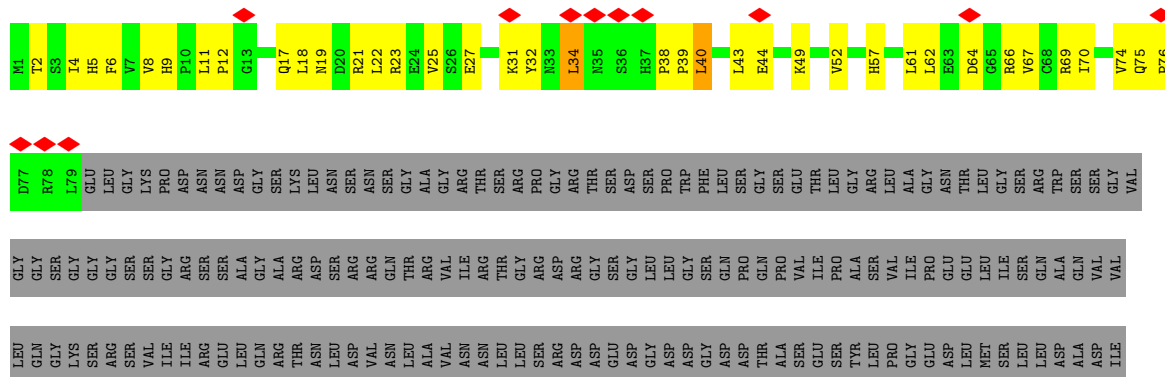
● Molecule 1: E3 ubiquitin-protein ligase UBR5





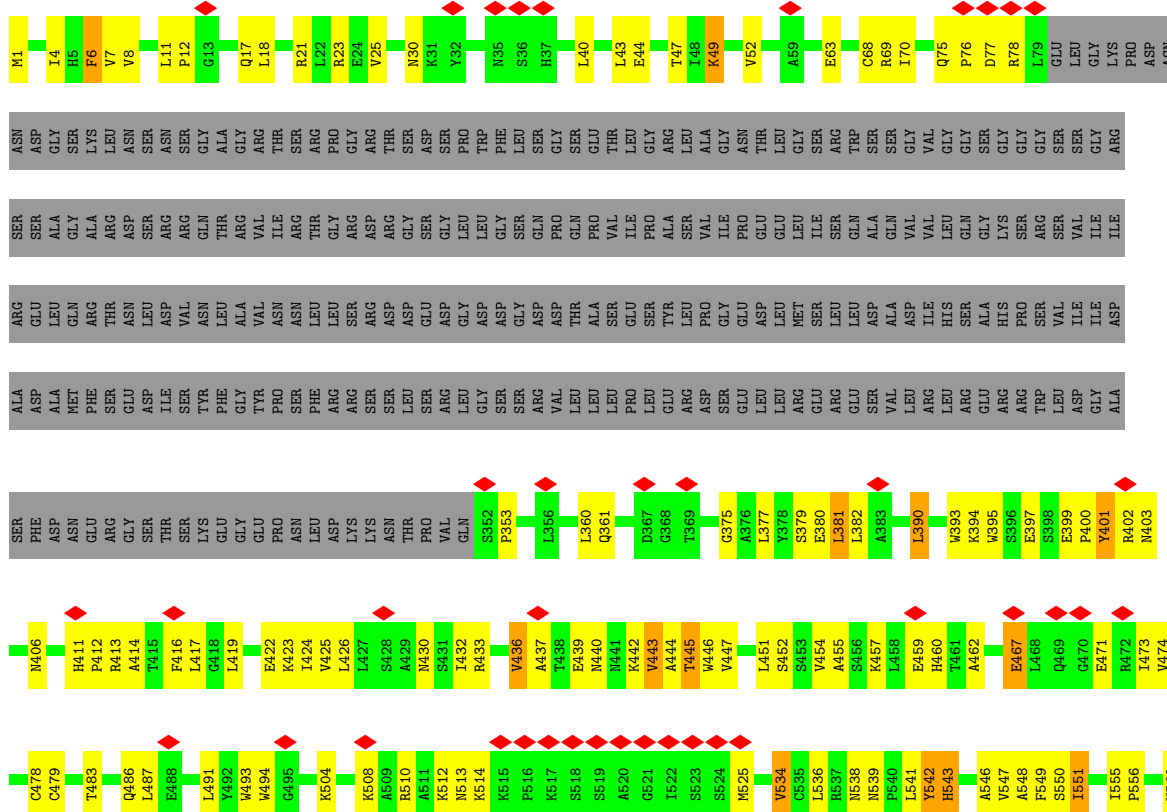
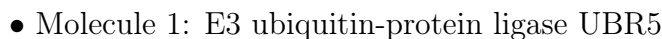


• Molecule 1: E3 ubiquitin-protein ligase UBR5



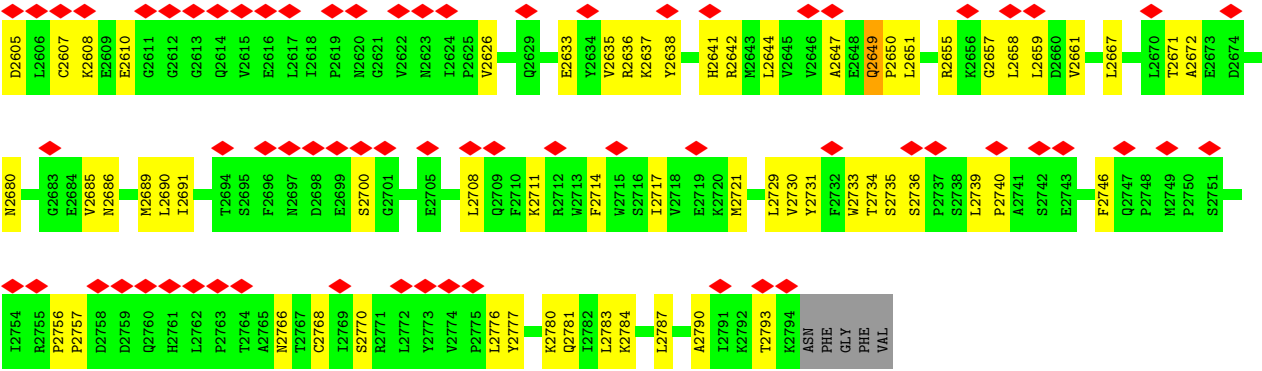








GLU	ASP	THR	L1819	ARG	LYS	A2045	ASN	L2186	H2272	GLU	GLU	ASP	R2530
LEU	SER	SER	N1826	ALA	ARG	E2046	ARG	L2187	A2273	ARG	ARG	SER	R2531
ASP	ASP	THR	L1827	ALA	THR	A2047	GLN	G2188	V2274	GLU	TYR	ILE	R2532
LEU	SER	ALA	Q1828	LEU	GLU	L2050	LYS	L2191	H2275	ARG	PRO	LEU	R2533
ALA	SER	ALA	N1829	LEU	LEU	Q2053	GLY	S2192	R2276	GLU	ARG	GLY	R2534
ALA	SER	SER	Y1830	SER	GLU	L2056	GLU	L2193	V2277	MET	VAL	LEU	R2535
ALA	GLN	SER	V1831	ALA	GLU	L2057	GLU	E2194	V2279	ARG	GLN	ALA	R2536
GLU	ASP	GLU	K1834	ARG	GLY	Q2058	PRO	L2195	T2280	ARG	ALA	ALA	R2537
THR	GLU	GLN	I1836	GLY	ILE	P2059	VAL	F2196	F2281	SER	MET	GLN	C2539
ASP	ILE	ASP	P1837	MET	ASN	N2060	LEU	G2197	R2282	GLY	PRO	GLY	L2545
SER	GLU	GLN	T1838	GLU	GLU	A2061	PRO	R2198	D2283	LEU	ALA	PHE	
GLU	THR	THR	W1839	ASP	ASP	R2062	GLU	E2202	E2284	ARG	ALA	ALA	T2548
THR	THR	THR	W1841	SER	SER	K2063	THR	V2204	P2285	ALA	SER	SER	T2549
ASN	PHE	ASN	T1845	GLU	HIS	E2064	GLU	D2065	G2286	GLY	LYS	GLY	L2550
HIS	M1690	ASN	M1846	GLU	GLU	D2066	SER	S2210	E2287	ARG	THR	ASN	N2551
SER	L1691	LEU	ARG	GLU	ASN	L2070	LYS	E2222	G2288	ARG	GLY	ARG	R2552
ASN	D1692	ARG	THR	ASP	ASP	P2070	PRO	E2226	S2289	ASP	MET	LYS	R2553
GLN	E1693	SER	T1849	S1926	ASP	Y2075	ALA	R2231	R2290	ARG	LEU	ARG	H2554
ASN	P1694	GLY	Q1852	H1928	ASP	S2076	HIS	L2232	V2291	ASP	LEU	ILE	I2555
ALA	L1695	THR	Y1855	N1929	ASN	S2077	ALA	Q2236	A2292	ARG	GLU	ALA	K2556
SER	E1696	ILE	G1856	D1930	GLN	S2078	LEU	Q2240	R2293	PHE	LEU	GLN	V2557
GLY	R1697	SER	P1865	E1931	ALA	A2079	ALA	L2241	S2294	ARG	ALA	ARG	L2558
ARG	T1698	ALA	Y1868	S1933	THR	S2080	ALA	E2242	F2295	GLN	GLN	THR	R2561
SER	T1699	ALA	H1869	D1934	LEU	S2081	GLN	L2243	V2296	LEU	LEU	SER	R2562
VAL	N1700	ALA	P1871	V1935	ASN	G2082	ALA	E2244	S2305	ILE	LEU	ASP	V2563
THR	S1701	ALA	H1870	L1936	ASP	K2083	LYS	D2247	R2306	THR	LEU	ASP	M2564
ALA	S1702	ALA	L1871	W1937	LYS	M2086	LYS	L2248	E2307	THR	LEU	ASP	H2565
THR	H1703	ALA	H1872	L1938	ASP	E2087	SER	Q2254	K2308	PRO	ALA	THR	D2566
ALA	A1704	LEU	H1873	L1939	ASP	V2088	LEU	T2255	L2309	PHE	GLY	THR	F2568
GLY	N1705	GLU	Q1876	V1941	SER	T2089	LEU	R2257	N2310	ARG	ASP	ASP	F2571
SER	G1706	ALA	N1877	S1943	LEU	D2091	LEU	Q2258	N2311	ARG	GLY	ASP	D2572
GLU	A1707	SER	S1878	V1950	PRO	R2092	LEU	L2259	L2312	PRO	GLU	ASP	Y2576
ALA	Q1708	GLY	A1879	F1951	ALA	L2095	ALA	N2260	E2314	ALA	ASP	VAL	L2579
ALA	A1710	ALA	R1880	Q1952	GLU	L2096	GLY	R2261	T2315	GLY	ASP	ASP	Q2587
SER	P1711	SER	R1881	L1954	THR	V2097	GLY	H2262	Q2316	ASN	GLU	GLU	S2588
VAL	R1712	VAL	T1779	W1957	M2029	K2101	THR	F2169	N2317	ASP	PRO	ASP	D2589
PRO	S1713	PRO	I1790	M1961	S2025	M2102	SER	L2166	ALA	ASP	PRO	ASP	A2591
ALA	M1714	ALA	V1791	N1962	D2027	S2103	GLY	T2167	THR	ASP	GLU	GLU	D2592
PHE	W1715	PHE	S1796	T1965	S2028	TYR	ALA	S2168	THR	GLY	PRO	ALA	A2593
PHE	W1716	SER	D1797	T1966	M2029	ALA	ASN	F2169	SER	LEU	ALA	HIS	F2594
GLU	R1719	GLU	L1798	LEU	G2033	ALA	ASN	W2176	LEU	GLN	GLY	GLY	G2596
ASP	N1720	ASP	M1799	ASP	C2034	ALA	LEU	T2180	THR	GLN	ARG	ARG	K2520
SER	THR	SER	L1808	THR	I2035	ALA	LEU	S2181	THR	ARG	GLU	GLU	N2521
GLN	H1S	GLN	I1813	PRO	P2036	ASN	LYS	R2266	THR	ARG	ASN	ASN	T2522
SER	GLN	SER	P1814	THR	P2037	ASN	VAL	C2267	SER	THR	GLY	GLY	R2525
ASN	ARG	ASN	A1815	LEU	V2042	MET	MET	T2270	LEU	ALA	ASP	ASP	
ALA	ALA	ALA	THR	GLY	P2043	GLN	GLN	P2271	ARG	GLY	ARG	ARG	
SER	THR	SER	GLY	ARG	L2044	GLN	GLN		THR	GLY	GLU	GLU	
ALA	ALA	ALA	ARG	ARG					ASP	GLY	ASP	ASP	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	401469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.408	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	364.32, 364.32, 364.32	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/14211	0.28	0/19260
1	B	0.12	0/14211	0.28	0/19260
1	C	0.15	1/14211 (0.0%)	0.30	0/19260
1	D	0.13	0/14211	0.30	0/19260
All	All	0.13	1/56844 (0.0%)	0.29	0/77040

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2090	VAL	C-O	-8.29	1.16	1.24

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	13924	0	13931	422	0
1	B	13924	0	13931	424	0
1	C	13924	0	13931	441	0
1	D	13924	0	13931	454	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
2	D	3	0	0	0	0
All	All	55708	0	55724	1632	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 15.

