



Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 06:25 AM EDT

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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

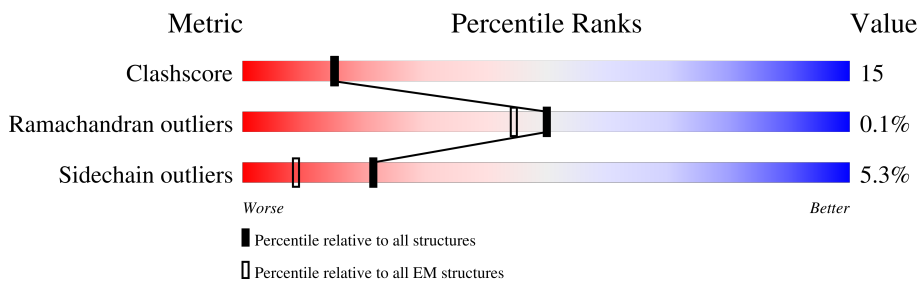
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>9%</div> <div>41%</div> <div>21%</div> <div>•</div> <div>37%</div> </div>
1	B	2799	<div> <div>10%</div> <div>41%</div> <div>20%</div> <div>•</div> <div>37%</div> </div>
1	C	2799	<div> <div>11%</div> <div>42%</div> <div>20%</div> <div>•</div> <div>37%</div> </div>
1	D	2799	<div> <div>11%</div> <div>40%</div> <div>21%</div> <div>•</div> <div>37%</div> </div>

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		

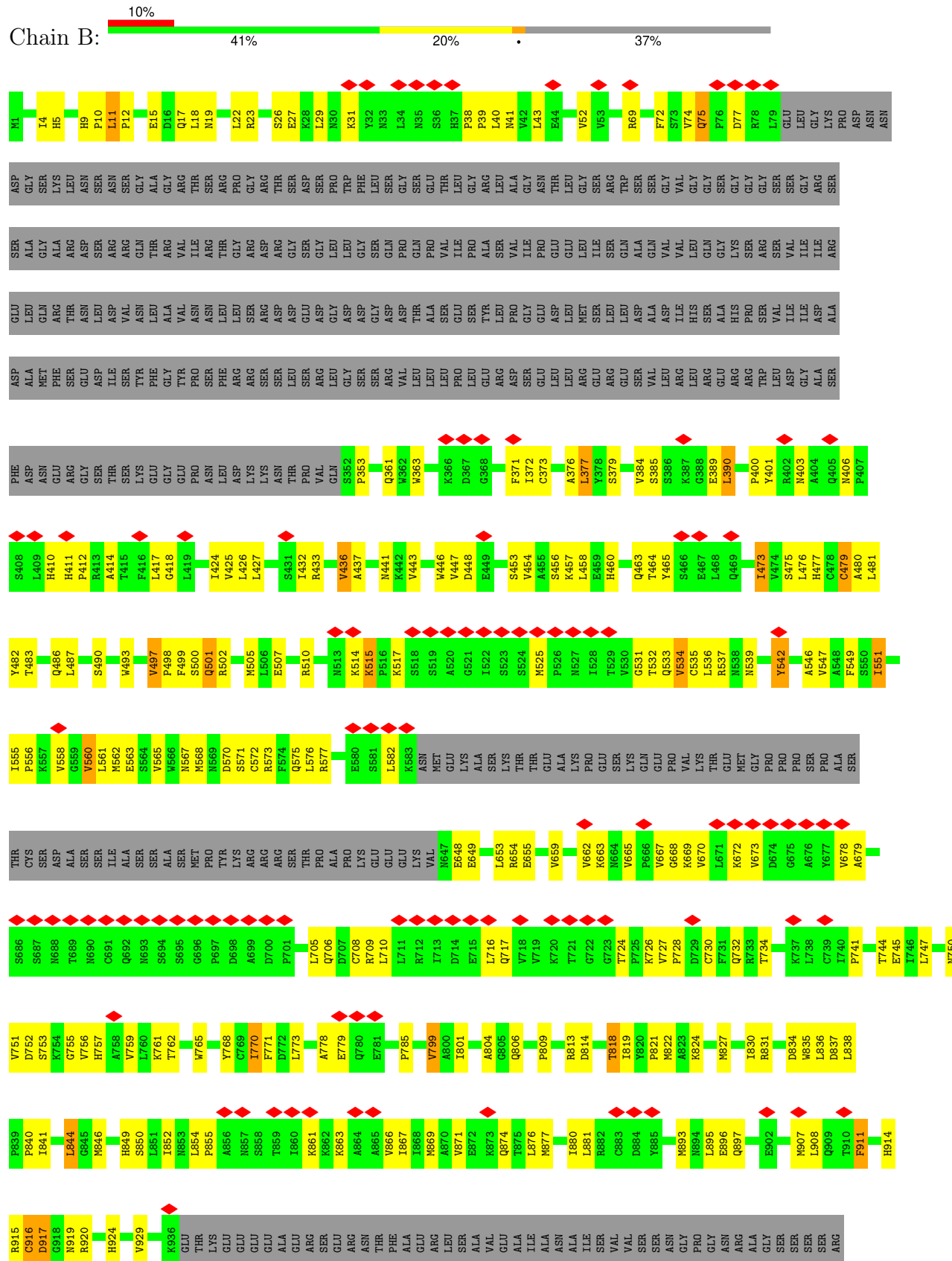
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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	

