



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:12 PM UTC

PDB ID : 9E12 / pdb\_00009e12  
EMDB ID : EMD-47381  
Title : Full-length human dynein-1 in phi conformation under Lis1 condition  
Authors : Yang, J.; Zhang, K.  
Deposited on : 2024-10-21  
Resolution : 4.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

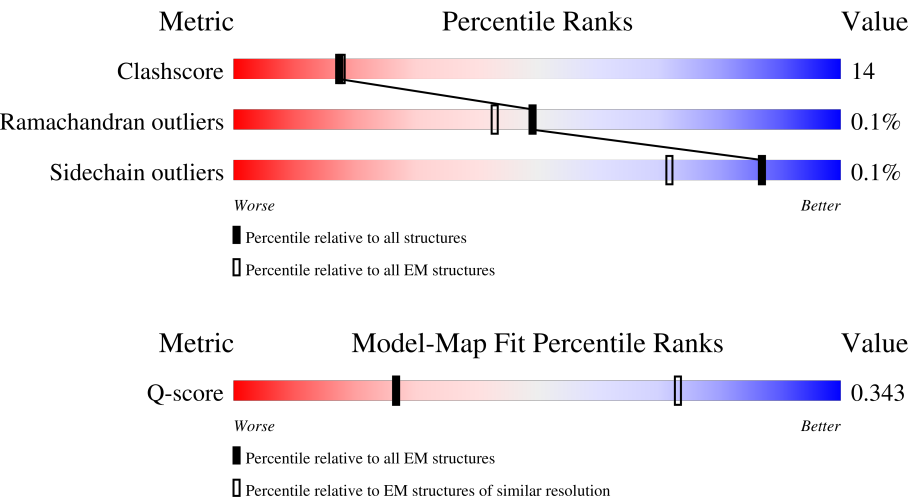
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 Å.

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




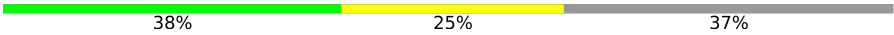






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 ( 4.00 - 5.00 )

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

Mol	Chain	Length	Quality of chain
1	A	4646	
1	B	4646	
2	C	638	
2	D	638	

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Mol	Chain	Length	Quality of chain
3	E	492	
3	F	492	
4	G	96	
4	H	96	
5	I	89	
5	J	89	
6	K	113	
6	L	113	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 89391 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4542	Total	C	N	O	S	0	0
			36692	23323	6381	6822	166		
1	B	4521	Total	C	N	O	S	0	0
			36527	23221	6349	6791	166		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		
2	D	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		

- Molecule 3 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		
3	F	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		

- Molecule 4 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
4	H	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

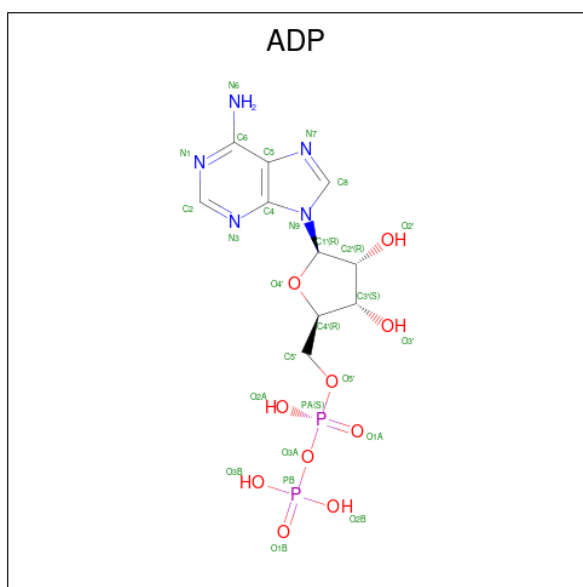
- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
5	J	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
6	L	113	Total	C	N	O	S	0	0
			872	548	142	175	7		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



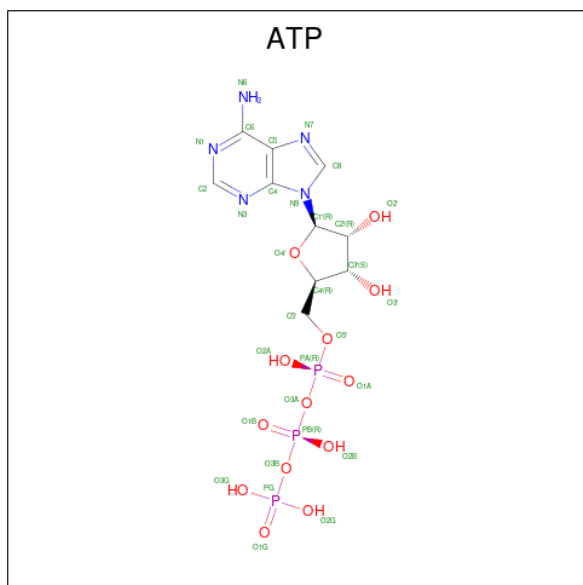
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

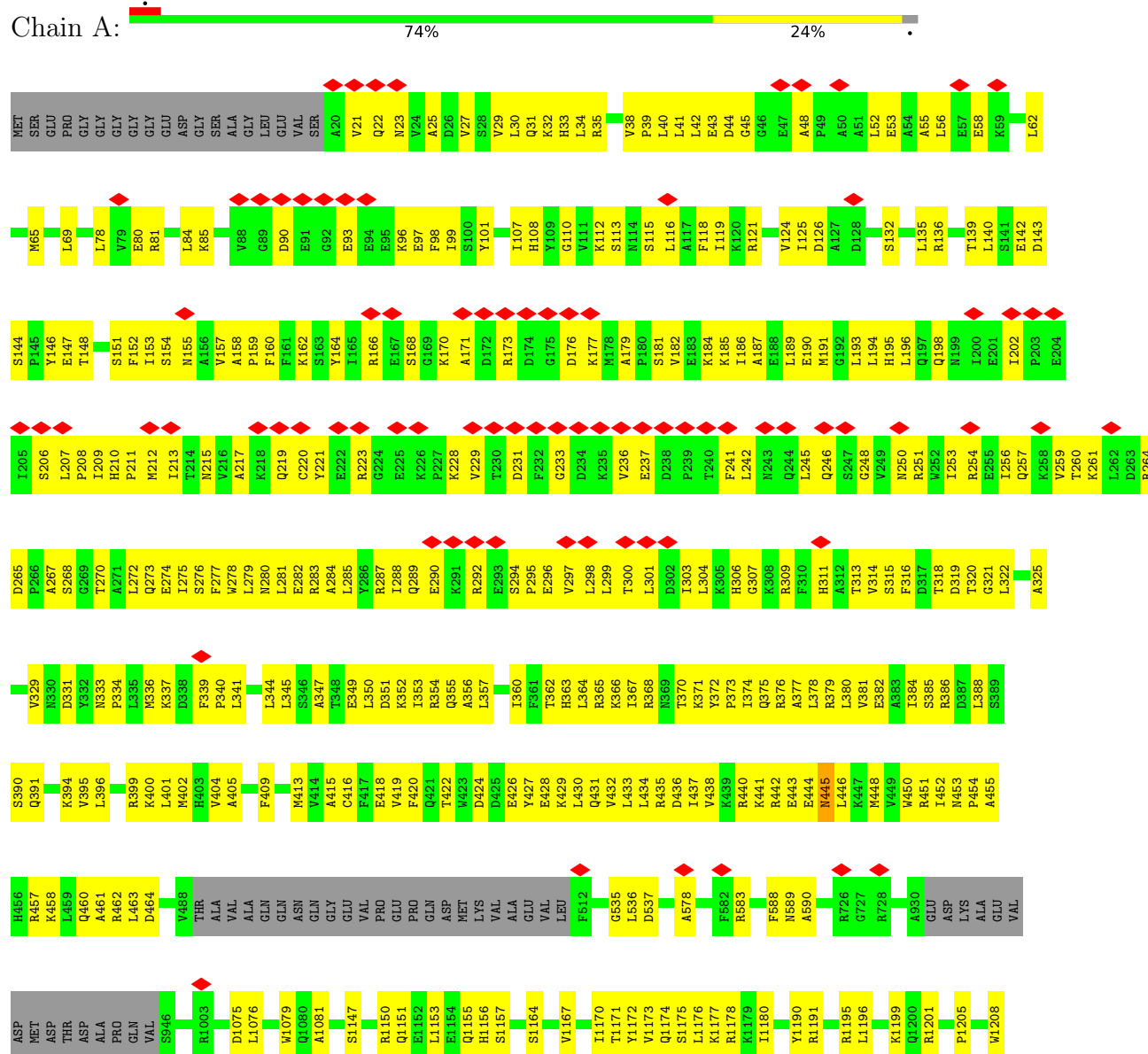
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Mg	0
			2	2	
9	B	2	Total	Mg	0
			2	2	

### 3 Residue-property plots

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

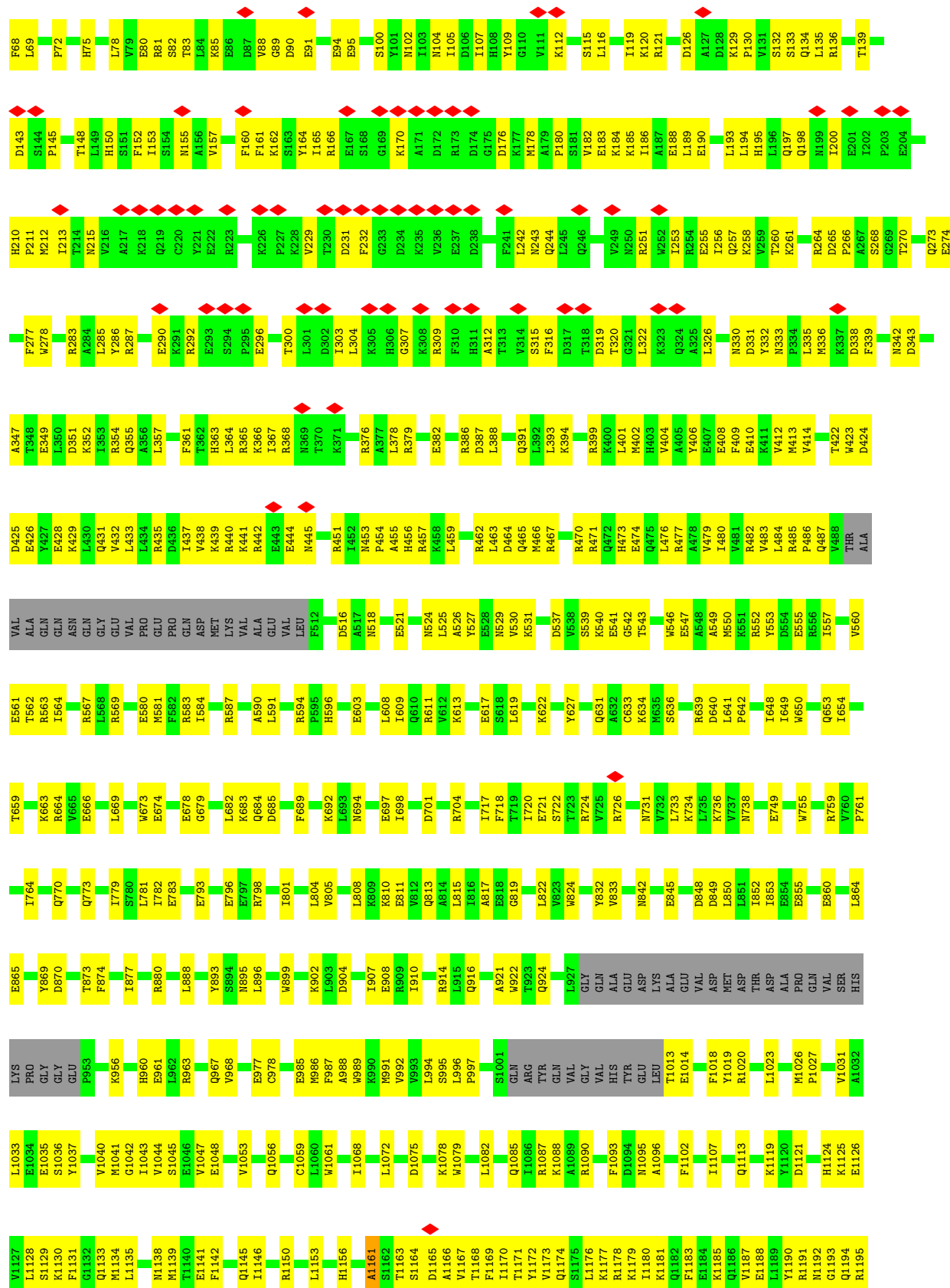
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1