All (1632) 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:C:2090:VAL:CG2	1:D:1374:GLN:HE22	1.80	0.95
1:C:744:THR:HA	1:C:761:LYS:O	1.69	0.92
1:B:371:PHE:HA	1:B:385:SER:HA	1.53	0.91
1:C:2090:VAL:HG22	1:D:1374:GLN:HE22	1.37	0.89
1:C:680:VAL:O	1:C:709:ARG:HB2	1.72	0.89
1:B:799:VAL:HA	1:B:813:ARG:O	1.76	0.86
1:A:1295:PRO:HG2	1:A:1297:ARG:HE	1.44	0.83
1:C:1333:LEU:HD13	1:C:1339:LEU:HD21	1.64	0.79
1:D:414:ALA:HB1	1:D:419:LEU:HB2	1.63	0.79
1:B:1199:CYS:SG	1:B:1216:HIS:HE1	2.03	0.79
1:B:531:GLY:HA2	1:B:669:LYS:HG3	1.65	0.78
1:A:1961:MET:HG2	1:A:2173:CYS:HB2	1.66	0.78
1:B:426:LEU:HB2	1:B:437:ALA:HB3	1.65	0.78
1:C:772:ASP:HB2	1:C:779:GLU:HB2	1.65	0.77
1:C:1917:PHE:HE2	1:D:1441:VAL:HG11	1.49	0.77
1:A:1933:SER:HB3	1:B:1376:GLY:HA2	1.67	0.77
1:D:1333:LEU:HD23	1:D:1339:LEU:HD21	1.67	0.77
1:C:426:LEU:HB2	1:C:437:ALA:HB3	1.66	0.76
1:D:671:LEU:HD11	1:D:681:LYS:HG2	1.66	0.76
1:B:18:LEU:HD22	1:B:809:PRO:HB2	1.68	0.76
1:B:498:PRO:HG3	1:B:773:LEU:HB2	1.67	0.75
1:D:2649:GLN:HG2	1:D:2650:PRO:HD3	1.69	0.75
1:D:473:ILE:HG22	1:D:487:LEU:HG	1.69	0.74
1:C:841:ILE:HA	1:C:871:VAL:HA	1.70	0.73
1:C:392:GLN:HE21	1:C:411:HIS:HA	1.52	0.73
1:B:453:SER:O	1:B:457:LYS:NZ	2.22	0.73
1:B:679:ALA:HB1	1:B:708:CYS:HB2	1.69	0.73
1:C:827:MET:HB2	1:C:1197:ARG:HH12	1.53	0.73
1:C:433:ARG:HD3	1:C:478:CYS:HB2	1.70	0.73
1:C:1408:GLU:O	1:C:1418:ARG:NH2	2.22	0.73
1:C:771:PHE:HA	1:C:778:ALA:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ILE:HG13	1:B:551:ILE:HD12	1.71	0.72
1:B:536:LEU:HB3	1:B:665:VAL:HG11	1.72	0.72
1:D:1177:ASP:H	1:D:1251:ARG:HH22	1.35	0.72
1:C:424:ILE:HG22	1:C:438:THR:HG22	1.71	0.72
1:C:1930:ASP:OD1	1:C:2090:VAL:HG23	1.90	0.71
1:C:62:LEU:HG	1:C:64:ASP:H	1.54	0.71
1:C:2102:MET:SD	1:C:2102:MET:N	2.60	0.71
1:A:2661:VAL:HG23	1:A:2662:LEU:HG	1.70	0.71
1:C:1933:SER:HB2	1:D:1376:GLY:HA2	1.71	0.71
1:C:799:VAL:HA	1:C:813:ARG:O	1.90	0.71
1:C:2040:PHE:HB3	1:C:2584:LEU:HD11	1.72	0.71
1:D:744:THR:HG22	1:D:762:THR:HB	1.73	0.71
1:A:2517:ARG:O	1:A:2525:ARG:NH2	2.24	0.71
1:D:1199:CYS:SG	1:D:1216:HIS:HE1	2.10	0.71
1:D:755:GLY:HA2	1:D:773:LEU:HD21	1.73	0.70
1:D:841:ILE:HG12	1:D:871:VAL:HG12	1.72	0.70
1:C:2093:ASN:HB2	1:D:1484:VAL:HG21	1.73	0.70
1:D:917:ASP:OD1	1:D:917:ASP:N	2.23	0.70
1:D:1124:ARG:HH21	1:D:1245:ALA:HA	1.57	0.70
1:A:2686:ASN:H	1:A:2689:MET:HE2	1.56	0.70
1:D:2028:SER:OG	1:D:2561:ARG:NH2	2.24	0.70
1:D:446:TRP:HB2	1:D:459:GLU:HG3	1.73	0.70
1:A:824:LYS:O	1:A:831:ARG:NH1	2.25	0.70
1:C:1205:LEU:HD13	1:C:1237:LYS:HE3	1.74	0.70
1:D:678:VAL:HG13	1:D:713:ILE:HG12	1.73	0.70
1:B:535:CYS:SG	1:B:536:LEU:N	2.64	0.70
1:D:2293:ARG:HB3	1:D:2736:SER:HB2	1.72	0.70
1:B:1819:LEU:HB3	1:B:2166:LEU:HD11	1.74	0.69
1:A:14:THR:H	1:A:17:GLN:HE22	1.40	0.69
1:A:680:VAL:O	1:A:709:ARG:HB2	1.92	0.69
1:C:554:GLY:HA3	1:C:850:SER:HB3	1.74	0.69
1:D:772:ASP:OD1	1:D:773:LEU:N	2.26	0.69
1:A:929:VAL:O	1:A:1081:ARG:NH1	2.26	0.68
1:C:915:ARG:NH2	1:C:919:ASN:O	2.25	0.68
1:B:750:ASN:ND2	1:B:801:ILE:O	2.26	0.68
1:A:1454:PRO:HB2	1:A:1456:PRO:HD2	1.74	0.68
1:C:424:ILE:HA	1:C:438:THR:HA	1.74	0.68
1:A:1854:ARG:NH1	1:B:1370:TYR:OH	2.26	0.68
1:B:2293:ARG:NH2	1:B:2770:SER:OG	2.26	0.68
1:A:534:VAL:HG12	1:A:718:VAL:HA	1.74	0.68
1:A:2766:ASN:O	1:A:2770:SER:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:VAL:HA	1:C:680:VAL:HG22	1.74	0.68
1:D:451:LEU:O	1:D:455:ALA:N	2.23	0.68
1:D:510:ARG:HA	1:D:513:ASN:HB2	1.75	0.68
1:D:2288:GLY:HA3	1:D:2768:CYS:HA	1.75	0.68
1:B:1846:MET:HE1	1:B:2196:PHE:HE2	1.59	0.68
1:D:1197:ARG:HB3	1:D:1220:ASP:HB3	1.74	0.68
1:C:2090:VAL:HG21	1:D:1374:GLN:HE22	1.57	0.67
1:D:1238:CYS:SG	1:D:1239:LYS:N	2.66	0.67
1:A:1697:ARG:HE	1:B:2691:ILE:HD12	1.58	0.67
1:B:1376:GLY:O	1:B:1427:ARG:NH2	2.26	0.67
1:D:568:MET:SD	1:D:568:MET:N	2.66	0.67
1:D:1171:TYR:O	1:D:1175:CYS:HB2	1.95	0.67
1:A:672:LYS:HB3	1:A:679:ALA:HB3	1.76	0.67
1:A:424:ILE:HG13	1:A:438:THR:HG22	1.75	0.67
1:A:2763:PRO:HA	1:A:2773:TYR:O	1.95	0.67
1:A:2092:ARG:HH11	1:B:1490:ILE:HD12	1.59	0.67
1:C:2248:ARG:NH1	1:C:2305:SER:OG	2.27	0.67
1:C:756:VAL:HG13	1:C:771:PHE:HB2	1.77	0.67
1:A:1916:ASP:OD1	1:B:1492:ARG:NH1	2.27	0.66
1:A:433:ARG:NH1	1:A:481:LEU:O	2.28	0.66
1:D:1280:VAL:HG22	1:D:1329:LEU:HD11	1.77	0.66
1:C:759:VAL:HG23	1:C:801:ILE:HD11	1.76	0.66
1:D:538:ASN:O	1:D:542:TYR:N	2.28	0.66
1:D:2766:ASN:O	1:D:2770:SER:HA	1.96	0.66
1:A:710:LEU:HD22	1:C:710:LEU:HD22	1.77	0.66
1:C:2083:LYS:NZ	1:C:2184:MET:SD	2.69	0.66
1:D:1836:ILE:HG13	1:D:1837:PRO:HD3	1.78	0.66
1:B:2290:GLY:HA3	1:B:2767:THR:HB	1.78	0.66
1:C:1494:THR:HG21	1:D:1917:PHE:HB2	1.78	0.66
1:D:447:VAL:HG21	1:D:454:VAL:HG12	1.78	0.66
1:A:562:MET:SD	1:A:563:GLU:N	2.68	0.65
1:B:2044:LEU:HD21	1:B:2051:ALA:HB3	1.77	0.65
1:D:857:ASN:HB3	1:D:862:LYS:HE3	1.78	0.65
1:D:771:PHE:HA	1:D:778:ALA:HA	1.78	0.65
1:D:1839:TRP:NE1	1:D:2176:MET:SD	2.59	0.65
1:B:536:LEU:O	1:B:539:ASN:ND2	2.30	0.65
1:A:2659:LEU:HD21	1:A:2667:LEU:HD22	1.78	0.65
1:B:535:CYS:HB2	1:B:667:VAL:HG22	1.78	0.65
1:A:2685:VAL:HG21	1:A:2730:VAL:HG21	1.79	0.65
1:B:1280:VAL:HG12	1:B:1329:LEU:HD11	1.79	0.65
1:A:1189:ILE:HD12	1:A:1292:GLN:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2186:LEU:HD13	1:B:2215:LEU:HD11	1.78	0.65
1:B:2505:PHE:HB3	1:B:2514:TYR:HB3	1.78	0.65
1:B:1439:LEU:HD21	1:B:1456:PRO:HB2	1.78	0.65
1:B:1712:ARG:HA	1:B:1715:GLN:HG2	1.78	0.65
1:D:11:LEU:HD13	1:D:863:LYS:HE3	1.79	0.65
1:D:799:VAL:HA	1:D:813:ARG:O	1.96	0.65
1:B:1333:LEU:HD23	1:B:1339:LEU:HD21	1.78	0.65
1:C:1847:ASP:OD2	1:C:2188:ARG:NH2	2.30	0.65
1:D:838:LEU:HD12	1:D:839:PRO:HD2	1.77	0.65
1:C:678:VAL:HG21	1:C:716:LEU:HD11	1.77	0.64
1:C:1851:ALA:HB2	1:C:2087:GLU:HB3	1.78	0.64
1:C:2062:ARG:NH1	1:D:1713:SER:OG	2.30	0.64
1:A:854:LEU:HD12	1:A:857:ASN:HA	1.79	0.64
1:D:543:HIS:HB3	1:D:665:VAL:HG11	1.79	0.64
1:D:1826:ASN:O	1:D:1829:ASN:ND2	2.30	0.64
1:C:795:ASN:OD1	1:C:797:ARG:NH1	2.30	0.64
1:B:2549:THR:OG1	1:B:2680:ASN:ND2	2.31	0.64
1:D:401:TYR:CZ	1:D:412:PRO:HD3	2.33	0.64
1:D:1871:PRO:HG3	1:D:1936:LEU:HD11	1.79	0.64
1:B:2222:GLU:OE1	1:B:2226:ARG:NH1	2.31	0.64
1:A:28:LYS:O	1:A:33:ASN:N	2.28	0.64
1:B:2178:MET:SD	1:B:2178:MET:N	2.70	0.64
1:A:394:LYS:HB2	1:A:397:GLU:HG3	1.80	0.64
1:D:2293:ARG:NH2	1:D:2770:SER:OG	2.31	0.64
1:B:69:ARG:HE	1:B:361:GLN:HE21	1.47	0.63
1:D:30:ASN:O	1:D:882:ARG:NH1	2.30	0.63
1:A:72:PHE:HA	1:A:356:LEU:HA	1.80	0.63
1:A:2550:LEU:O	1:A:2676:ARG:NH1	2.26	0.63
1:B:2633:GLU:OE1	1:B:2636:ARG:NH2	2.29	0.63
1:C:2293:ARG:NH2	1:C:2767:THR:O	2.32	0.63
1:D:474:VAL:N	1:D:486:GLN:O	2.30	0.63
1:C:2505:PHE:HB3	1:C:2514:TYR:HB3	1.80	0.63
1:B:363:TRP:HE1	1:B:400:PRO:HB3	1.63	0.63
1:B:2028:SER:OG	1:B:2561:ARG:NH2	2.31	0.63
1:C:1379:ARG:NH1	1:C:1517:GLU:OE1	2.31	0.63
1:B:747:LEU:HD21	1:B:761:LYS:HB2	1.81	0.63
1:B:1334:GLN:HA	1:B:1404:THR:HG21	1.81	0.63
1:D:1155:MET:HA	1:D:1158:VAL:HG12	1.79	0.63
1:C:373:CYS:HB2	1:C:384:VAL:HB	1.81	0.63
1:D:2294:SER:HB3	1:D:2735:SER:HB2	1.81	0.63
1:D:2690:LEU:HG	1:D:2739:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:PHE:HB2	1:C:811:ILE:HB	1.80	0.62
1:C:555:ILE:O	1:C:557:LYS:NZ	2.31	0.62
1:D:426:LEU:HG	1:D:437:ALA:HB3	1.82	0.62
1:D:2686:ASN:HD21	1:D:2689:MET:HG3	1.63	0.62
1:D:2766:ASN:ND2	1:D:2768:CYS:SG	2.72	0.62
1:A:1378:ILE:HD11	1:B:1935:VAL:HG23	1.82	0.62
1:B:1166:ASP:HB3	1:B:1217:LYS:HD2	1.81	0.62
1:B:1171:TYR:OH	1:B:1271:ARG:NH2	2.32	0.62
1:C:750:ASN:ND2	1:C:801:ILE:O	2.32	0.62
1:D:1181:PHE:HB2	1:D:1232:CYS:HB3	1.82	0.62
1:D:1943:SER:O	1:D:1943:SER:OG	2.15	0.62
1:C:6:PHE:HD2	1:C:868:ILE:HD12	1.65	0.62
1:D:1440:SER:HB2	1:D:1790:ILE:HG21	1.81	0.62
1:D:1941:VAL:HG12	1:D:2196:PHE:HE1	1.64	0.62
1:D:2027:ASP:OD1	1:D:2561:ARG:NH2	2.33	0.62
1:A:2240:LEU:HD11	1:A:2277:VAL:HA	1.82	0.62
1:C:748:ALA:HB3	1:C:801:ILE:HG13	1.81	0.62
1:D:473:ILE:HA	1:D:487:LEU:HA	1.82	0.62
1:D:2549:THR:OG1	1:D:2680:ASN:ND2	2.33	0.62
1:A:708:CYS:O	1:C:672:LYS:NZ	2.33	0.61
1:A:1438:ILE:HG23	1:B:1918:LEU:HD12	1.81	0.61
1:A:2721:MET:O	1:A:2726:ARG:NH2	2.33	0.61
1:B:2027:ASP:OD1	1:B:2561:ARG:NH2	2.32	0.61
1:B:2724:THR:OG1	1:B:2725:GLU:OE1	2.15	0.61
1:C:2226:ARG:HA	1:C:2229:MET:HG2	1.81	0.61
1:A:2562:LYS:NZ	1:A:2563:VAL:O	2.33	0.61
1:C:1441:VAL:HG11	1:D:1917:PHE:HE2	1.66	0.61
1:A:2637:LYS:HA	1:A:2640:GLU:HB3	1.81	0.61
1:B:818:THR:HA	1:B:840:PRO:HA	1.82	0.61
1:B:2552:ARG:NH1	1:B:2567:ASP:OD1	2.33	0.61
1:A:1367:GLU:OE2	1:B:2069:ARG:NH1	2.34	0.61
1:C:384:VAL:HG23	1:C:427:LEU:HD12	1.81	0.61
1:D:850:SER:HA	1:D:863:LYS:HA	1.83	0.61
1:A:2635:VAL:O	1:A:2638:TYR:HB3	2.01	0.61
1:B:1461:LYS:NZ	1:B:1794:GLN:OE1	2.33	0.61
1:A:62:LEU:HG	1:A:64:ASP:H	1.66	0.61
1:A:1494:THR:HG21	1:B:1917:PHE:HB2	1.83	0.61
1:B:482:TYR:CZ	1:B:773:LEU:HD11	2.36	0.61
1:B:2616:GLU:HG3	1:B:2622:VAL:HG23	1.82	0.61
1:D:1191:GLN:HG3	1:D:1193:ILE:HD11	1.83	0.61
1:D:1385:HIS:NE2	1:D:1510:SER:OG	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PRO:HD2	1:A:861:LYS:HD3	1.83	0.61
1:B:4:ILE:HG12	1:B:40:LEU:HD22	1.83	0.60
1:A:1331:ARG:NH1	1:A:1331:ARG:O	2.33	0.60
1:D:18:LEU:HD22	1:D:809:PRO:HB2	1.81	0.60
1:A:854:LEU:HD23	1:A:854:LEU:H	1.65	0.60
1:A:1697:ARG:HB3	1:B:2691:ILE:HG23	1.82	0.60
1:C:1718:VAL:HG13	1:D:1942:CYS:HB2	1.83	0.60
1:A:825:ASP:OD1	1:A:829:GLY:N	2.34	0.60
1:C:62:LEU:HD23	1:C:66:ARG:HB2	1.84	0.60
1:C:750:ASN:HB3	1:C:803:THR:HG22	1.82	0.60
1:D:414:ALA:HA	1:D:417:LEU:HB2	1.84	0.60
1:A:380:GLU:HB3	1:A:394:LYS:HD3	1.82	0.60
1:A:2240:LEU:HD12	1:A:2241:SER:H	1.66	0.60
1:B:706:GLN:O	1:D:672:LYS:NZ	2.35	0.60
1:C:52:VAL:HG11	1:C:375:GLY:HA2	1.83	0.60
1:A:732:GLN:NE2	1:A:734:THR:O	2.30	0.60
1:A:765:TRP:HE1	1:A:783:ASN:HD22	1.48	0.60
1:B:2087:GLU:O	1:B:2089:THR:N	2.35	0.60
1:C:1713:SER:OG	1:D:2062:ARG:NH1	2.35	0.60
1:A:1124:ARG:NH2	1:A:1177:ASP:O	2.34	0.60
1:A:1258:LEU:HD11	1:A:1264:LEU:HD12	1.82	0.60
1:B:2198:ARG:NH1	1:B:2219:GLU:OE1	2.35	0.60
1:C:795:ASN:ND2	1:C:798:ASN:OD1	2.33	0.60
1:D:1796:SER:HG	1:D:1957:TRP:CD1	2.20	0.60
1:C:544:ALA:HA	1:C:561:LEU:HG	1.83	0.60
1:A:2035:ILE:HD12	1:A:2036:PRO:HD2	1.83	0.60
1:B:744:THR:HG22	1:B:762:THR:HB	1.83	0.60
1:D:1259:LEU:HD11	1:D:1332:VAL:HG22	1.82	0.60
1:C:1928:HIS:HA	1:C:2091:ASP:HB2	1.84	0.60
1:A:930:CYS:HA	1:A:1081:ARG:HH12	1.67	0.59
1:A:1484:VAL:HG21	1:B:2093:ASN:HB2	1.83	0.59
1:A:2721:MET:HG3	1:A:2726:ARG:HH21	1.67	0.59
1:B:814:ASP:OD1	1:B:818:THR:N	2.32	0.59
1:C:2089:THR:HG23	1:D:1373:GLN:HE22	1.65	0.59
1:C:2686:ASN:HB3	1:C:2689:MET:HB2	1.84	0.59
1:D:1173:LEU:HD12	1:D:1258:LEU:HD22	1.84	0.59
1:D:2522:THR:HG23	1:D:2525:ARG:H	1.67	0.59
1:A:1929:ASN:OD1	1:B:1430:ARG:NH1	2.35	0.59
1:A:417:LEU:HG	1:A:444:ALA:HB1	1.84	0.59
1:A:2253:GLN:NE2	1:A:2311:ASN:O	2.33	0.59
1:D:809:PRO:HG2	1:D:846:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:LYS:HE2	1:A:674:ASP:HB2	1.83	0.59
1:A:1412:LYS:HZ1	1:A:1418:ARG:HH21	1.51	0.59
1:B:475:SER:HB2	1:B:486:GLN:HE21	1.68	0.59
1:D:360:LEU:HD23	1:D:360:LEU:H	1.68	0.59
1:C:678:VAL:HG13	1:C:713:ILE:HG12	1.83	0.59
1:B:771:PHE:HA	1:B:778:ALA:HA	1.84	0.59
1:B:1495:ALA:HA	1:B:1775:SER:H	1.68	0.59
1:D:491:LEU:HD21	1:D:749:VAL:HG11	1.84	0.59
1:C:76:PRO:HG3	1:C:851:LEU:HB3	1.85	0.59
1:C:379:SER:OG	1:C:380:GLU:OE1	2.19	0.59
1:D:785:PRO:HG2	1:D:833:PRO:HD3	1.85	0.59
1:D:927:VAL:HG21	1:D:1120:ALA:HB2	1.85	0.59
1:B:1793:ARG:HG3	1:B:1956:TYR:HE2	1.68	0.58
1:D:2075:TYR:HB2	1:D:2086:MET:HE3	1.85	0.58
1:C:516:PRO:HG2	1:C:717:GLN:HB2	1.84	0.58
1:C:2062:ARG:NH2	1:C:2064:GLU:OE1	2.35	0.58
1:C:1434:ARG:HH21	1:D:1926:ARG:HA	1.67	0.58
1:B:1231:TYR:HD1	1:B:1231:TYR:H	1.50	0.58
1:B:497:VAL:O	1:B:502:ARG:NH1	2.34	0.58
1:C:1485:PRO:HG3	1:D:2092:ARG:HD2	1.85	0.58
1:C:2568:PHE:HZ	1:C:2642:ARG:HD3	1.69	0.58
1:A:1363:LEU:O	1:A:1368:GLN:NE2	2.37	0.58
1:A:1711:PRO:HD3	1:B:2198:ARG:HG2	1.86	0.58
1:B:433:ARG:HH12	1:B:458:LEU:HD13	1.69	0.58
1:B:577:ARG:HD3	1:B:582:LEU:HD21	1.84	0.58
1:B:916:CYS:SG	1:B:917:ASP:N	2.76	0.58
1:C:66:ARG:HB3	1:C:362:TRP:HZ2	1.69	0.58
1:C:2515:THR:HB	1:C:2551:ASN:HD22	1.68	0.58
1:D:2552:ARG:NH1	1:D:2567:ASP:OD1	2.37	0.58
1:A:685:THR:OG1	1:C:672:LYS:NZ	2.37	0.58
1:C:537:ARG:NE	1:C:537:ARG:O	2.35	0.58
1:A:2549:THR:OG1	1:A:2680:ASN:ND2	2.36	0.58
1:B:1331:ARG:O	1:B:1331:ARG:NH1	2.37	0.58
1:C:6:PHE:CD2	1:C:868:ILE:HD12	2.39	0.58
1:C:854:LEU:HD12	1:C:855:PRO:HD2	1.86	0.58
1:C:1930:ASP:OD1	1:C:2090:VAL:CG2	2.51	0.58
1:C:2087:GLU:O	1:C:2089:THR:N	2.36	0.58
1:C:2090:VAL:HG22	1:D:1374:GLN:NE2	2.15	0.58
1:C:2250:LEU:HA	1:C:2253:GLN:HG2	1.85	0.58
1:C:2571:PHE:HE2	1:C:2642:ARG:HB3	1.68	0.58
1:D:673:VAL:HG22	1:D:678:VAL:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2222:GLU:OE1	1:D:2226:ARG:NH1	2.37	0.58
1:B:15:GLU:OE2	1:B:824:LYS:NZ	2.37	0.58
1:B:52:VAL:HB	1:B:376:ALA:HB2	1.86	0.58
1:B:705:LEU:HA	1:D:705:LEU:HB3	1.86	0.58
1:B:850:SER:HA	1:B:863:LYS:HA	1.86	0.58
1:D:560:VAL:O	1:D:574:PHE:HA	2.04	0.58
1:B:432:ILE:HD11	1:B:556:PRO:HG3	1.85	0.57
1:C:551:ILE:HG23	1:C:556:PRO:HB3	1.85	0.57
1:D:75:GLN:HG3	1:D:78:ARG:HB2	1.86	0.57
1:D:1409:LEU:HD11	1:D:1425:THR:HG21	1.86	0.57
1:A:1273:GLU:HB2	1:A:1277:LEU:HD23	1.86	0.57
1:A:2072:GLN:HB2	1:A:2074:LEU:HD13	1.85	0.57
1:B:2536:LEU:HD11	1:B:2548:ILE:HD11	1.86	0.57
1:C:448:ASP:OD1	1:C:449:GLU:N	2.37	0.57
1:C:2766:ASN:O	1:C:2770:SER:N	2.37	0.57
1:D:1429:LEU:HA	1:D:1432:VAL:HG12	1.86	0.57
1:B:515:LYS:NZ	1:B:517:LYS:O	2.37	0.57
1:B:2306:ASN:HA	1:B:2503:PRO:HB3	1.85	0.57
1:B:2718:VAL:HA	1:B:2721:MET:HE3	1.84	0.57
1:C:1472:VAL:HG21	1:C:1827:LEU:HD21	1.86	0.57
1:D:2290:GLY:O	1:D:2735:SER:OG	2.20	0.57
1:A:32:TYR:HB3	1:A:34:LEU:HD23	1.87	0.57
1:B:741:PRO:HG2	1:B:744:THR:HG21	1.86	0.57
1:B:2052:ASP:OD2	1:B:2053:GLN:NE2	2.38	0.57
1:C:18:LEU:HD22	1:C:809:PRO:HB2	1.87	0.57
1:A:1368:GLN:O	1:A:1372:ASN:ND2	2.32	0.57
1:A:2088:VAL:HG13	1:B:1373:GLN:HG3	1.86	0.57
1:A:2503:PRO:O	1:A:2517:ARG:NE	2.28	0.57
1:B:2530:ARG:HE	1:B:2653:ALA:HB1	1.68	0.57
1:D:884:ASP:HB3	1:D:887:ALA:HB3	1.86	0.57
1:A:1179:CYS:SG	1:A:1180:SER:N	2.77	0.57
1:C:2663:PRO:O	1:C:2666:SER:OG	2.20	0.57
1:D:1265:VAL:HG23	1:D:1275:LEU:HD23	1.86	0.57
1:A:360:LEU:HD23	1:A:360:LEU:H	1.70	0.57
1:A:1828:GLN:HE22	1:A:2171:PRO:HB3	1.70	0.57
1:A:1851:ALA:HB2	1:A:2087:GLU:HB3	1.86	0.57
1:B:1154:PHE:HD1	1:B:1157:MET:HE3	1.69	0.57
1:B:2216:GLY:O	1:B:2221:LYS:NZ	2.37	0.57
1:C:1918:LEU:HB3	1:D:1513:LEU:HD22	1.85	0.57
1:D:52:VAL:HG11	1:D:375:GLY:HA2	1.87	0.57
1:D:430:ASN:ND2	1:D:478:CYS:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2062:ARG:NH2	1:D:2064:GLU:OE1	2.38	0.57
1:D:2248:ARG:NH2	1:D:2249:ASP:OD1	2.37	0.57
1:A:1253:ASP:O	1:A:1257:ARG:HG2	2.05	0.57
1:B:924:HIS:CD2	1:B:1116:PRO:HG3	2.40	0.57
1:C:2721:MET:HB3	1:C:2725:GLU:HB2	1.86	0.57
1:B:385:SER:OG	1:B:389:GLU:OE1	2.22	0.57
1:C:682:PHE:O	1:C:685:THR:OG1	2.21	0.57
1:C:2598:MET:HB2	1:C:2600:LEU:HD13	1.87	0.57
1:A:782:ASN:HB3	1:A:830:ILE:HG12	1.87	0.57
1:A:2226:ARG:NH1	1:A:2543:ASN:OD1	2.36	0.57
1:B:929:VAL:O	1:B:1082:LYS:NZ	2.37	0.57
1:D:536:LEU:HG	1:D:538:ASN:H	1.70	0.57
1:D:547:VAL:H	1:D:660:GLU:HB3	1.70	0.57
1:D:663:LYS:HB3	1:D:726:LYS:HB2	1.86	0.57
1:A:1238:CYS:SG	1:A:1239:LYS:N	2.77	0.56
1:C:377:LEU:O	1:C:395:TRP:NE1	2.38	0.56
1:C:2259:LEU:HD22	1:C:2534:ARG:HH21	1.70	0.56
1:C:1916:ASP:OD2	1:D:1719:ARG:NH1	2.38	0.56
1:A:1177:ASP:H	1:A:1251:ARG:HH22	1.51	0.56
1:A:2087:GLU:O	1:A:2089:THR:N	2.39	0.56
1:B:479:CYS:SG	1:B:481:LEU:N	2.78	0.56
1:C:2253:GLN:HA	1:C:2312:LEU:HD21	1.86	0.56
1:D:445:THR:HG23	1:D:460:HIS:HB2	1.86	0.56
1:D:1493:PRO:O	1:D:1719:ARG:NH2	2.38	0.56
1:D:1839:TRP:HE3	1:D:1954:LEU:HD13	1.70	0.56
1:B:1271:ARG:NH1	1:B:1273:GLU:OE2	2.38	0.56
1:B:2631:VAL:HG13	1:B:2632:TYR:HD1	1.71	0.56
1:C:473:ILE:HA	1:C:487:LEU:HD13	1.88	0.56
1:A:799:VAL:HA	1:A:813:ARG:O	2.06	0.56
1:A:1925:MET:HB3	1:B:1434:ARG:HG2	1.87	0.56
1:B:893:MET:O	1:B:896:GLU:HG3	2.06	0.56
1:C:2037:PRO:HG3	1:C:2070:PRO:HA	1.87	0.56
1:C:2240:LEU:HD23	1:C:2277:VAL:HG22	1.87	0.56
1:C:2716:SER:OG	1:C:2720:LYS:NZ	2.38	0.56
1:D:2035:ILE:HD12	1:D:2036:PRO:HD2	1.87	0.56
1:A:1124:ARG:HH21	1:A:1245:ALA:HA	1.71	0.56
1:A:2539:CYS:HA	1:A:2544:GLU:HB2	1.87	0.56
1:B:705:LEU:HD22	1:D:704:LEU:HB3	1.88	0.56
1:B:1173:LEU:HD12	1:B:1258:LEU:HD12	1.87	0.56
1:B:2545:LEU:HD13	1:B:2738:SER:HB2	1.86	0.56
1:B:2662:LEU:HD12	1:B:2663:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:MET:SD	1:C:568:MET:N	2.79	0.56
1:C:813:ARG:NH1	1:C:842:SER:O	2.37	0.56
1:C:2035:ILE:HD12	1:C:2036:PRO:HD2	1.88	0.56
1:C:2507:GLN:HE22	1:C:2512:GLY:H	1.52	0.56
1:D:1475:LEU:HD22	1:D:1791:VAL:HG23	1.87	0.56
1:A:2561:ARG:NH2	1:A:2670:LEU:O	2.38	0.56
1:B:753:SER:HB3	1:B:806:GLN:HB3	1.88	0.56
1:B:2035:ILE:HD12	1:B:2036:PRO:HD2	1.86	0.56
1:D:1169:PRO:HD2	1:D:1264:LEU:HD11	1.87	0.56
1:A:377:LEU:HD21	1:A:434:ALA:HB2	1.87	0.56
1:C:1709:GLN:O	1:D:2198:ARG:NH2	2.39	0.56
1:C:2274:VAL:H	1:C:2541:LEU:HD21	1.70	0.56
1:C:2517:ARG:NH1	1:C:2518:PRO:O	2.38	0.56
1:B:2240:LEU:HB2	1:B:2274:VAL:HG11	1.87	0.56
1:D:2556:LYS:HE3	1:D:2561:ARG:HE	1.71	0.56
1:A:935:ASN:OD1	1:A:1245:ALA:N	2.38	0.56
1:C:1855:TYR:OH	1:C:1933:SER:O	2.24	0.56
1:C:2198:ARG:NH2	1:C:2219:GLU:OE2	2.39	0.56
1:D:536:LEU:HG	1:D:538:ASN:N	2.20	0.56
1:B:1181:PHE:HZ	1:B:1314:MET:HE2	1.71	0.55
1:D:467:GLU:HG3	1:D:735:PRO:HB2	1.88	0.55
1:A:1917:PHE:HB2	1:B:1494:THR:HG21	1.86	0.55
1:A:2038:ASN:HD22	1:A:2041:GLU:H	1.53	0.55
1:A:2252:ILE:HB	1:A:2310:PRO:HG2	1.88	0.55
1:B:757:HIS:ND1	1:B:768:TYR:OH	2.36	0.55
1:C:380:GLU:O	1:C:395:TRP:NE1	2.39	0.55
1:C:565:VAL:HG11	1:C:653:LEU:HD23	1.87	0.55
1:C:2520:LYS:H	1:C:2525:ARG:HH12	1.54	0.55
1:D:1272:GLY:HA3	1:D:1354:LEU:HB2	1.89	0.55
1:B:1253:ASP:O	1:B:1257:ARG:HG2	2.06	0.55
1:C:1265:VAL:O	1:C:1274:HIS:NE2	2.39	0.55
1:A:1329:LEU:HD23	1:A:1397:LEU:HD13	1.88	0.55
1:A:2236:GLN:NE2	1:A:2273:ALA:O	2.39	0.55
1:B:2723:MET:SD	1:B:2723:MET:N	2.78	0.55
1:C:1082:LYS:O	1:C:1086:HIS:ND1	2.36	0.55
1:C:1411:ASN:O	1:C:1418:ARG:NH1	2.39	0.55
1:D:1352:ASP:OD1	1:D:1352:ASP:N	2.39	0.55
1:D:2037:PRO:HG3	1:D:2070:PRO:HA	1.88	0.55
1:D:2500:ASP:HB2	1:D:2520:LYS:HD2	1.88	0.55
1:A:1855:TYR:OH	1:A:1933:SER:O	2.24	0.55
1:B:750:ASN:HB2	1:B:801:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:PHE:HA	1:C:385:SER:HA	1.88	0.55
1:C:401:TYR:HE1	1:C:403:ASN:HB2	1.72	0.55
1:A:46:ALA:HB1	1:A:62:LEU:HD13	1.89	0.55
1:A:2598:MET:HE3	1:A:2626:VAL:HG21	1.89	0.55
1:C:9:HIS:CD2	1:C:865:ALA:HB3	2.42	0.55
1:D:915:ARG:NH1	1:D:921:ASN:OD1	2.40	0.55
1:D:1799:MET:HE1	1:D:1831:VAL:HG21	1.89	0.55
1:B:1820:THR:OG1	1:B:1823:ASP:OD1	2.24	0.55
1:B:2054:PRO:HG3	1:B:2510:LYS:HG2	1.89	0.55
1:C:724:THR:HG23	1:C:727:VAL:HG22	1.88	0.55
1:D:1291:CYS:O	1:D:1294:ARG:NH2	2.39	0.55
1:D:2248:ARG:NH2	1:D:2308:LYS:O	2.39	0.55
1:A:704:LEU:HD12	1:C:701:PRO:HB2	1.88	0.55
1:A:2257:ARG:HD3	1:A:2315:ILE:HA	1.89	0.55
1:D:2708:LEU:HD13	1:D:2711:LYS:HD2	1.88	0.55
1:A:2244:VAL:HG11	1:A:2295:PHE:HE1	1.72	0.55
1:B:1952:GLN:NE2	1:B:2210:SER:OG	2.38	0.55
1:C:2536:LEU:HD21	1:C:2548:ILE:HD13	1.89	0.55
1:D:413:ARG:HH12	1:D:416:PHE:HB3	1.72	0.55
1:B:542:TYR:O	1:B:565:VAL:N	2.31	0.54
1:B:837:ASP:OD1	1:B:920:ARG:NH2	2.38	0.54
1:C:534:VAL:HG12	1:C:718:VAL:HA	1.88	0.54
1:D:2242:LEU:HD11	1:D:2279:VAL:HA	1.89	0.54
1:D:2734:THR:HG22	1:D:2770:SER:HB3	1.89	0.54
1:B:854:LEU:HD12	1:B:855:PRO:HD2	1.88	0.54
1:B:1468:LEU:O	1:B:1472:VAL:HG22	2.06	0.54
1:C:1934:ASP:HB2	1:D:1518:PRO:HB3	1.88	0.54
1:D:1690:MET:SD	1:D:1690:MET:N	2.80	0.54
1:D:2633:GLU:OE1	1:D:2636:ARG:NH2	2.30	0.54
1:A:19:ASN:ND2	1:A:822:MET:O	2.39	0.54
1:A:43:LEU:HD12	1:A:46:ALA:HB3	1.88	0.54
1:B:441:ASN:O	1:B:464:THR:OG1	2.21	0.54
1:B:1385:HIS:CE1	1:B:1389:VAL:HG11	2.43	0.54
1:C:510:ARG:HB2	1:C:541:LEU:HD11	1.88	0.54
1:C:1911:MET:SD	1:C:1911:MET:N	2.80	0.54
1:A:1170:LEU:HD13	1:A:1258:LEU:HD23	1.89	0.54
1:B:915:ARG:NH2	1:B:919:ASN:O	2.37	0.54
1:D:2637:LYS:O	1:D:2641:HIS:N	2.40	0.54
1:A:672:LYS:NZ	1:C:708:CYS:O	2.36	0.54
1:A:841:ILE:HG22	1:A:871:VAL:HG12	1.89	0.54
1:A:1690:MET:N	1:A:1690:MET:SD	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:ARG:NE	1:A:2742:SER:OG	2.40	0.54
1:C:1522:ARG:HD3	1:D:1865:PRO:HD3	1.90	0.54
1:A:27:GLU:O	1:A:31:LYS:N	2.34	0.54
1:B:1131:THR:O	1:B:1134:GLU:HG3	2.07	0.54
1:C:1352:ASP:OD1	1:C:1352:ASP:N	2.40	0.54
1:A:1472:VAL:HG21	1:A:1827:LEU:HD21	1.89	0.54
1:C:2180:ILE:HG23	1:C:2185:LEU:HD21	1.90	0.54
1:D:2536:LEU:HD21	1:D:2548:ILE:HB	1.90	0.54
1:A:1711:PRO:HA	1:B:2060:ASN:HD21	1.71	0.54
1:B:411:HIS:CD2	1:B:414:ALA:HB2	2.42	0.54
1:B:1839:TRP:HE3	1:B:1954:LEU:HD13	1.72	0.54
1:B:2098:LEU:HB2	1:B:2099:PRO:HD3	1.90	0.54
1:B:2553:HIS:HB3	1:B:2567:ASP:HB3	1.90	0.54
1:C:838:LEU:N	1:C:917:ASP:OD2	2.37	0.54
1:C:2521:ASN:H	1:C:2525:ARG:HH22	1.55	0.54
1:A:895:LEU:HG	1:A:908:LEU:HD21	1.90	0.54
1:A:1704:ALA:O	1:A:1705:ASN:ND2	2.41	0.54
1:C:1131:THR:O	1:C:1134:GLU:HG2	2.08	0.54
1:B:747:LEU:HB2	1:B:759:VAL:HG23	1.89	0.54
1:C:817:GLY:HA3	1:C:840:PRO:HB3	1.90	0.54
1:C:837:ASP:N	1:C:917:ASP:OD2	2.41	0.54
1:A:836:LEU:HD13	1:A:838:LEU:HD12	1.90	0.53
1:B:493:TRP:CZ2	1:B:773:LEU:HB3	2.43	0.53
1:B:2309:LEU:HD12	1:B:2310:PRO:HD2	1.90	0.53
1:C:69:ARG:HH22	1:C:395:TRP:HA	1.73	0.53
1:A:2199:VAL:HG22	1:B:1710:ALA:HB2	1.89	0.53
1:C:923:LEU:HD23	1:C:1105:LEU:HB3	1.91	0.53
1:B:572:CYS:SG	1:B:573:ARG:N	2.81	0.53
1:B:1124:ARG:NH1	1:B:1177:ASP:O	2.42	0.53
1:C:27:GLU:O	1:C:31:LYS:N	2.33	0.53
1:C:747:LEU:HD23	1:C:759:VAL:HG12	1.90	0.53
1:C:882:ARG:NH1	1:C:884:ASP:OD2	2.40	0.53
1:C:2506:TYR:CD1	1:C:2517:ARG:HB2	2.44	0.53
1:A:1396:LEU:HD23	1:A:1396:LEU:H	1.73	0.53
1:B:479:CYS:SG	1:B:806:GLN:NE2	2.68	0.53
1:B:510:ARG:NH2	1:B:539:ASN:H	2.06	0.53
1:C:1839:TRP:HZ3	1:C:1958:ILE:HD11	1.74	0.53
1:D:811:ILE:HG21	1:D:844:LEU:HD21	1.91	0.53
1:D:2515:THR:HG23	1:D:2551:ASN:HD22	1.72	0.53
1:C:760:LEU:HD11	1:C:771:PHE:HZ	1.74	0.53
1:D:803:THR:HA	1:D:846:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1375:SER:HG	1:D:1427:ARG:HH22	1.51	0.53
1:D:1379:ARG:NH2	1:D:1517:GLU:OE1	2.41	0.53
1:C:747:LEU:HB3	1:C:799:VAL:HG21	1.89	0.53
1:D:504:LYS:O	1:D:508:LYS:N	2.41	0.53
1:D:549:PHE:H	1:D:657:VAL:HG12	1.74	0.53
1:D:1320:GLU:HB2	1:D:1323:ARG:HH21	1.73	0.53
1:D:2021:PRO:HA	1:D:2024:ARG:HE	1.74	0.53
1:B:476:LEU:O	1:B:477:HIS:ND1	2.42	0.53
1:B:1195:GLU:OE2	1:B:1224:LYS:NZ	2.36	0.53
1:B:2245:ASP:OD1	1:B:2245:ASP:N	2.42	0.53
1:B:2604:ILE:HD11	1:B:2615:VAL:HB	1.91	0.53
1:C:19:ASN:ND2	1:C:822:MET:O	2.42	0.53
1:D:1197:ARG:NH1	1:D:1220:ASP:OD2	2.41	0.53
1:A:1247:GLN:HG3	1:A:1250:ALA:H	1.72	0.53
1:B:1381:ASP:OD1	1:B:1434:ARG:NH1	2.42	0.53
1:D:7:VAL:HG12	1:D:867:ILE:HB	1.90	0.53
1:A:1262:THR:OG1	1:A:1263:ASN:N	2.42	0.53
1:A:2572:ASP:OD1	1:A:2572:ASP:N	2.40	0.53
1:B:1449:LYS:HD2	1:B:1451:ASN:HD21	1.73	0.53
1:C:1492:ARG:NE	1:D:1940:ASP:OD1	2.38	0.53
1:D:2102:MET:HG2	1:D:2176:MET:HE3	1.90	0.53
1:D:1201:LEU:HA	1:D:1205:LEU:HB2	1.90	0.53
1:D:2242:LEU:HD21	1:D:2279:VAL:HG22	1.91	0.53
1:A:411:HIS:HB3	1:A:414:ALA:HB2	1.90	0.52
1:A:1480:GLU:OE1	1:B:1928:HIS:NE2	2.42	0.52
1:A:2505:PHE:HD1	1:A:2516:PRO:HA	1.74	0.52
1:B:75:GLN:NE2	1:B:353:PRO:O	2.42	0.52
1:C:1110:ASP:OD1	1:C:1112:ARG:N	2.33	0.52
1:D:2087:GLU:HG2	1:D:2188:ARG:HH21	1.72	0.52
1:A:1508:GLN:OE1	1:A:1509:GLY:N	2.42	0.52
1:B:2765:ALA:HB2	1:B:2772:LEU:HD23	1.91	0.52
1:C:390:LEU:HD11	1:C:436:VAL:HG21	1.91	0.52
1:C:2564:ASN:N	1:C:2567:ASP:OD2	2.40	0.52
1:A:498:PRO:HG3	1:A:773:LEU:HB2	1.90	0.52
1:B:846:MET:HG3	1:B:867:ILE:HG12	1.91	0.52
1:B:1860:ALA:HB2	1:B:1871:PRO:HG2	1.89	0.52
1:C:1921:ALA:O	1:C:1925:MET:HG3	2.09	0.52
1:A:915:ARG:NH2	1:A:919:ASN:OD1	2.42	0.52
1:A:2734:THR:HG22	1:A:2770:SER:HB2	1.90	0.52
1:B:426:LEU:HD23	1:B:476:LEU:HD12	1.91	0.52
1:D:1082:LYS:O	1:D:1086:HIS:ND1	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2731:TYR:O	1:D:2735:SER:HA	2.10	0.52
1:A:1379:ARG:HH12	1:A:1517:GLU:HG3	1.74	0.52
1:B:1690:MET:SD	1:B:1690:MET:N	2.83	0.52
1:B:2517:ARG:O	1:B:2525:ARG:NH2	2.41	0.52
1:C:2537:GLY:HA3	1:C:2661:VAL:HG21	1.91	0.52
1:D:1099:GLN:OE1	1:D:1099:GLN:N	2.42	0.52
1:D:2248:ARG:NH1	1:D:2307:GLU:OE1	2.42	0.52
1:C:49:LYS:O	1:C:49:LYS:NZ	2.33	0.52
1:D:30:ASN:ND2	1:D:837:ASP:O	2.41	0.52
1:D:1215:CYS:SG	1:D:1242:THR:OG1	2.68	0.52
1:A:393:TRP:HB3	1:A:400:PRO:HA	1.91	0.52
1:C:893:MET:O	1:C:896:GLU:HG3	2.10	0.52
1:D:1194:PHE:O	1:D:1207:CYS:N	2.36	0.52
1:A:379:SER:HB2	1:A:450:THR:HG23	1.90	0.52
1:A:2724:THR:O	1:A:2727:GLN:HG3	2.10	0.52
1:B:2025:ARG:HB2	1:B:2030:THR:HG23	1.92	0.52
1:C:4:ILE:HB	1:C:40:LEU:HD13	1.90	0.52
1:C:363:TRP:CZ2	1:C:391:TYR:HB3	2.45	0.52
1:C:1710:ALA:HA	1:D:2198:ARG:HB3	1.91	0.52
1:C:2259:LEU:HB3	1:C:2534:ARG:HE	1.75	0.52
1:C:2598:MET:HE1	1:C:2626:VAL:HG23	1.92	0.52
1:D:753:SER:OG	1:D:754:LYS:NZ	2.38	0.52
1:D:837:ASP:N	1:D:917:ASP:OD2	2.43	0.52
1:D:2780:LYS:O	1:D:2784:LYS:HG2	2.10	0.52
1:A:75:GLN:NE2	1:A:353:PRO:O	2.43	0.52