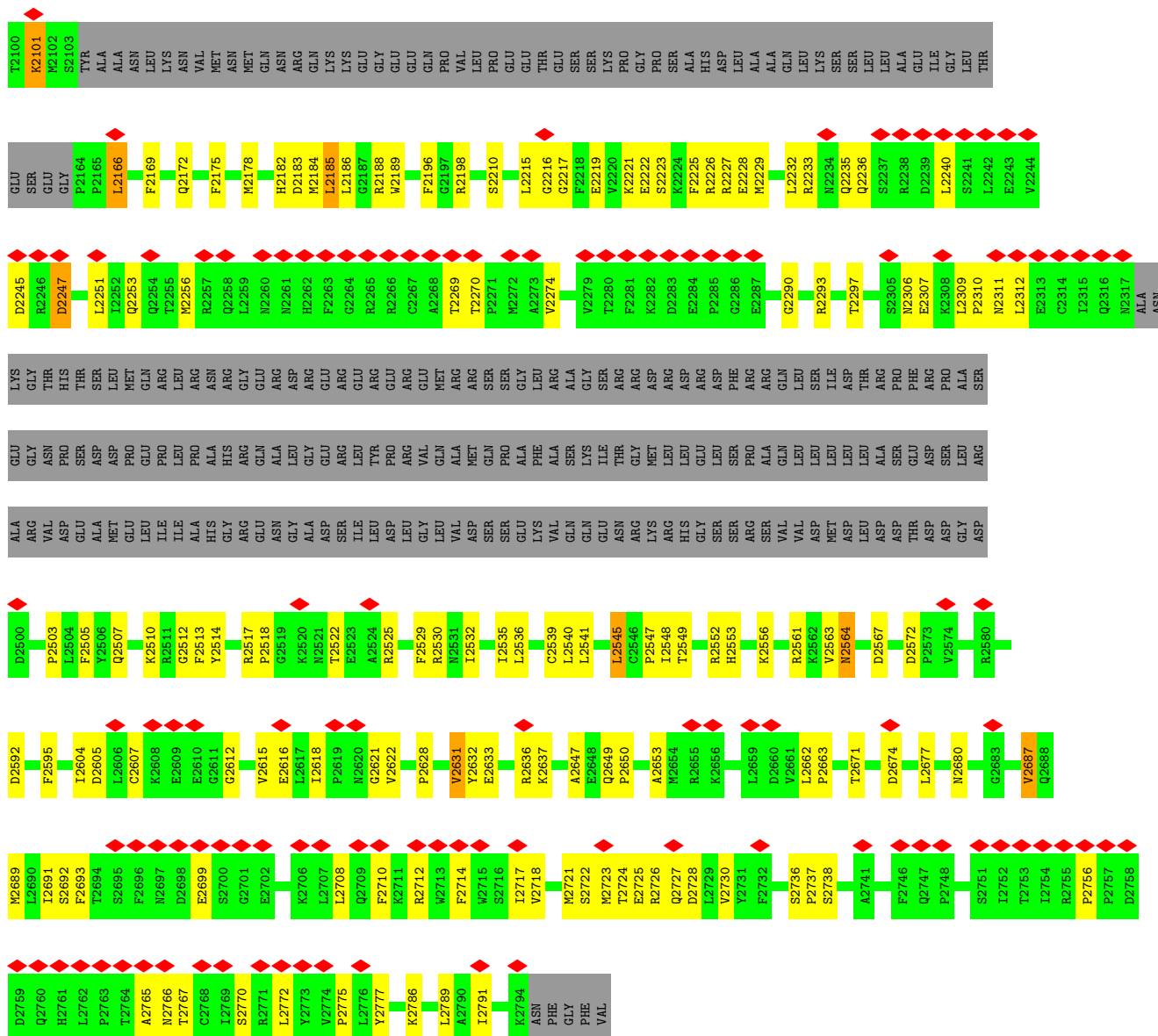




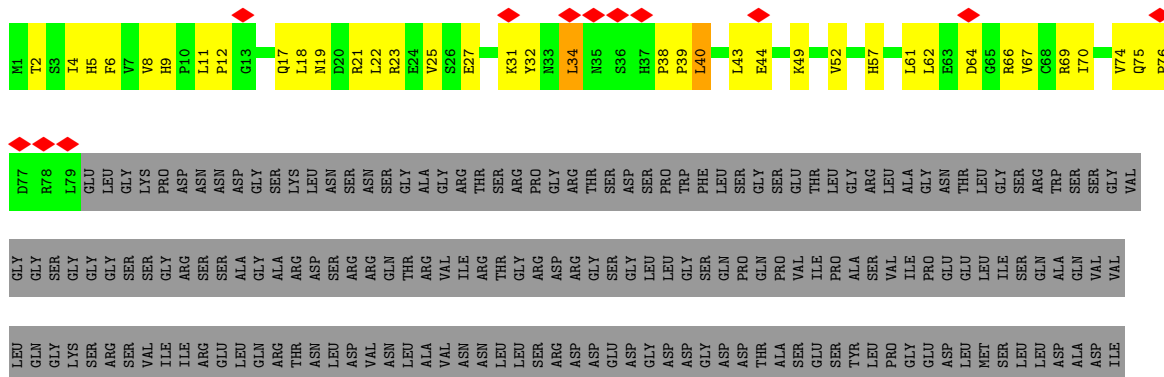
● Molecule 1: E3 ubiquitin-protein ligase UBR5