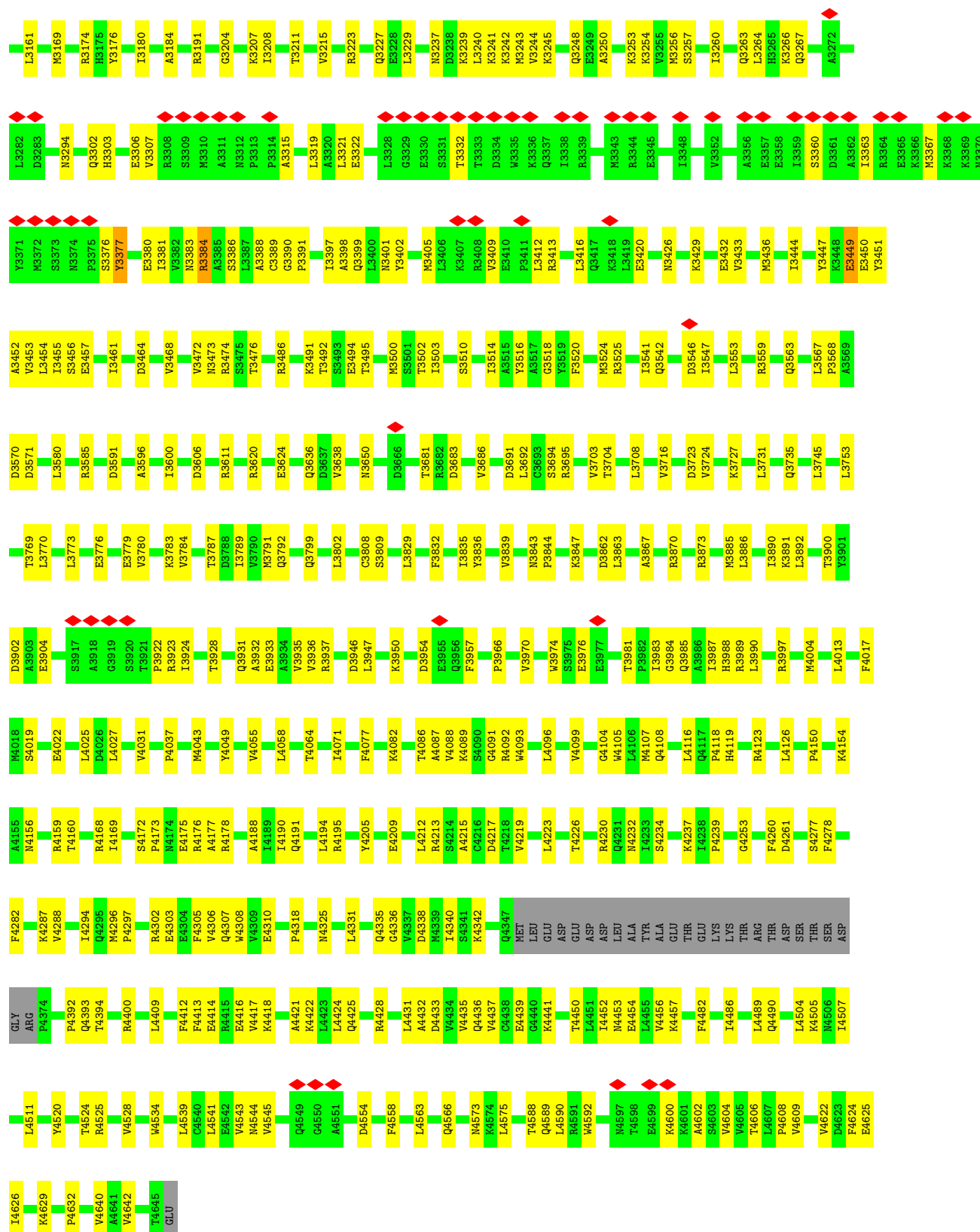
L1209	L1439	A1555	G1728	D1847	C2142	D2304	I2415	V2569	K2721	K2898	Q3038	R3174
E1215	Q1440	K1568	K1729	F1848	I1997	D2308	Q2416	T2570	P2722	D2917	Q3043	R3175
G1219	K1441	P1562	D1734	Q1850	L2001	N2314	I2422	T2572	L2723	D2917	L3044	Y3176
F1221	B1442	Q1566	T1737	V1853	V2006	L2319	M2423	T2574	R2726	I2922	D3045	L3177
M1222	A1444	R1567	Q1746	Q1856	N2012	D2321	S2429	R2576	P2732	L2933	L3180	L3180
M1225	D1448	A1577	A1747	M1861	T2017	D2324	E2444	R2576	V2733	L2934	E3048	R3191
R1226	M1457	K1580	Q1748	A1862	L2039	L2324	H2445	L2581	S2743	G2937	L3050	S3192
K1228	A1458	L1749	V1750	Q1876	S2026	E2331	L2449	V2582	I2747	T2944	Y3051	S3192
L1459	L1459	K1581	V1751	D1877	L2157	S2334	L2452	T2583	R2753	R2948	Q3057	R3196
D1229	E1461	V1582	L1752	K1878	T2042	N2338	R2453	L2583	L2769	M2953	R3060	E3196
I1232	K1464	S1583	Q1755	L1890	Q2047	F2343	L2458	L2583	M2773	L2956	M3068	R3197
Q1233	Q1465	L1584	I1756	P1907	N2053	Q2346	M2461	L2592	F2776	T2961	P3070	Q3198
E1262	V1469	V1591	E1760	G1911	T2061	D2347	L2462	L2592	Y2779	Y2967	T3081	V3212
M1270	L1477	L1619	E1763	S1915	E2062	L2348	H2463	L2605	M2779	T2968	L3085	V3212
L1306	V1478	R1623	T1764	E1765	E2063	C2359	Q2464	L2614	F2784	G2969	T3085	Q3214
D1308	L1486	V1632	M1769	E1934	L2065	G2360	A2465	E2615	Y2794	D2973	T3099	Q3214
R1357	I1487	D1633	G1770	D1937	N2067	N2361	Q2482	E2616	M2799	E2974	E3100	V3215
P1374	D1491	D1634	G1772	F1945	K2068	D2372	Q2486	L2620	L2813	D2975	Q3104	E3217
A1375	D1492	D1634	G1773	G1947	V2070	L2382	E2487	L2623	L2816	L2976	T3110	R3219
Q1378	L1493	L1638	A1775	Q1950	P2071	L2382	Q2491	P2628	E2819	R2977	M3113	E3228
Y1380	V1497	V1647	A1776	V1951	F2072	D2388	R2492	E2629	G2820	K2989	D3114	L3229
A1381	I1501	L1650	P1777	D1959	K2073	E2389	Y2493	L2630	L2824	N2998	L3115	E3230
R1388	V1504	M1657	S1780	E1959	L2075	GLY	D2505	T2634	L2824	L3008	D3124	V3231
M1398	M1507	V1661	V1785	F1960	Q2079	GLU	K2509	K2667	L2837	D3001	Y3125	K3242
L1399	Y1513	I1676	M1798	M1961	R2091	ASP	M2510	V2660	V2837	S3002	V3129	K3242
V1400	F1516	P1679	E1799	L1963	K2094	ALA	E2513	C2663	V2838	G3003	Y3130	M3243
E1517	E1517	E1680	Q1800	E1964	S2094	ARG	E2517	E2665	E2839	F3004	D3131	V3244
D1519	D1518	E1680	P1802	R1965	V2096	ARG	Y2517	L2666	R2843	L3005	K3132	K3245
W1523	D1525	K1707	L1803	M1967	L2097	LYS	P2517	I2667	E2848	M3008	L3133	Q3248
E1524	K1526	K1707	R1806	Q1973	V2098	LYS	I2521	L2668	T2852	L3011	Q3135	E3249
W1537	W1537	V1711	K1807	Q1977	K2104	GLU	P2527	M2671	L2855	L3012	P3136	E3251
I1538	W1537	V1711	H1810	I1978	R2107	ASP	N2531	D2672	R2863	E3016	R3140	K3252
D1539	W1537	E1719	L1815	H1985	T2108	GLU	E2538	K2673	A2866	V3017	E3141	K3253
V1540	I1538	S1720	F1836	S1986	E2120	GLU	W2545	T2676	K2879	L3020	V3148	V3255
R1543	I1538	V1721	E1837	N1987	E2133	ALA	W2548	F2682	K2892	Y3026	F3149	K3256
Y1546	D1539	E1722	M1838	N1988	Q2134	ALA	W2548	Q2698	Y2896	R3030	Q3257	Q3257
	V1540	V1724	L1839	Y1990	E2135	P2411	Q2554	Q2707	R2896	T3031	V3150	Q3258
			S1840	D1991	L2136	M2412				L3153	T3153	E3259
			R1843	K1992	L2137					L3154	L3154	T3260
				T1993	T2138					E3035	Q3263	L3264