1:A:655:GLU:N	1:A:655:GLU:OE1	2.43	0.52
1:A:770:ILE:O	1:A:779:GLU:N	2.43	0.52
1:B:1114:MET:HA	1:B:1118:MET:HE3	1.92	0.52
1:C:75:GLN:OE1	1:C:75:GLN:N	2.43	0.52
1:D:571:SER:HB3	1:D:651:TRP:HE3	1.73	0.52
1:A:41:ASN:O	1:A:44:GLU:HB2	2.10	0.51
1:A:2229:MET:HE2	1:A:2232:LEU:HD21	1.93	0.51
1:B:2618:ILE:HG13	1:B:2621:GLY:HA3	1.92	0.51
1:C:2603:ALA:HB1	1:C:2614:GLN:HE21	1.76	0.51
1:D:893:MET:O	1:D:896:GLU:HG3	2.10	0.51
1:A:7:VAL:HG21	1:A:21:ARG:HB3	1.93	0.51
1:A:2086:MET:HG3	1:A:2088:VAL:HG23	1.92	0.51
1:B:2233:ARG:HB3	1:B:2541:LEU:HD11	1.91	0.51
1:C:411:HIS:O	1:C:414:ALA:N	2.35	0.51
1:C:474:VAL:N	1:C:486:GLN:O	2.43	0.51
1:C:1411:ASN:HB3	1:C:1418:ARG:HH12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1253:ASP:OD1	1:D:1257:ARG:NH1	2.37	0.51
1:B:498:PRO:O	1:B:501:GLN:NE2	2.41	0.51
1:B:2522:THR:HG23	1:B:2525:ARG:H	1.76	0.51
1:C:2069:ARG:NH1	1:D:1367:GLU:OE2	2.44	0.51
1:C:2267:CYS:SG	1:C:2268:ALA:N	2.84	0.51
1:D:400:PRO:HG2	1:D:402:ARG:HE	1.75	0.51
1:D:1077:GLU:O	1:D:1081:ARG:N	2.39	0.51
1:C:515:LYS:HG3	1:C:516:PRO:HD3	1.92	0.51
1:D:433:ARG:HG2	1:D:447:VAL:HG12	1.93	0.51
1:D:390:LEU:HD13	1:D:411:HIS:CD2	2.46	0.51
1:D:1855:TYR:OH	1:D:1934:ASP:N	2.43	0.51
1:D:2089:THR:HB	1:D:2095:LEU:HD11	1.93	0.51
1:A:2199:VAL:HG13	1:B:1707:ALA:HA	1.91	0.51
1:B:575:GLN:NE2	1:B:648:GLU:OE1	2.43	0.51
1:C:74:VAL:H	1:C:849:HIS:HE1	1.56	0.51
1:C:493:TRP:HE1	1:C:736:LYS:HE2	1.76	0.51
1:D:424:ILE:HG23	1:D:436:VAL:HG13	1.92	0.51
1:D:2558:LEU:HD22	1:D:2658:LEU:HD13	1.92	0.51
1:A:4:ILE:O	1:A:5:HIS:ND1	2.43	0.51
1:A:1444:ALA:HA	1:A:1499:LEU:HG	1.92	0.51
1:A:2184:MET:HG3	1:A:2185:LEU:HD22	1.91	0.51
1:A:2761:HIS:HB3	1:A:2775:PRO:HG3	1.92	0.51
1:B:27:GLU:HG2	1:B:31:LYS:HD2	1.92	0.51
1:B:1193:ILE:HB	1:B:1206:CYS:HB3	1.93	0.51
1:B:1333:LEU:HA	1:B:1339:LEU:HD21	1.92	0.51
1:B:1496:PRO:HA	1:B:1779:THR:HG21	1.93	0.51
1:C:4:ILE:O	1:C:5:HIS:ND1	2.44	0.51
1:D:1841:TRP:CZ3	1:D:1950:VAL:HG21	2.46	0.51
1:A:837:ASP:OD1	1:A:920:ARG:NH2	2.44	0.51
1:A:1475:LEU:HD22	1:A:1791:VAL:HG23	1.91	0.51
1:B:414:ALA:O	1:B:418:GLY:N	2.44	0.51
1:C:2602:PHE:HD2	1:C:2617:LEU:HB2	1.75	0.51
1:D:2766:ASN:O	1:D:2770:SER:CA	2.59	0.51
1:A:49:LYS:HD3	1:A:63:GLU:HG3	1.93	0.51
1:A:1859:LEU:HG	1:B:1519:LEU:HD23	1.92	0.51
1:A:2605:ASP:HA	1:A:2614:GLN:HA	1.92	0.51
1:B:473:ILE:HA	1:B:487:LEU:HD13	1.93	0.51
1:B:822:MET:HE3	1:B:830:ILE:HD12	1.93	0.51
1:B:1220:ASP:OD1	1:B:1222:LYS:NZ	2.33	0.51
1:C:433:ARG:NE	1:C:483:THR:OG1	2.39	0.51
1:D:745:GLU:HG2	1:D:746:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1290:HIS:HE1	1:D:1322:PRO:HG2	1.76	0.51
1:D:2026:SER:OG	1:D:2556:LYS:NZ	2.39	0.51
1:D:2700:SER:HB3	1:D:2756:PRO:HG3	1.93	0.51
1:A:70:ILE:HD13	1:A:360:LEU:HA	1.93	0.51
1:A:2534:ARG:NH1	1:A:2660:ASP:OD2	2.44	0.51
1:A:2781:GLN:HA	1:A:2784:LYS:HZ3	1.74	0.51
1:B:549:PHE:HA	1:B:558:VAL:HA	1.93	0.51
1:B:1444:ALA:HA	1:B:1786:ARG:HH22	1.76	0.51
1:C:389:GLU:HB2	1:C:391:TYR:CE2	2.46	0.51
1:C:514:LYS:HA	1:C:537:ARG:HH12	1.75	0.51
1:C:1340:LYS:NZ	1:C:1420:GLU:OE2	2.44	0.51
1:D:1868:PRO:HA	1:D:1873:HIS:CE1	2.45	0.51
1:D:2074:LEU:HD13	1:D:2086:MET:HA	1.92	0.51
1:A:1410:GLN:OE1	1:A:1818:LYS:NZ	2.44	0.50
1:A:1916:ASP:OD2	1:B:1492:ARG:NH2	2.40	0.50
1:B:499:PHE:HB3	1:B:654:ARG:CZ	2.41	0.50
1:B:679:ALA:HA	1:B:709:ARG:O	2.11	0.50
1:C:673:VAL:HG22	1:C:678:VAL:HG12	1.93	0.50
1:D:361:GLN:OE1	1:D:361:GLN:N	2.42	0.50
1:D:930:CYS:HA	1:D:1082:LYS:HD2	1.93	0.50
1:D:2165:PRO:HB2	1:D:2167:THR:HG22	1.92	0.50
1:D:2721:MET:HE1	1:D:2729:LEU:HB2	1.93	0.50
1:A:1276:LEU:O	1:A:1280:VAL:HG23	2.11	0.50
1:A:2279:VAL:HG11	1:A:2295:PHE:HB2	1.94	0.50
1:B:390:LEU:HD13	1:B:411:HIS:CD2	2.47	0.50
1:B:500:SER:OG	1:B:654:ARG:NH2	2.42	0.50
1:C:912:ILE:HG23	1:C:1105:LEU:HD21	1.93	0.50
1:C:1201:LEU:HG	1:C:1237:LYS:HD2	1.93	0.50
1:D:379:SER:OG	1:D:380:GLU:OE1	2.17	0.50
1:D:854:LEU:HD12	1:D:855:PRO:HD2	1.92	0.50
1:A:2290:GLY:H	1:A:2768:CYS:HA	1.76	0.50
1:B:533:GLN:OE1	1:B:669:LYS:N	2.44	0.50
1:B:2607:CYS:O	1:B:2612:GLY:N	2.42	0.50
1:C:57:HIS:HD2	1:C:69:ARG:HH21	1.58	0.50
1:C:1106:LEU:HD22	1:C:1132:ILE:HD11	1.93	0.50
1:D:762:THR:HG23	1:D:765:TRP:HB3	1.92	0.50
1:D:1712:ARG:HA	1:D:1715:GLN:HG2	1.93	0.50
1:A:1225:ARG:H	1:A:1225:ARG:HD3	1.77	0.50
1:A:1716:TRP:CZ2	1:B:1856:GLY:HA3	2.45	0.50
1:B:2235:GLN:NE2	1:B:2236:GLN:OE1	2.44	0.50
1:D:2053:GLN:HB2	1:D:2056:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:TYR:OH	1:A:755:GLY:O	2.29	0.50
1:B:2097:VAL:HG13	1:B:2101:LYS:HD2	1.92	0.50
1:C:1711:PRO:O	1:C:1715:GLN:HG2	2.11	0.50
1:C:1928:HIS:NE2	1:D:1480:GLU:OE2	2.45	0.50
1:D:2050:LEU:HD22	1:D:2066:LEU:HG	1.93	0.50
1:D:2604:ILE:HG21	1:D:2638:TYR:HE2	1.76	0.50
1:A:487:LEU:HB2	1:A:490:SER:HB2	1.94	0.50
1:B:499:PHE:CD1	1:B:654:ARG:HD2	2.47	0.50
1:C:18:LEU:HD21	1:C:811:ILE:HD11	1.93	0.50
1:C:2572:ASP:N	1:C:2572:ASP:OD1	2.43	0.50
1:D:680:VAL:O	1:D:708:CYS:HA	2.12	0.50
1:D:1276:LEU:O	1:D:1280:VAL:HG23	2.11	0.50
1:A:52:VAL:HG22	1:A:374:ILE:HD12	1.94	0.50
1:A:2238:ARG:NH2	1:A:2262:HIS:O	2.44	0.50
1:A:2607:CYS:O	1:A:2612:GLY:N	2.43	0.50
1:A:2729:LEU:HD13	1:A:2787:LEU:HD21	1.94	0.50
1:C:487:LEU:HB2	1:C:490:SER:HB2	1.93	0.50
1:C:514:LYS:HA	1:C:537:ARG:HH22	1.77	0.50
1:C:1279:LEU:HB3	1:C:1329:LEU:HD13	1.93	0.50
1:A:1164:ASN:OD1	1:A:1164:ASN:N	2.44	0.50
1:A:2075:TYR:HB2	1:A:2086:MET:HE3	1.93	0.50
1:B:844:LEU:HD13	1:B:869:MET:HG2	1.93	0.50
1:D:493:TRP:O	1:D:736:LYS:HB3	2.12	0.50
1:A:654:ARG:H	1:A:654:ARG:HD3	1.77	0.50
1:A:1197:ARG:HH22	1:A:1202:LEU:HB2	1.76	0.50
1:B:1932:HIS:HD2	1:B:1937:PRO:HG3	1.77	0.50
1:C:1926:ARG:HA	1:D:1434:ARG:HH21	1.76	0.50
1:C:2016:THR:HA	1:C:2020:HIS:CD2	2.46	0.50
1:D:2232:LEU:O	1:D:2235:GLN:NE2	2.44	0.50
1:D:2545:LEU:HD21	1:D:2740:PRO:HA	1.94	0.50
1:A:560:VAL:HG22	1:A:575:GLN:HB2	1.93	0.49
1:A:2193:LEU:HD22	1:A:2215:LEU:HD21	1.92	0.49
1:B:2532:ILE:O	1:B:2535:ILE:HG13	2.11	0.49
1:C:501:GLN:HA	1:C:504:LYS:HE2	1.94	0.49
1:C:1334:GLN:HA	1:C:1404:THR:HG21	1.94	0.49
1:C:2042:VAL:HG23	1:C:2047:ALA:HB2	1.94	0.49
1:C:2184:MET:HG3	1:C:2185:LEU:HD22	1.94	0.49
1:D:17:GLN:O	1:D:21:ARG:HG2	2.12	0.49
1:D:2563:VAL:HG11	1:D:2644:LEU:HD11	1.94	0.49
1:A:445:THR:HB	1:A:494:TRP:HH2	1.76	0.49
1:A:710:LEU:HD21	1:C:679:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:PRO:HD2	1:A:1264:LEU:HD13	1.94	0.49
1:A:1514:PHE:HE1	1:B:1922:LEU:HD21	1.77	0.49
1:A:1841:TRP:O	1:A:1845:ILE:HG12	2.11	0.49
1:B:1082:LYS:O	1:B:1086:HIS:ND1	2.35	0.49
1:B:1095:SER:O	1:B:1099:GLN:NE2	2.45	0.49
1:C:821:PRO:HG3	1:C:836:LEU:HD21	1.94	0.49
1:C:886:GLU:OE1	1:C:889:ARG:NH2	2.45	0.49
1:C:1202:LEU:H	1:C:1205:LEU:HB2	1.77	0.49
1:C:2178:MET:SD	1:C:2178:MET:N	2.81	0.49
1:C:2504:LEU:O	1:C:2517:ARG:N	2.45	0.49
1:A:2055:HIS:O	1:A:2058:GLN:NE2	2.32	0.49
1:A:2518:PRO:HB3	1:A:2650:PRO:HG2	1.95	0.49
1:C:401:TYR:CE1	1:C:403:ASN:HB2	2.47	0.49
1:C:1215:CYS:HB2	1:C:1216:HIS:CD2	2.48	0.49
1:C:1276:LEU:O	1:C:1280:VAL:HG23	2.12	0.49
1:C:2240:LEU:HB2	1:C:2277:VAL:HG13	1.94	0.49
1:A:1202:LEU:HG	1:A:1203:GLU:HG2	1.93	0.49
1:A:1492:ARG:NH1	1:B:1916:ASP:OD1	2.32	0.49
1:C:57:HIS:HB2	1:C:395:TRP:CE3	2.47	0.49
1:C:1842:MET:HE3	1:C:1951:PHE:HD1	1.78	0.49
1:D:818:THR:OG1	1:D:838:LEU:O	2.28	0.49
1:B:26:SER:HB3	1:B:838:LEU:HG	1.95	0.49
1:B:536:LEU:HA	1:B:717:GLN:OE1	2.11	0.49
1:C:1922:LEU:HG	1:D:1513:LEU:HD21	1.95	0.49
1:C:2274:VAL:HG23	1:C:2542:GLN:HE22	1.78	0.49
1:D:563:GLU:HG2	1:D:573:ARG:HB2	1.94	0.49
1:D:1194:PHE:N	1:D:1207:CYS:O	2.40	0.49
1:A:672:LYS:HG3	1:C:706:GLN:HA	1.94	0.49
1:B:1464:PHE:HB3	1:B:1798:LEU:HD11	1.95	0.49
1:C:502:ARG:HA	1:C:505:MET:HE3	1.94	0.49
1:C:2195:LEU:HD22	1:D:1714:MET:HE2	1.95	0.49
1:C:2546:CYS:O	1:C:2680:ASN:HA	2.12	0.49
1:D:534:VAL:HA	1:D:719:VAL:H	1.77	0.49
1:D:2579:LEU:HD12	1:D:2635:VAL:HG13	1.93	0.49
1:A:7:VAL:HG12	1:A:867:ILE:HB	1.95	0.49
1:A:1370:TYR:OH	1:B:1854:ARG:HD2	2.12	0.49
1:B:456:SER:H	1:B:457:LYS:HZ2	1.60	0.49
1:B:1799:MET:HE1	1:B:2169:PHE:HE2	1.76	0.49
1:C:4:ILE:HG13	1:C:43:LEU:HD23	1.94	0.49
1:C:1705:ASN:HA	1:C:1720:ASN:HD21	1.78	0.49
1:D:1519:LEU:HD12	1:D:1520:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2267:CYS:SG	1:A:2268:ALA:N	2.85	0.49
1:A:2689:MET:HE3	1:A:2739:LEU:HD12	1.95	0.49
1:B:1437:VAL:HG11	1:B:1482:LEU:HD11	1.94	0.49
1:B:2228:GLU:HG3	1:B:2232:LEU:HD23	1.95	0.49
1:C:540:PRO:HG3	1:C:566:TRP:CH2	2.48	0.49
1:C:2247:ASP:OD2	1:C:2250:LEU:N	2.42	0.49
1:D:1201:LEU:HD21	1:D:1237:LYS:HG2	1.95	0.49
1:D:1469:PRO:HG3	1:D:1819:LEU:HD13	1.95	0.49
1:D:2601:ALA:HA	1:D:2626:VAL:H	1.78	0.49
1:A:573:ARG:HG2	1:A:650:GLN:HG2	1.93	0.49
1:A:573:ARG:NH1	1:A:648:GLU:OE2	2.46	0.49
1:A:2201:MET:HE1	1:A:2212:LEU:HB3	1.94	0.49
1:B:2517:ARG:HD3	1:B:2518:PRO:HD2	1.95	0.49
1:C:455:ALA:HA	1:C:458:LEU:HB2	1.94	0.49
1:D:1841:TRP:O	1:D:1845:ILE:HG12	2.13	0.49
1:D:2647:ALA:HB1	1:D:2651:LEU:HD23	1.95	0.49
1:A:1364:LEU:HD22	1:B:2069:ARG:HH11	1.77	0.49
1:B:425:VAL:HG13	1:B:426:LEU:HD13	1.95	0.49
1:B:505:MET:HE2	1:B:728:PRO:HG2	1.94	0.49
1:B:2766:ASN:O	1:B:2770:SER:HA	2.12	0.49
1:C:394:LYS:HB2	1:C:397:GLU:HG3	1.95	0.49
1:D:534:VAL:HG13	1:D:718:VAL:HA	1.94	0.49
1:D:549:PHE:HZ	1:D:551:ILE:HG23	1.76	0.49
1:D:1117:PHE:HZ	1:D:1258:LEU:HD11	1.78	0.49
1:D:1331:ARG:O	1:D:1331:ARG:NH1	2.37	0.49
1:D:1348:GLN:NE2	1:D:1372:ASN:O	2.36	0.49
1:D:1375:SER:OG	1:D:1427:ARG:NH2	2.32	0.49
1:D:70:ILE:HD13	1:D:360:LEU:HA	1.93	0.48
1:D:422:GLU:N	1:D:422:GLU:OE1	2.46	0.48
1:D:846:MET:HG2	1:D:867:ILE:HG23	1.94	0.48
1:D:1087:PHE:O	1:D:1090:LYS:HG2	2.12	0.48
1:D:1122:SER:HA	1:D:1172:VAL:HG11	1.95	0.48
1:A:2677:LEU:O	1:A:2741:ALA:HB2	2.13	0.48
1:B:663:LYS:HB3	1:B:727:VAL:HG23	1.94	0.48
1:B:1914:ARG:O	1:B:1918:LEU:HD23	2.12	0.48
1:B:2592:ASP:OD1	1:B:2592:ASP:N	2.46	0.48
1:C:17:GLN:O	1:C:21:ARG:HG2	2.14	0.48
1:C:1856:GLY:HA3	1:D:1716:TRP:CZ2	2.48	0.48
1:C:1941:VAL:HG11	1:C:2195:LEU:HG	1.94	0.48
1:C:2733:TRP:CD1	1:C:2734:THR:HG23	2.47	0.48
1:D:1091:LEU:O	1:D:1095:SER:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1388:ILE:HG12	1:D:1398:LEU:HD11	1.95	0.48
1:A:387:LYS:O	1:A:423:LYS:HA	2.13	0.48
1:A:2304:LEU:HD21	1:A:2548:ILE:HA	1.95	0.48
1:B:510:ARG:HA	1:B:510:ARG:HH11	1.78	0.48
1:C:32:TYR:HB3	1:C:34:LEU:HD23	1.95	0.48
1:C:384:VAL:HG13	1:C:424:ILE:HG13	1.93	0.48
1:C:1396:LEU:HD23	1:C:1396:LEU:H	1.77	0.48
1:D:2309:LEU:HD12	1:D:2310:PRO:HD2	1.95	0.48
1:D:2555:ILE:HA	1:D:2558:LEU:HB2	1.95	0.48
1:A:2240:LEU:HA	1:A:2262:HIS:CE1	2.48	0.48
1:B:534:VAL:HG21	1:B:716:LEU:HD13	1.96	0.48
1:C:529:THR:O	1:C:532:THR:OG1	2.27	0.48
1:C:1870:HIS:HD2	1:D:1519:LEU:HD21	1.78	0.48
1:D:394:LYS:HB2	1:D:397:GLU:OE1	2.14	0.48
1:D:2714:PHE:O	1:D:2717:ILE:HG13	2.13	0.48
1:A:539:ASN:N	1:A:540:PRO:HD3	2.29	0.48
1:A:2102:MET:HG2	1:A:2176:MET:SD	2.53	0.48
1:B:403:ASN:ND2	1:B:406:ASN:O	2.46	0.48
1:B:510:ARG:O	1:B:510:ARG:NH1	2.46	0.48
1:B:2605:ASP:OD1	1:B:2605:ASP:N	2.44	0.48
1:C:1828:GLN:HE22	1:C:2171:PRO:HB3	1.78	0.48
1:C:2083:LYS:O	1:C:2188:ARG:NH1	2.46	0.48
1:D:493:TRP:CZ2	1:D:736:LYS:HD2	2.48	0.48
1:D:874:GLN:HG2	1:D:914:HIS:CE1	2.48	0.48
1:D:1464:PHE:HB3	1:D:1798:LEU:HD11	1.96	0.48
1:D:2607:CYS:SG	1:D:2608:LYS:N	2.87	0.48
1:A:14:THR:N	1:A:17:GLN:HE22	2.09	0.48
1:A:1839:TRP:HZ3	1:A:1958:ILE:HD11	1.78	0.48
1:B:533:GLN:HA	1:B:668:GLY:C	2.38	0.48
1:B:1429:LEU:HA	1:B:1432:VAL:HG12	1.96	0.48
1:B:2297:THR:HA	1:B:2547:PRO:HG2	1.94	0.48
1:B:2529:PHE:CD2	1:B:2650:PRO:HB3	2.49	0.48
1:C:2557:VAL:HG21	1:C:2651:LEU:HD13	1.96	0.48
1:A:1207:CYS:HB3	1:A:1234:CYS:HB2	1.95	0.48
1:A:2606:LEU:N	1:A:2613:GLY:O	2.44	0.48
1:A:2714:PHE:O	1:A:2717:ILE:HG13	2.13	0.48
1:B:732:GLN:NE2	1:B:734:THR:O	2.45	0.48
1:C:18:LEU:O	1:C:22:LEU:HG	2.13	0.48
1:C:1138:LYS:O	1:C:1141:LYS:NZ	2.46	0.48
1:C:1174:CYS:HA	1:C:1324:PHE:HE2	1.79	0.48
1:C:2279:VAL:H	1:C:2291:VAL:HG11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1334:GLN:HA	1:D:1404:THR:HG21	1.95	0.48
1:B:510:ARG:NH2	1:B:537:ARG:O	2.38	0.48
1:B:1395:ILE:HD13	1:B:1459:LYS:HE3	1.96	0.48
1:B:2074:LEU:HD23	1:B:2086:MET:HA	1.95	0.48
1:C:747:LEU:HD12	1:C:799:VAL:HG21	1.94	0.48
1:C:1193:ILE:HG23	1:C:1206:CYS:HB2	1.96	0.48
1:C:2088:VAL:HG12	1:D:1373:GLN:CD	2.38	0.48
1:A:2020:HIS:CD2	1:A:2022:PHE:H	2.31	0.48
1:C:1711:PRO:HA	1:D:2060:ASN:HD21	1.78	0.48
1:D:1255:LEU:HD11	1:D:1324:PHE:CE1	2.49	0.48
1:D:1272:GLY:O	1:D:1379:ARG:NH1	2.47	0.48
1:D:1423:ALA:O	1:D:1426:MET:HG2	2.13	0.48
1:A:394:LYS:N	1:A:397:GLU:OE2	2.46	0.48
1:A:2277:VAL:HG23	1:A:2542:GLN:HG3	1.96	0.48
1:B:39:PRO:HG2	1:B:40:LEU:HD12	1.95	0.48
1:C:773:LEU:H	1:C:773:LEU:HD22	1.79	0.48
1:C:1352:ASP:O	1:C:1355:SER:OG	2.27	0.48
1:D:6:PHE:HA	1:D:867:ILE:O	2.14	0.48
1:D:2513:PHE:HD2	1:D:2551:ASN:HA	1.78	0.48
1:A:823:ALA:HB3	1:A:831:ARG:HB3	1.95	0.47
1:A:1856:GLY:HA2	1:A:1936:LEU:HD12	1.96	0.47
1:B:757:HIS:HB3	1:B:768:TYR:HE1	1.79	0.47
1:B:1387:LEU:HD11	1:B:1397:LEU:HB3	1.96	0.47
1:B:1469:PRO:HG3	1:B:1819:LEU:HD13	1.95	0.47
1:B:1475:LEU:HA	1:B:1478:VAL:HG12	1.95	0.47
1:B:1846:MET:HE2	1:B:1846:MET:HA	1.96	0.47
1:B:2775:PRO:HD2	1:B:2777:TYR:HE1	1.78	0.47
1:C:513:ASN:HD21	1:C:726:LYS:HA	1.79	0.47
1:C:2520:LYS:N	1:C:2525:ARG:HH12	2.10	0.47
1:D:1179:CYS:SG	1:D:1180:SER:N	2.87	0.47
1:A:69:ARG:HD2	1:A:395:TRP:CZ3	2.49	0.47
1:A:491:LEU:HB2	1:A:738:LEU:HB2	1.95	0.47
1:A:670:VAL:HG13	1:A:680:VAL:HG22	1.95	0.47
1:A:923:LEU:HD23	1:A:1105:LEU:HB3	1.97	0.47
1:A:1713:SER:OG	1:B:2062:ARG:NH1	2.47	0.47
1:A:2531:ASN:HA	1:A:2534:ARG:HG2	1.96	0.47
1:B:17:GLN:OE1	1:B:17:GLN:N	2.40	0.47
1:B:532:THR:O	1:B:670:VAL:HG23	2.14	0.47
1:B:2507:GLN:NE2	1:B:2512:GLY:H	2.12	0.47
1:C:52:VAL:HG22	1:C:374:ILE:HD12	1.95	0.47
1:C:549:PHE:CE2	1:C:657:VAL:HG11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:CYS:N	1:C:776:GLY:O	2.46	0.47
1:C:818:THR:HG21	1:C:917:ASP:HB3	1.95	0.47
1:C:1114:MET:HB3	1:C:1118:MET:HB2	1.95	0.47
1:C:2733:TRP:HD1	1:C:2734:THR:HG23	1.80	0.47
1:D:4:ILE:HG21	1:D:43:LEU:HD23	1.96	0.47
1:D:895:LEU:HD11	1:D:908:LEU:HD13	1.96	0.47
1:D:1841:TRP:HZ3	1:D:1950:VAL:HG21	1.78	0.47
1:D:1927:SER:O	1:D:2091:ASP:HB3	2.13	0.47
1:A:6:PHE:CZ	1:A:356:LEU:HD11	2.49	0.47
1:A:2309:LEU:HG	1:A:2501:ASN:HA	1.97	0.47
1:B:547:VAL:O	1:B:659:VAL:HG12	2.14	0.47
1:B:717:GLN:OE1	1:B:717:GLN:N	2.47	0.47
1:B:834:ASP:OD1	1:B:834:ASP:N	2.47	0.47
1:B:1467:LEU:HD13	1:B:1817:VAL:HG21	1.96	0.47
1:C:931:PHE:CZ	1:C:1123:GLY:HA3	2.50	0.47
1:C:2718:VAL:HA	1:C:2721:MET:SD	2.54	0.47
1:D:536:LEU:O	1:D:539:ASN:HB2	2.15	0.47
1:D:561:LEU:HD22	1:D:563:GLU:H	1.79	0.47
1:D:2610:GLU:OE1	1:D:2610:GLU:N	2.43	0.47
1:A:75:GLN:OE1	1:A:75:GLN:N	2.47	0.47
1:A:813:ARG:HH12	1:A:842:SER:C	2.22	0.47
1:A:1276:LEU:HD13	1:A:1342:MET:HB2	1.96	0.47
1:A:1498:THR:OG1	1:A:1499:LEU:N	2.47	0.47
1:B:2529:PHE:HD2	1:B:2650:PRO:HB3	1.79	0.47
1:C:551:ILE:HA	1:C:556:PRO:HA	1.96	0.47
1:C:1931:GLU:OE1	1:D:1434:ARG:NH2	2.47	0.47
1:C:2044:LEU:HB2	1:C:2576:TYR:CE2	2.49	0.47
1:C:2529:PHE:HA	1:C:2532:ILE:HG22	1.95	0.47
1:D:2605:ASP:OD1	1:D:2605:ASP:N	2.43	0.47
1:A:2765:ALA:HB2	1:A:2772:LEU:HD23	1.95	0.47
1:B:401:TYR:CZ	1:B:412:PRO:HD3	2.50	0.47
1:B:1828:GLN:HB2	1:B:2169:PHE:HZ	1.80	0.47
1:B:2256:MET:HE1	1:B:2312:LEU:HG	1.96	0.47
1:C:540:PRO:HB3	1:C:564:SER:HB3	1.97	0.47
1:D:702:SER:HA	1:D:705:LEU:HD21	1.97	0.47
1:A:1177:ASP:HA	1:A:1251:ARG:HH12	1.80	0.47
1:A:2087:GLU:OE2	1:A:2188:ARG:NH1	2.47	0.47
1:A:2623:ASN:OD1	1:A:2623:ASN:N	2.42	0.47
1:A:2698:ASP:OD1	1:A:2698:ASP:N	2.48	0.47
1:B:567:ASN:HB3	1:B:570:ASP:HB3	1.97	0.47
1:B:1286:GLN:HG3	1:B:1290:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2725:GLU:OE1	1:B:2725:GLU:N	2.43	0.47
1:B:2786:LYS:HD2	1:B:2789:LEU:HD21	1.97	0.47
1:C:667:VAL:HG13	1:C:683:PRO:HD2	1.95	0.47
1:C:768:TYR:HB2	1:C:784:PHE:CZ	2.50	0.47
1:C:1234:CYS:SG	1:C:1240:CYS:HB2	2.54	0.47
1:D:1092:LEU:O	1:D:1095:SER:OG	2.31	0.47
1:D:2777:TYR:HB2	1:D:2783:LEU:HD22	1.96	0.47
1:A:762:THR:HG23	1:A:765:TRP:HB3	1.97	0.47
1:A:813:ARG:NH1	1:A:841:ILE:O	2.48	0.47
1:A:2504:LEU:HD13	1:A:2532:ILE:HD11	1.96	0.47
1:A:2530:ARG:O	1:A:2534:ARG:HG2	2.14	0.47
1:B:23:ARG:NH1	1:B:835:TRP:O	2.47	0.47
1:B:571:SER:HA	1:B:653:LEU:HB2	1.97	0.47
1:B:1126:TYR:HB2	1:B:1127:PRO:HD3	1.97	0.47
1:B:1962:ASN:O	1:B:1965:THR:OG1	2.25	0.47
1:B:2097:VAL:O	1:B:2101:LYS:HB2	2.14	0.47
1:C:1488:MET:HG3	1:D:1841:TRP:CD1	2.50	0.47
1:C:1845:ILE:HD12	1:D:1490:ILE:HD12	1.96	0.47
1:D:895:LEU:HG	1:D:907:MET:HE1	1.95	0.47
1:D:1089:LEU:HD23	1:D:1092:LEU:HD23	1.95	0.47
1:A:1839:TRP:CZ3	1:A:1958:ILE:HD11	2.50	0.47
1:C:818:THR:HG22	1:C:819:ILE:H	1.79	0.47
1:C:1097:VAL:HG13	1:C:1098:LEU:HG	1.96	0.47
1:C:1343:ILE:HG21	1:C:1424:VAL:HG13	1.97	0.47
1:C:1821:TYR:OH	1:C:2168:SER:O	2.22	0.47
1:A:1952:GLN:HE22	1:A:2207:GLU:HB2	1.79	0.47
1:A:2279:VAL:HB	1:A:2291:VAL:HG22	1.97	0.47
1:A:2766:ASN:HB2	1:A:2769:ILE:HG12	1.96	0.47
1:B:463:GLN:HB3	1:B:465:TYR:HE1	1.78	0.47
1:C:827:MET:HB2	1:C:1197:ARG:NH1	2.27	0.47
1:C:1173:LEU:O	1:C:1251:ARG:NH2	2.37	0.47
1:C:2095:LEU:HD13	1:C:2095:LEU:HA	1.67	0.47
1:A:22:LEU:O	1:A:25:VAL:HG12	2.14	0.47
1:B:372:ILE:N	1:B:384:VAL:O	2.40	0.47
1:B:487:LEU:N	1:B:490:SER:O	2.41	0.47
1:B:2217:GLY:O	1:B:2221:LYS:NZ	2.42	0.47
1:C:4:ILE:HG12	1:C:44:GLU:HG2	1.95	0.47
1:C:1201:LEU:HD21	1:C:1234:CYS:HA	1.97	0.47
1:C:1280:VAL:HG22	1:C:1329:LEU:HD21	1.95	0.47
1:D:2044:LEU:HB2	1:D:2576:TYR:CE2	2.50	0.47
1:A:38:PRO:N	1:A:39:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:SER:OG	1:A:486:GLN:HB3	2.15	0.46
1:A:1378:ILE:HD12	1:A:1518:PRO:HB3	1.98	0.46
1:A:1832:GLU:O	1:A:1836:ILE:HG12	2.14	0.46
1:A:2178:MET:SD	1:A:2178:MET:N	2.88	0.46
1:A:2671:THR:OG1	1:A:2674:ASP:OD2	2.32	0.46
1:B:2718:VAL:O	1:B:2721:MET:HG2	2.16	0.46
1:C:1171:TYR:OH	1:C:1271:ARG:NH2	2.32	0.46
1:D:805:GLY:O	1:D:808:SER:OG	2.33	0.46
1:D:1376:GLY:O	1:D:1427:ARG:NH1	2.49	0.46
1:D:1402:LEU:HD11	1:D:1463:VAL:HG22	1.96	0.46
1:A:371:PHE:HA	1:A:384:VAL:O	2.16	0.46
1:A:924:HIS:CE1	1:A:1110:ASP:HB3	2.49	0.46
1:B:821:PRO:HD2	1:B:835:TRP:CZ3	2.49	0.46
1:B:1841:TRP:CZ3	1:B:1950:VAL:HG11	2.50	0.46
1:B:2091:ASP:OD1	1:B:2092:ARG:N	2.48	0.46
1:B:2311:ASN:OD1	1:B:2312:LEU:N	2.47	0.46
1:C:12:PRO:HD2	1:C:861:LYS:HD3	1.97	0.46
1:C:1842:MET:SD	1:C:1951:PHE:HA	2.55	0.46
1:D:18:LEU:HD11	1:D:811:ILE:HD11	1.97	0.46
1:D:1317:HIS:O	1:D:1317:HIS:ND1	2.49	0.46
1:D:2044:LEU:HB2	1:D:2576:TYR:HE2	1.80	0.46
1:D:2279:VAL:HG21	1:D:2295:PHE:HB3	1.96	0.46
1:D:2572:ASP:OD1	1:D:2572:ASP:N	2.47	0.46
1:A:397:GLU:OE1	1:A:399:GLU:N	2.24	0.46
1:A:530:VAL:HG13	1:A:673:VAL:HB	1.96	0.46
1:B:1431:SER:HA	1:B:1434:ARG:NH1	2.31	0.46
1:B:1705:ASN:HD22	1:B:1705:ASN:H	1.63	0.46
1:C:411:HIS:O	1:C:413:ARG:N	2.47	0.46
1:D:23:ARG:HB2	1:D:836:LEU:HD22	1.96	0.46
1:D:575:GLN:OE1	1:D:647:ASN:ND2	2.49	0.46
1:D:825:ASP:OD1	1:D:829:GLY:N	2.49	0.46
1:A:482:TYR:OH	1:A:752:ASP:O	2.28	0.46
1:A:2240:LEU:HD21	1:A:2277:VAL:HG22	1.98	0.46
1:C:818:THR:HG23	1:C:839:PRO:O	2.15	0.46
1:C:2222:GLU:OE1	1:C:2226:ARG:NH1	2.48	0.46
1:D:2507:GLN:OE1	1:D:2511:ARG:HA	2.16	0.46
1:A:1385:HIS:CD2	1:A:1514:PHE:HD2	2.33	0.46
1:A:2093:ASN:HB2	1:B:1484:VAL:HG21	1.97	0.46
1:B:2054:PRO:HB2	1:B:2513:PHE:CZ	2.50	0.46
1:C:61:LEU:HD22	1:C:374:ILE:HG23	1.98	0.46
1:C:2197:GLY:HA2	1:C:2212:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2539:CYS:SG	1:C:2540:LEU:N	2.89	0.46
1:D:76:PRO:HB3	1:D:860:ILE:HD13	1.97	0.46
1:D:536:LEU:HD21	1:D:538:ASN:HB3	1.98	0.46
1:D:1388:ILE:HD11	1:D:1432:VAL:HG23	1.97	0.46
1:A:754:LYS:H	1:A:754:LYS:HD2	1.81	0.46
1:A:1195:GLU:O	1:A:1221:CYS:HA	2.16	0.46
1:A:1340:LYS:HZ1	1:A:1420:GLU:HB3	1.81	0.46
1:A:1929:ASN:O	1:A:1929:ASN:ND2	2.44	0.46
1:B:662:VAL:HA	1:B:726:LYS:HB2	1.96	0.46
1:B:1958:ILE:O	1:B:1961:MET:HG3	2.15	0.46
1:C:509:ALA:HA	1:C:512:LYS:HG2	1.96	0.46
1:C:561:LEU:H	1:C:561:LEU:HD23	1.79	0.46
1:C:2601:ALA:HA	1:C:2625:PRO:HA	1.96	0.46
1:C:2708:LEU:HD13	1:C:2711:LYS:HD2	1.97	0.46
1:D:575:GLN:HA	1:D:647:ASN:ND2	2.31	0.46
1:D:794:GLN:HE22	1:D:913:SER:HB3	1.80	0.46
1:D:2191:LEU:O	1:D:2194:GLU:HG3	2.16	0.46
1:A:36:SER:OG	1:A:44:GLU:OE2	2.22	0.46
1:A:806:GLN:N	1:A:806:GLN:OE1	2.49	0.46
1:A:2299:ILE:HG21	1:A:2535:ILE:HD13	1.97	0.46
1:A:2556:LYS:HG2	1:A:2672:ALA:HB2	1.97	0.46
1:A:2583:ILE:HG23	1:A:2632:TYR:HE1	1.81	0.46
1:B:479:CYS:SG	1:B:480:ALA:N	2.89	0.46
1:B:861:LYS:H	1:B:861:LYS:HD2	1.81	0.46
1:B:1429:LEU:HB2	1:B:1474:GLU:HG3	1.98	0.46
1:D:413:ARG:HE	1:D:459:GLU:HG2	1.81	0.46
1:D:1472:VAL:HG21	1:D:1827:LEU:HD21	1.97	0.46
1:A:5:HIS:O	1:A:869:MET:HG2	2.16	0.46
1:A:673:VAL:HG22	1:A:678:VAL:HG12	1.98	0.46
1:A:741:PRO:HB2	1:A:744:THR:HG21	1.98	0.46
1:A:1468:LEU:HD13	1:A:1805:TYR:HE2	1.79	0.46
1:D:1130:ILE:HG12	1:D:1254:LEU:HD13	1.97	0.46
1:D:2203:ASP:OD1	1:D:2204:VAL:N	2.48	0.46
1:A:540:PRO:HD2	1:A:566:TRP:CH2	2.50	0.46
1:A:2027:ASP:HA	1:A:2030:THR:HG22	1.98	0.46
1:B:1869:ASN:OD1	1:B:1869:ASN:N	2.48	0.46
1:A:1381:ASP:OD2	1:B:1926:ARG:NH2	2.47	0.46
1:A:2060:ASN:OD1	1:A:2060:ASN:N	2.48	0.46
1:B:10:PRO:HB3	1:B:861:LYS:HG2	1.97	0.46
1:B:770:ILE:O	1:B:779:GLU:N	2.49	0.46
1:C:17:GLN:OE1	1:C:17:GLN:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1109:LYS:HB3	1:C:1114:MET:N	2.31	0.46
1:D:1828:GLN:O	1:D:1831:VAL:HG12	2.15	0.46
1:D:2564:ASN:HD21	1:D:2566:HIS:HB2	1.80	0.46
1:D:2780:LYS:HE2	1:D:2781:GLN:HE22	1.81	0.46
1:A:790:ALA:HB3	1:A:1111:ALA:HA	1.99	0.45
1:A:1188:HIS:HB3	1:A:1229:THR:OG1	2.16	0.45
1:A:1422:ILE:O	1:A:1426:MET:HG2	2.16	0.45
1:A:2561:ARG:HG2	1:A:2562:LYS:H	1.81	0.45
1:B:1177:ASP:H	1:B:1251:ARG:NH2	2.14	0.45
1:B:1262:THR:OG1	1:B:1263:ASN:N	2.49	0.45
1:B:2723:MET:HA	1:B:2726:ARG:HD2	1.98	0.45
1:C:413:ARG:HH11	1:C:449:GLU:HA	1.81	0.45
1:C:912:ILE:HG13	1:C:1101:TYR:CD1	2.52	0.45
1:C:1098:LEU:HA	1:C:1101:TYR:CD2	2.51	0.45
1:C:1864:ASP:HB3	1:D:1520:PRO:HG2	1.97	0.45
1:C:2507:GLN:NE2	1:C:2512:GLY:H	2.13	0.45
1:C:2698:ASP:OD1	1:C:2698:ASP:N	2.46	0.45
1:D:77:ASP:OD1	1:D:77:ASP:N	2.46	0.45
1:D:766:VAL:HG11	1:D:791:PHE:CD2	2.51	0.45
1:A:1718:VAL:HG13	1:B:1942:CYS:HB3	1.98	0.45
1:B:1947:VAL:HA	1:B:1950:VAL:HG12	1.98	0.45
1:B:2699:GLU:HG3	1:B:2756:PRO:HD3	1.97	0.45
1:C:38:PRO:N	1:C:39:PRO:HD2	2.30	0.45
1:C:841:ILE:HG22	1:C:871:VAL:HG12	1.98	0.45
1:D:705:LEU:HD23	1:D:705:LEU:H	1.81	0.45
1:A:502:ARG:NH1	1:A:730:CYS:O	2.50	0.45
1:A:2095:LEU:HD13	1:A:2095:LEU:HA	1.76	0.45
1:B:74:VAL:HG12	1:B:849:HIS:CD2	2.51	0.45
1:B:414:ALA:HA	1:B:417:LEU:HB2	1.99	0.45
1:B:1807:HIS:O	1:B:1811:SER:OG	2.27	0.45
1:C:2644:LEU:O	1:C:2648:GLU:N	2.50	0.45
1:D:423:LYS:HB3	1:D:439:GLU:HB3	1.99	0.45
1:A:445:THR:O	1:A:459:GLU:HG2	2.17	0.45
1:A:1493:PRO:HD2	1:B:1940:ASP:OD2	2.16	0.45
1:B:72:PHE:HE2	1:B:866:VAL:HG21	1.81	0.45
1:B:761:LYS:HA	1:B:765:TRP:O	2.16	0.45
1:B:1714:MET:HE3	1:B:1714:MET:HB2	1.90	0.45
1:B:2689:MET:O	1:B:2692:SER:OG	2.33	0.45
1:D:563:GLU:HB3	1:D:573:ARG:HD3	1.98	0.45
1:D:1235:TRP:CD2	1:D:1315:PRO:HD3	2.52	0.45
1:D:1339:LEU:HD22	1:D:1339:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2279:VAL:HB	1:D:2291:VAL:HG22	1.97	0.45
1:D:2649:GLN:CD	1:D:2649:GLN:H	2.23	0.45
1:A:816:ASN:HD21	1:A:915:ARG:HG3	1.82	0.45
1:A:834:ASP:OD2	1:A:1239:LYS:NZ	2.49	0.45
1:A:1499:LEU:HD21	1:A:1786:ARG:HH22	1.82	0.45
1:C:738:LEU:HD13	1:C:756:VAL:HG11	1.98	0.45
1:C:1711:PRO:HD3	1:D:2198:ARG:HG3	1.99	0.45
1:C:2531:ASN:O	1:C:2534:ARG:HG2	2.16	0.45
1:D:548:ALA:HB1	1:D:657:VAL:H	1.82	0.45
1:D:1333:LEU:HD22	1:D:1401:LEU:HD13	1.97	0.45
1:D:2534:ARG:HG2	1:D:2661:VAL:HG11	1.97	0.45
1:A:494:TRP:HB3	1:A:735:PRO:HA	1.99	0.45
1:B:40:LEU:HD23	1:B:43:LEU:HD23	1.99	0.45
1:B:2687:VAL:O	1:B:2691:ILE:HG12	2.16	0.45
1:C:1841:TRP:O	1:C:1845:ILE:HG12	2.16	0.45
1:D:549:PHE:CZ	1:D:551:ILE:HG23	2.50	0.45
1:D:1244:ILE:HD13	1:D:1244:ILE:HA	1.77	0.45
1:A:1438:ILE:HD12	1:B:1918:LEU:HD13	1.99	0.45
1:B:460:HIS:ND1	1:B:465:TYR:OH	2.50	0.45
1:B:535:CYS:SG	1:B:665:VAL:HB	2.56	0.45
1:B:1335:ASP:OD1	1:B:1337:ASN:N	2.49	0.45
1:C:495:GLY:O	1:C:732:GLN:HB3	2.16	0.45
1:C:929:VAL:HG23	1:C:1085:ALA:HB1	1.98	0.45
1:C:1237:LYS:HE2	1:C:1237:LYS:HB2	1.81	0.45
1:C:2247:ASP:OD1	1:C:2251:LEU:N	2.49	0.45
1:D:834:ASP:OD1	1:D:834:ASP:N	2.40	0.45
1:A:802:PHE:HB2	1:A:811:ILE:HB	1.99	0.45
1:A:935:ASN:ND2	1:A:1244:ILE:HA	2.31	0.45
1:B:1360:ILE:HD12	1:B:1368:GLN:HA	1.99	0.45
1:B:1839:TRP:CE3	1:B:1954:LEU:HD13	2.51	0.45
1:C:540:PRO:HG2	1:C:543:HIS:NE2	2.32	0.45
1:C:1370:TYR:CD1	1:D:2088:VAL:HG12	2.52	0.45
1:C:1519:LEU:HD21	1:D:1870:HIS:HD2	1.81	0.45
1:C:2740:PRO:HB3	1:C:2745:GLY:HA3	1.99	0.45
1:D:393:TRP:HB3	1:D:400:PRO:HA	1.98	0.45
1:D:510:ARG:HA	1:D:514:LYS:H	1.82	0.45
1:D:671:LEU:HB2	1:D:679:ALA:O	2.17	0.45
1:D:2086:MET:HG3	1:D:2088:VAL:HG22	1.99	0.45
1:D:2757:PRO:HB3	1:D:2776:LEU:O	2.17	0.45
1:A:547:VAL:HG21	1:A:577:ARG:HE	1.82	0.45
1:A:924:HIS:CD2	1:A:1116:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2219:GLU:O	1:A:2222:GLU:HG3	2.16	0.45