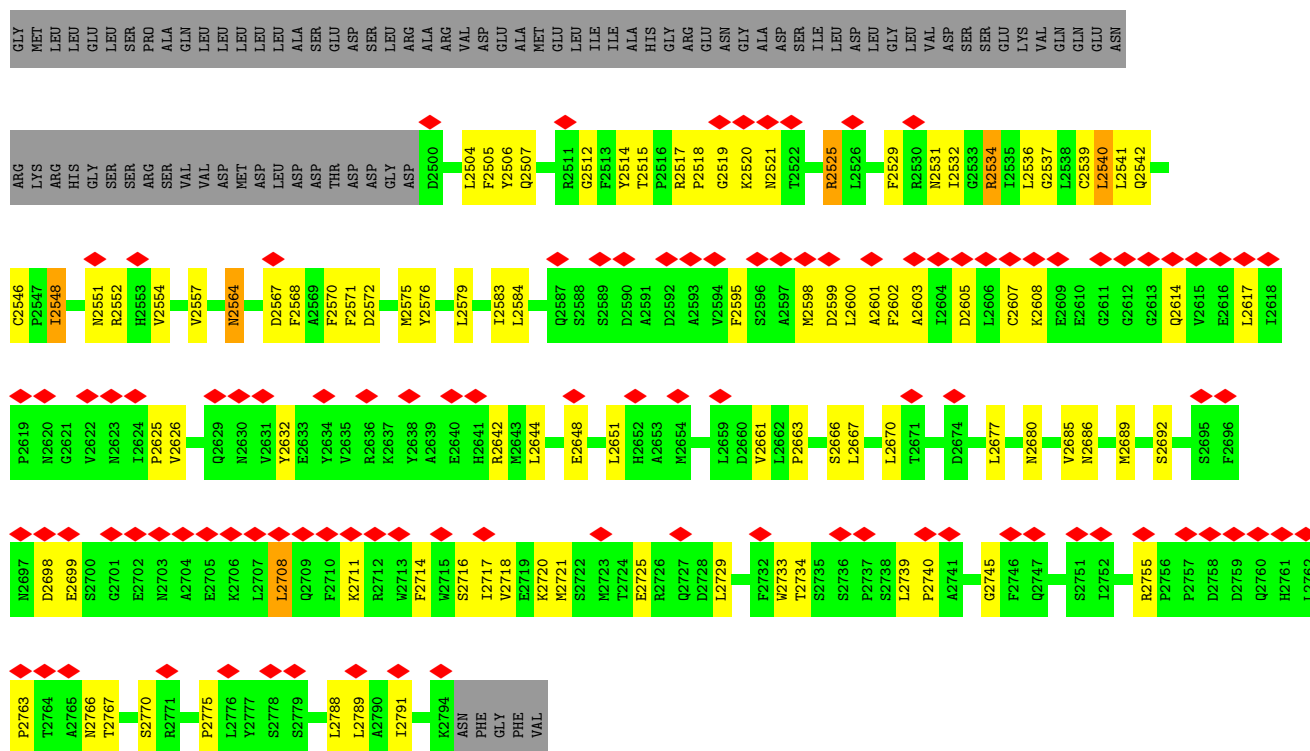


• Molecule 1: E3 ubiquitin-protein ligase UBR5

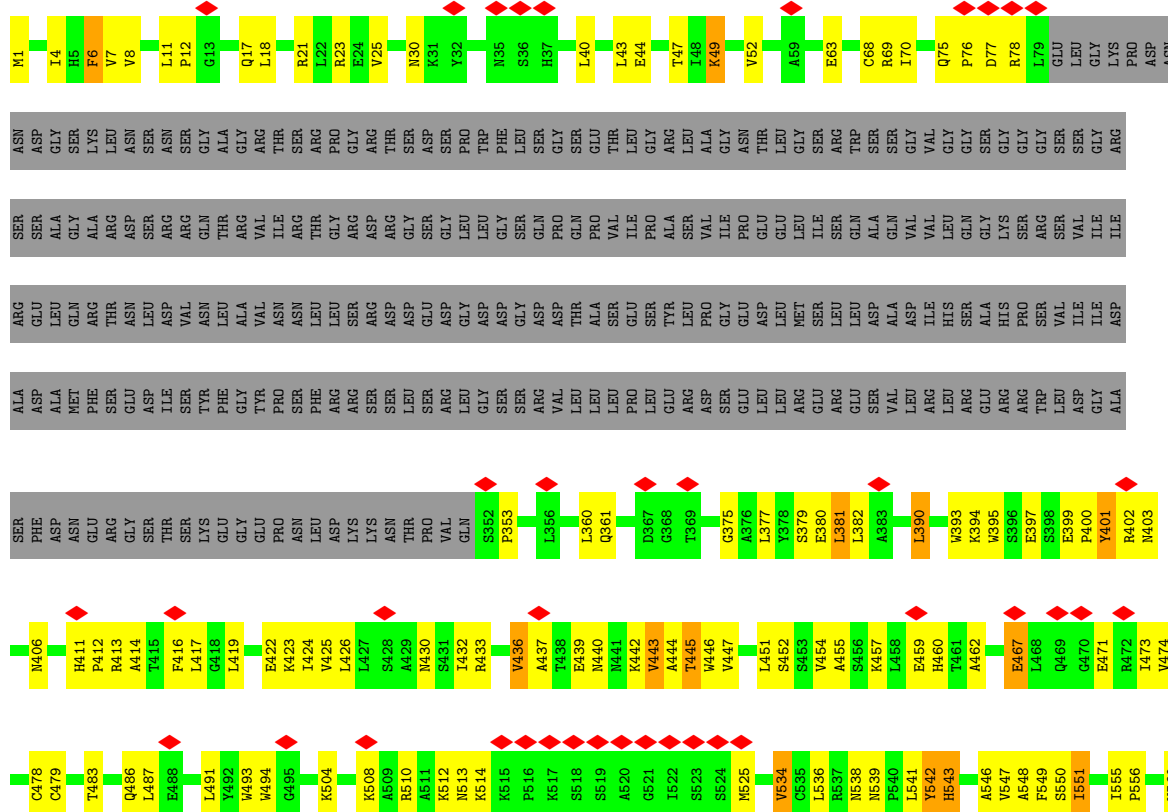


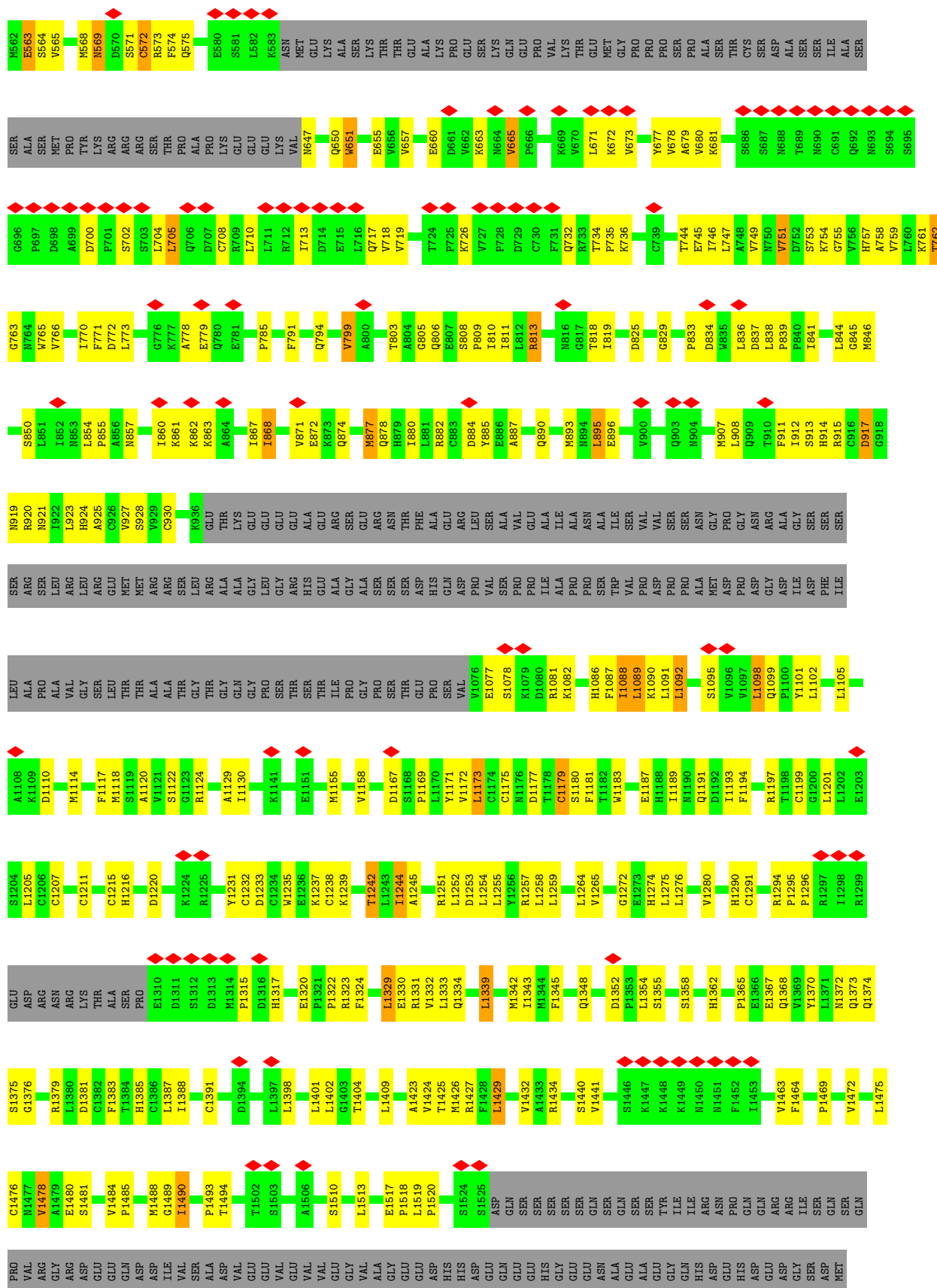




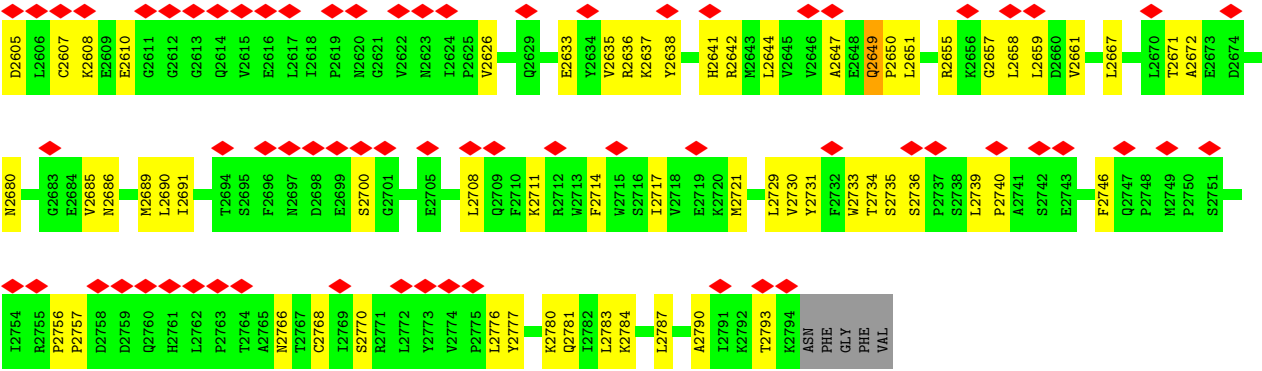


• Molecule 1: E3 ubiquitin-protein ligase UBR5





GLU	ASP	THR	L1819	ARG	LYS	A2045	ASN	L2186	H2272	GLU	GLU	ASP	R2530
LEU	SER	SER	N1826	ARG	ARG	E2046	ARG	G2187	A2273	ARG	ARG	SER	R2531
ASP	ASP	THR	L1827	ALA	THR	A2047	GLN	R2188	V2274	GLU	GLU	ASP	T2532
LEU	SER	ALA	Q1828	LEU	GLU	L2050	LYS	L2191	H2275	ARG	ARG	LEU	G2533
ALA	SER	ALA	N1829	LEU	LEU	Q2053	GLY	S2192	R2276	GLU	GLU	LEU	T2535
ALA	SER	SER	Y1830	SER	GLU	L2056	GLY	L2193	V2277	ARG	MET	GLY	L2536
ALA	GLN	SER	V1831	ALA	GLU	L2057	GLU	E2194	V2279	ARG	ARG	LEU	G2537
GLU	ASP	GLU	K1834	ARG	GLY	Q2058	GLU	L2195	T2280	GLU	GLU	GLU	C2538
THR	GLU	GLN	I1835	GLN	ILE	P2059	PRO	F2196	F2281	SER	SER	ASP	C2539
ASP	ILE	ILE	I1836	MET	ASN	N2060	VAL	G2197	R2282	GLY	GLY	SER	L2545
ASP	GLU	TYR	P1837	GLU	ASN	A2061	LEU	R2198	D2283	LEU	PHE	GLU	L2546
SER	GLN	ILE	T1838	GLU	GLU	E2202	PRO	E2202	T2284	ARG	ALA	ARG	T2548
GLU	THR	ASP	W1839	ASP	ASP	R2062	GLU	L2199	P2285	ARG	ALA	SER	T2549
SER	THR	ASP	W1841	SER	GLU	K2063	THR	V2204	G2286	GLY	GLY	GLN	L2550
ASN	PHE	GLU	T1845	GLU	HIS	E2064	GLU	D2065	E2287	SER	ARG	ASN	N2551
HIS	M1690	LEU	M1846	GLU	ASN	L2066	SER	S2210	G2288	GLU	ARG	THR	R2552
SER	L1691	ARG	T1849	GLU	ASN	P2070	LYS	E2222	ASP	ARG	GLY	GLY	T2553
ASN	D1692	ARG	Q1852	ASP	ASP	L2075	PRO	R2226	ASP	ARG	MET	LEU	H2554
ASN	E1693	SER	Y1855	ASP	ASP	S2076	ALA	K2231	R2293	ARG	LEU	LEU	T2555
ALA	P1694	GLY	G1856	THR	GLN	S2077	HIS	L2232	S2294	PHE	SER	GLU	K2556
ALA	L1695	ILE	P1865	ASN	ASN	S2078	LEU	Q2236	F2295	ARG	PRO	LEU	V2557
GLY	E1696	SER	Y1868	GLN	ALA	A2079	ALA	L2240	T2296	ARG	GLN	ALA	L2558
ARG	R1697	THR	N1869	ALA	ALA	S2080	LEU	R2241	S2305	GLN	ARG	GLN	R2561
SER	T1698	ALA	H1870	THR	THR	S2081	ALA	L2242	N2306	SER	ILE	SER	V2562
VAL	T1699	ALA	P1871	LEU	ASN	G2082	GLN	E2243	E2307	ILE	LEU	LEU	N2564
VAL	N1700	ALA	H1873	ASP	LYS	K2083	LYS	V2244	K2308	THR	LEU	LEU	H2565
THR	S1701	ALA	Q1876	ASP	ASP	M2086	SER	D2247	L2309	PRO	GLU	ASP	T2566
ALA	S1702	ALA	N1877	ASP	ASP	E2087	LEU	R2248	P2310	ARG	ASP	THR	D2567
THR	H1703	LEU	A1878	LEU	LEU	V2088	LEU	L2250	N2311	ARG	GLY	ASP	F2571
ALA	A1704	ALA	S1879	PRO	PRO	T2089	ALA	L2251	L2312	PRO	ALA	ASP	D2572