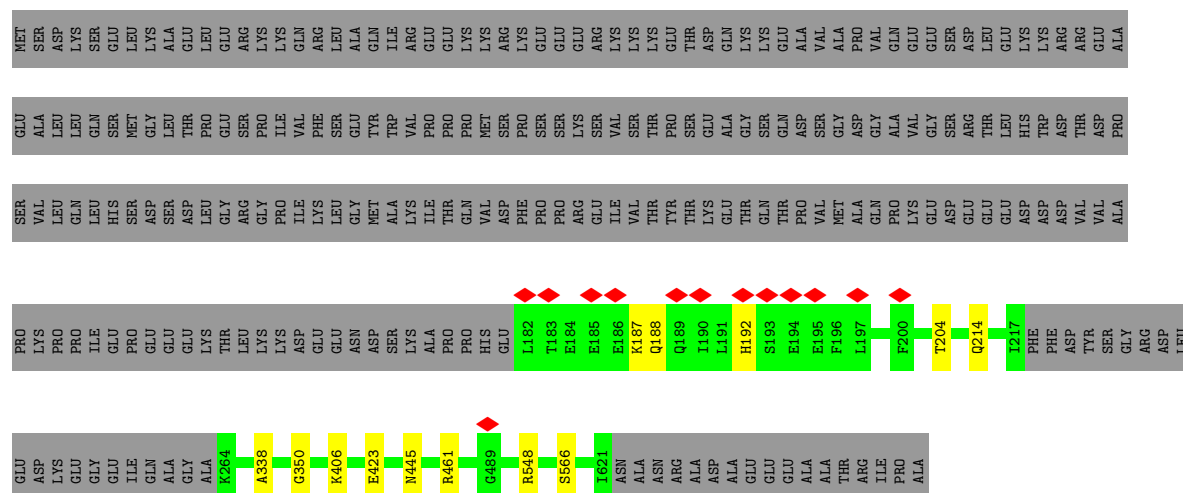






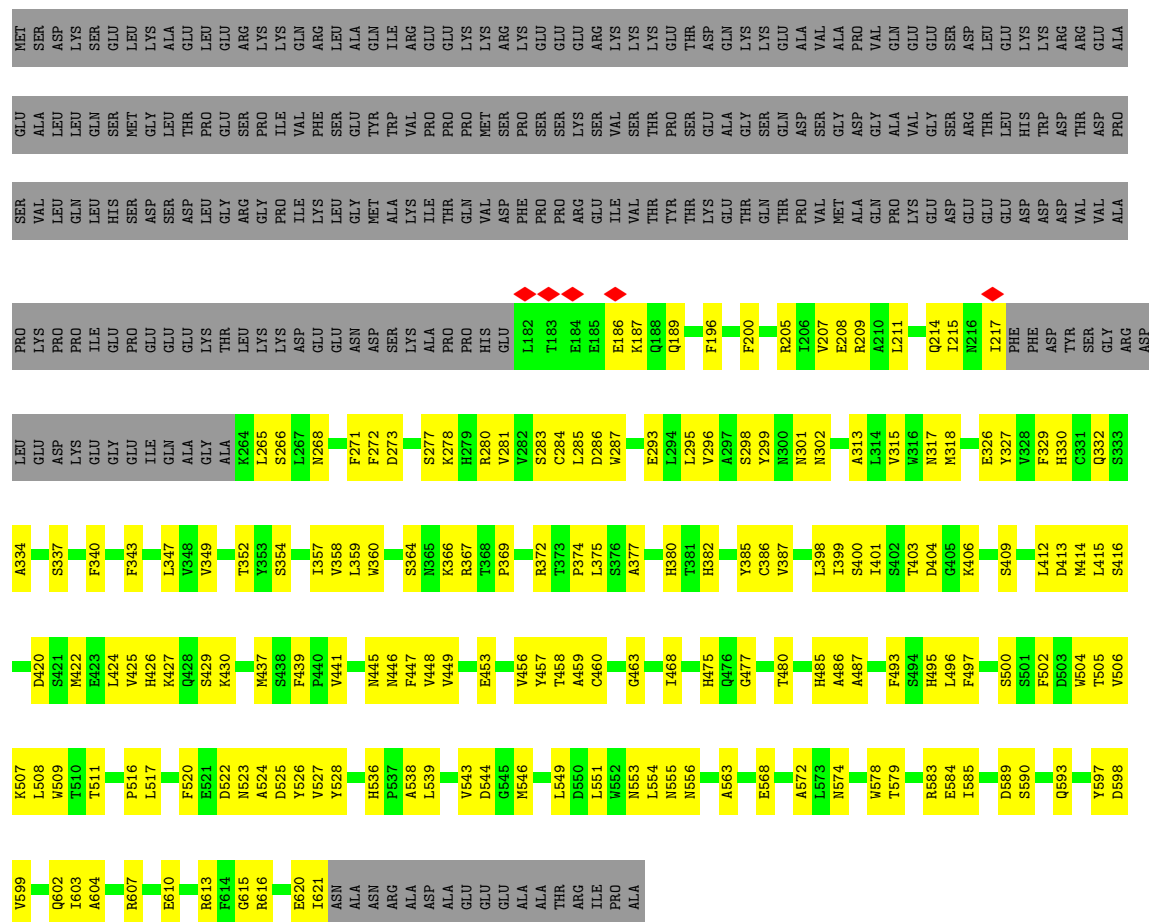
• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

Chain C: 60% 38%



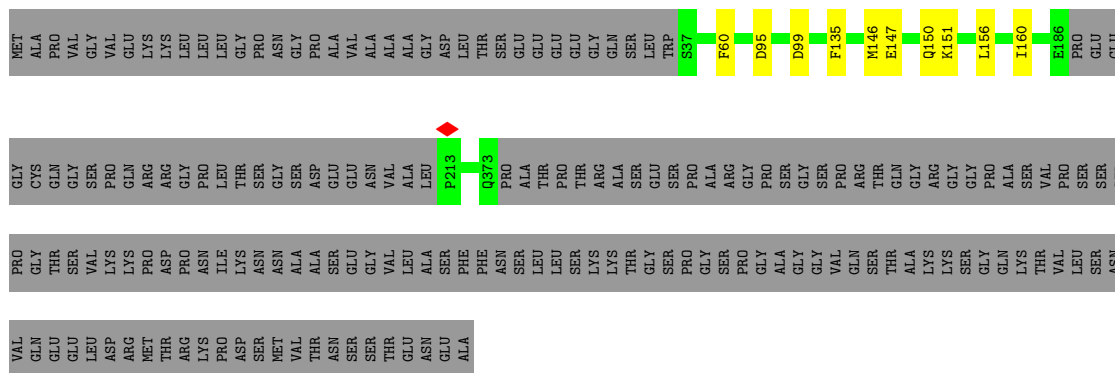
• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

Chain D: 35% 27% 38%

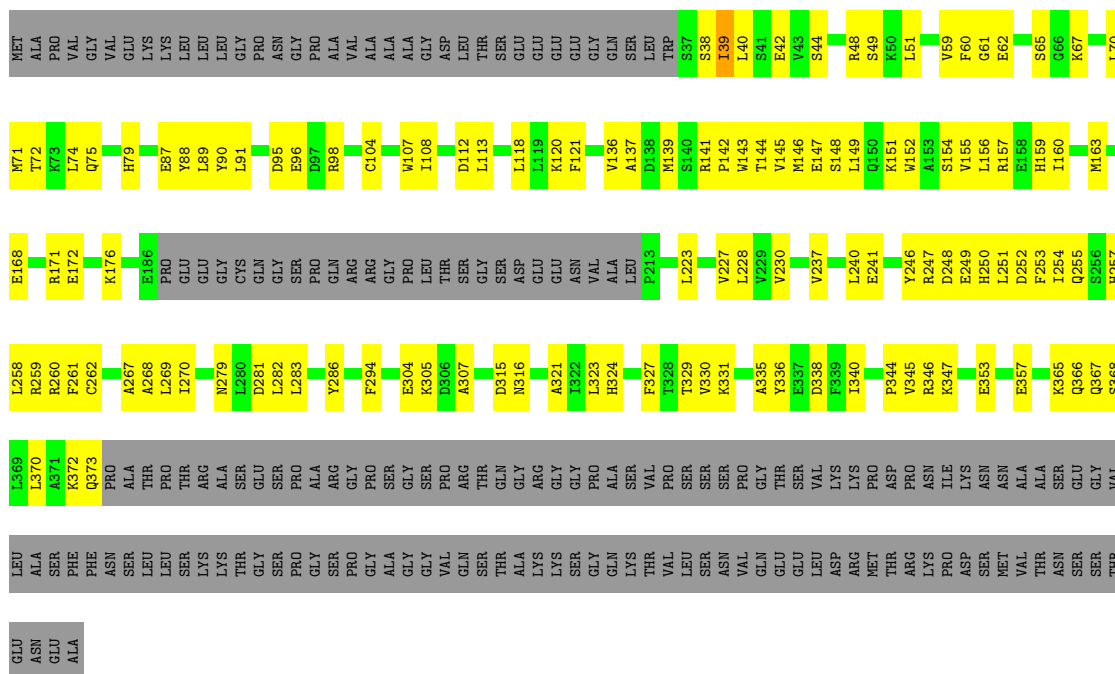
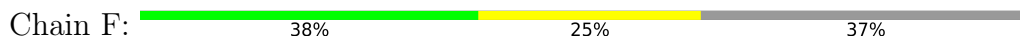


• Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

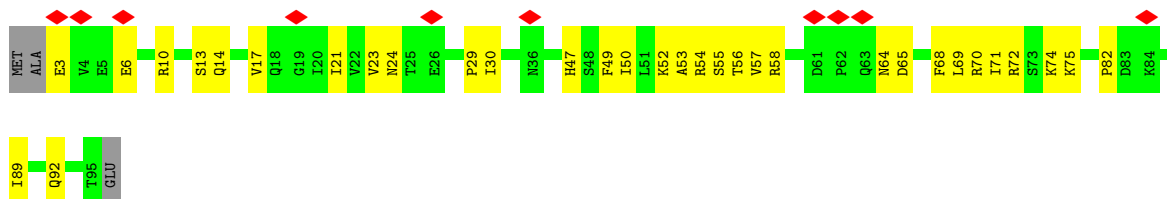
Chain E: 61% 37%



- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

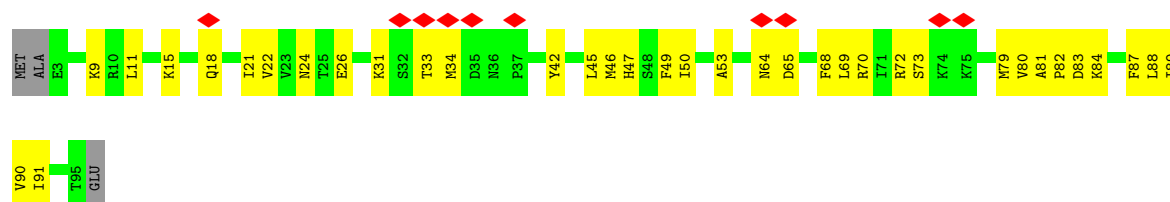


- Molecule 4: Dynein light chain roadblock-type 1

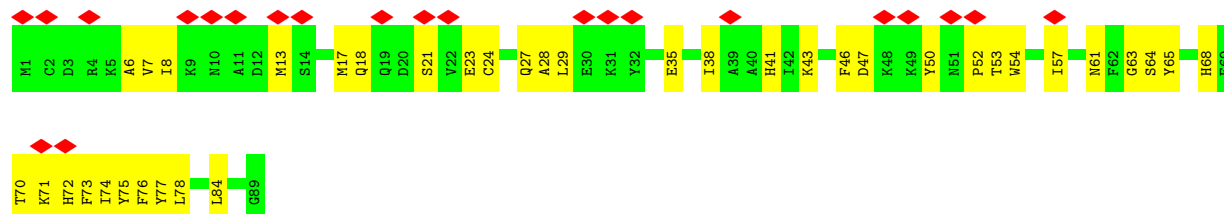


- Molecule 4: Dynein light chain roadblock-type 1

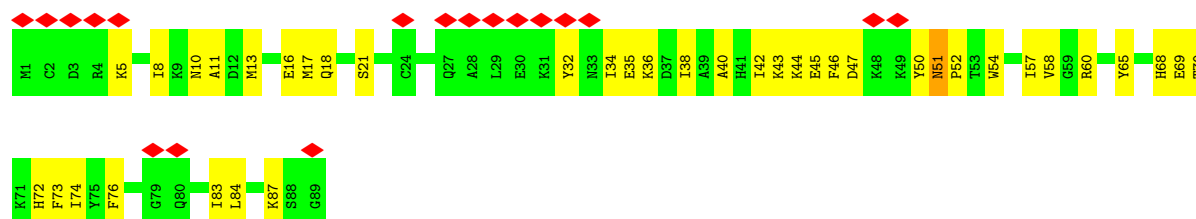




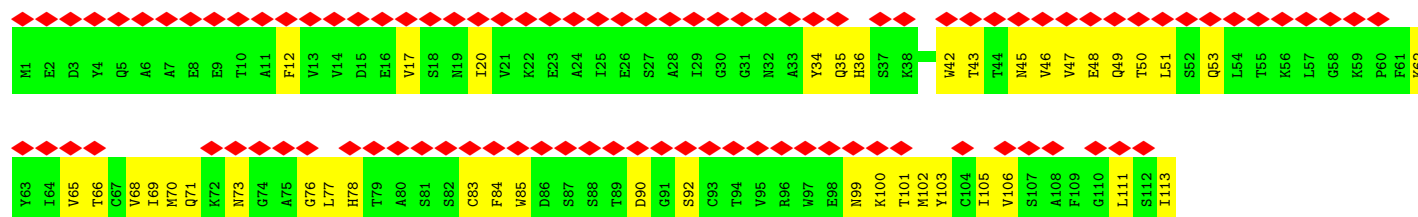
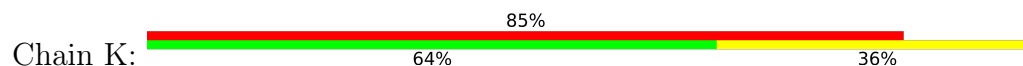
• Molecule 5: Dynein light chain 1, cytoplasmic