1:B:546:ALA:HB3	1:B:561:LEU:HB3	1.98	0.45
1:B:1793:ARG:HG3	1:B:1956:TYR:CE2	2.51	0.45
1:B:1806:ASN:OD1	1:B:1806:ASN:N	2.49	0.45
1:C:1429:LEU:HD13	1:C:1471:ALA:HA	1.99	0.45
1:A:772:ASP:HB2	1:A:779:GLU:HB2	1.99	0.45
1:B:673:VAL:HG22	1:B:678:VAL:HG12	1.99	0.45
1:B:1402:LEU:HD22	1:B:1467:LEU:HD23	1.98	0.45
1:B:2083:LYS:O	1:B:2188:ARG:NH1	2.50	0.45
1:C:2025:ARG:NH1	1:C:2067:PHE:O	2.48	0.45
1:D:536:LEU:HB3	1:D:539:ASN:CG	2.42	0.45
1:D:542:TYR:HE2	1:D:546:ALA:H	1.64	0.45
1:D:1098:LEU:HA	1:D:1101:TYR:HD2	1.81	0.45
1:D:2790:ALA:O	1:D:2793:THR:OG1	2.33	0.45
1:A:424:ILE:HA	1:A:438:THR:HA	1.99	0.44
1:A:935:ASN:HD21	1:A:1244:ILE:HA	1.83	0.44
1:A:1507:MET:O	1:A:1511:GLU:HG2	2.16	0.44
1:A:2500:ASP:HB2	1:A:2520:LYS:HD2	1.97	0.44
1:B:22:LEU:HB3	1:B:836:LEU:HD13	1.97	0.44
1:C:2504:LEU:HB3	1:C:2529:PHE:HE1	1.82	0.44
1:C:2583:ILE:HG23	1:C:2632:TYR:CE1	2.51	0.44
1:D:549:PHE:CE1	1:D:556:PRO:HB2	2.52	0.44
1:D:1201:LEU:HD22	1:D:1205:LEU:HB3	1.99	0.44
1:D:2029:MET:HE1	1:D:2566:HIS:HB2	1.99	0.44
1:A:1514:PHE:CE1	1:B:1922:LEU:HD11	2.53	0.44
1:A:2189:TRP:HB3	1:A:2192:SER:OG	2.16	0.44
1:A:2555:ILE:HD11	1:A:2675:PHE:HB3	1.99	0.44
1:B:417:LEU:HD11	1:B:446:TRP:HB3	2.00	0.44
1:B:447:VAL:HG21	1:B:454:VAL:HG13	1.99	0.44
1:B:841:ILE:HA	1:B:871:VAL:HG12	1.98	0.44
1:B:1197:ARG:NH2	1:B:1198:THR:OG1	2.50	0.44
1:B:1473:GLU:O	1:B:1477:ASN:ND2	2.51	0.44
1:B:1475:LEU:HD22	1:B:1791:VAL:HG23	1.99	0.44
1:C:1464:PHE:HB3	1:C:1798:LEU:HD11	1.99	0.44
1:C:1697:ARG:HB3	1:D:2691:ILE:HG23	1.98	0.44
1:C:2085:LEU:O	1:C:2188:ARG:NH1	2.47	0.44
1:C:2568:PHE:CZ	1:C:2642:ARG:HD3	2.50	0.44
1:A:2752:ILE:HG12	1:A:2772:LEU:HB2	2.00	0.44
1:B:482:TYR:OH	1:B:752:ASP:O	2.21	0.44
1:B:2671:THR:HG23	1:B:2674:ASP:H	1.82	0.44
1:C:924:HIS:ND1	1:C:1110:ASP:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:HIS:CD2	1:D:414:ALA:HB2	2.51	0.44
1:A:37:HIS:HB3	1:A:39:PRO:HD2	2.00	0.44
1:A:1334:GLN:HA	1:A:1404:THR:HG21	2.00	0.44
1:A:1961:MET:HG3	1:A:2171:PRO:HB2	2.00	0.44
1:A:2044:LEU:HB2	1:A:2576:TYR:CD2	2.53	0.44
1:A:2094:CYS:HA	1:A:2097:VAL:HG12	1.99	0.44
1:A:2577:GLU:OE1	1:A:2580:ARG:NH1	2.50	0.44
1:A:2763:PRO:HG3	1:A:2775:PRO:HD2	1.98	0.44
1:B:38:PRO:HA	1:B:41:ASN:ND2	2.32	0.44
1:C:497:VAL:HG23	1:C:502:ARG:HG2	2.00	0.44
1:C:747:LEU:HD21	1:C:761:LYS:HB2	2.00	0.44
1:D:452:SER:HA	1:D:455:ALA:HB3	2.00	0.44
1:D:1078:SER:O	1:D:1082:LYS:HG2	2.17	0.44
1:D:1342:MET:HB3	1:D:1342:MET:HE2	1.77	0.44
1:D:1962:ASN:ND2	1:D:2180:ILE:O	2.48	0.44
1:A:1150:GLU:HA	1:A:1153:VAL:HG12	1.99	0.44
1:A:1922:LEU:HD11	1:B:1514:PHE:CE1	2.53	0.44
1:A:1934:ASP:HB2	1:B:1518:PRO:HB3	2.00	0.44
1:B:576:LEU:HD21	1:B:649:GLU:HB3	2.00	0.44
1:C:1408:GLU:OE1	1:C:1417:ARG:NH1	2.50	0.44
1:C:2598:MET:HG3	1:C:2599:ASP:N	2.32	0.44
1:D:12:PRO:HG3	1:D:861:LYS:HG2	2.00	0.44
1:D:397:GLU:HG2	1:D:399:GLU:H	1.81	0.44
1:D:423:LYS:HB2	1:D:423:LYS:HE3	1.76	0.44
1:D:747:LEU:HB2	1:D:759:VAL:HB	2.00	0.44
1:D:1252:LEU:HA	1:D:1255:LEU:HD12	1.99	0.44
1:D:2232:LEU:HG	1:D:2235:GLN:HE22	1.82	0.44
1:A:703:SER:O	1:A:707:ASP:HB2	2.17	0.44
1:A:876:LEU:HB2	1:A:891:TYR:CE2	2.53	0.44
1:A:2513:PHE:HD2	1:A:2551:ASN:HA	1.82	0.44
1:B:379:SER:OG	1:B:448:ASP:OD1	2.24	0.44
1:B:2727:GLN:HB3	1:B:2737:PRO:HB3	1.98	0.44
1:B:2728:ASP:HB3	1:B:2791:ILE:HB	1.99	0.44
1:C:66:ARG:HB3	1:C:362:TRP:CZ2	2.49	0.44
1:C:1124:ARG:NH2	1:C:1177:ASP:O	2.49	0.44
1:C:2595:PHE:HA	1:C:2598:MET:HG2	1.98	0.44
1:D:1952:GLN:CD	1:D:2210:SER:HA	2.43	0.44
1:A:1777:TYR:HB2	1:B:1778:LEU:HD23	2.00	0.44
1:B:11:LEU:N	1:B:12:PRO:HD2	2.33	0.44
1:B:482:TYR:OH	1:B:755:GLY:O	2.36	0.44
1:B:874:GLN:NE2	1:B:877:MET:SD	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2053:GLN:HB3	1:B:2055:HIS:CE1	2.52	0.44
1:B:2730:VAL:HG12	1:B:2736:SER:O	2.17	0.44
1:C:2248:ARG:NH2	1:C:2308:LYS:O	2.51	0.44
1:D:49:LYS:HB2	1:D:63:GLU:HG3	2.00	0.44
1:D:890:GLN:HA	1:D:893:MET:HG2	1.98	0.44
1:D:1331:ARG:HA	1:D:1331:ARG:HD2	1.82	0.44
1:D:1365:PRO:O	1:D:1368:GLN:HG2	2.17	0.44
1:D:1929:ASN:O	1:D:1931:GLU:HG3	2.18	0.44
1:D:2256:MET:SD	1:D:2257:ARG:N	2.90	0.44
1:A:1206:CYS:N	1:A:1233:ASP:OD1	2.49	0.44
1:A:1231:TYR:HD1	1:A:1231:TYR:H	1.65	0.44
1:A:1962:ASN:O	1:A:1965:THR:OG1	2.22	0.44
1:A:2602:PHE:CE2	1:A:2634:TYR:HB2	2.53	0.44
1:D:1:MET:HE2	1:D:47:THR:HG22	2.00	0.44
1:D:861:LYS:H	1:D:861:LYS:HD2	1.83	0.44
1:A:1125:ALA:HB1	1:A:1128:ALA:HB3	2.00	0.44
1:A:1856:GLY:HA3	1:B:1716:TRP:CZ2	2.53	0.44
1:B:532:THR:HG22	1:B:534:VAL:HG13	1.99	0.44
1:B:1868:PRO:HA	1:B:1873:HIS:CE1	2.53	0.44
1:B:2247:ASP:OD1	1:B:2251:LEU:N	2.50	0.44
1:C:2017:GLY:HA2	1:C:2632:TYR:HD2	1.83	0.44
1:D:915:ARG:NH1	1:D:919:ASN:OD1	2.51	0.44
1:D:2083:LYS:HG3	1:D:2188:ARG:NH1	2.33	0.44
1:A:1370:TYR:HE1	1:B:2088:VAL:HA	1.83	0.43
1:A:2316:GLN:HG2	1:A:2317:ASN:H	1.83	0.43
1:B:1373:GLN:OE1	1:B:1374:GLN:NE2	2.50	0.43
1:B:1868:PRO:HA	1:B:1873:HIS:ND1	2.32	0.43
1:D:885:TYR:HA	1:D:1088:ILE:HD11	2.00	0.43
1:D:1387:LEU:HA	1:D:1391:CYS:SG	2.58	0.43
1:D:1813:ILE:HG22	1:D:1815:ALA:H	1.83	0.43
1:D:2240:LEU:HD23	1:D:2277:VAL:HG22	2.00	0.43
1:A:835:TRP:CD1	1:A:835:TRP:H	2.35	0.43
1:A:1439:LEU:HB3	1:A:1457:ILE:HD11	2.00	0.43
1:A:1499:LEU:HD12	1:A:1499:LEU:HA	1.89	0.43
1:B:804:ALA:HB2	1:B:846:MET:HE3	2.00	0.43
1:B:1805:TYR:HE1	1:B:1809:VAL:HG11	1.83	0.43
1:B:1836:ILE:HG23	1:B:1837:PRO:HD3	1.99	0.43
1:C:817:GLY:O	1:C:841:ILE:N	2.42	0.43
1:C:925:ALA:O	1:C:929:VAL:HG22	2.17	0.43
1:C:1272:GLY:HA3	1:C:1354:LEU:HB2	2.00	0.43
1:D:390:LEU:HB3	1:D:411:HIS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1343:ILE:HG21	1:D:1424:VAL:HG13	2.00	0.43
1:A:747:LEU:HB3	1:A:799:VAL:HB	2.01	0.43
1:A:1194:PHE:CE1	1:A:1223:LEU:HB2	2.54	0.43
1:A:2690:LEU:O	1:A:2694:THR:OG1	2.31	0.43
1:B:75:GLN:HB2	1:B:77:ASP:OD1	2.18	0.43
1:B:1124:ARG:NH2	1:B:1176:ASN:O	2.52	0.43
1:B:1784:LEU:HD12	1:B:1784:LEU:HA	1.87	0.43
1:B:2183:ASP:OD1	1:B:2184:MET:N	2.51	0.43
1:C:381:LEU:HG	1:C:382:LEU:N	2.34	0.43
1:C:917:ASP:N	1:C:917:ASP:OD1	2.50	0.43
1:C:2763:PRO:HG3	1:C:2775:PRO:HD3	2.00	0.43
1:D:443:VAL:HG21	1:D:494:TRP:HZ2	1.82	0.43
1:D:471:GLU:HB2	1:D:487:LEU:HD23	2.00	0.43
1:D:844:LEU:HD12	1:D:845:GLY:N	2.33	0.43
1:D:1961:MET:O	1:D:1965:THR:HG23	2.18	0.43
1:D:2272:MET:SD	1:D:2272:MET:N	2.84	0.43
1:D:2571:PHE:CE2	1:D:2642:ARG:HD3	2.53	0.43
1:A:478:CYS:HA	1:A:483:THR:HA	2.00	0.43
1:A:1834:LYS:HD3	1:A:1834:LYS:HA	1.92	0.43
1:A:2515:THR:HG22	1:A:2551:ASN:HB2	2.00	0.43
1:C:662:VAL:HB	1:C:663:LYS:HD3	1.99	0.43
1:C:1120:ALA:HA	1:C:1125:ALA:HB3	1.99	0.43
1:C:2721:MET:HE1	1:C:2729:LEU:HB2	1.99	0.43
1:D:877:MET:O	1:D:880:ILE:HG13	2.19	0.43
1:A:52:VAL:HB	1:A:376:ALA:HB2	2.00	0.43
1:A:682:PHE:HD2	1:A:709:ARG:HG3	1.83	0.43
1:A:922:ILE:HG13	1:A:923:LEU:HD22	2.01	0.43
1:A:2616:GLU:OE1	1:A:2621:GLY:N	2.42	0.43
1:B:497:VAL:HG12	1:B:498:PRO:HD2	2.01	0.43
1:B:741:PRO:O	1:B:744:THR:OG1	2.31	0.43
1:B:2633:GLU:O	1:B:2637:LYS:HG2	2.18	0.43
1:C:76:PRO:HB3	1:C:851:LEU:HD22	2.00	0.43
1:C:1411:ASN:HB3	1:C:1418:ARG:NH1	2.34	0.43
1:D:21:ARG:O	1:D:25:VAL:HG23	2.18	0.43
1:D:924:HIS:CD2	1:D:1110:ASP:HB3	2.53	0.43
1:D:1846:MET:HE1	1:D:2192:SER:HB3	2.01	0.43
1:D:1937:PRO:HB2	1:D:1939:LEU:HD22	2.00	0.43
1:A:68:CYS:SG	1:A:69:ARG:N	2.91	0.43
1:A:492:TYR:CD1	1:A:737:LYS:HA	2.53	0.43
1:A:775:THR:O	1:A:777:LYS:NZ	2.52	0.43
1:A:908:LEU:HA	1:A:908:LEU:HD23	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PRO:N	1:B:39:PRO:HD2	2.33	0.43
1:B:2221:LYS:HD2	1:B:2674:ASP:OD2	2.19	0.43
1:B:2595:PHE:CG	1:B:2628:PRO:HG3	2.54	0.43
1:C:491:LEU:HB2	1:C:738:LEU:HB2	2.00	0.43
1:C:827:MET:HE2	1:C:1197:ARG:CZ	2.49	0.43
1:C:1787:ALA:O	1:C:1791:VAL:HG23	2.19	0.43
1:D:838:LEU:HD21	1:D:841:ILE:HD11	2.01	0.43
1:A:1110:ASP:OD1	1:A:1111:ALA:N	2.52	0.43
1:A:2256:MET:HE3	1:A:2303:PHE:HZ	1.83	0.43
1:B:377:LEU:HD21	1:B:432:ILE:O	2.19	0.43
1:B:479:CYS:HB3	1:B:751:VAL:CG1	2.48	0.43
1:B:2714:PHE:O	1:B:2717:ILE:HG13	2.18	0.43
1:C:1438:ILE:HD12	1:D:1918:LEU:HD22	2.01	0.43
1:D:541:LEU:O	1:D:565:VAL:N	2.52	0.43
1:D:749:VAL:HG12	1:D:758:ALA:HA	2.01	0.43
1:B:895:LEU:HD11	1:B:908:LEU:HD13	1.99	0.43
1:C:23:ARG:NH1	1:C:27:GLU:OE2	2.52	0.43
1:C:790:ALA:HB1	1:C:919:ASN:HB2	2.00	0.43
1:C:2199:VAL:HG13	1:D:1707:ALA:HA	2.00	0.43
1:C:2607:CYS:SG	1:C:2608:LYS:N	2.92	0.43
1:C:2766:ASN:O	1:C:2770:SER:CA	2.67	0.43
1:D:561:LEU:HD21	1:D:572:CYS:SG	2.59	0.43
1:D:819:ILE:HD12	1:D:819:ILE:HA	1.88	0.43
1:D:1485:PRO:O	1:D:1489:GLY:N	2.49	0.43
1:D:2074:LEU:HB3	1:D:2086:MET:HB3	2.00	0.43
1:A:1340:LYS:NZ	1:A:1420:GLU:HB3	2.34	0.43
1:A:1691:LEU:HB2	1:B:2712:ARG:HH12	1.84	0.43
1:A:1854:ARG:HE	1:A:2191:LEU:HD13	1.83	0.43
1:A:1924:LEU:HD13	1:B:1485:PRO:HG3	2.00	0.43
1:A:2708:LEU:HA	1:A:2711:LYS:HG2	2.00	0.43
1:B:401:TYR:HD2	1:B:410:HIS:HD2	1.67	0.43
1:B:1155:MET:HA	1:B:1158:VAL:HG12	2.01	0.43
1:B:2182:HIS:O	1:B:2186:LEU:HG	2.18	0.43
1:C:2714:PHE:O	1:C:2717:ILE:HG13	2.18	0.43
1:D:920:ARG:HB3	1:D:924:HIS:HB3	2.01	0.43
1:D:1962:ASN:O	1:D:1965:THR:OG1	2.22	0.43
1:D:2655:ARG:CZ	1:D:2659:LEU:HD11	2.49	0.43
1:A:2239:ASP:OD1	1:A:2275:HIS:HB3	2.19	0.43
1:A:2297:THR:HG22	1:A:2301:GLN:OE1	2.19	0.43
1:B:15:GLU:H	1:B:15:GLU:CD	2.26	0.43
1:B:655:GLU:N	1:B:655:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1197:ARG:HE	1:B:1220:ASP:HB3	1.84	0.43
1:B:1940:ASP:OD1	1:B:1940:ASP:N	2.52	0.43
1:B:2552:ARG:NH1	1:B:2556:LYS:HG3	2.34	0.43
1:B:2721:MET:HB2	1:B:2725:GLU:HG3	2.01	0.43
1:C:1917:PHE:HB2	1:D:1494:THR:HG21	2.00	0.43
1:C:2203:ASP:OD1	1:C:2204:VAL:HG23	2.19	0.43
1:D:479:CYS:HB3	1:D:751:VAL:HG12	2.00	0.43
1:D:761:LYS:NZ	1:D:763:GLY:O	2.41	0.43
1:D:1839:TRP:CE3	1:D:1954:LEU:HD13	2.52	0.43
1:D:2182:HIS:O	1:D:2186:LEU:HG	2.19	0.43
1:A:451:LEU:O	1:A:454:VAL:HG22	2.19	0.42
1:A:1366:GLU:O	1:A:1369:VAL:HG12	2.18	0.42
1:A:1520:PRO:HG2	1:B:1864:ASP:HB3	2.01	0.42
1:A:2252:ILE:O	1:A:2256:MET:HG2	2.19	0.42
1:B:876:LEU:HD23	1:B:911:PHE:CE1	2.54	0.42
1:B:2253:GLN:HE21	1:B:2310:PRO:HB2	1.84	0.42
1:C:509:ALA:O	1:C:513:ASN:N	2.43	0.42
1:C:2219:GLU:O	1:C:2222:GLU:HG3	2.18	0.42
1:D:403:ASN:HB3	1:D:406:ASN:O	2.19	0.42
1:D:569:ASN:N	1:D:569:ASN:OD1	2.52	0.42
1:D:2558:LEU:HD23	1:D:2655:ARG:HA	2.00	0.42
1:A:70:ILE:HD11	1:A:357:GLY:HA3	2.00	0.42
1:A:711:LEU:HD13	1:A:716:LEU:HD11	2.01	0.42
1:A:1226:THR:O	1:A:1228:PRO:HD3	2.19	0.42
1:B:2253:GLN:HA	1:B:2256:MET:HE2	1.99	0.42
1:C:1481:SER:HB2	1:D:1928:HIS:ND1	2.34	0.42
1:C:2552:ARG:HD3	1:C:2570:PHE:CG	2.54	0.42
1:C:2575:MET:HE3	1:C:2579:LEU:HD22	2.01	0.42
1:D:565:VAL:HA	1:D:572:CYS:SG	2.59	0.42
1:D:655:GLU:N	1:D:655:GLU:OE1	2.52	0.42
1:D:770:ILE:O	1:D:779:GLU:HG3	2.19	0.42
1:D:1117:PHE:CE1	1:D:1129:ALA:HB1	2.54	0.42
1:D:1714:MET:HA	1:D:1716:TRP:CD1	2.55	0.42
1:D:1852:GLN:HE22	1:D:1939:LEU:HB3	1.83	0.42
1:A:687:SER:HB3	1:A:706:GLN:HB3	2.01	0.42
1:B:560:VAL:HG13	1:B:575:GLN:HB3	2.01	0.42
1:B:705:LEU:HD21	1:D:671:LEU:HD13	2.00	0.42
1:B:1871:PRO:HG3	1:B:1936:LEU:HD21	1.99	0.42
1:B:2223:SER:O	1:B:2227:ARG:HG2	2.19	0.42
1:B:2710:PHE:HE1	1:B:2777:TYR:HB2	1.85	0.42
1:B:2766:ASN:O	1:B:2770:SER:CA	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2050:LEU:HD13	1:C:2066:LEU:HD11	2.02	0.42
1:D:510:ARG:HB3	1:D:514:LYS:HB3	2.02	0.42
1:D:549:PHE:CG	1:D:550:SER:N	2.87	0.42
1:D:1180:SER:HA	1:D:1183:TRP:HE1	1.85	0.42
1:A:443:VAL:HG12	1:A:476:LEU:HD11	2.02	0.42
1:A:1475:LEU:HA	1:A:1478:VAL:HG12	2.02	0.42
1:A:2230:GLU:HA	1:A:2233:ARG:HG2	2.00	0.42
1:B:22:LEU:HD13	1:B:819:ILE:HG12	2.02	0.42
1:B:1402:LEU:HD13	1:B:1466:ALA:HB3	2.01	0.42
1:C:1125:ALA:HB1	1:C:1128:ALA:HB3	2.02	0.42
1:C:1269:ASN:HD21	1:C:1273:GLU:HG3	1.83	0.42
1:C:1707:ALA:HB1	1:C:1718:VAL:HG12	2.01	0.42
1:C:1955:ILE:HD13	1:C:1958:ILE:HD12	2.01	0.42
1:B:562:MET:N	1:B:562:MET:SD	2.92	0.42
1:C:1170:LEU:HD12	1:C:1170:LEU:HA	1.82	0.42
1:C:1475:LEU:HD22	1:C:1791:VAL:HG13	2.02	0.42
1:C:2519:GLY:H	1:C:2525:ARG:CZ	2.32	0.42
1:C:2554:VAL:HA	1:C:2557:VAL:HG22	2.02	0.42
1:D:1102:LEU:HD23	1:D:1105:LEU:HD12	2.01	0.42
1:D:2083:LYS:HG3	1:D:2188:ARG:HH11	1.84	0.42
1:A:686:SER:HA	1:A:707:ASP:CG	2.44	0.42
1:A:1197:ARG:NH2	1:A:1202:LEU:HB2	2.35	0.42
1:A:1791:VAL:O	1:A:1795:ILE:HG23	2.20	0.42
1:A:2671:THR:OG1	1:A:2673:GLU:OE2	2.26	0.42
1:A:2763:PRO:HB3	1:A:2774:VAL:HG12	2.01	0.42
1:B:1115:THR:OG1	1:B:1118:MET:HG3	2.20	0.42
1:B:1170:LEU:HB2	1:B:1264:LEU:HD23	2.02	0.42
1:C:352:SER:HA	1:C:353:PRO:HD3	1.85	0.42
1:C:726:LYS:O	1:C:727:VAL:HB	2.18	0.42
1:C:752:ASP:HB3	1:C:803:THR:HG21	2.02	0.42
1:D:2595:PHE:CD1	1:D:2600:LEU:HB2	2.55	0.42
1:D:2671:THR:OG1	1:D:2672:ALA:N	2.53	0.42
1:A:385:SER:HB3	1:A:391:TYR:HE2	1.84	0.42
1:A:492:TYR:HD1	1:A:737:LYS:HA	1.85	0.42
1:A:2102:MET:SD	1:A:2103:SER:N	2.92	0.42
1:A:2534:ARG:HH11	1:A:2660:ASP:HB2	1.85	0.42
1:A:2686:ASN:N	1:A:2689:MET:HE2	2.30	0.42
1:B:497:VAL:HG23	1:B:730:CYS:O	2.19	0.42
1:C:442:LYS:HB3	1:C:462:ALA:HB1	2.00	0.42
1:C:1117:PHE:CE1	1:C:1129:ALA:HB1	2.55	0.42
1:C:1177:ASP:H	1:C:1251:ARG:HH22	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1331:ARG:O	1:C:1331:ARG:NH1	2.53	0.42
1:C:1941:VAL:HG21	1:C:2195:LEU:HD23	2.00	0.42
1:D:1488:MET:HE3	1:D:1488:MET:HB2	1.98	0.42
1:D:2532:ILE:O	1:D:2535:ILE:HG12	2.19	0.42
1:A:551:ILE:HA	1:A:556:PRO:HA	2.01	0.42
1:A:667:VAL:O	1:A:669:LYS:NZ	2.39	0.42
1:A:1402:LEU:HD11	1:A:1463:VAL:HA	2.01	0.42
1:A:1500:ALA:HB1	1:A:1505:ASP:HB3	2.01	0.42
1:A:1828:GLN:HB2	1:A:2169:PHE:HZ	1.84	0.42
1:A:2294:SER:OG	1:A:2735:SER:HB2	2.19	0.42
1:A:2715:TRP:HA	1:A:2718:VAL:HG22	2.01	0.42
1:B:568:MET:HE3	1:B:568:MET:HB3	1.82	0.42
1:B:804:ALA:HB2	1:B:846:MET:HG2	2.02	0.42
1:C:432:ILE:HG21	1:C:551:ILE:HD12	2.00	0.42
1:C:501:GLN:HA	1:C:504:LYS:HG2	2.00	0.42
1:C:1925:MET:HE1	1:D:1434:ARG:HA	2.00	0.42
1:D:380:GLU:HA	1:D:394:LYS:HA	2.01	0.42
1:D:1362:HIS:CD2	1:D:1362:HIS:H	2.36	0.42
1:D:2784:LYS:O	1:D:2787:LEU:HG	2.20	0.42
1:A:536:LEU:HD23	1:A:716:LEU:HG	2.01	0.42
1:A:881:LEU:HA	1:A:929:VAL:HG11	2.02	0.42
1:A:893:MET:O	1:A:896:GLU:HG3	2.19	0.42
1:A:1266:THR:HA	1:A:1274:HIS:HE1	1.85	0.42
1:A:1927:SER:OG	1:A:2090:VAL:HG13	2.19	0.42
1:A:2792:LYS:HB3	1:A:2792:LYS:HE3	1.83	0.42
1:B:1235:TRP:CE3	1:B:1315:PRO:HD3	2.54	0.42
1:B:1259:LEU:HD11	1:B:1332:VAL:HG22	2.01	0.42
1:B:1470:TYR:HA	1:B:1473:GLU:HG3	2.02	0.42
1:C:427:LEU:HD23	1:C:428:SER:N	2.34	0.42
1:C:885:TYR:CZ	1:C:1087:PHE:HB3	2.55	0.42
1:C:1917:PHE:CE2	1:D:1441:VAL:HG11	2.41	0.42
1:C:2605:ASP:OD1	1:C:2605:ASP:N	2.45	0.42
1:A:679:ALA:HB2	1:C:710:LEU:HD11	2.02	0.42
1:A:1102:LEU:HA	1:A:1105:LEU:HB2	2.01	0.42
1:A:1367:GLU:OE1	1:A:1367:GLU:N	2.53	0.42
1:A:1842:MET:SD	1:A:1951:PHE:HA	2.60	0.42
1:A:2064:GLU:HG2	1:A:2190:ARG:HH12	1.85	0.42
1:A:2766:ASN:HD21	1:A:2773:TYR:HE2	1.66	0.42
1:B:745:GLU:N	1:B:745:GLU:OE1	2.53	0.42
1:B:1124:ARG:NH1	1:B:1244:ILE:O	2.53	0.42
1:B:2572:ASP:OD1	1:B:2572:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1348:GLN:NE2	1:C:1372:ASN:O	2.53	0.42
1:C:1386:CYS:HA	1:C:1390:LYS:HG2	2.02	0.42
1:C:2229:MET:HA	1:C:2232:LEU:HG	2.01	0.42
1:D:377:LEU:HD11	1:D:382:LEU:HD11	2.00	0.42
1:D:457:LYS:HE2	1:D:457:LYS:HB3	1.87	0.42
1:D:1476:CYS:SG	1:D:1831:VAL:HG23	2.60	0.42
1:D:1846:MET:HA	1:D:1849:THR:HG22	2.01	0.42
1:A:69:ARG:NH1	1:A:395:TRP:HA	2.35	0.41
1:A:1201:LEU:HD21	1:A:1234:CYS:HA	2.02	0.41
1:A:2763:PRO:CA	1:A:2773:TYR:O	2.68	0.41
1:B:2232:LEU:O	1:B:2235:GLN:NE2	2.38	0.41
1:C:74:VAL:HG12	1:C:849:HIS:ND1	2.34	0.41
1:C:1513:LEU:HD21	1:D:1919:ASN:HA	2.02	0.41
1:D:11:LEU:N	1:D:12:PRO:HD2	2.34	0.41
1:D:1709:GLN:OE1	1:D:1709:GLN:N	2.47	0.41
1:A:2580:ARG:NH1	1:A:2581:GLN:OE1	2.52	0.41
1:A:2726:ARG:O	1:A:2730:VAL:HG23	2.20	0.41
1:B:710:LEU:HD11	1:D:679:ALA:HB2	2.01	0.41
1:B:1364:LEU:O	1:B:1368:GLN:HG3	2.20	0.41
1:B:2552:ARG:HH11	1:B:2556:LYS:HG3	1.85	0.41
1:C:2:THR:OG1	1:C:871:VAL:O	2.24	0.41
1:C:22:LEU:O	1:C:25:VAL:HG12	2.19	0.41
1:C:441:ASN:ND2	1:C:441:ASN:O	2.53	0.41
1:C:750:ASN:OD1	1:C:803:THR:N	2.52	0.41
1:C:840:PRO:O	1:C:872:GLU:N	2.41	0.41
1:C:1716:TRP:CZ2	1:D:1856:GLY:HA3	2.54	0.41
1:C:2788:LEU:HD13	1:C:2791:ILE:HD11	2.01	0.41
1:D:1776:SER:O	1:D:1779:THR:HG22	2.20	0.41
1:D:2097:VAL:HB	1:D:2101:LYS:HE3	2.00	0.41
1:A:493:TRP:CD1	1:A:736:LYS:HB3	2.54	0.41
1:B:463:GLN:HB3	1:B:465:TYR:CE1	2.55	0.41
1:B:846:MET:HA	1:B:866:VAL:O	2.21	0.41
1:B:916:CYS:HG	1:B:920:ARG:HE	1.63	0.41
1:C:1336:TRP:CD1	1:C:1408:GLU:HG3	2.54	0.41
1:C:2265:ARG:HD3	1:C:2266:ARG:H	1.85	0.41
1:D:381:LEU:HB2	1:D:395:TRP:CH2	2.55	0.41
1:D:440:ASN:HB3	1:D:442:LYS:HE2	2.02	0.41
1:D:2554:VAL:HG13	1:D:2651:LEU:HD11	2.01	0.41
1:A:908:LEU:O	1:A:912:ILE:HG12	2.19	0.41
1:A:1871:PRO:HB3	1:B:1716:TRP:CD1	2.55	0.41
1:B:1164:ASN:OD1	1:B:1164:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2058:GLN:OE1	1:B:2060:ASN:N	2.39	0.41
1:C:381:LEU:HG	1:C:382:LEU:H	1.86	0.41
1:D:2730:VAL:HA	1:D:2733:TRP:HB2	2.03	0.41
1:A:2600:LEU:O	1:A:2626:VAL:N	2.54	0.41
1:B:1099:GLN:OE1	1:B:1099:GLN:N	2.54	0.41
1:B:1438:ILE:HD13	1:B:1438:ILE:HA	1.90	0.41
1:B:2556:LYS:HD3	1:B:2556:LYS:HA	1.90	0.41
1:C:502:ARG:NH1	1:C:657:VAL:HA	2.36	0.41
1:C:784:PHE:HD2	1:C:820:TYR:CZ	2.38	0.41
1:C:1156:GLY:HA2	1:C:1160:PRO:HA	2.02	0.41
1:C:1714:MET:HE2	1:C:1716:TRP:HE1	1.86	0.41
1:C:1716:TRP:CE3	1:D:1936:LEU:HD13	2.55	0.41
1:C:1936:LEU:HD12	1:C:1936:LEU:HA	1.94	0.41
1:D:432:ILE:HD12	1:D:451:LEU:HD11	2.02	0.41
1:D:542:TYR:HB3	1:D:564:SER:HA	2.03	0.41
1:D:543:HIS:CB	1:D:665:VAL:HG11	2.48	0.41
1:D:1102:LEU:HD23	1:D:1102:LEU:HA	1.91	0.41
1:D:1834:LYS:HA	1:D:1834:LYS:HD3	1.76	0.41
1:A:1259:LEU:HD21	1:A:1332:VAL:HG22	2.02	0.41
1:B:752:ASP:CG	1:B:757:HIS:HE2	2.28	0.41
1:B:1340:LYS:O	1:B:1344:MET:HB2	2.20	0.41
1:C:1169:PRO:HD2	1:C:1264:LEU:HD13	2.01	0.41
1:C:1339:LEU:HA	1:C:1339:LEU:HD22	1.86	0.41
1:C:1403:GLY:O	1:C:1407:LYS:HG2	2.21	0.41
1:C:1821:TYR:CE1	1:C:2164:PRO:HB2	2.55	0.41
1:C:1941:VAL:HG13	1:C:2196:PHE:HE1	1.86	0.41
1:D:68:CYS:SG	1:D:69:ARG:N	2.94	0.41
1:A:495:GLY:O	1:A:732:GLN:HB3	2.20	0.41
1:B:907:MET:HE2	1:B:907:MET:HB2	1.97	0.41
1:B:1179:CYS:SG	1:B:1180:SER:N	2.93	0.41
1:C:441:ASN:O	1:C:464:THR:OG1	2.39	0.41
1:C:1187:GLU:H	1:C:1187:GLU:HG3	1.71	0.41
1:C:1710:ALA:HB3	1:C:1715:GLN:CD	2.46	0.41
1:D:757:HIS:NE2	1:D:810:ILE:HG13	2.36	0.41
1:A:2087:GLU:OE2	1:A:2188:ARG:HG2	2.21	0.41
1:B:896:GLU:OE2	1:B:897:GLN:NE2	2.53	0.41
1:B:1201:LEU:HD22	1:B:1205:LEU:HB3	2.03	0.41
1:C:8:VAL:HG12	1:C:866:VAL:HG22	2.01	0.41
1:C:851:LEU:HD12	1:C:851:LEU:H	1.85	0.41
1:C:917:ASP:O	1:C:920:ARG:HG3	2.20	0.41
1:C:1170:LEU:HD11	1:C:1255:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2238:ARG:HD3	1:C:2238:ARG:HA	1.89	0.41
1:D:1114:MET:HB3	1:D:1118:MET:HB2	2.03	0.41
1:D:1478:VAL:O	1:D:1481:SER:OG	2.23	0.41
1:D:2247:ASP:OD1	1:D:2251:LEU:N	2.54	0.41
1:D:2257:ARG:NH2	1:D:2314:CYS:SG	2.94	0.41
1:A:63:GLU:OE1	1:A:63:GLU:N	2.54	0.41
1:A:813:ARG:NH1	1:A:842:SER:O	2.41	0.41
1:A:917:ASP:OD1	1:A:917:ASP:N	2.54	0.41
1:A:921:ASN:ND2	1:A:1108:ALA:HB3	2.36	0.41
1:A:1089:LEU:HD13	1:A:1089:LEU:HA	1.91	0.41
1:A:1203:GLU:O	1:A:1204:SER:OG	2.33	0.41
1:A:1317:HIS:O	1:A:1317:HIS:ND1	2.52	0.41
1:A:1376:GLY:O	1:A:1427:ARG:NH2	2.44	0.41
1:A:1484:VAL:HG13	1:A:1488:MET:HE2	2.03	0.41
1:A:1492:ARG:HG3	1:B:1940:ASP:OD2	2.21	0.41
1:A:2186:LEU:HD22	1:A:2193:LEU:HD11	2.03	0.41
1:A:2257:ARG:HA	1:A:2257:ARG:NH1	2.36	0.41
1:A:2601:ALA:HA	1:A:2625:PRO:HA	2.03	0.41
1:B:5:HIS:CE1	1:B:29:LEU:HD13	2.56	0.41
1:B:514:LYS:O	1:B:515:LYS:HG2	2.21	0.41
1:B:710:LEU:HD22	1:D:710:LEU:HD13	2.02	0.41
1:B:1431:SER:HA	1:B:1434:ARG:CZ	2.50	0.41
1:B:1480:GLU:HA	1:B:1483:ILE:HG22	2.03	0.41
1:B:2185:LEU:HD12	1:B:2189:TRP:CZ3	2.56	0.41
1:B:2689:MET:HE2	1:B:2689:MET:HB3	1.95	0.41
1:C:880:ILE:HA	1:C:1088:ILE:HD13	2.02	0.41
1:C:1189:ILE:HD13	1:C:1189:ILE:HA	1.82	0.41
1:C:1329:LEU:HA	1:C:1332:VAL:HG12	2.02	0.41
1:C:1404:THR:O	1:C:1408:GLU:HG2	2.21	0.41
1:C:2519:GLY:H	1:C:2525:ARG:NH2	2.17	0.41
1:C:2564:ASN:ND2	1:C:2567:ASP:OD1	2.53	0.41
1:D:40:LEU:O	1:D:44:GLU:HG2	2.20	0.41
1:D:413:ARG:O	1:D:417:LEU:HG	2.21	0.41
1:D:1819:LEU:O	1:D:2166:LEU:HD11	2.20	0.41
1:A:433:ARG:HH12	1:A:495:GLY:CA	2.33	0.41
1:A:1930:ASP:CG	1:B:1373:GLN:HE22	2.29	0.41
1:A:2585:ALA:O	1:A:2588:SER:OG	2.30	0.41
1:B:2564:ASN:N	1:B:2567:ASP:OD2	2.44	0.41
1:C:49:LYS:HD2	1:C:49:LYS:HA	1.81	0.41
1:C:401:TYR:CE1	1:C:410:HIS:HA	2.56	0.41
1:C:530:VAL:HG22	1:C:673:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:751:VAL:O	1:C:805:GLY:HA2	2.20	0.41
1:C:2099:PRO:O	1:C:2176:MET:HE3	2.20	0.41
1:D:1927:SER:C	1:D:2091:ASP:HB3	2.46	0.41
1:A:69:ARG:HD2	1:A:395:TRP:CE3	2.57	0.40
1:A:490:SER:HB3	1:A:492:TYR:CZ	2.56	0.40
1:B:424:ILE:HG23	1:B:436:VAL:HG13	2.03	0.40
1:B:515:LYS:O	1:B:517:LYS:HD3	2.21	0.40
1:B:852:ILE:H	1:B:852:ILE:HG13	1.64	0.40
1:B:2185:LEU:HD13	1:B:2185:LEU:HA	1.84	0.40
1:B:2269:THR:OG1	1:B:2270:THR:N	2.54	0.40
1:C:377:LEU:HA	1:C:430:ASN:O	2.21	0.40
1:C:753:SER:HB3	1:C:806:GLN:HA	2.02	0.40
1:C:766:VAL:HG11	1:C:791:PHE:CD2	2.56	0.40
1:C:1187:GLU:OE1	1:C:1189:ILE:HG12	2.20	0.40
1:C:2699:GLU:OE2	1:C:2755:ARG:NE	2.50	0.40
1:D:732:GLN:NE2	1:D:734:THR:O	2.53	0.40
1:D:1355:SER:HB3	1:D:1358:SER:HB2	2.03	0.40
1:D:1480:GLU:O	1:D:1484:VAL:HG23	2.21	0.40
1:D:2505:PHE:HD1	1:D:2516:PRO:HA	1.85	0.40
1:A:411:HIS:O	1:A:413:ARG:N	2.53	0.40
1:A:474:VAL:HB	1:A:486:GLN:O	2.21	0.40
1:A:2504:LEU:HA	1:A:2525:ARG:NH2	2.36	0.40
1:A:2790:ALA:O	1:A:2793:THR:OG1	2.33	0.40
1:B:19:ASN:ND2	1:B:822:MET:O	2.50	0.40
1:B:672:LYS:HB3	1:B:679:ALA:HB3	2.03	0.40
1:B:1102:LEU:HD23	1:B:1102:LEU:HA	1.89	0.40
1:B:1235:TRP:CZ2	1:B:1314:MET:HG3	2.56	0.40
1:B:2225:PHE:O	1:B:2229:MET:HG2	2.21	0.40
1:C:2026:SER:OG	1:C:2027:ASP:N	2.54	0.40
1:C:2199:VAL:HG22	1:D:1710:ALA:HB2	2.03	0.40
1:C:2667:LEU:HA	1:C:2670:LEU:HD12	2.03	0.40
1:D:75:GLN:NE2	1:D:353:PRO:O	2.45	0.40
1:D:494:TRP:HB3	1:D:735:PRO:HA	2.02	0.40
1:D:923:LEU:HD22	1:D:1092:LEU:HD21	2.04	0.40
1:D:1345:PHE:CE1	1:D:1352:ASP:HB3	2.56	0.40
1:D:1345:PHE:CZ	1:D:1352:ASP:HB3	2.56	0.40
1:D:2757:PRO:HD3	1:D:2776:LEU:HB3	2.02	0.40
1:A:502:ARG:O	1:A:505:MET:HG3	2.21	0.40
1:A:1961:MET:O	1:A:1965:THR:HG23	2.22	0.40
1:A:2059:PRO:HA	1:A:2677:LEU:HD21	2.03	0.40
1:A:2647:ALA:C	1:A:2650:PRO:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:CYS:SG	1:B:427:LEU:HB3	2.62	0.40
1:B:517:LYS:HB2	1:B:517:LYS:HE2	1.83	0.40
1:B:827:MET:HB2	1:B:1197:ARG:NH1	2.36	0.40
1:B:924:HIS:ND1	1:B:1110:ASP:HB3	2.37	0.40
1:B:2095:LEU:HD12	1:B:2095:LEU:HA	1.82	0.40
1:C:787:SER:OG	1:C:1111:ALA:O	2.33	0.40
1:C:1197:ARG:HH21	1:C:1220:ASP:CG	2.30	0.40
1:C:1202:LEU:N	1:C:1205:LEU:HB2	2.36	0.40
1:C:1422:ILE:O	1:C:1426:MET:HG2	2.22	0.40
1:C:2225:PHE:O	1:C:2228:GLU:HG3	2.22	0.40
1:D:444:ALA:HB2	1:D:462:ALA:HB2	2.04	0.40
1:D:1233:ASP:OD1	1:D:1233:ASP:N	2.44	0.40
1:D:2530:ARG:NH2	1:D:2657:GLY:HA2	2.37	0.40
1:A:1196:CYS:SG	1:A:1198:THR:OG1	2.76	0.40
1:A:2256:MET:SD	1:A:2531:ASN:ND2	2.81	0.40
1:A:2700:SER:HB3	1:A:2756:PRO:HA	2.03	0.40
1:B:433:ARG:HD2	1:B:483:THR:OG1	2.22	0.40
1:B:2079:ALA:HB1	1:B:2084:CYS:HB3	2.02	0.40
1:B:2647:ALA:C	1:B:2650:PRO:HD2	2.46	0.40
1:C:11:LEU:HA	1:C:11:LEU:HD23	1.83	0.40
1:C:1240:CYS:SG	1:C:1242:THR:OG1	2.76	0.40
1:C:1436:PHE:HB2	1:C:1460:CYS:SG	2.62	0.40
1:C:1854:ARG:NH1	1:D:1370:TYR:OH	2.46	0.40
1:C:2288:GLY:O	1:C:2291:VAL:HG12	2.21	0.40
1:C:2677:LEU:HA	1:C:2677:LEU:HD12	1.84	0.40
1:D:925:ALA:HA	1:D:928:SER:HB3	2.03	0.40
1:D:1295:PRO:HA	1:D:1296:PRO:HD3	1.88	0.40
1:A:433:ARG:NH1	1:A:482:TYR:HA	2.37	0.40
1:A:562:MET:H	1:A:562:MET:HG3	1.62	0.40
1:A:574:PHE:HD2	1:A:651:TRP:HB2	1.87	0.40
1:A:1483:ILE:HD12	1:A:1483:ILE:HA	1.93	0.40
1:A:1841:TRP:HZ3	1:A:1950:VAL:HG21	1.86	0.40
1:A:2240:LEU:HD23	1:A:2274:VAL:HG11	2.03	0.40
1:B:785:PRO:HG3	1:B:831:ARG:O	2.21	0.40
1:B:1432:VAL:HA	1:B:1435:VAL:HG12	2.03	0.40
1:B:1846:MET:HE1	1:B:2196:PHE:CE2	2.48	0.40
1:C:752:ASP:HA	1:C:805:GLY:HA2	2.04	0.40
1:C:872:GLU:N	1:C:872:GLU:OE1	2.54	0.40
1:C:2228:GLU:O	1:C:2232:LEU:HG	2.21	0.40
1:C:2685:VAL:HG13	1:C:2739:LEU:HD12	2.03	0.40
1:D:6:PHE:HD1	1:D:868:ILE:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:THR:O	1:D:493:TRP:HA	2.21	0.40
1:D:1280:VAL:HG21	1:D:1383:PHE:CD1	2.56	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	1753/2799 (63%)	1658 (95%)	94 (5%)	1 (0%)	48	79
1	B	1753/2799 (63%)	1654 (94%)	97 (6%)	2 (0%)	48	79
1	C	1753/2799 (63%)	1658 (95%)	93 (5%)	2 (0%)	48	79
1	D	1753/2799 (63%)	1635 (93%)	117 (7%)	1 (0%)	48	79
All	All	7012/11196 (63%)	6605 (94%)	401 (6%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	727	VAL
1	B	515	LYS
1	B	2088	VAL
1	D	542	TYR
1	A	662	VAL
1	C	2088	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1561/2419 (64%)	1480 (95%)	81 (5%)	21	47
1	B	1561/2419 (64%)	1479 (95%)	82 (5%)	20	47
1	C	1561/2419 (64%)	1483 (95%)	78 (5%)	22	48
1	D	1561/2419 (64%)	1474 (94%)	87 (6%)	19	46
All	All	6244/9676 (64%)	5916 (95%)	328 (5%)	22	47