GLY	N1705	ALA	R1880	ALA	ALA	D2091	ILE	L2255	E2313	ALA	GLU	GLY	Y2576
SER	G1706	SER	R1881	S1943	ALA	R2092	GLY	Q2254	C2314	SER	ASP	ASP	L2579
GLU	A1707	ALA	GLU	V1950	ALA	L2095	SER	T2255	T2315	GLY	ASN	VAL	F2587
ALA	Q1708	GLY	ARG	F1951	GLU	E2096	GLY	R2257	Q2316	ASN	ASP	ASP	Q2588
ALA	A1710	ALA	ALA	Q1952	GLU	V2097	THR	Q2258	N2317	GLY	ASP	GLU	S2589
SER	P1711	SER	THR	L1954	TYR	K2101	GLY	L2259	ALA	ASN	ASP	GLU	D2590
VAL	R1712	VAL	ALA	T1965	M2029	M2102	GLY	N2260	THR	THR	PRO	GLU	A2591
PRO	S1713	PRO	ARG	T1966	G2033	S2103	THR	N2261	THR	THR	ALA	ILE	D2592
ALA	M1714	ALA	ALA	LEU	C2034	ALA	ALA	H2262	SER	SER	PRO	ALA	A2593
PHE	Q1715	PHE	GLU	ASP	C2035	ALA	ASN	G2264	LEU	LEU	HIS	GLY	P2594
PHE	W1716	PHE	GLU	THR	P2036	TYR	LEU	R2265	MET	GLN	ARG	ARG	F2595
SER	R1719	SER	ALA	GLU	P2037	ALA	ASN	R2266	THR	GLN	GLY	THR	S2596
ASP	N1720	ASP	ALA	LEU	G2036	ALA	LEU	C2267	GLY	GLY	GLU	ASP	K2597
GLN	THR	GLN	ALA	ASP	P2037	ALA	LEU	A2268	ARG	ASN	ASN	GLY	N2598
SER	H1S	SER	ALA	THR	P2037	ALA	ASN	T2269	GLY	GLY	GLY	THR	D2599
GLN	GLN	GLN	ALA	PRO	P2037	ALA	ASN	T2270	ASP	ASP	ASP	ALA	L2600
ASN	ARG	ASN	LEU	GLN	P2037	ALA	ASN	T2271	ARG	ARG	ARG	ALA	A2601
ASN	ALA	ALA	LEU	LEU	P2037	ALA	ASN	T2271	GLY	GLY	GLY	ALA	F2602
SER	ALA	ALA	GLY	ARG	P2037	ALA	ASN	T2271	GLY	GLY	GLY	ALA	A2603
SER	THR	THR	GLY	ARG	P2037	ALA	ASN	T2271	GLY	GLY	GLY	ALA	I2604
ALA	ALA	ALA	GLY	ARG	P2037	ALA	ASN	T2271	GLY	GLY	GLY	ALA	



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 (\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 (\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%)	50	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%)	19	47
1	B	1561/2419 (64%)	1479 (95%)	82 (5%)	19	46
1	C	1561/2419 (64%)	1483 (95%)	78 (5%)	20	49
1	D	1561/2419 (64%)	1474 (94%)	87 (6%)	17	45
All	All	6244/9676 (64%)	5916 (95%)	328 (5%)	21	46

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.

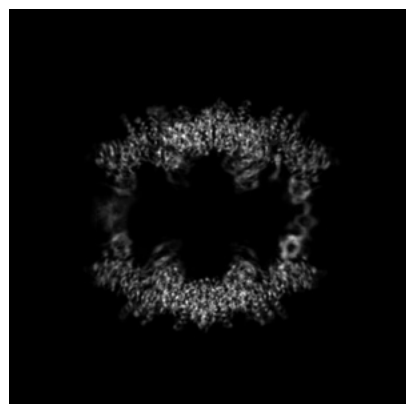
6 Map visualisation [i](#)

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.

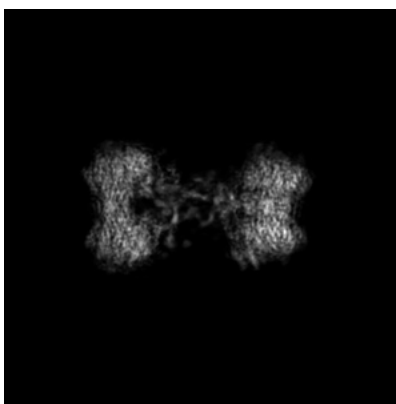
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

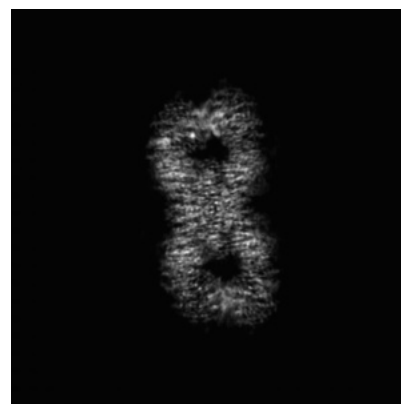
6.1.1 Primary map



X

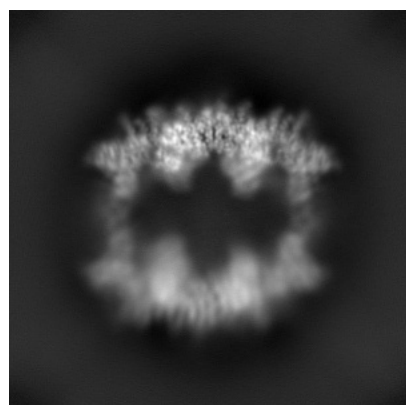


Y

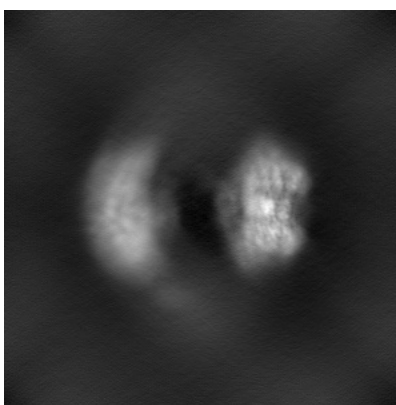


Z

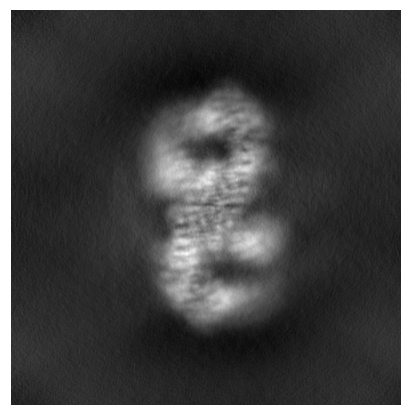
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