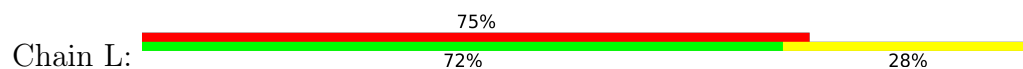
• Molecule 5: Dynein light chain 1, cytoplasmic

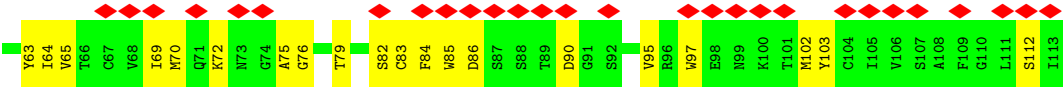


• Molecule 6: Dynein light chain Tctex-type 1



• Molecule 6: Dynein light chain Tctex-type 1







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103097	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.240	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	729.12, 729.12, 729.12	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.736, 1.736, 1.736	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ATP

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	0.19	0/37419	0.42	1/50625 (0.0%)
1	B	0.15	0/37249	0.37	2/50395 (0.0%)
2	C	0.18	0/3195	0.40	0/4351
2	D	0.15	0/3195	0.41	0/4351
3	E	0.16	0/2573	0.38	0/3473
3	F	0.16	0/2573	0.38	0/3473
4	G	0.14	0/752	0.37	0/1017
4	H	0.15	0/752	0.42	0/1017
5	I	0.21	0/744	0.48	0/997
5	J	0.17	0/744	0.47	0/997
6	K	0.15	0/888	0.40	0/1203
6	L	0.15	0/888	0.38	0/1203
All	All	0.17	0/90972	0.40	3/123102 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3449	GLU	CA-C-N	-7.56	108.82	120.31
1	B	3449	GLU	C-N-CA	-7.56	108.82	120.31
1	A	1402	GLU	N-CA-C	-6.67	106.35	114.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3438	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36692	0	36962	848	0
1	B	36527	0	36809	988	0
2	C	3112	0	2964	10	0
2	D	3112	0	2964	129	0
3	E	2518	0	2525	5	0
3	F	2518	0	2525	99	0
4	G	742	0	768	29	0
4	H	742	0	768	32	0
5	I	728	0	714	41	0
5	J	728	0	714	51	0
6	K	872	0	846	37	0
6	L	872	0	846	32	0
7	A	81	0	36	2	0
7	B	81	0	36	2	0
8	A	31	0	12	0	0
8	B	31	0	12	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
All	All	89391	0	89501	2182	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 14.