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	VAL
1	A	18	LEU
1	A	60	PHE
1	A	74	VAL
1	A	377	LEU
1	A	411	HIS
1	A	436	VAL
1	A	461	THR
1	A	501	GLN
1	A	541	LEU
1	A	547	VAL
1	A	551	ILE
1	A	560	VAL
1	A	710	LEU
1	A	756	VAL
1	A	762	THR
1	A	773	LEU
1	A	784	PHE
1	A	803	THR
1	A	806	GLN
1	A	836	LEU
1	A	849	HIS
1	A	854	LEU
1	A	872	GLU
1	A	895	LEU
1	A	1097	VAL
1	A	1110	ASP
1	A	1153	VAL
1	A	1164	ASN

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Mol	Chain	Res	Type
1	A	1209	THR
1	A	1231	TYR
1	A	1238	CYS
1	A	1262	THR
1	A	1267	LEU
1	A	1367	GLU
1	A	1389	VAL
1	A	1405	LEU
1	A	1409	LEU
1	A	1429	LEU
1	A	1438	ILE
1	A	1439	LEU
1	A	1441	VAL
1	A	1453	ILE
1	A	1480	GLU
1	A	1490	ILE
1	A	1513	LEU
1	A	1517	GLU
1	A	1522	ARG
1	A	1823	ASP
1	A	1846	MET
1	A	1922	LEU
1	A	1929	ASN
1	A	1932	HIS
1	A	1941	VAL
1	A	1961	MET
1	A	2041	GLU
1	A	2042	VAL
1	A	2044	LEU
1	A	2089	THR
1	A	2095	LEU
1	A	2166	LEU
1	A	2201	MET
1	A	2204	VAL
1	A	2211	ILE
1	A	2240	LEU
1	A	2242	LEU
1	A	2253	GLN
1	A	2269	THR
1	A	2540	LEU
1	A	2548	ILE
1	A	2554	VAL