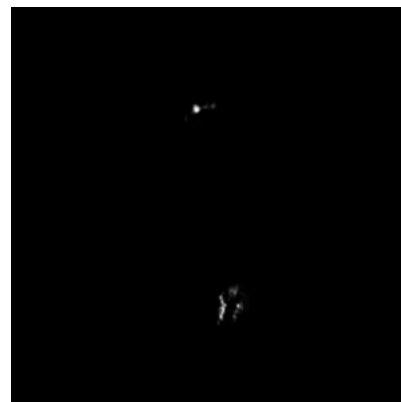
6.2.1 Primary map



X Index: 220

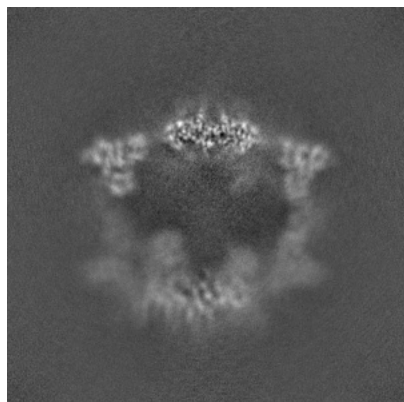


Y Index: 220

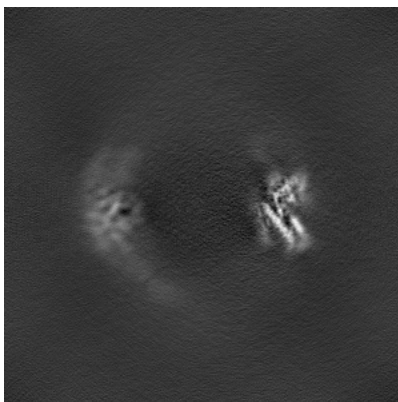


Z Index: 220

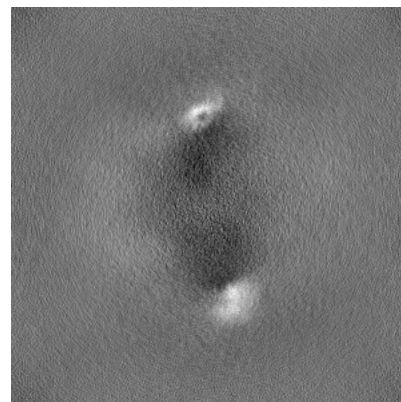
6.2.2 Raw map



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

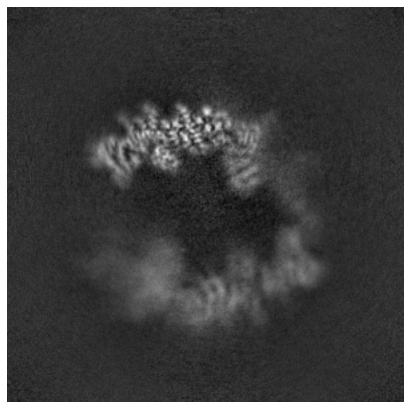


Y Index: 257

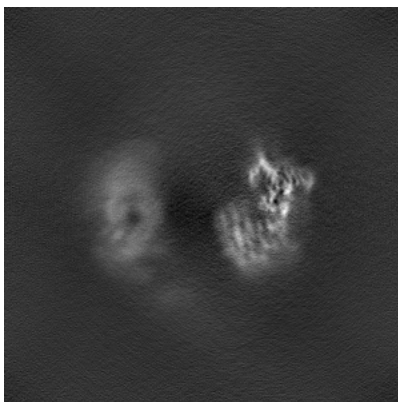


Z Index: 297

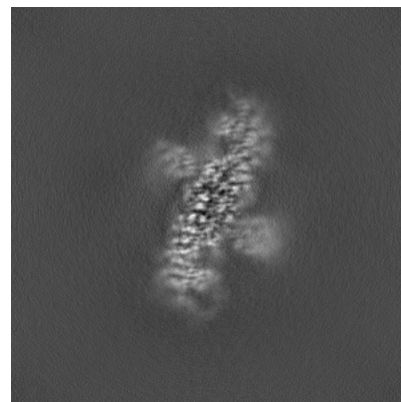
6.3.2 Raw map



X Index: 196



Y Index: 262

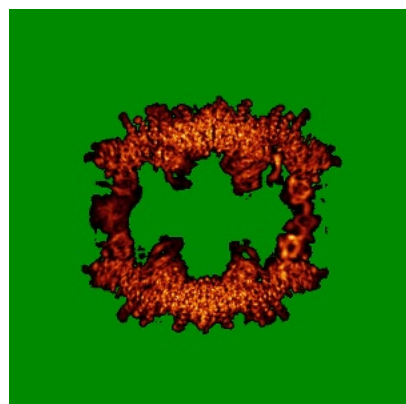


Z Index: 297

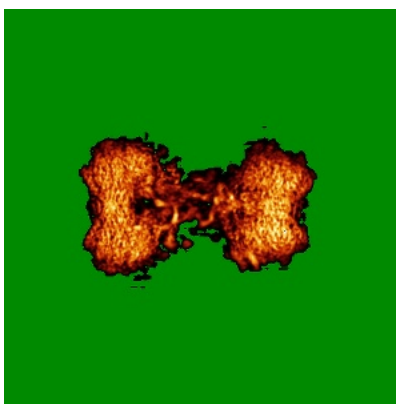
The images above show the largest variance slices of the map in three orthogonal directions.

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

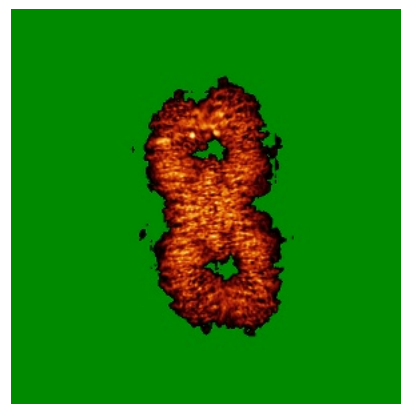
6.4.1 Primary map



X

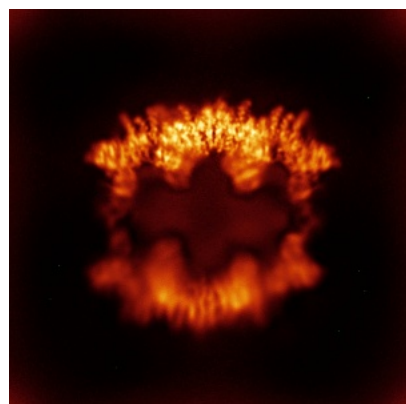


Y

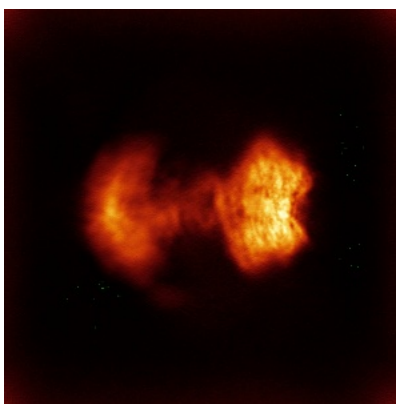


Z

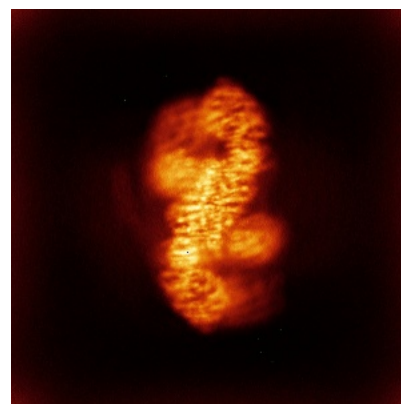
6.4.2 Raw map



X



Y

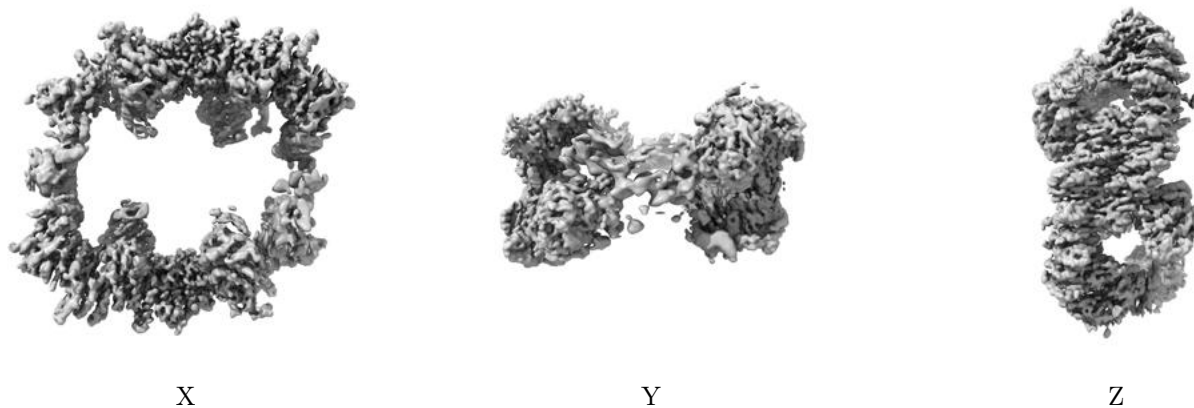


Z

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.