All (2182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3257:SER:HA	1:A:3260:ILE:HD12	1.20	1.10
1:A:185:LYS:HE3	1:B:189:LEU:HD13	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3441:GLU:HA	1:A:3444:ILE:HD12	1.54	0.89
1:B:333:ASN:HA	1:B:336:MET:HE3	1.56	0.88
1:A:457:ARG:O	1:A:461:ALA:N	2.08	0.87
1:A:3256:MET:HG2	1:A:3433:VAL:HG21	1.57	0.86
1:A:1567:ARG:NH1	1:B:3043:MET:SD	2.48	0.86
1:A:4600:LYS:HZ3	1:A:4604:VAL:HB	1.41	0.85
1:A:378:LEU:HD23	1:A:450:TRP:CD1	2.12	0.84
1:A:1478:VAL:HG21	1:A:1488:ARG:HE	1.44	0.83
1:A:164:TYR:HE1	1:B:145:PRO:HG2	1.41	0.83
1:A:1174:GLN:HA	1:A:1177:LYS:HG2	1.62	0.82
1:B:3257:SER:HA	1:B:3260:ILE:HD12	1.60	0.82
1:A:2423:MET:HE3	1:A:2462:LEU:HD13	1.60	0.81
1:B:3044:LEU:HD22	1:B:3049:GLU:HG3	1.61	0.81
1:A:1222:ASN:HA	1:A:1225:MET:HE3	1.62	0.81
1:B:853:ILE:HG21	1:B:888:LEU:HD21	1.62	0.81
1:B:2686:MET:HE2	1:B:2708:PHE:HZ	1.45	0.81
1:B:526:ALA:O	1:B:553:TYR:OH	1.99	0.80
1:B:4092:ARG:HE	1:B:4093:TRP:H	1.26	0.80
4:G:57:VAL:HG21	4:G:64:ASN:HD22	1.46	0.79
1:A:182:VAL:HA	1:A:185:LYS:HG2	1.65	0.78
1:B:91:GLU:OE1	1:B:243:ASN:ND2	2.15	0.78
3:F:160:ILE:HA	3:F:163:MET:HE3	1.65	0.78
1:A:441:LYS:HA	1:A:445:ASN:H	1.48	0.78
5:I:13:MET:HE2	5:I:74:ILE:HB	1.66	0.77
1:A:285:LEU:HA	1:A:288:ILE:HG22	1.65	0.77
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.67	0.77
1:A:1229:ASP:O	1:A:1233:GLN:NE2	2.18	0.76
1:A:3194:LEU:HD12	1:A:3197:GLN:HE21	1.49	0.76
1:B:874:PHE:HB3	1:B:996:LEU:HD21	1.68	0.76
1:B:484:LEU:HD13	1:B:564:ILE:HG12	1.67	0.76
2:D:315:VAL:HB	2:D:327:TYR:HB2	1.66	0.76
1:B:669:LEU:HD22	1:B:673:TRP:HB3	1.68	0.76
1:B:399:ARG:NH2	1:B:408:GLU:OE1	2.19	0.76
1:B:1460:GLU:OE1	1:B:1464:LYS:NZ	2.19	0.76
1:B:1514:LYS:HA	1:B:1517:GLU:HG3	1.68	0.76
1:A:314:VAL:O	1:A:318:THR:N	2.20	0.75
1:A:147:GLU:HA	1:A:196:LEU:HD13	1.69	0.75
1:A:426:GLU:HA	1:A:429:LYS:HB2	1.68	0.75
1:A:290:GLU:HA	1:A:321:GLY:HA2	1.69	0.75
1:A:1460:GLU:OE1	1:A:1464:LYS:NZ	2.18	0.75
1:B:801:ILE:HD11	1:B:850:LEU:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:GLN:NE2	1:B:685:ASP:OD1	2.21	0.74
1:A:115:SER:H	1:A:140:LEU:HB3	1.51	0.74
3:F:72:THR:HG21	3:F:79:HIS:HA	1.69	0.74
1:B:3970:VAL:HB	1:B:3989:ARG:HD3	1.70	0.74
1:A:378:LEU:HD12	1:A:381:VAL:HB	1.69	0.74
1:A:333:ASN:HD21	1:A:366:LYS:HG3	1.51	0.74
1:B:78:LEU:HD11	1:B:115:SER:HB2	1.68	0.73
1:A:132:SER:O	1:A:136:ARG:NH2	2.20	0.73
1:B:4600:LYS:HD3	1:B:4602:ALA:H	1.53	0.73
1:A:160:PHE:HB2	1:B:107:ILE:HD12	1.70	0.73
1:A:84:LEU:HB3	1:A:98:PHE:HB3	1.70	0.73
1:B:483:VAL:O	1:B:567:ARG:NH1	2.22	0.72
1:B:4453:ASN:OD1	1:B:4457:LYS:NZ	2.22	0.72
1:B:4541:LEU:HD11	1:B:4590:LEU:HB3	1.71	0.72
1:A:375:GLN:HA	1:A:450:TRP:HB3	1.71	0.72
1:A:1225:MET:HG3	1:A:1226:ARG:HH21	1.53	0.72
1:B:266:PRO:HB3	1:B:376:ARG:HG3	1.72	0.72
1:B:3745:LEU:HD11	1:B:3776:GLU:HG2	1.71	0.72
1:B:3223:ARG:O	1:B:3227:GLN:NE2	2.23	0.72
1:B:4432:ALA:O	1:B:4436:GLN:NE2	2.23	0.72
1:B:4421:ALA:O	1:B:4425:GLN:NE2	2.23	0.72
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.71	0.71
1:B:413:MET:HE1	1:B:463:LEU:HB3	1.70	0.71
1:A:44:ASP:HB2	1:B:130:PRO:HB3	1.72	0.71
1:B:162:LYS:HG2	1:B:166:ARG:HE	1.56	0.71
1:B:1196:LEU:HD23	1:B:1199:LYS:HE2	1.72	0.71
1:B:3451:TYR:HA	1:B:3454:LEU:HG	1.72	0.71
1:B:649:ILE:O	1:B:653:GLN:HG2	1.90	0.71
1:B:130:PRO:HB2	1:B:133:SER:HB2	1.70	0.71
2:D:553:ASN:ND2	2:D:556:ASN:OD1	2.23	0.71
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.24	0.71
1:B:4303:GLU:O	1:B:4307:GLN:NE2	2.23	0.71
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.72	0.71
1:B:516:ASP:HA	1:B:563:ARG:HH12	1.55	0.71
1:A:81:ARG:HD3	1:A:99:ILE:HG13	1.73	0.71
6:L:25:ILE:HG23	6:L:29:ILE:HD12	1.73	0.70
1:A:4052:SER:HA	1:A:4095:MET:HE1	1.73	0.70
5:I:43:LYS:NZ	5:I:47:ASP:OD2	2.24	0.70
1:B:3239:LYS:HG2	1:B:3451:TYR:CZ	2.25	0.70
1:B:1037:TYR:HB3	3:F:121:PHE:CZ	2.27	0.70
1:A:378:LEU:HB3	1:A:450:TRP:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1085:GLN:HE22	3:F:39:ILE:HD12	1.57	0.70
1:B:1596:GLY:HA2	1:B:1599:ARG:HH12	1.56	0.70
1:B:119:ILE:O	1:B:136:ARG:HB3	1.91	0.70
1:B:722:SER:HB3	1:B:731:ASN:HD21	1.56	0.70
1:A:1195:ARG:NH2	3:F:96:GLU:O	2.24	0.70
1:A:378:LEU:HD23	1:A:450:TRP:HD1	1.57	0.69
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.73	0.69
1:B:243:ASN:OD1	1:B:309:ARG:NH2	2.25	0.69
1:B:266:PRO:HB2	1:B:379:ARG:HB2	1.72	0.69
1:B:399:ARG:HH22	1:B:404:VAL:HG11	1.57	0.69
1:B:150:HIS:HB2	1:B:193:LEU:HB3	1.74	0.69
1:B:1973:GLN:NE2	1:B:1977:CYS:SG	2.66	0.69
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.26	0.69
3:F:259:ARG:HH11	3:F:323:LEU:HD22	1.58	0.69
4:G:54:ARG:HH12	4:G:65:ASP:HA	1.56	0.69
6:L:29:ILE:O	6:L:32:ASN:ND2	2.24	0.69
1:B:639:ARG:HH22	2:D:574:ASN:HD21	1.41	0.69
1:B:2481:MET:HE1	1:B:2485:GLN:HG2	1.73	0.69
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.24	0.69
1:B:456:HIS:HA	1:B:459:LEU:HB2	1.73	0.69
1:B:3559:ARG:O	1:B:3563:GLN:NE2	2.25	0.69
4:H:21:ILE:HG12	4:H:89:ILE:HD11	1.75	0.69
1:A:159:PRO:HD2	1:B:107:ILE:HD11	1.75	0.69
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.74	0.69
1:A:193:LEU:HD13	1:B:182:VAL:HG11	1.75	0.68
1:B:1173:VAL:HG22	1:B:1177:LYS:HE3	1.75	0.68
1:B:3580:LEU:HD13	1:B:3600:ILE:HD11	1.73	0.68
1:A:368:ARG:NH2	1:A:436:ASP:O	2.22	0.68
2:D:445:ASN:HD21	2:D:463:GLY:H	1.41	0.68
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.26	0.68
1:B:386:ARG:NH2	1:B:453:ASN:O	2.27	0.68
1:B:1567:ARG:O	1:B:1571:ILE:HG12	1.93	0.68
1:B:2185:VAL:HG22	1:B:2243:ARG:HH21	1.58	0.68
1:A:374:ILE:HD11	1:A:440:ARG:NH1	2.07	0.68
1:A:418:GLU:O	1:A:422:THR:OG1	2.04	0.68
1:A:331:ASP:HA	1:A:370:THR:HB	1.76	0.68
1:A:364:LEU:HA	1:A:367:ILE:HG22	1.75	0.68
1:B:466:MET:HE3	1:B:470:ARG:HG3	1.76	0.68
1:B:798:ARG:HH12	1:B:855:GLU:HB3	1.59	0.68
1:B:2623:SER:OG	1:B:3081:THR:O	2.12	0.68
1:A:1562:PRO:O	1:A:1566:GLN:NE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:PRO:HD2	1:B:764:ILE:HD12	1.76	0.67
2:D:347:LEU:HD23	2:D:359:LEU:HD11	1.76	0.67
1:A:3872:ALA:HB1	1:A:3880:HIS:CD2	2.29	0.67
1:B:2000:GLU:OE1	1:B:2005:GLN:NE2	2.27	0.67
1:B:4150:PRO:O	1:B:4195:ARG:NH2	2.24	0.67
1:B:2816:LEU:HD12	1:B:2817:PRO:HD2	1.77	0.67
3:F:113:LEU:HD21	3:F:151:LYS:HD2	1.76	0.67
1:B:482:ARG:O	1:B:487:GLN:NE2	2.28	0.67
1:B:441:LYS:O	1:B:445:ASN:N	2.26	0.67
1:B:3360:SER:HA	1:B:3363:ILE:HD12	1.76	0.67
1:B:3638:VAL:HG12	1:B:3681:THR:HB	1.77	0.67
5:I:57:ILE:HD13	5:J:57:ILE:HD12	1.76	0.67
1:A:195:HIS:CE1	1:A:265:ASP:HB2	2.30	0.67
1:A:3257:SER:CA	1:A:3260:ILE:HD12	2.12	0.67
1:B:2488:ARG:NH2	1:B:2544:GLU:OE2	2.27	0.67
5:J:58:VAL:HG22	5:J:83:ILE:HG12	1.77	0.67
1:B:3983:ILE:O	1:B:3987:ILE:HD12	1.94	0.67
1:A:337:LYS:HZ3	1:A:363:HIS:HB3	1.60	0.67
1:A:2660:VAL:HG22	1:A:2707:GLN:HB3	1.77	0.67
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.76	0.67
1:A:2623:SER:OG	1:A:3081:THR:O	2.13	0.66
1:B:569:ARG:NH1	1:B:603:GLU:OE1	2.28	0.66
1:A:42:LEU:HB3	1:A:81:ARG:HH21	1.58	0.66
1:B:960:HIS:ND1	1:B:978:CYS:SG	2.68	0.66
2:D:349:VAL:HG21	2:D:398:LEU:HD11	1.75	0.66
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.76	0.66
1:B:1218:TRP:O	1:B:1222:ASN:ND2	2.28	0.66
1:B:3799:GLN:HA	1:B:3802:LEU:HD23	1.77	0.66
1:B:4037:PRO:HB2	1:B:4118:PRO:HG2	1.78	0.66
1:B:4511:LEU:HD12	1:B:4563:LEU:HD21	1.76	0.66
3:F:62:GLU:HG3	3:F:65:SER:HB2	1.76	0.66
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.77	0.66
1:B:343:ASP:OD1	1:B:352:LYS:NZ	2.29	0.66
1:B:1769:MET:HE2	1:B:1776:ALA:HA	1.77	0.66
1:A:119:ILE:HD12	1:B:155:ASN:HB2	1.77	0.66
1:A:2776:PHE:HA	1:A:2779:MET:HE2	1.76	0.66
1:A:2091:ARG:NH2	7:A:4701:ADP:O2A	2.29	0.66
1:A:2672:ASP:OD2	1:A:2673:LYS:N	2.29	0.66
1:B:1486:LEU:HD22	1:B:1541:GLN:HG3	1.78	0.66
1:B:2447:MET:HE1	1:B:2723:LEU:HD12	1.76	0.66
1:A:337:LYS:HZ1	1:A:364:LEU:N	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1680:GLU:OE1	1:A:1680:GLU:N	2.27	0.66
1:B:379:ARG:NH2	1:B:451:ARG:O	2.28	0.66
1:B:2686:MET:HE2	1:B:2708:PHE:CZ	2.28	0.66
1:B:3114:ASP:O	1:B:3140:ARG:NH2	2.28	0.66