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Mol	Chain	Res	Type
1	A	2563	VAL
1	A	2565	TRP
1	A	2581	GLN
1	A	2592	ASP
1	A	2623	ASN
1	A	2721	MET
1	A	2746	PHE
1	A	2752	ILE
1	A	2766	ASN
1	B	9	HIS
1	B	11	LEU
1	B	75	GLN
1	B	377	LEU
1	B	390	LEU
1	B	436	VAL
1	B	443	VAL
1	B	473	ILE
1	B	479	CYS
1	B	497	VAL
1	B	501	GLN
1	B	507	GLU
1	B	525	MET
1	B	534	VAL
1	B	542	TYR
1	B	551	ILE
1	B	555	ILE
1	B	560	VAL
1	B	563	GLU
1	B	724	THR
1	B	756	VAL
1	B	770	ILE
1	B	799	VAL
1	B	818	THR
1	B	844	LEU
1	B	880	ILE
1	B	881	LEU
1	B	911	PHE
1	B	914	HIS
1	B	916	CYS
1	B	917	ASP
1	B	1089	LEU
1	B	1114	MET

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Mol	Chain	Res	Type
1	B	1153	VAL
1	B	1173	LEU
1	B	1189	ILE
1	B	1193	ILE
1	B	1207	CYS
1	B	1229	THR
1	B	1231	TYR
1	B	1233	ASP
1	B	1255	LEU
1	B	1276	LEU
1	B	1286	GLN
1	B	1329	LEU
1	B	1457	ILE
1	B	1473	GLU
1	B	1480	GLU
1	B	1484	VAL
1	B	1784	LEU
1	B	1806	ASN
1	B	1832	GLU
1	B	1838	THR
1	B	1869	ASN
1	B	1924	LEU
1	B	1941	VAL
1	B	1961	MET
1	B	2030	THR
1	B	2044	LEU
1	B	2056	LEU
1	B	2088	VAL
1	B	2090	VAL
1	B	2095	LEU
1	B	2101	LYS
1	B	2166	LEU
1	B	2172	GLN
1	B	2175	PHE
1	B	2185	LEU
1	B	2247	ASP
1	B	2307	GLU
1	B	2539	CYS
1	B	2540	LEU
1	B	2545	LEU
1	B	2563	VAL
1	B	2564	ASN