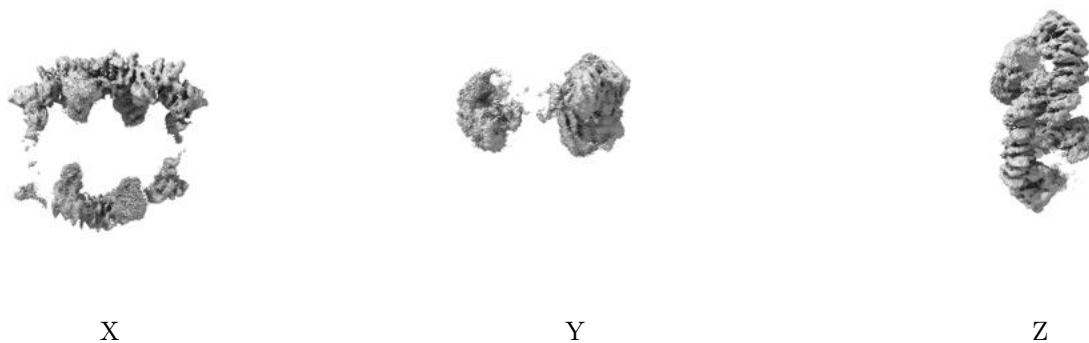
6.5 Orthogonal surface views [i](#)

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.

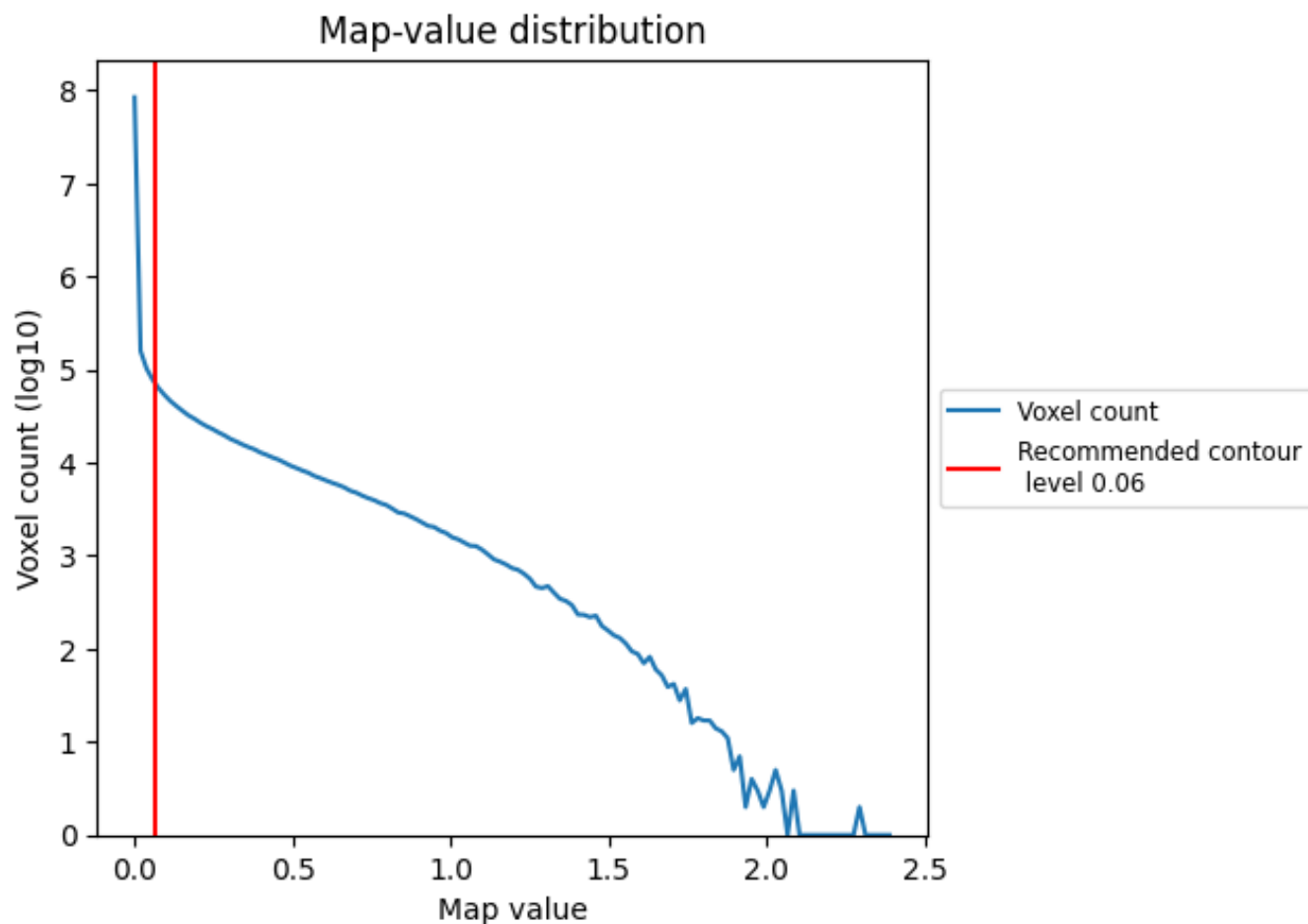
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

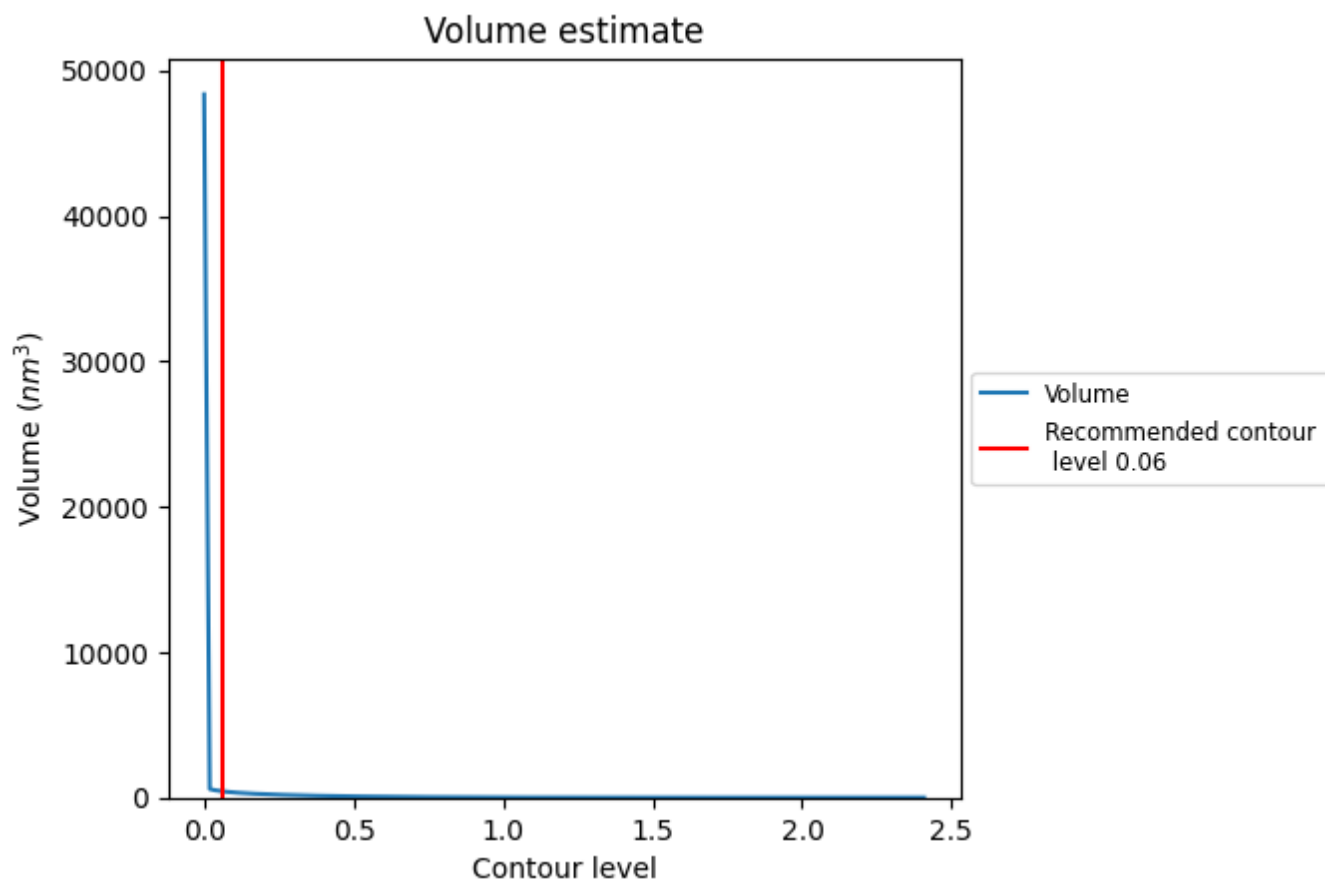
This section contains the results of statistical analysis of the map.

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.