1:A:2934:LEU:HD11	1:A:3068:MET:HE3	1.78	0.66
1:B:195:HIS:O	1:B:198:GLN:NE2	2.29	0.66
1:B:330:ASN:HA	1:B:333:ASN:HB2	1.77	0.66
1:A:285:LEU:HD21	1:A:329:VAL:HG11	1.77	0.66
1:A:370:THR:O	1:A:440:ARG:NH2	2.29	0.66
1:A:3239:LYS:HG2	1:A:3451:TYR:CE2	2.31	0.66
1:A:265:ASP:OD1	1:A:376:ARG:NH2	2.28	0.66
1:A:3257:SER:HA	1:A:3260:ILE:CD1	2.13	0.66
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.78	0.66
1:B:4104:GLY:HA2	1:B:4107:MET:HE3	1.77	0.66
1:A:1962:ARG:NH2	1:A:2314:ASN:OD1	2.30	0.65
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.78	0.65
1:A:1191:ARG:NH2	1:A:1215:GLU:OE2	2.28	0.65
1:A:4541:LEU:HD21	1:A:4590:LEU:HD22	1.79	0.65
2:D:187:LYS:HE3	4:H:24:ASN:H	1.60	0.65
1:B:365:ARG:NH2	1:B:429:LYS:O	2.29	0.65
1:B:581:MET:HG2	1:B:611:ARG:HH21	1.62	0.65
2:C:188:GLN:O	2:C:192:HIS:ND1	2.29	0.65
1:A:337:LYS:HE2	1:A:363:HIS:HD2	1.62	0.65
1:A:350:LEU:HB3	1:A:419:VAL:HG21	1.79	0.65
1:B:1213:ASN:HB3	5:J:11:ALA:HB3	1.77	0.65
1:B:2558:GLU:OE1	1:B:2561:LYS:NZ	2.29	0.64
1:B:3256:MET:HG2	1:B:3433:VAL:HG21	1.78	0.64
1:B:4504:LEU:HA	1:B:4507:ILE:HD12	1.79	0.64
4:G:54:ARG:NH2	4:G:64:ASN:O	2.28	0.64
1:A:2839:GLU:OE1	1:A:2839:GLU:N	2.29	0.64
1:B:88:VAL:HB	1:B:95:GLU:HA	1.79	0.64
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.79	0.64
2:D:313:ALA:HB3	2:D:329:PHE:HB3	1.79	0.64
5:J:43:LYS:NZ	5:J:47:ASP:OD2	2.29	0.64
1:B:1090:ARG:HH21	1:B:1121:ASP:HA	1.62	0.64
1:B:1133:GLN:OE1	1:B:1133:GLN:N	2.30	0.64
1:B:2149:LEU:HD11	1:B:2157:LEU:HD22	1.80	0.64
1:B:3057:GLN:OE1	1:B:3060:ARG:NH1	2.30	0.64
1:B:2304:ASP:OD1	1:B:2726:ARG:NH2	2.31	0.64
1:B:2590:PRO:HA	1:B:2708:PHE:O	1.96	0.64
1:A:2480:PRO:O	1:A:2482:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3360:SER:HA	1:A:3363:ILE:HD12	1.80	0.64
1:B:781:LEU:HD21	1:B:833:VAL:HG22	1.80	0.64
1:B:1087:ARG:HH21	1:B:1200:GLN:HE22	1.44	0.64
1:B:3243:MET:HE1	1:B:3444:ILE:HA	1.80	0.64
2:C:445:ASN:O	2:C:461:ARG:N	2.28	0.64
3:F:253:PHE:HZ	3:F:336:TYR:HA	1.62	0.64
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.31	0.64
5:I:8:ILE:HG23	5:I:76:PHE:HB3	1.80	0.64
1:B:3787:THR:O	1:B:3791:MET:HG2	1.99	0.63
2:D:332:GLN:OE1	2:D:372:ARG:NH1	2.32	0.63
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.27	0.63
1:B:242:LEU:HB3	1:B:309:ARG:HE	1.63	0.63
1:B:4091:GLY:HA2	1:B:4119:HIS:HB3	1.80	0.63
1:A:334:PRO:HG3	1:A:367:ILE:HD11	1.79	0.63
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.80	0.63
1:B:916:GLN:HB2	1:B:1026:MET:SD	2.39	0.63
3:F:89:LEU:HG	3:F:90:TYR:H	1.62	0.63
1:A:3732:LEU:HD22	1:A:3791:MET:HE1	1.80	0.63
1:B:285:LEU:HB2	1:B:322:LEU:HD11	1.80	0.63
1:B:3946:ASP:OD1	1:B:3950:LYS:NZ	2.31	0.63
2:D:377:ALA:O	2:D:406:LYS:NZ	2.29	0.63
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.32	0.63
1:A:4600:LYS:NZ	1:A:4604:VAL:HB	2.13	0.63
1:B:2837:LEU:HD13	1:B:2842:GLU:HB3	1.80	0.63
1:B:3161:LEU:HD21	1:B:3524:MET:HE3	1.81	0.63
2:D:358:VAL:HG13	2:D:369:PRO:HB3	1.81	0.63
1:A:1965:GLU:HG2	1:A:2026:SER:HB3	1.80	0.62
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.81	0.62
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.34	0.62
1:B:1962:ARG:NH2	1:B:2314:ASN:OD1	2.32	0.62
1:B:3839:VAL:HG21	1:B:3863:LEU:HA	1.81	0.62
1:A:1167:VAL:HA	1:A:1170:ILE:HG12	1.82	0.62
1:B:1170:ILE:O	1:B:1174:GLN:NE2	2.32	0.62
1:A:264:ARG:O	1:A:376:ARG:NH2	2.28	0.62
1:B:1457:MET:HA	1:B:1460:GLU:HG3	1.82	0.62
1:B:3454:LEU:HA	1:B:3457:GLU:HG2	1.80	0.62
2:D:607:ARG:NH1	2:D:610:GLU:OE2	2.32	0.62
1:A:113:SER:H	1:A:142:GLU:HG3	1.63	0.62
1:A:3933:GLU:HG3	1:A:3937:ARG:HE	1.65	0.62
1:A:3983:ILE:O	1:A:3987:ILE:HD12	1.99	0.62
1:B:88:VAL:HG22	1:B:90:ASP:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:GLN:NE2	3:F:357:GLU:OE1	2.32	0.62
1:B:1126:GLU:OE1	1:B:1130:LYS:NZ	2.33	0.62
1:A:3044:LEU:HD22	1:A:3049:GLU:HG3	1.82	0.62
4:G:74:LYS:NZ	4:H:65:ASP:OD1	2.31	0.62
5:I:64:SER:H	5:J:36:LYS:HD3	1.65	0.62
1:B:255:GLU:HA	1:B:258:LYS:HE3	1.81	0.62
1:A:401:LEU:HD23	1:A:536:LEU:HA	1.81	0.62
1:A:1724:VAL:HA	1:A:1727:PHE:HD2	1.65	0.62
1:A:3253:LYS:HZ3	1:A:3436:MET:HB2	1.65	0.62
1:B:343:ASP:O	1:B:352:LYS:NZ	2.33	0.62
1:B:613:LYS:HE2	1:B:682:LEU:HB2	1.81	0.62
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.65	0.61
1:A:428:GLU:HA	1:A:431:GLN:HG2	1.82	0.61
1:B:260:THR:HG23	1:B:261:LYS:HD3	1.82	0.61
1:B:530:VAL:HG12	1:B:549:ALA:HB1	1.83	0.61
1:B:961:GLU:OE2	1:B:963:ARG:NH2	2.33	0.61
2:D:459:ALA:HB2	2:D:468:ILE:HD13	1.82	0.61
1:A:264:ARG:HB3	1:A:277:PHE:CD2	2.35	0.61
1:A:315:SER:O	1:A:321:GLY:N	2.28	0.61
1:A:4395:LEU:HD21	1:A:4489:LEU:HD22	1.81	0.61
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.65	0.61
1:B:4088:VAL:HG11	1:B:4116:LEU:HD21	1.81	0.61
1:A:62:LEU:HA	1:A:65:MET:HE3	1.82	0.61
1:A:2589:LYS:HD3	1:A:2590:PRO:HD2	1.82	0.61
1:B:1965:GLU:OE1	1:B:1965:GLU:N	2.23	0.61
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	1.83	0.61
1:A:4393:GLN:HG3	1:A:4428:ARG:HH12	1.65	0.61
5:I:75:TYR:HD1	5:I:84:LEU:HB2	1.65	0.61
5:J:40:ALA:HB1	5:J:44:LYS:NZ	2.15	0.61
5:J:50:TYR:HB2	5:J:54:TRP:CH2	2.36	0.61
6:L:85:TRP:CD1	6:L:90:ASP:HB2	2.36	0.61
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.30	0.61
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.18	0.61
1:B:3174:ARG:NH1	1:B:3650:ASN:OD1	2.33	0.61
1:A:3113:MET:HE2	1:A:3115:LEU:HD21	1.81	0.61
1:B:1041:MET:HE1	3:F:121:PHE:CZ	2.35	0.61
1:B:4414:GLU:HG3	1:B:4418:LYS:NZ	2.16	0.61
1:B:264:ARG:HD3	1:B:274:GLU:HG2	1.83	0.61
1:B:3253:LYS:HD3	1:B:3436:MET:HG3	1.83	0.61
1:A:96:LYS:NZ	1:A:97:GLU:O	2.33	0.61
1:A:1806:ARG:O	1:A:1810:HIS:ND1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.34	0.61
2:D:583:ARG:NH1	2:D:599:VAL:O	2.21	0.61
1:A:121:ARG:NH1	1:B:143:ASP:OD2	2.33	0.60
1:A:2481:MET:HE1	1:A:2486:LEU:HA	1.83	0.60
1:B:1959:GLU:HB3	1:B:1962:ARG:HD3	1.83	0.60
1:B:3242:LYS:HA	1:B:3245:LYS:HD2	1.83	0.60
1:A:4002:LEU:HD11	1:A:4335:GLN:HB3	1.83	0.60
1:B:1636:ASP:O	1:B:1640:ILE:HD12	2.01	0.60
1:B:4175:GLU:N	1:B:4175:GLU:OE1	2.33	0.60
1:A:210:HIS:NE2	1:A:212:MET:HE2	2.16	0.60
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.82	0.60
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.33	0.60
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	1.83	0.60
1:A:1155:GLN:HE22	1:A:1157:SER:HB2	1.66	0.60
1:A:3016:GLU:OE2	1:A:3051:TYR:OH	2.17	0.60
1:A:3244:VAL:O	1:A:3248:GLN:HG2	2.01	0.60
1:B:1543:ARG:NH1	1:B:1612:GLN:OE1	2.33	0.60
2:C:187:LYS:HB3	4:G:30:ILE:HG13	1.82	0.60
1:B:3981:THR:HG23	1:B:3984:GLY:H	1.66	0.60
1:B:869:TYR:HB2	1:B:914:ARG:HH21	1.67	0.60
1:B:1168:THR:O	1:B:1171:THR:OG1	2.16	0.60
1:B:3386:SER:OG	1:B:3389:CYS:SG	2.60	0.60
5:I:46:PHE:HB3	5:I:54:TRP:CD1	2.37	0.60
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.35	0.60
1:B:264:ARG:NH2	1:B:268:SER:O	2.34	0.60
1:B:264:ARG:O	1:B:376:ARG:NH1	2.33	0.60
1:B:4099:VAL:HG11	1:B:4126:LEU:HD22	1.83	0.60
1:A:3817:SER:O	1:A:4346:MET:HE1	2.01	0.60
1:B:251:ARG:NH1	1:B:251:ARG:O	2.34	0.60
1:B:2969:GLY:HA2	1:B:3004:PHE:HE1	1.67	0.60
1:B:153:ILE:O	1:B:157:VAL:HG12	2.01	0.60
1:B:4400:ARG:HD3	1:B:4414:GLU:OE2	2.02	0.60
5:I:13:MET:SD	5:I:17:MET:HG3	2.42	0.60
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.84	0.60
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.35	0.60
1:B:1455:GLY:HA3	1:B:1512:TYR:HE2	1.66	0.60
1:B:1519:ASP:OD1	1:B:1520:ALA:N	2.34	0.60
1:B:1721:VAL:HA	1:B:1724:VAL:HG12	1.83	0.60
2:D:543:VAL:HB	2:D:549:LEU:HD12	1.82	0.60
1:A:315:SER:HA	1:A:319:ASP:H	1.67	0.59
1:B:1043:ILE:HA	1:B:1102:PHE:HE2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:568:GLU:N	2:D:568:GLU:OE2	2.35	0.59
1:B:1756:ILE:O	1:B:1760:GLU:HG2	2.02	0.59
1:B:2974:GLU:OE1	1:B:2977:ARG:NH1	2.35	0.59
6:K:48:GLU:OE2	6:K:49:GLN:NE2	2.35	0.59
1:A:386:ARG:NH1	1:A:452:ILE:O	2.35	0.59
1:B:464:ASP:HA	1:B:467:ARG:HG2	1.84	0.59
1:B:1033:LEU:O	1:B:1036:SER:OG	2.16	0.59
6:K:73:ASN:HD21	6:L:75:ALA:HB2	1.67	0.59
1:A:440:ARG:HA	1:A:443:GLU:HG2	1.85	0.59