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Mol	Chain	Res	Type
1	B	2631	VAL
1	B	2649	GLN
1	B	2677	LEU
1	B	2687	VAL
1	B	2693	PHE
1	B	2708	LEU
1	B	2722	SER
1	C	34	LEU
1	C	40	LEU
1	C	67	VAL
1	C	70	ILE
1	C	369	THR
1	C	425	VAL
1	C	430	ASN
1	C	432	ILE
1	C	484	CYS
1	C	497	VAL
1	C	504	LYS
1	C	653	LEU
1	C	662	VAL
1	C	685	THR
1	C	705	LEU
1	C	724	THR
1	C	749	VAL
1	C	750	ASN
1	C	756	VAL
1	C	767	ARG
1	C	773	LEU
1	C	794	GLN
1	C	798	ASN
1	C	810	ILE
1	C	818	THR
1	C	836	LEU
1	C	841	ILE
1	C	872	GLU
1	C	881	LEU
1	C	916	CYS
1	C	1099	GLN
1	C	1109	LYS
1	C	1173	LEU
1	C	1189	ILE
1	C	1202	LEU

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Mol	Chain	Res	Type
1	C	1209	THR
1	C	1214	VAL
1	C	1234	CYS
1	C	1256	TYR
1	C	1279	LEU
1	C	1339	LEU
1	C	1373	GLN
1	C	1398	LEU
1	C	1405	LEU
1	C	1431	SER
1	C	1482	LEU
1	C	1490	ILE
1	C	1507	MET
1	C	1697	ARG
1	C	1714	MET
1	C	1799	MET
1	C	1832	GLU
1	C	1838	THR
1	C	1839	TRP
1	C	1846	MET
1	C	1922	LEU
1	C	1932	HIS
1	C	1941	VAL
1	C	1959	LYS
1	C	2035	ILE
1	C	2062	ARG
1	C	2089	THR
1	C	2090	VAL
1	C	2095	LEU
1	C	2098	LEU
1	C	2203	ASP
1	C	2211	ILE
1	C	2215	LEU
1	C	2269	THR
1	C	2291	VAL
1	C	2525	ARG
1	C	2534	ARG
1	C	2540	LEU
1	C	2548	ILE
1	C	2564	ASN
1	C	2692	SER
1	C	2708	LEU

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Mol	Chain	Res	Type
1	C	2789	LEU
1	D	6	PHE
1	D	8	VAL
1	D	49	LYS
1	D	381	LEU
1	D	390	LEU
1	D	401	TYR
1	D	425	VAL
1	D	436	VAL
1	D	443	VAL
1	D	445	THR
1	D	467	GLU
1	D	512	LYS
1	D	525	MET
1	D	534	VAL
1	D	543	HIS
1	D	551	ILE
1	D	555	ILE
1	D	561	LEU
1	D	563	GLU
1	D	569	ASN
1	D	572	CYS
1	D	650	GLN
1	D	651	TRP
1	D	665	VAL
1	D	677	TYR
1	D	700	ASP
1	D	705	LEU
1	D	717	GLN
1	D	751	VAL
1	D	762	THR
1	D	799	VAL
1	D	806	GLN
1	D	813	ARG
1	D	868	ILE
1	D	872	GLU
1	D	877	MET
1	D	878	GLN
1	D	895	LEU
1	D	911	PHE
1	D	912	ILE
1	D	917	ASP

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Mol	Chain	Res	Type
1	D	1088	ILE
1	D	1089	LEU
1	D	1092	LEU
1	D	1098	LEU
1	D	1167	ASP
1	D	1173	LEU
1	D	1179	CYS
1	D	1187	GLU
1	D	1189	ILE
1	D	1211	CYS
1	D	1231	TYR
1	D	1242	THR
1	D	1244	ILE
1	D	1274	HIS
1	D	1329	LEU
1	D	1330	GLU
1	D	1339	LEU
1	D	1381	ASP
1	D	1429	LEU
1	D	1478	VAL
1	D	1490	ILE
1	D	1829	ASN
1	D	1846	MET
1	D	1869	ASN
1	D	1924	LEU
1	D	1932	HIS
1	D	1941	VAL
1	D	1943	SER
1	D	2035	ILE
1	D	2042	VAL
1	D	2058	GLN
1	D	2089	THR
1	D	2092	ARG
1	D	2102	MET
1	D	2232	LEU
1	D	2240	LEU
1	D	2247	ASP
1	D	2307	GLU
1	D	2538	LEU
1	D	2539	CYS
1	D	2545	LEU
1	D	2558	LEU

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Mol	Chain	Res	Type
1	D	2649	GLN
1	D	2667	LEU
1	D	2685	VAL
1	D	2746	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	392	GLN
1	A	421	ASN
1	A	469	GLN
1	A	477	HIS
1	A	501	GLN
1	A	782	ASN
1	A	783	ASN
1	A	798	ASN
1	A	816	ASN
1	A	914	HIS
1	A	924	HIS
1	A	1263	ASN
1	A	1411	ASN
1	A	1451	ASN
1	A	1794	GLN
1	A	1952	GLN
1	A	2038	ASN
1	A	2072	GLN
1	A	2182	HIS
1	A	2260	ASN
1	A	2262	HIS
1	A	2527	ASN
1	A	2553	HIS
1	A	2680	ASN
1	B	9	HIS
1	B	75	GLN
1	B	361	GLN
1	B	410	HIS
1	B	411	HIS
1	B	486	GLN
1	B	575	GLN
1	B	780	GLN
1	B	782	ASN

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Mol	Chain	Res	Type
1	B	806	GLN
1	B	849	HIS
1	B	874	GLN
1	B	878	GLN
1	B	879	HIS
1	B	924	HIS
1	B	1281	GLN
1	B	1286	GLN
1	B	1362	HIS
1	B	1368	GLN
1	B	1451	ASN
1	B	1508	GLN
1	B	1705	ASN
1	B	1773	ASN
1	B	1807	HIS
1	B	1963	GLN
1	B	2019	ASN
1	B	2060	ASN
1	B	2093	ASN
1	B	2253	GLN
1	B	2527	ASN
1	B	2566	HIS
1	B	2587	GLN
1	B	2629	GLN
1	B	2680	ASN
1	C	50	GLN
1	C	392	GLN
1	C	421	ASN
1	C	430	ASN
1	C	441	ASN
1	C	469	GLN
1	C	501	GLN
1	C	513	ASN
1	C	539	ASN
1	C	664	ASN
1	C	782	ASN
1	C	794	GLN
1	C	849	HIS
1	C	1176	ASN
1	C	1373	GLN
1	C	1385	HIS
1	C	1773	ASN

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Mol	Chain	Res	Type
1	C	1822	GLN
1	C	1932	HIS
1	C	2093	ASN
1	C	2172	GLN
1	C	2253	GLN
1	C	2564	ASN
1	C	2614	GLN
1	D	41	ASN
1	D	392	GLN
1	D	411	HIS
1	D	647	ASN
1	D	794	GLN
1	D	874	GLN
1	D	914	HIS
1	D	1084	ASN
1	D	1137	GLN
1	D	1274	HIS
1	D	1281	GLN
1	D	1350	ASN
1	D	1368	GLN
1	D	1372	ASN
1	D	1374	GLN
1	D	1508	GLN
1	D	1794	GLN
1	D	1852	GLN
1	D	1919	ASN
1	D	2301	GLN
1	D	2551	ASN
1	D	2566	HIS
1	D	2587	GLN
1	D	2629	GLN
1	D	2641	HIS
1	D	2680	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

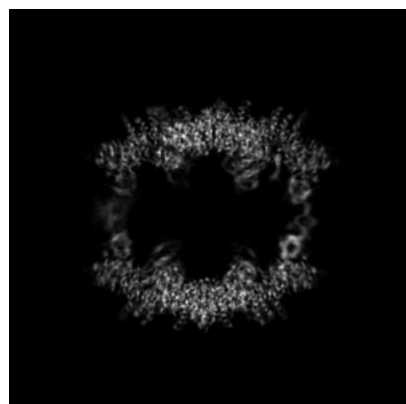
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28646. These allow visual inspection of the internal detail of the map and identification of artifacts.

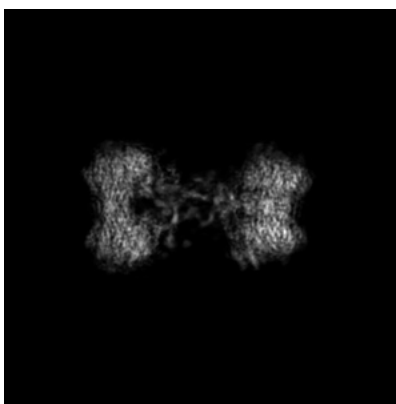
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

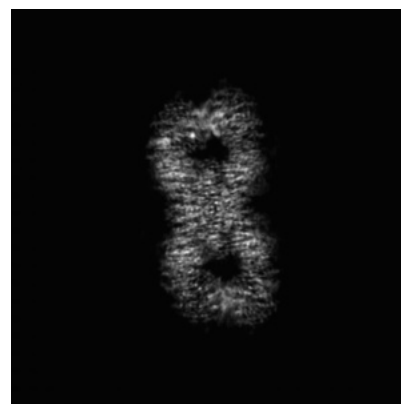
6.1.1 Primary map



X

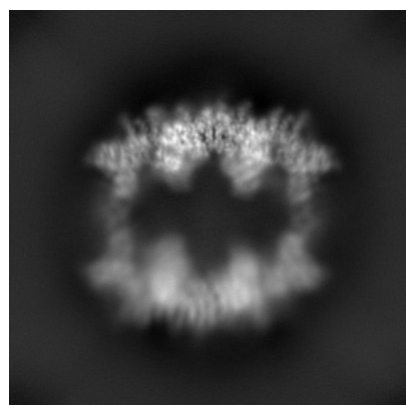


Y

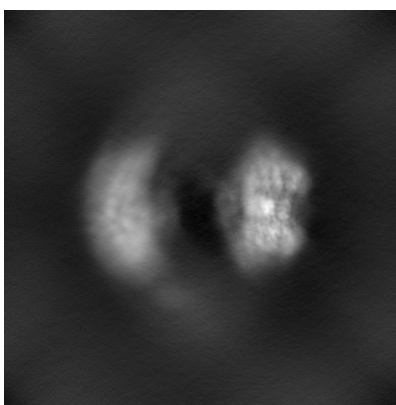


Z

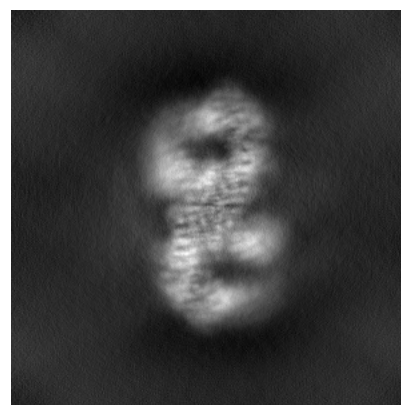
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

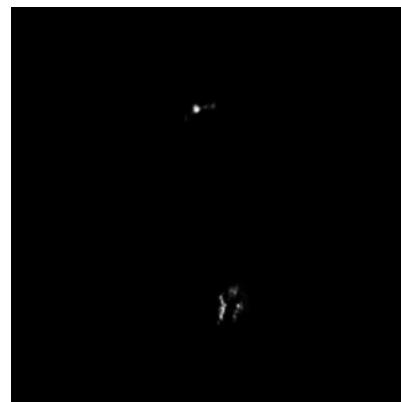
6.2.1 Primary map



X Index: 220

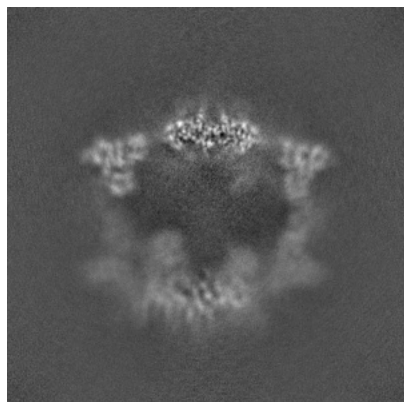


Y Index: 220

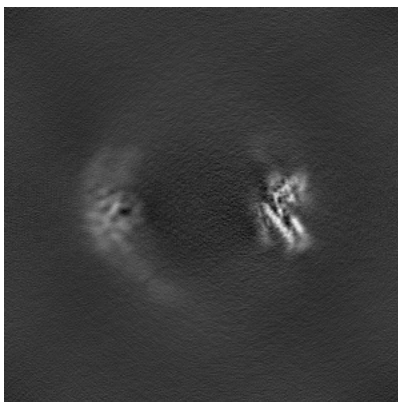


Z Index: 220

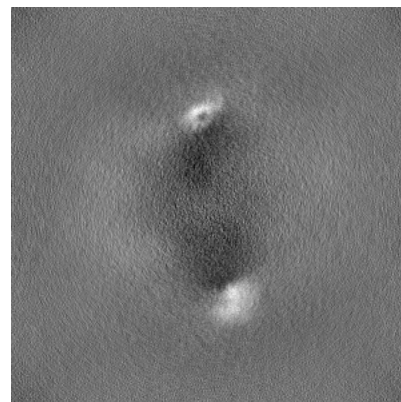
6.2.2 Raw map



X Index: 220



Y Index: 220



Z Index: 220

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: 195

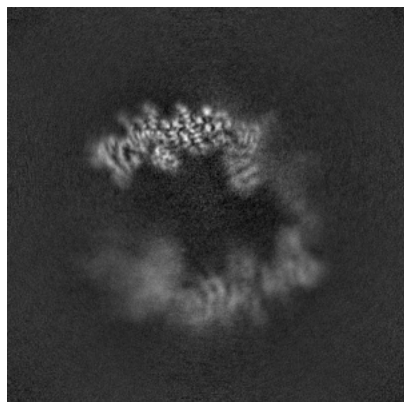


Y Index: 257

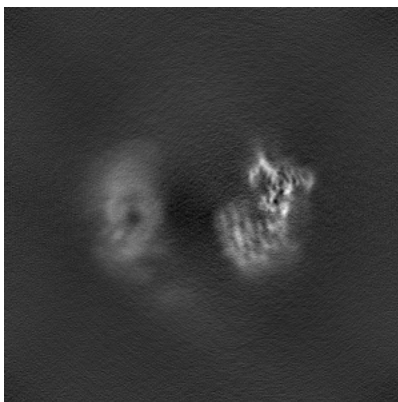


Z Index: 297

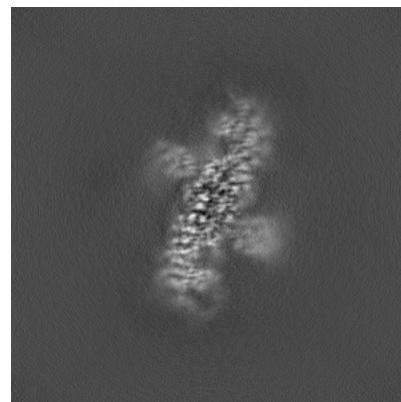
6.3.2 Raw map



X Index: 196



Y Index: 262

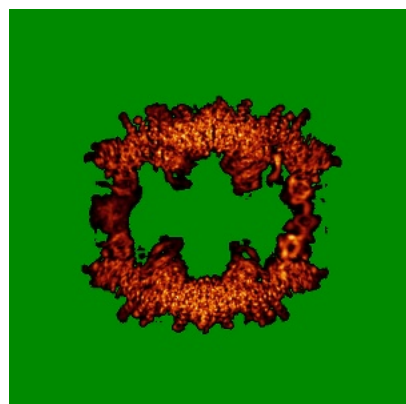


Z Index: 297

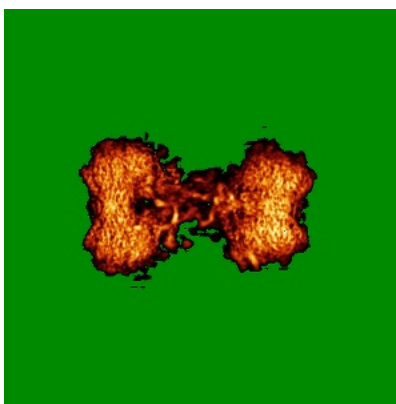
The images above show the largest variance slices of the map in three orthogonal directions.

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

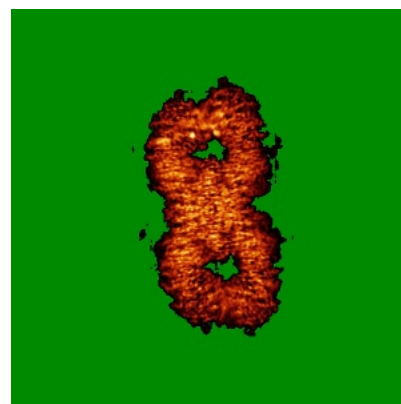
6.4.1 Primary map



X

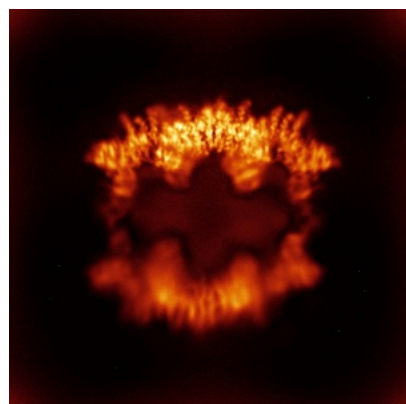


Y

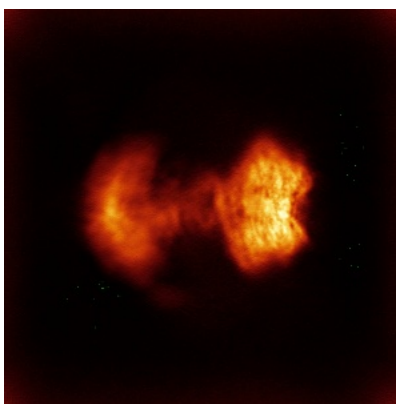


Z

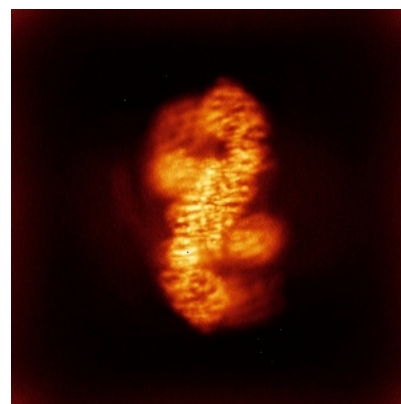
6.4.2 Raw map



X



Y

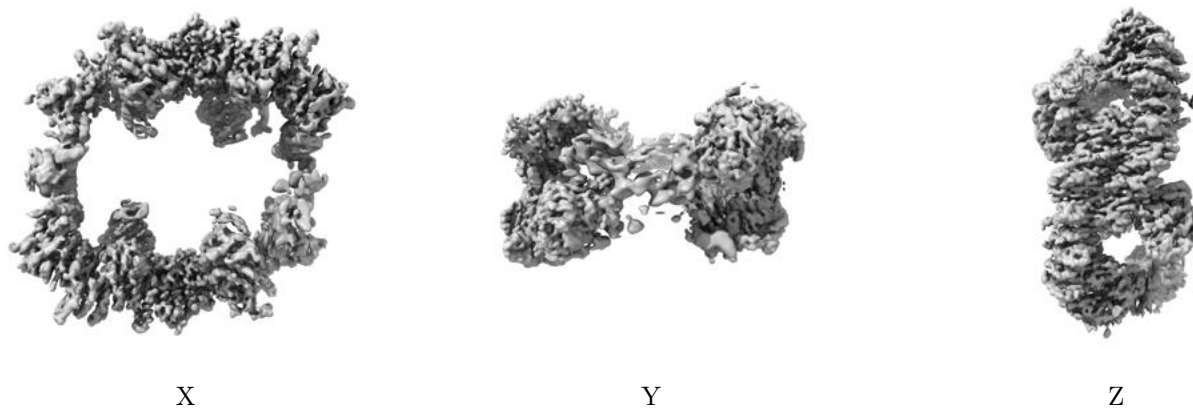


Z

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

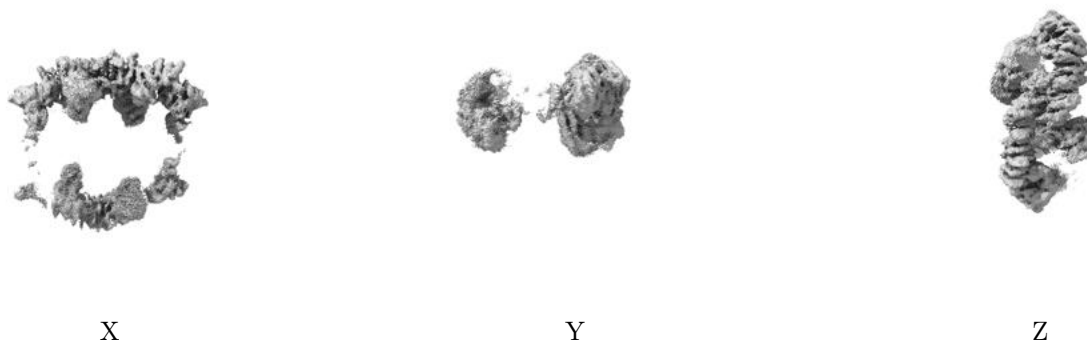
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