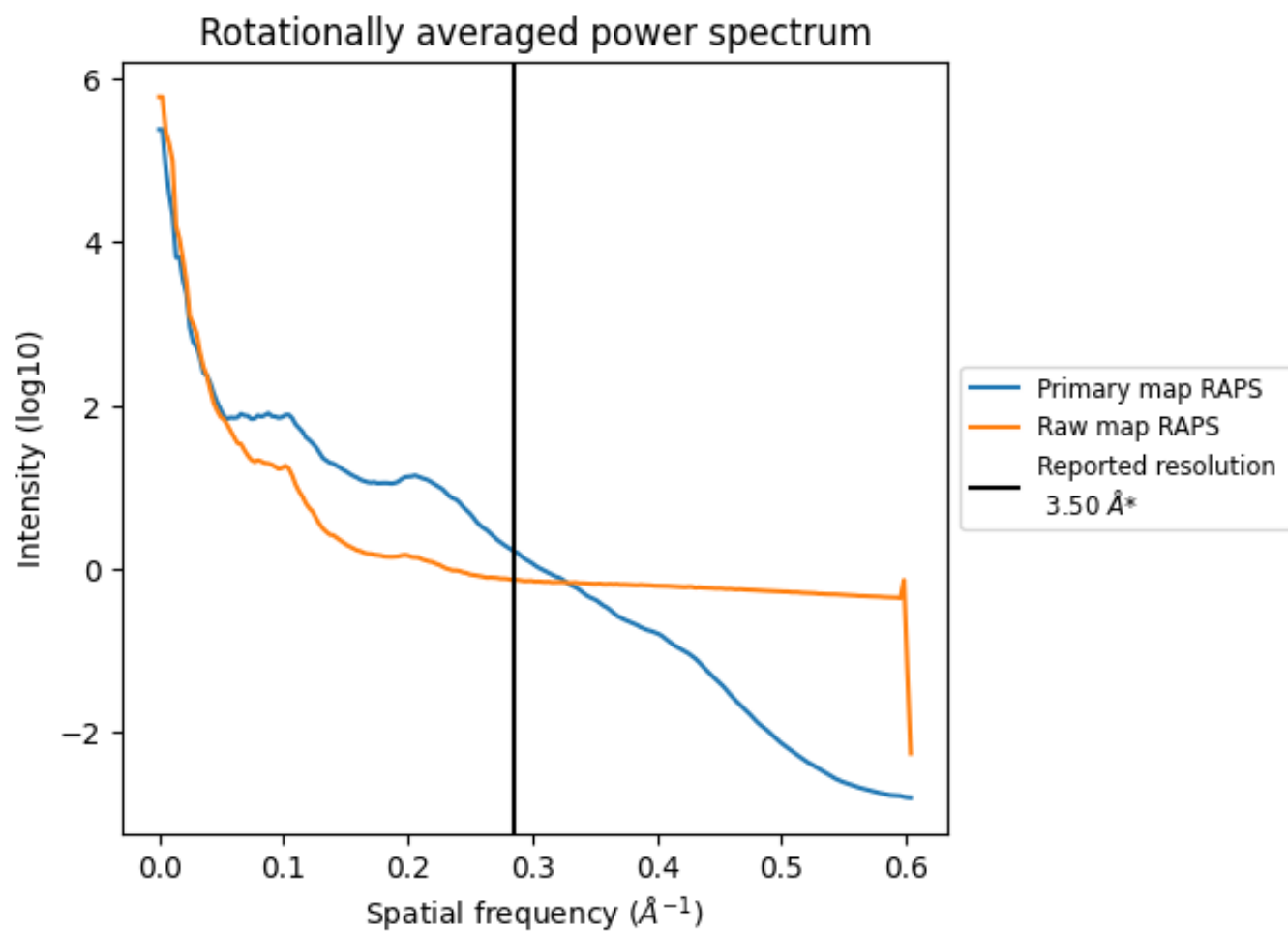
7.2 Volume estimate [i](#)



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 ⓘ

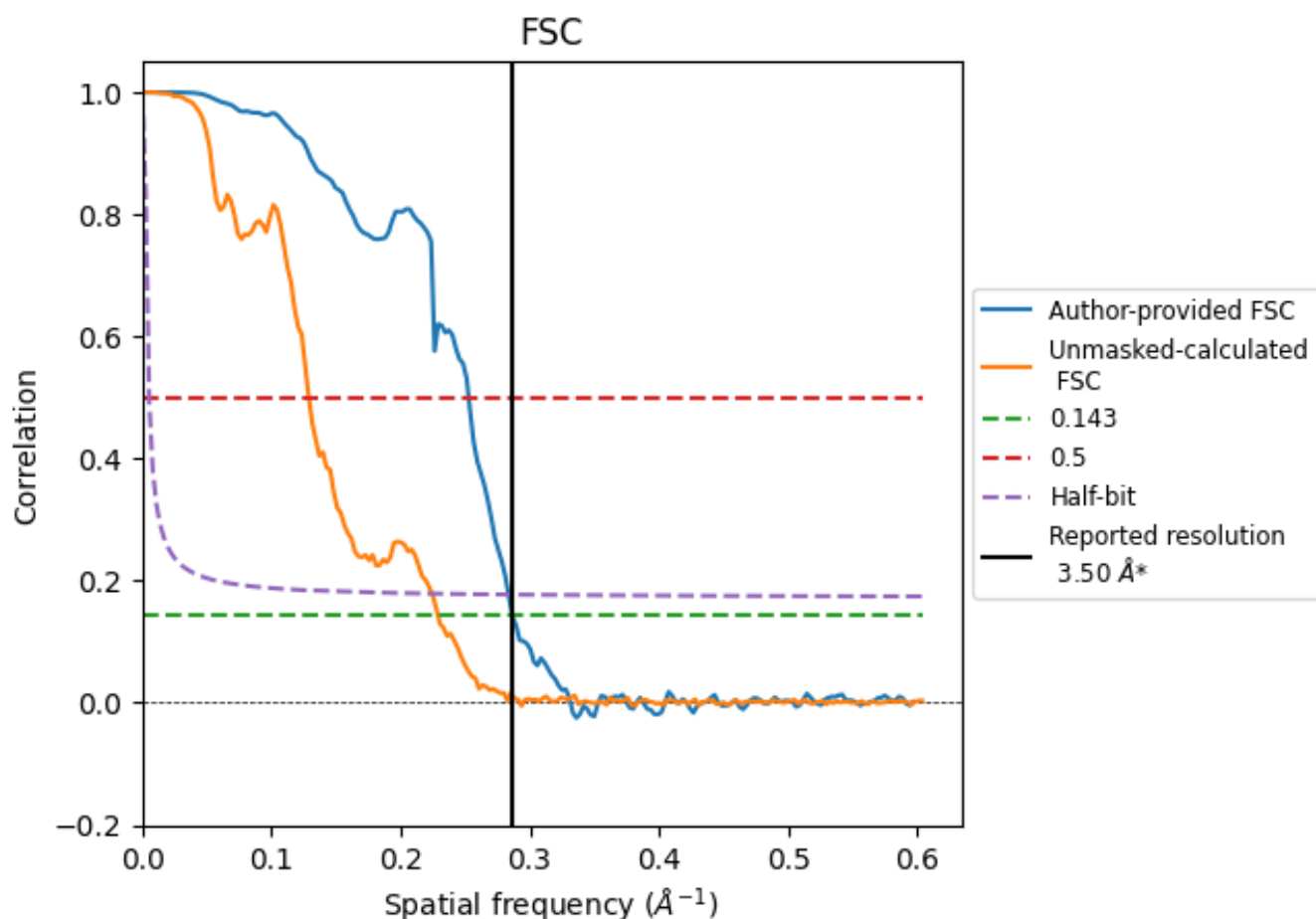


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

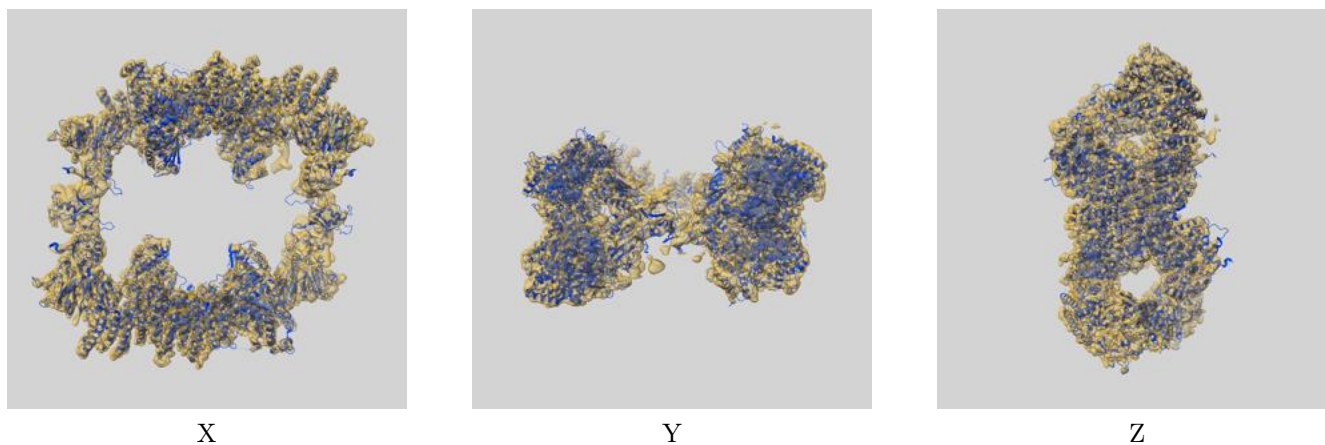
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.96	3.53
Unmasked-calculated*	4.37	7.75	4.46