1:A:2320:ASP:OD1	1:A:2321:ASP:N	2.31	0.59
1:B:442:ARG:O	1:B:445:ASN:ND2	2.35	0.59
1:B:2848:GLU:O	1:B:2852:THR:HG23	2.03	0.59
2:D:357:ILE:HD11	2:D:380:HIS:HD2	1.66	0.59
5:I:8:ILE:HG21	5:I:18:GLN:HE22	1.67	0.59
1:A:40:LEU:O	1:B:132:SER:OG	2.14	0.59
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.26	0.59
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.33	0.59
1:A:3251:GLU:HA	1:A:3254:LYS:HD2	1.84	0.59
1:B:270:THR:HG23	1:B:273:GLN:H	1.67	0.59
1:B:2125:GLY:O	1:B:2128:ALA:N	2.35	0.59
1:A:162:LYS:HE2	1:A:166:ARG:CZ	2.33	0.59
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.83	0.59
1:A:3249:GLU:HA	1:A:3252:LYS:HD2	1.85	0.59
1:B:80:GLU:HB3	1:B:102:ASN:HB2	1.83	0.59
1:B:3034:LYS:NZ	1:B:3044:LEU:O	2.29	0.59
5:I:8:ILE:HG21	5:I:18:GLN:NE2	2.16	0.59
1:A:1810:HIS:HD2	1:A:1878:LYS:HB2	1.67	0.59
1:B:717:ILE:HA	1:B:824:TRP:HE3	1.68	0.59
6:K:50:THR:HG21	6:K:65:VAL:HG21	1.83	0.59
1:A:4436:GLN:HG3	1:A:4441:LYS:HE2	1.85	0.59
2:D:551:LEU:HB2	2:D:563:ALA:HB3	1.84	0.59
1:A:4453:ASN:OD1	1:A:4457:LYS:NZ	2.35	0.59
1:B:121:ARG:NH1	1:B:133:SER:O	2.36	0.59
1:B:755:TRP:CG	2:D:453:GLU:HG3	2.38	0.59
1:B:3691:ASP:OD1	1:B:3692:LEU:N	2.36	0.59
1:A:3731:LEU:HB3	1:A:3791:MET:HE2	1.85	0.59
3:F:38:SER:O	3:F:40:LEU:N	2.35	0.59
4:H:33:THR:HG23	4:H:34:MET:SD	2.43	0.58
1:A:292:ARG:HA	1:A:297:VAL:HG12	1.85	0.58
1:A:1946:VAL:HG13	1:A:2006:VAL:HG21	1.85	0.58
1:A:391:GLN:HA	1:A:394:LYS:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HE	1:A:453:ASN:HB3	1.67	0.58
1:A:3877:HIS:HA	1:A:3880:HIS:CE1	2.39	0.58
4:H:83:ASP:OD1	4:H:84:LYS:N	2.36	0.58
1:A:3386:SER:OG	1:A:3389:CYS:SG	2.61	0.58
6:K:47:VAL:HG21	6:L:82:SER:H	1.67	0.58
1:A:116:LEU:HD22	1:A:139:THR:HG22	1.86	0.58
1:A:275:ILE:HA	1:A:278:TRP:HD1	1.68	0.58
1:A:1171:THR:HA	1:A:1174:GLN:HG2	1.84	0.58
1:B:185:LYS:O	1:B:189:LEU:HD23	2.03	0.58
1:B:264:ARG:NH1	1:B:265:ASP:O	2.36	0.58
1:B:423:TRP:HH2	1:B:454:PRO:HG3	1.68	0.58
1:B:1061:TRP:HB2	1:B:1119:LYS:NZ	2.18	0.58
1:B:1188:GLU:O	1:B:1191:ARG:HG2	2.02	0.58
1:A:2848:GLU:O	1:A:2852:THR:HG23	2.03	0.58
1:A:3877:HIS:HA	1:A:3880:HIS:ND1	2.19	0.58
1:B:332:TYR:CD2	1:B:336:MET:HE2	2.38	0.58
1:B:648:ILE:HD11	1:B:698:ILE:HB	1.86	0.58
1:B:3789:ILE:O	1:B:3792:GLN:HG3	2.02	0.58
6:K:78:HIS:CE1	6:L:69:ILE:H	2.22	0.58
1:A:43:GLU:HG3	1:A:81:ARG:HH22	1.68	0.58
1:A:415:ALA:O	1:A:418:GLU:HG3	2.04	0.58
2:D:607:ARG:HG2	2:D:610:GLU:HG2	1.85	0.58
3:F:336:TYR:CZ	3:F:340:ILE:HD11	2.39	0.58
5:I:8:ILE:HD13	5:I:18:GLN:HE21	1.68	0.58
1:A:164:TYR:CE1	1:B:145:PRO:HG2	2.30	0.58
1:A:246:GLN:HB2	1:A:309:ARG:HE	1.69	0.58
1:B:1468:GLU:O	1:B:1472:THR:HG22	2.04	0.58
4:G:50:ILE:HD11	4:G:82:PRO:HG3	1.86	0.58
1:A:93:GLU:HB2	1:A:211:PRO:HB2	1.86	0.58
1:A:162:LYS:HE2	1:A:166:ARG:NE	2.19	0.58
1:A:1763:GLU:OE2	1:A:1838:TRP:NE1	2.34	0.58
1:A:3057:GLN:OE1	1:A:3060:ARG:NH1	2.34	0.58
1:B:1170:ILE:O	1:B:1173:VAL:HG12	2.04	0.58
1:B:3933:GLU:O	1:B:3937:ARG:HG3	2.03	0.58
1:A:264:ARG:NH2	1:A:268:SER:O	2.36	0.58
1:B:2557:VAL:O	1:B:2757:ARG:NH2	2.36	0.58
1:B:3502:THR:HG22	1:B:3542:GLN:HB3	1.84	0.58
1:B:1211:ILE:O	1:B:1214:ILE:HG12	2.04	0.57
1:B:1850:GLN:HB3	1:B:1856:GLN:HG2	1.86	0.57
1:B:1914:GLU:HG3	7:B:4701:ADP:H2'	1.86	0.57
1:B:2138:ILE:HD12	1:B:2161:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4544:ASN:OD1	1:B:4573:ASN:ND2	2.31	0.57
1:A:337:LYS:NZ	1:A:360:ILE:O	2.37	0.57
1:A:2152:GLU:OE2	1:A:2152:GLU:N	2.28	0.57
1:B:1774:ASP:OD1	1:B:1775:ALA:N	2.35	0.57
1:B:1806:ARG:O	1:B:1810:HIS:ND1	2.31	0.57
1:B:1989:ASN:OD1	1:B:1990:TYR:N	2.37	0.57
1:B:3735:GLN:NE2	1:B:3791:MET:HG3	2.19	0.57
5:I:24:CYS:HA	5:I:27:GLN:CD	2.29	0.57
1:A:264:ARG:NH1	1:A:267:ALA:O	2.35	0.57
1:B:78:LEU:HB3	1:B:104:ASN:HB2	1.87	0.57
1:B:3322:GLU:OE2	1:B:3377:TYR:OH	2.22	0.57
1:A:181:SER:HA	1:A:184:LYS:HD2	1.86	0.57
1:A:3263:GLN:CD	1:A:3426:ASN:HB3	2.29	0.57
1:A:3433:VAL:HA	1:A:3436:MET:HG2	1.86	0.57
1:B:58:GLU:HG3	1:B:61:ALA:H	1.69	0.57
1:B:1760:GLU:O	1:B:1764:THR:HG23	2.04	0.57
5:J:8:ILE:HG23	5:J:76:PHE:HB3	1.87	0.57
1:A:1727:PHE:HE1	1:A:1737:THR:HG23	1.69	0.57
1:A:3904:GLU:OE1	1:A:3904:GLU:N	2.35	0.57
1:A:4544:ASN:OD1	1:A:4573:ASN:ND2	2.32	0.57
1:B:85:LYS:HE3	1:B:95:GLU:HB2	1.87	0.57
1:B:530:VAL:HG22	1:B:553:TYR:OH	2.04	0.57
1:B:2290:SER:HB2	1:B:2295:LEU:HG	1.87	0.57
1:A:460:GLN:HA	1:A:463:LEU:HB2	1.86	0.57
4:G:74:LYS:HG3	4:G:75:LYS:HD2	1.85	0.57
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.05	0.57
1:B:922:TRP:CH2	1:B:986:MET:HB2	2.40	0.57
1:B:3886:LEU:O	1:B:3890:ILE:HG12	2.04	0.57
1:B:4287:LYS:HA	1:B:4287:LYS:HE3	1.87	0.57
5:J:50:TYR:HB2	5:J:54:TRP:HH2	1.70	0.57
1:A:1959:GLU:HB3	1:A:1962:ARG:HD3	1.86	0.57
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.04	0.57
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.38	0.57
1:B:170:LYS:NZ	1:B:176:ASP:O	2.38	0.57
1:B:2851:ASP:HA	1:B:2867:MET:HE1	1.86	0.57
6:L:22:LYS:HE3	6:L:95:VAL:HG11	1.85	0.57
1:A:55:ALA:HB3	1:A:101:TYR:HD2	1.70	0.57
1:A:424:ASP:HA	1:A:427:TYR:HB3	1.87	0.57
1:B:3904:GLU:OE1	1:B:3904:GLU:N	2.36	0.57
5:I:8:ILE:HD13	5:I:18:GLN:NE2	2.19	0.57
1:B:423:TRP:HZ3	1:B:457:ARG:HH12	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:ILE:HG13	1:B:1212:ASP:N	2.19	0.57
1:B:3377:TYR:HB3	1:B:3397:ILE:HD11	1.87	0.57
1:A:438:VAL:HA	1:A:441:LYS:HG2	1.85	0.56
1:A:1810:HIS:CD2	1:A:1878:LYS:HB2	2.39	0.56
3:F:118:LEU:O	3:F:121:PHE:HB3	2.05	0.56
1:A:3877:HIS:HA	1:A:3880:HIS:HD1	1.68	0.56
1:B:956:LYS:N	1:B:985:GLU:OE2	2.34	0.56
4:H:46:MET:O	4:H:50:ILE:HG12	2.05	0.56
1:A:3191:ARG:HG2	1:A:3503:ILE:HD13	1.86	0.56
1:B:357:LEU:HD11	1:B:423:TRP:HB2	1.86	0.56
1:B:1079:TRP:CZ3	1:B:1134:MET:HE3	2.41	0.56
1:B:1518:GLU:HG2	1:B:1519:ASP:N	2.19	0.56
1:B:2388:ASP:OD1	1:B:2389:GLU:N	2.38	0.56
1:B:2495:VAL:HA	1:B:2498:ILE:HD12	1.87	0.56
1:B:4169:ILE:HG21	1:B:4302:ARG:HE	1.70	0.56
4:G:49:PHE:HA	4:G:52:LYS:HG2	1.87	0.56
1:B:2478:ASP:OD1	1:B:2479:PHE:N	2.37	0.56
2:D:427:LYS:O	2:D:430:LYS:HG3	2.05	0.56
3:F:281:ASP:OD1	3:F:282:LEU:N	2.38	0.56
1:A:189:LEU:HD22	1:B:185:LYS:HE2	1.87	0.56
1:B:1755:GLN:HG2	1:B:1814:GLU:OE2	2.04	0.56
1:B:4105:TRP:CD1	1:B:4108:GLN:HE21	2.24	0.56
1:A:3923:ARG:HH12	1:A:3925:GLN:HA	1.71	0.56
1:B:1174:GLN:OE1	1:B:1233:GLN:NE2	2.39	0.56
1:B:3923:ARG:NH1	1:B:3924:ILE:O	2.39	0.56
2:D:215:ILE:HG13	2:D:217:ILE:H	1.69	0.56
3:E:147:GLU:O	3:E:151:LYS:N	2.38	0.56
6:K:85:TRP:CD1	6:K:90:ASP:HB2	2.40	0.56
1:A:413:MET:HA	1:A:416:CYS:SG	2.46	0.56
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.88	0.56
1:B:242:LEU:HB3	1:B:309:ARG:NE	2.21	0.56
1:B:3253:LYS:HB3	1:B:3433:VAL:HG13	1.87	0.56
1:B:1958:ASP:HA	1:B:2017:THR:HB	1.88	0.56
6:K:68:VAL:HG22	6:L:79:THR:HG22	1.88	0.56
1:A:78:LEU:HB2	1:A:107:ILE:HG22	1.87	0.56
1:B:148:THR:HG23	1:B:152:PHE:CE2	2.39	0.56
1:B:2514:LEU:O	1:B:2518:ILE:HG12	2.06	0.56
1:B:2943:LYS:N	7:B:4704:ADP:O1B	2.37	0.56
1:A:354:ARG:HD3	1:A:419:VAL:HG22	1.87	0.56
1:A:368:ARG:HA	1:A:440:ARG:NH1	2.21	0.56
1:A:2478:ASP:OD1	1:A:2479:PHE:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:PHE:HA	1:B:738:ASN:H	1.70	0.56
1:B:4505:LYS:NZ	1:B:4554:ASP:O	2.35	0.56
1:A:3257:SER:O	1:A:3260:ILE:HB	2.06	0.55
1:A:4082:LYS:O	1:A:4086:THR:HG23	2.06	0.55
1:B:80:GLU:O	1:B:102:ASN:N	2.39	0.55
1:B:354:ARG:NH1	1:B:422:THR:OG1	2.40	0.55
1:B:613:LYS:HG3	1:B:682:LEU:HD12	1.88	0.55
1:B:864:LEU:HB2	1:B:877:ILE:HG21	1.87	0.55
1:B:987:PHE:HB3	1:B:991:MET:HE1	1.87	0.55
1:B:2596:PRO:HB2	1:B:2738:TYR:CE1	2.41	0.55
1:B:3263:GLN:CD	1:B:3426:ASN:HB3	2.30	0.55
2:D:448:VAL:HG21	2:D:497:PHE:CZ	2.40	0.55
2:D:613:ARG:HA	2:D:616:ARG:HG2	1.88	0.55
3:F:59:VAL:HG12	3:F:108:ILE:HA	1.88	0.55
1:A:187:ALA:O	1:A:191:MET:HG3	2.06	0.55
1:A:3124:ASP:OD1	1:A:3125:TYR:N	2.39	0.55
1:A:4173:PRO:HG2	1:A:4176:ARG:HH21	1.71	0.55
1:B:332:TYR:HD2	1:B:336:MET:HE2	1.71	0.55
1:B:4082:LYS:O	1:B:4086:THR:HG23	2.06	0.55
2:D:272:PHE:HD2	2:D:593:GLN:HB2	1.71	0.55
2:D:445:ASN:OD1	2:D:446:ASN:N	2.34	0.55
1:A:202:ILE:HG23	1:A:259:VAL:HG12	1.88	0.55