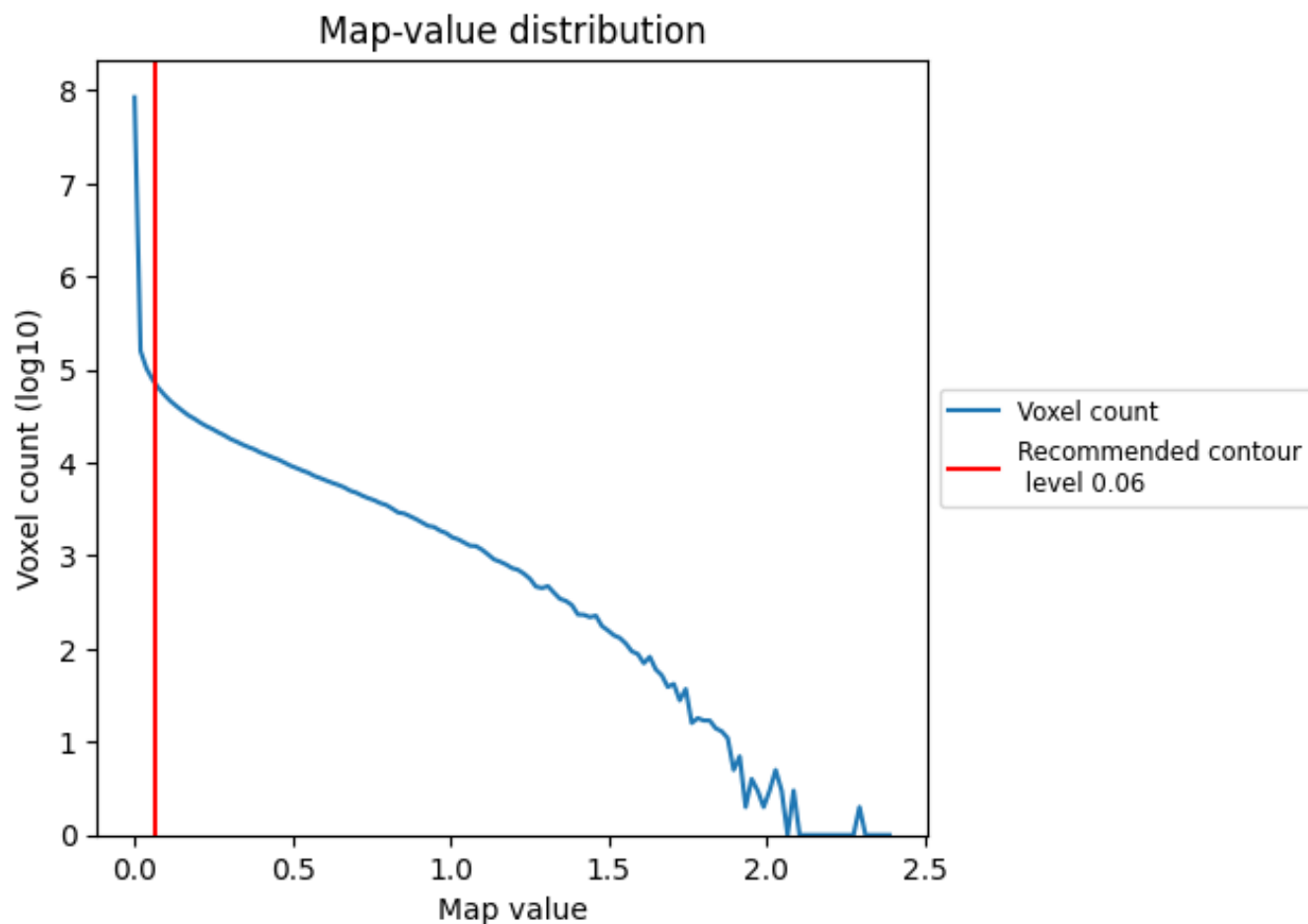
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

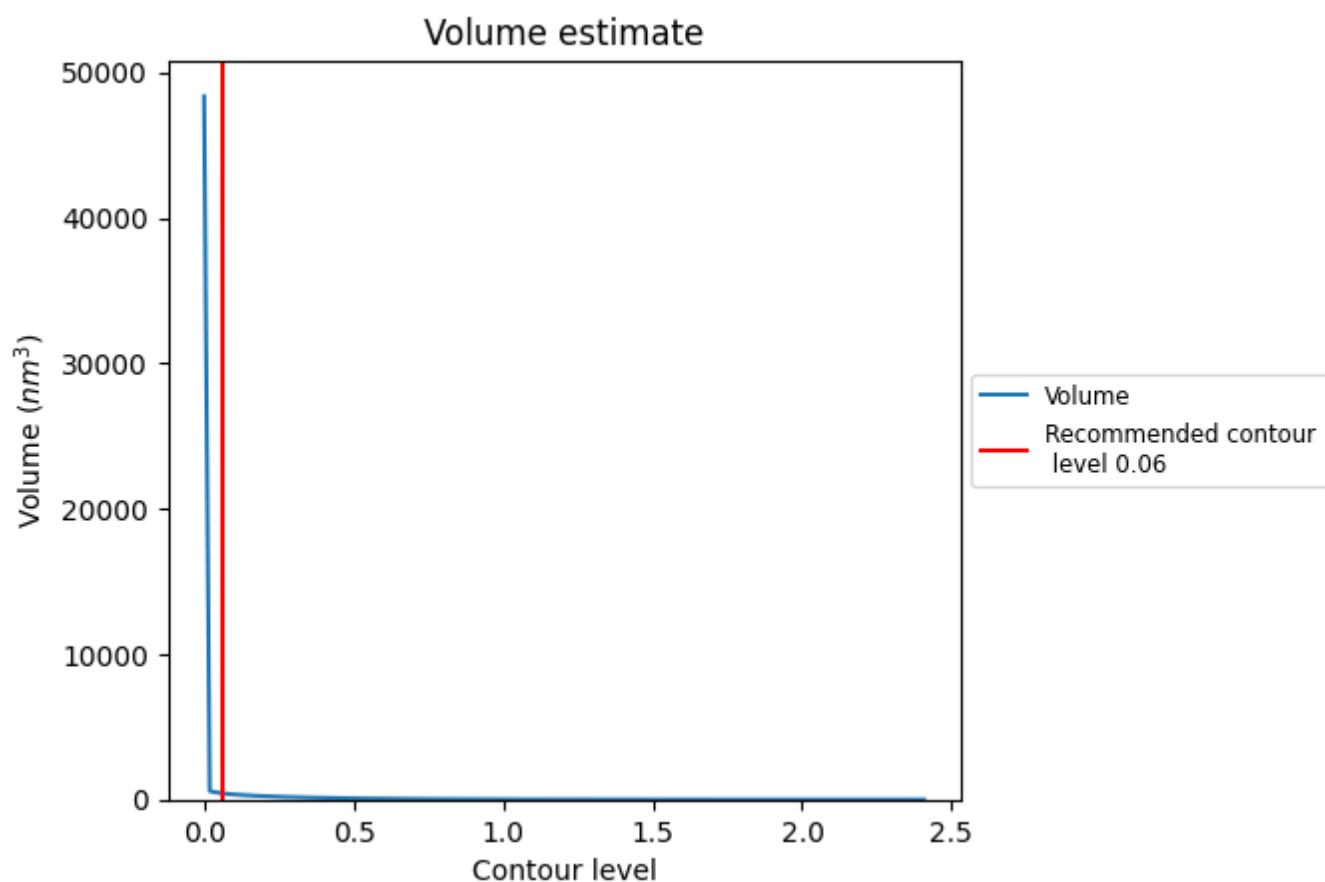
This section contains the results of statistical analysis of the map.

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.

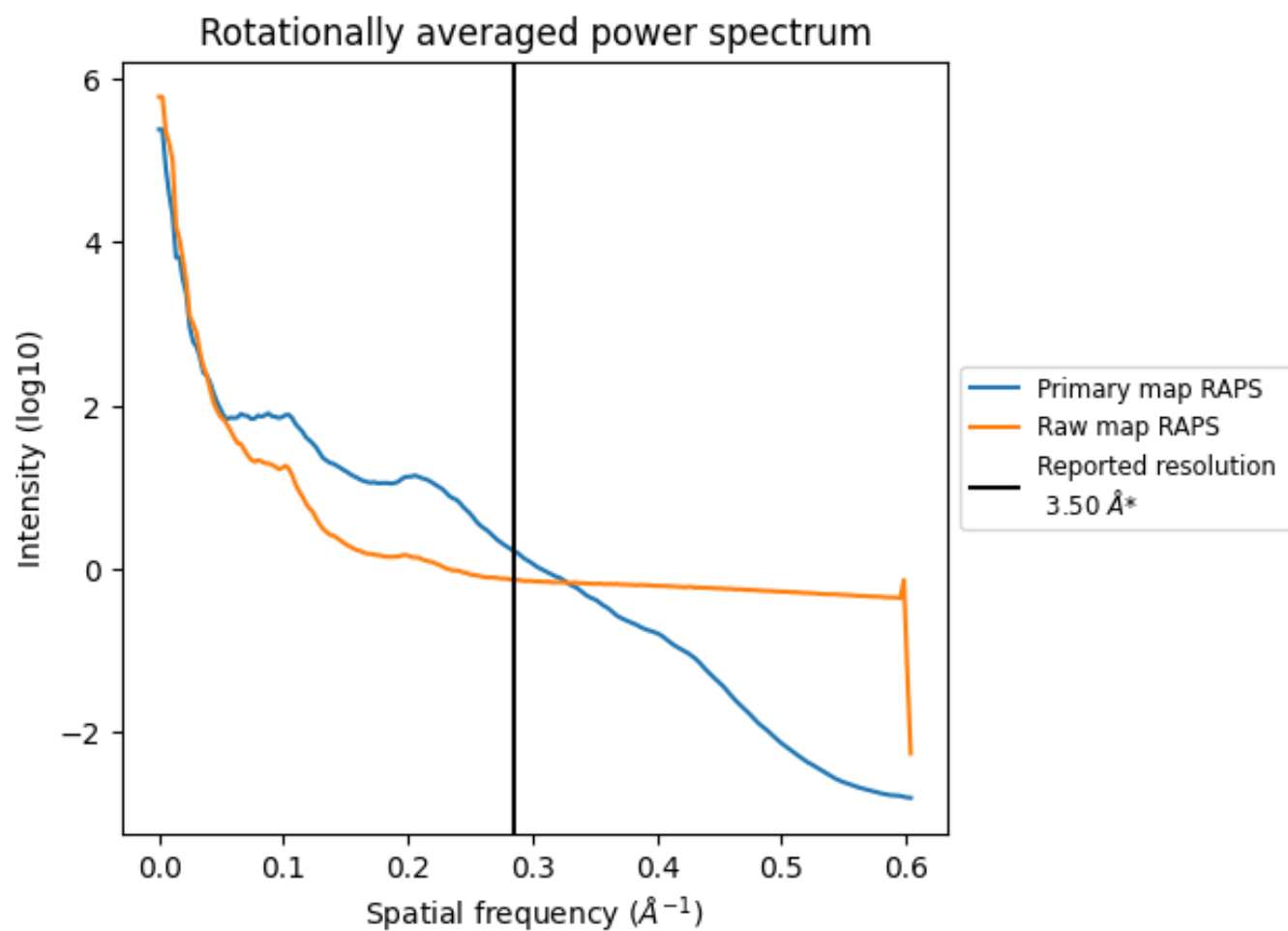
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm^3 ; this corresponds to an approximate mass of 388 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 ⓘ

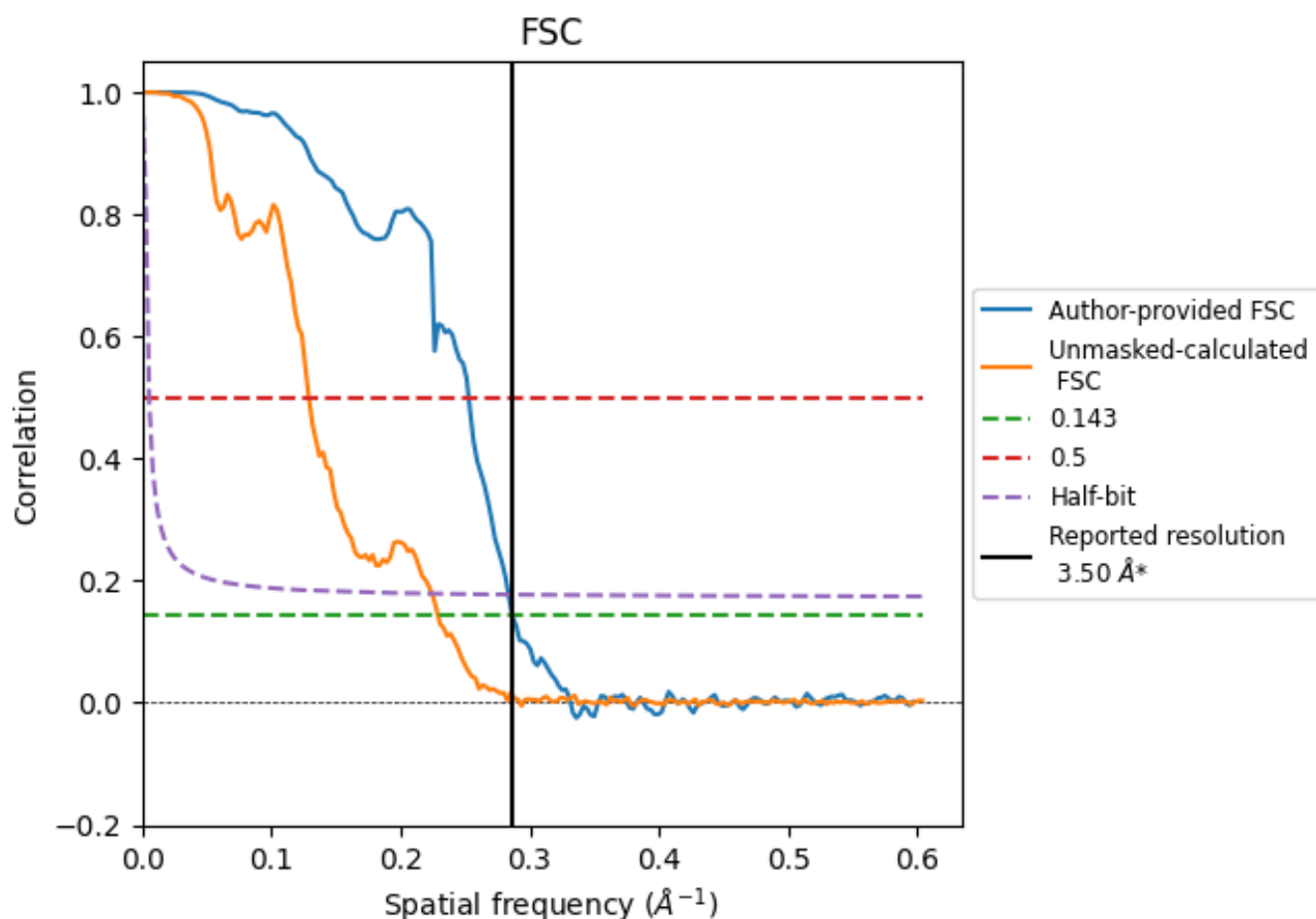


*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

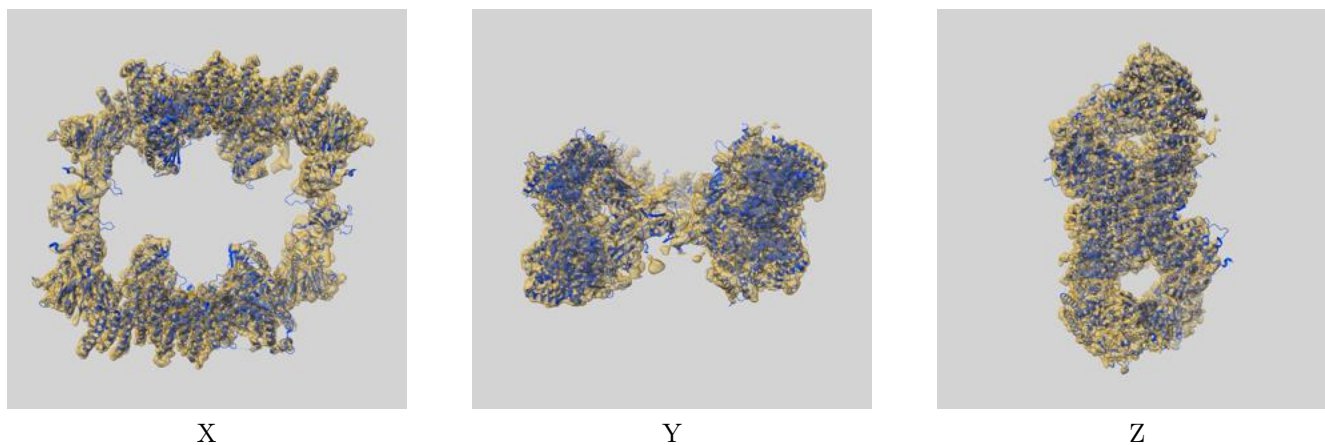
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.96	3.53
Unmasked-calculated*	4.37	7.75	4.46

*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 4.37 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

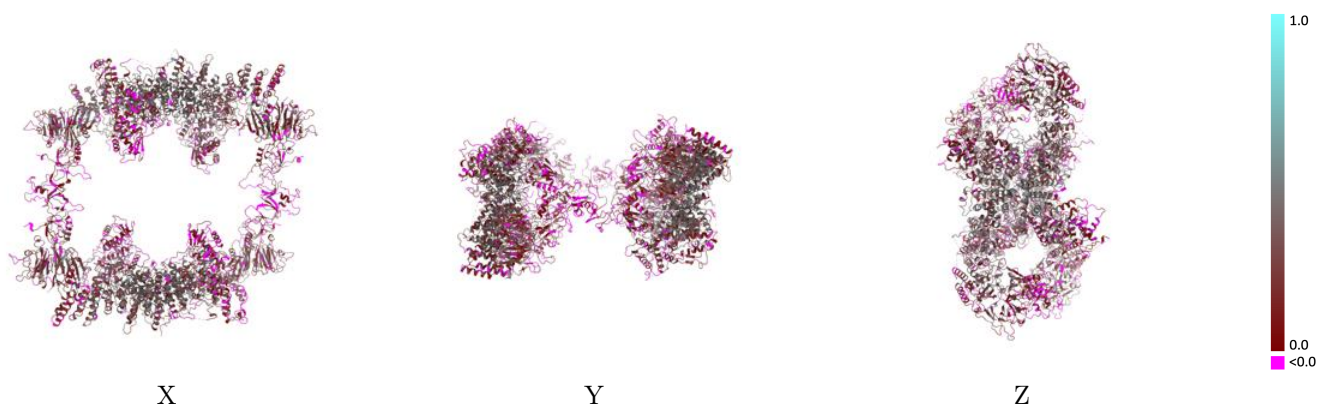
This section contains information regarding the fit between EMDB map EMD-28646 and PDB model 8EWI. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



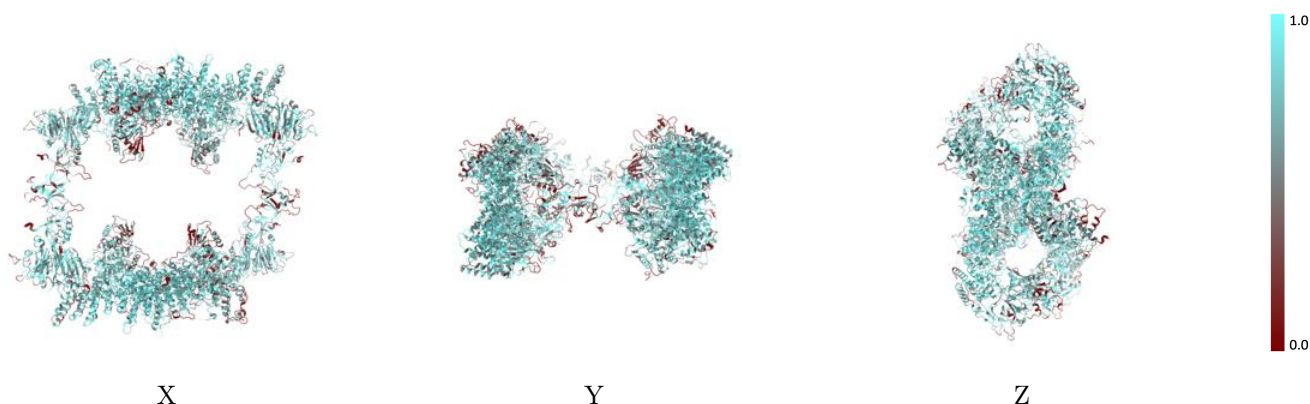
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



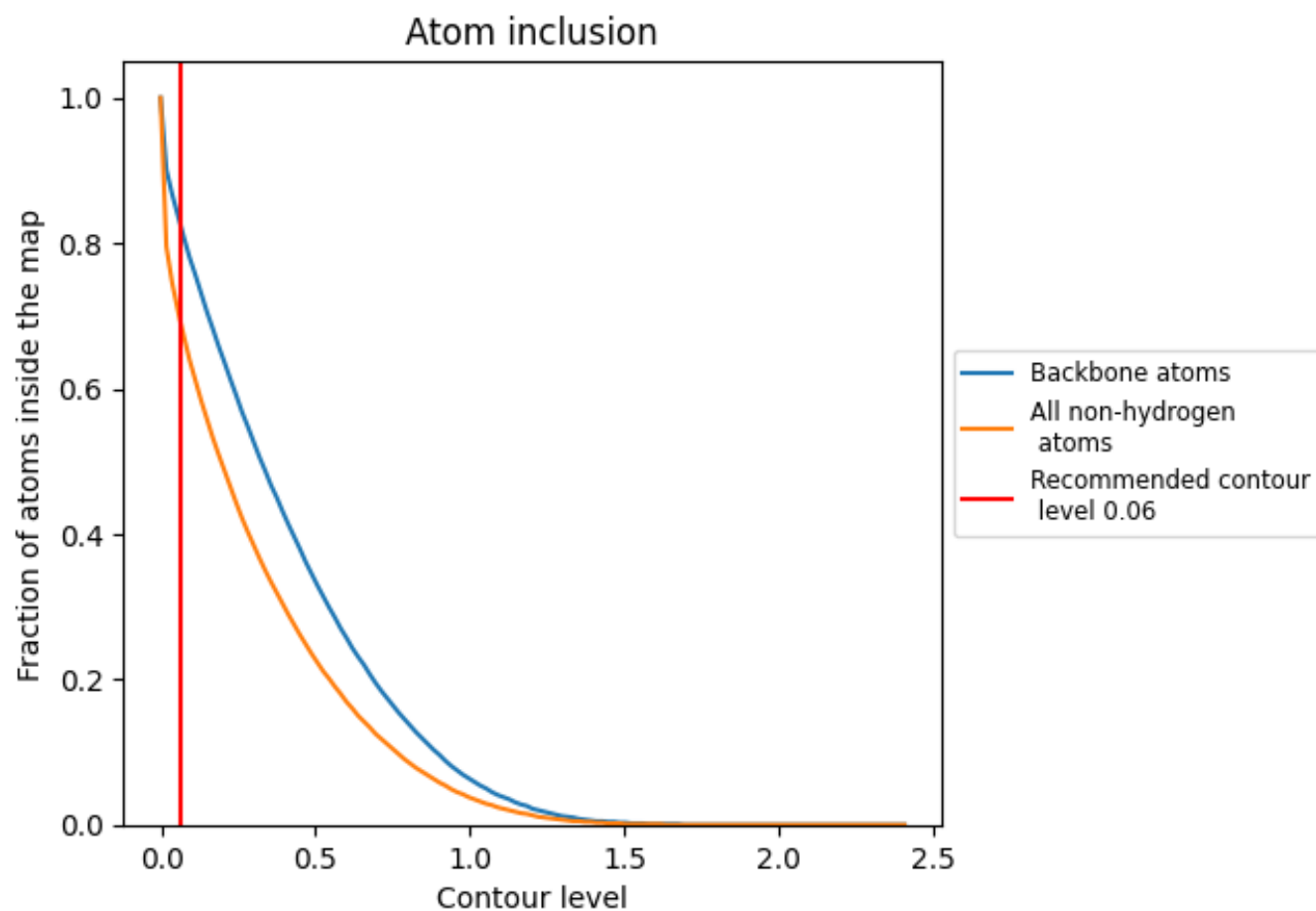
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 70% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.2480
A	0.7200	0.2670
B	0.6930	0.2540
C	0.6820	0.2390
D	0.6870	0.2330