*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](#)

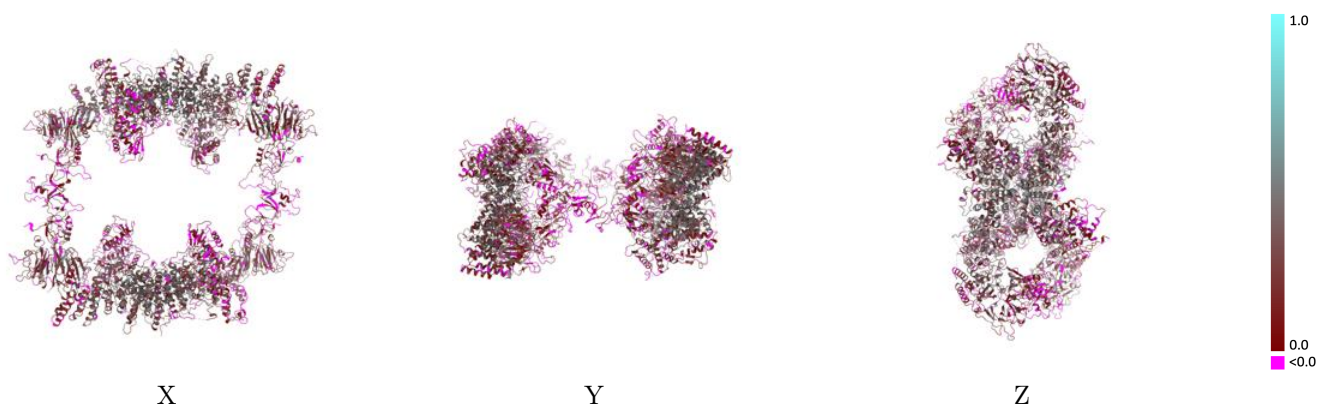
This section contains information regarding the fit between EMDB map EMD-28646 and PDB model 8EWI. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



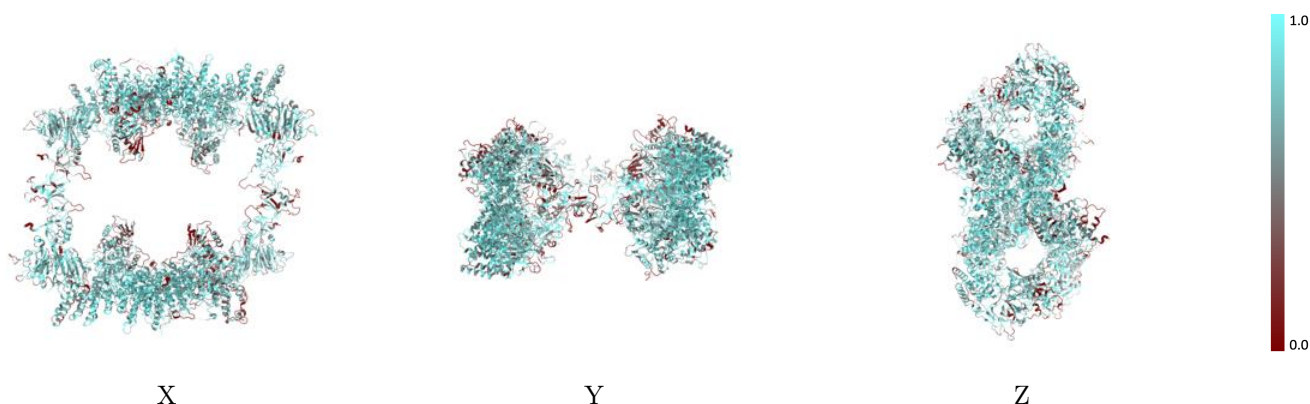
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



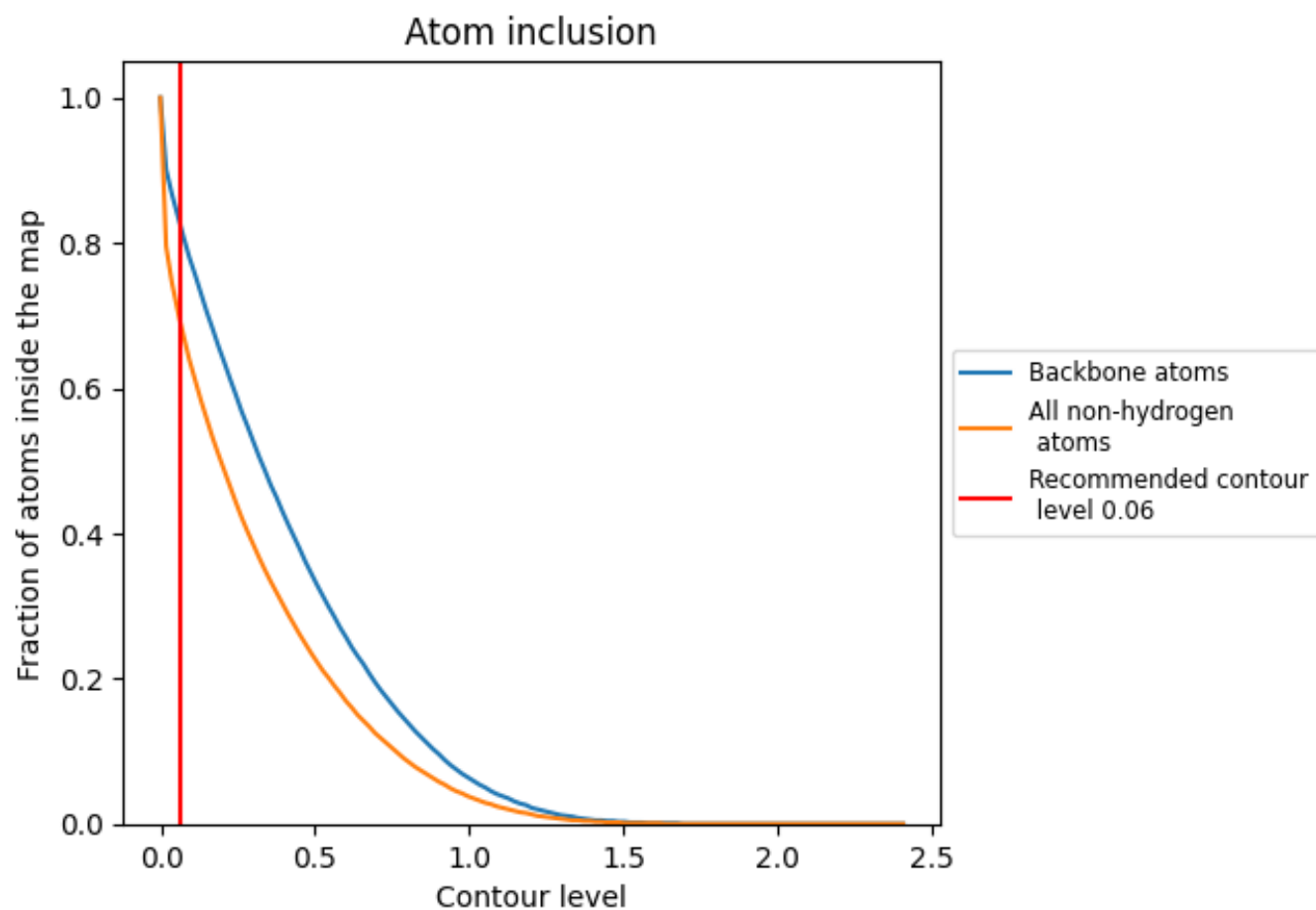
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.6960	<div></div> 0.2480
A	<div></div> 0.7200	<div></div> 0.2670
B	<div></div> 0.6930	<div></div> 0.2540
C	<div></div> 0.6820	<div></div> 0.2390
D	<div></div> 0.6870	<div></div> 0.2330