1:A:207:LEU:HG	1:A:209:ILE:HG12	1.87	0.55
1:B:994:LEU:HD11	1:B:1020:ARG:HA	1.88	0.55
1:B:2484:GLU:O	1:B:2488:ARG:HG3	2.06	0.55
1:B:3984:GLY:O	1:B:3988:HIS:ND1	2.36	0.55
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.87	0.55
1:A:4525:ARG:HD3	1:A:4536:LEU:HD23	1.88	0.55
1:B:312:ALA:O	1:B:315:SER:OG	2.20	0.55
1:B:1041:MET:HE1	3:F:121:PHE:CE1	2.42	0.55
1:B:2437:LEU:HD21	1:B:2451:ARG:HG3	1.88	0.55
2:D:439:PHE:HB3	2:D:447:PHE:CE2	2.42	0.55
3:F:87:GLU:HB2	3:F:108:ILE:HG23	1.88	0.55
1:A:434:LEU:O	1:A:438:VAL:HG23	2.06	0.55
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.06	0.55
5:J:13:MET:SD	5:J:73:PHE:N	2.79	0.55
1:A:38:VAL:HG21	1:A:52:LEU:HD22	1.88	0.55
1:B:1213:ASN:HD22	5:J:10:ASN:C	2.15	0.55
2:D:555:ASN:ND2	2:D:610:GLU:OE1	2.28	0.55
5:I:70:THR:O	5:I:72:HIS:ND1	2.33	0.55
1:A:325:ALA:O	1:A:329:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2572:LEU:O	1:A:2576:ARG:HG3	2.06	0.55
1:A:453:ASN:OD1	1:A:457:ARG:NH2	2.40	0.55
1:B:988:ALA:O	1:B:992:VAL:HG23	2.07	0.55
3:F:321:ALA:HA	3:F:324:HIS:NE2	2.22	0.55
1:A:260:THR:HG21	1:A:322:LEU:HD21	1.89	0.55
1:A:1760:GLU:O	1:A:1764:THR:HG23	2.07	0.55
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.41	0.55
1:A:4043:MET:HE2	1:A:4051:ALA:HB1	1.89	0.55
1:A:4566:GLN:O	1:A:4640:VAL:HA	2.07	0.55
1:B:242:LEU:HD21	1:B:307:GLY:HA3	1.89	0.55
1:B:977:GLU:HA	3:F:90:TYR:OH	2.06	0.55
1:A:158:ALA:HB3	1:A:159:PRO:HD3	1.88	0.55
1:A:4031:VAL:HG11	1:A:4058:LEU:HD21	1.88	0.55
1:B:332:TYR:CE1	1:B:335:LEU:HD22	2.42	0.55
1:B:336:MET:HA	1:B:339:PHE:HE2	1.72	0.55
1:B:1595:GLN:OE1	1:B:1595:GLN:N	2.38	0.55
1:A:1785:VAL:HG13	1:A:1815:LEU:HD12	1.89	0.54
1:A:2372:ASP:OD2	1:A:2429:SER:OG	2.25	0.54
1:A:4604:VAL:HG13	1:A:4624:PHE:C	2.32	0.54
1:A:29:VAL:O	1:A:33:HIS:ND1	2.40	0.54
1:B:3158:ASN:ND2	1:B:3169:MET:O	2.41	0.54
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.89	0.54
1:A:3485:GLU:OE2	1:A:3774:LYS:NZ	2.39	0.54
1:A:4557:SER:HB3	1:A:4591:ARG:HD3	1.90	0.54
1:B:666:GLU:OE1	1:B:673:TRP:NE1	2.39	0.54
1:B:721:GLU:OE2	1:B:736:LYS:NZ	2.37	0.54
1:B:3723:ASP:OD1	1:B:3724:VAL:N	2.40	0.54
2:D:456:VAL:HG21	2:D:509:TRP:HZ2	1.72	0.54
3:F:60:PHE:HE2	3:F:148:SER:HB2	1.71	0.54
1:A:228:LYS:N	1:A:231:ASP:OD2	2.38	0.54
1:A:1774:ASP:OD1	1:A:1775:ALA:N	2.37	0.54
1:A:3872:ALA:HB1	1:A:3880:HIS:HD2	1.70	0.54
1:B:210:HIS:HB3	1:B:213:ILE:HG22	1.89	0.54
1:B:257:GLN:NE2	1:B:319:ASP:OD1	2.40	0.54
1:B:2289:ASP:OD1	1:B:2290:SER:N	2.40	0.54
1:B:2885:ASP:OD1	1:B:2886:GLN:N	2.37	0.54
5:I:35:GLU:HA	5:I:38:ILE:HD12	1.90	0.54
1:A:374:ILE:HG21	1:A:437:ILE:HG21	1.89	0.54
1:A:420:PHE:CD1	1:A:460:GLN:HG3	2.42	0.54
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	1.90	0.54
1:B:724:ARG:HD2	1:B:726:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1161:ALA:C	1:B:1163:THR:H	2.14	0.54
1:B:1810:HIS:HD2	1:B:1878:LYS:HB2	1.72	0.54
5:J:34:ILE:O	5:J:38:ILE:HG12	2.08	0.54
1:A:3928:THR:HG22	1:A:3931:GLN:HG3	1.89	0.54
1:B:2839:GLU:OE1	1:B:2841:GLU:HB2	2.07	0.54
1:A:4417:VAL:HA	1:A:4489:LEU:HD21	1.89	0.54
1:B:186:ILE:O	1:B:190:GLU:HG2	2.08	0.54
1:B:342:ASN:OD1	1:B:343:ASP:N	2.41	0.54
1:B:3028:THR:O	1:B:3032:GLN:HG3	2.08	0.54
1:B:4393:GLN:HG3	1:B:4428:ARG:HH12	1.73	0.54
2:D:495:HIS:HB2	2:D:511:THR:HG22	1.90	0.54
1:A:179:ALA:HA	1:A:182:VAL:HG22	1.88	0.54
1:A:438:VAL:O	1:A:442:ARG:HG2	2.08	0.54
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	1.88	0.54
1:B:720:ILE:HG13	3:F:367:GLN:NE2	2.23	0.54
1:B:3376:SER:HA	1:B:3380:GLU:OE1	2.08	0.54
3:F:71:MET:HG3	3:F:89:LEU:HD23	1.89	0.54
1:A:209:ILE:HA	1:A:248:GLY:HA3	1.90	0.54
1:A:329:VAL:C	1:A:331:ASP:H	2.15	0.54
1:A:3433:VAL:HG22	1:A:3436:MET:HE2	1.88	0.54
2:D:386:CYS:HB3	2:D:401:ILE:HG22	1.89	0.54
5:J:13:MET:HB2	5:J:18:GLN:HE21	1.72	0.54
5:J:32:TYR:HB2	5:J:38:ILE:HD13	1.90	0.54
1:A:208:PRO:HG2	1:A:251:ARG:HG3	1.90	0.54
1:A:347:ALA:HA	1:A:352:LYS:HD3	1.90	0.54
1:B:4031:VAL:HG11	1:B:4058:LEU:HD21	1.90	0.54
1:A:3239:LYS:HG2	1:A:3451:TYR:CZ	2.43	0.53
1:A:3654:ARG:HG2	1:A:3656:THR:HG23	1.89	0.53
1:A:3910:ARG:HG2	1:A:3910:ARG:O	2.08	0.53
1:B:1125:LYS:HA	1:B:1128:LEU:HD12	1.89	0.53
1:B:1497:VAL:O	1:B:1501:ILE:HG13	2.07	0.53
1:B:1504:VAL:HG11	1:B:1524:GLU:HB2	1.89	0.53
1:A:118:PHE:HB3	1:A:135:LEU:HD21	1.90	0.53
1:B:150:HIS:CE1	1:B:194:LEU:HB3	2.43	0.53
1:B:1059:CYS:SG	3:F:44:SER:HB2	2.48	0.53
3:F:241:GLU:HA	3:F:246:TYR:H	1.73	0.53
1:A:295:PRO:HA	1:A:298:LEU:HD12	1.89	0.53
1:B:129:LYS:HD2	1:B:130:PRO:HD2	1.89	0.53
1:B:229:VAL:HG12	1:B:303:ILE:HG22	1.90	0.53
1:B:561:GLU:OE1	1:B:594:ARG:NH1	2.42	0.53
1:B:2262:ASP:OD1	1:B:2263:HIS:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3753:LEU:HD11	1:B:3770:LEU:HD21	1.89	0.53
1:A:1911:GLY:O	1:A:1915:SER:OG	2.25	0.53
1:A:1973:GLN:NE2	1:A:1977:CYS:SG	2.80	0.53
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.42	0.53
1:A:3276:MET:HE1	1:A:3412:LEU:HD13	1.89	0.53
1:A:3451:TYR:HA	1:A:3454:LEU:HG	1.91	0.53
1:B:908:GLU:HB2	1:B:1019:TYR:CZ	2.43	0.53
2:D:382:HIS:CG	2:D:404:ASP:HB2	2.44	0.53
5:I:13:MET:HA	5:I:71:LYS:HD2	1.89	0.53
1:A:121:ARG:HD2	1:A:136:ARG:HG2	1.90	0.53
1:A:213:ILE:HB	1:A:241:PHE:CZ	2.44	0.53
1:A:1751:VAL:HG11	1:A:1878:LYS:HE3	1.91	0.53
1:B:904:ASP:HA	1:B:907:ILE:HG22	1.91	0.53
1:B:1085:GLN:HA	1:B:1088:LYS:HE3	1.91	0.53
1:B:3974:TRP:NE1	1:B:3976:GLU:OE2	2.36	0.53
1:B:4452:ILE:O	1:B:4456:VAL:HG13	2.09	0.53
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.44	0.53
1:B:1679:ARG:NH2	1:B:1680:GLU:OE2	2.42	0.53
1:B:2438:GLU:O	1:B:2442:GLN:NE2	2.40	0.53
1:B:2967:TYR:OH	1:B:2975:ASP:OD2	2.22	0.53
1:B:3546:ASP:OD1	1:B:3547:ILE:N	2.41	0.53
1:B:4422:LYS:HE2	1:B:4422:LYS:HA	1.91	0.53
2:D:480:THR:OG1	2:D:500:SER:O	2.19	0.53
1:A:195:HIS:ND1	1:A:198:GLN:OE1	2.41	0.53
1:A:253:ILE:HA	1:A:256:ILE:HG12	1.89	0.53
1:A:311:HIS:HA	1:A:314:VAL:HG22	1.91	0.53
4:G:14:GLN:NE2	4:G:92:GLN:OE1	2.41	0.53
6:K:77:LEU:HD12	6:K:78:HIS:N	2.24	0.53
1:A:3043:MET:HG3	1:B:1567:ARG:NH1	2.24	0.53
1:A:3253:LYS:HE2	1:A:3436:MET:HE3	1.90	0.53
1:A:3444:ILE:O	1:A:3445:ALA:C	2.51	0.53
1:A:4505:LYS:NZ	1:A:4557:SER:O	2.39	0.53
1:B:485:ARG:NH1	1:B:486:PRO:O	2.42	0.53
1:B:2453:ARG:NH1	1:B:2505:ASP:OD2	2.31	0.53
1:A:3229:LEU:HD12	1:A:3461:ILE:HG23	1.89	0.53
1:A:3783:LYS:O	1:A:3787:THR:HG23	2.09	0.53
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.44	0.53
2:D:287:TRP:CE2	2:D:295:LEU:HD12	2.44	0.53
5:J:17:MET:HE2	5:J:50:TYR:CG	2.43	0.53
6:K:51:LEU:HD13	6:L:84:PHE:CZ	2.44	0.53
1:A:3241:LYS:HG3	1:A:3245:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:HD2	1:B:56:LEU:HD11	1.91	0.53
1:B:689:PHE:HA	1:B:692:LYS:HE3	1.90	0.53
1:A:354:ARG:HD2	1:A:422:THR:HB	1.91	0.52
1:B:480:ILE:HD12	1:B:564:ILE:HD13	1.92	0.52
3:F:172:GLU:O	3:F:176:LYS:HG2	2.10	0.52
1:A:186:ILE:O	1:A:190:GLU:HG2	2.10	0.52
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.43	0.52
1:A:4600:LYS:HG3	1:A:4602:ALA:H	1.73	0.52
1:B:674:GLU:HB2	1:B:683:LYS:HD3	1.91	0.52
1:B:1165:ASP:O	1:B:1168:THR:HB	2.09	0.52
2:D:352:THR:HG23	2:D:354:SER:H	1.75	0.52
3:F:120:LYS:HA	3:F:159:HIS:HE1	1.74	0.52
1:A:588:PHE:O	1:A:590:ALA:N	2.42	0.52
1:A:2571:THR:H	1:A:2574:THR:HB	1.75	0.52
1:A:3409:VAL:HA	1:A:3412:LEU:HD12	1.90	0.52
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.91	0.52
1:A:4541:LEU:HB2	1:A:4592:TRP:CZ3	2.45	0.52
1:B:438:VAL:HA	1:B:441:LYS:HB2	1.92	0.52
1:B:2210:LEU:O	1:B:2214:THR:HG23	2.09	0.52
1:A:282:GLU:HA	1:A:285:LEU:HG	1.92	0.52
1:A:1153:LEU:HD11	1:A:1228:LYS:HG3	1.91	0.52
1:A:1196:LEU:HA	1:A:1199:LYS:HG2	1.91	0.52
1:A:1497:VAL:O	1:A:1501:ILE:HG13	2.09	0.52
1:A:3427:GLN:O	1:A:3431:ASN:ND2	2.43	0.52
1:B:349:GLU:OE1	1:B:349:GLU:N	2.43	0.52
2:D:359:LEU:HB2	2:D:415:LEU:HD22	1.92	0.52
1:B:231:ASP:OD1	1:B:232:PHE:N	2.43	0.52
1:B:552:ARG:O	1:B:555:GLU:HG2	2.10	0.52
1:B:1150:ARG:HG3	5:J:70:THR:HG21	1.91	0.52
1:B:4450:THR:O	1:B:4454:GLU:HG3	2.09	0.52
2:D:293:GLU:HB3	2:D:318:MET:HB2	1.92	0.52
6:L:90:ASP:OD1	6:L:112:SER:N	2.30	0.52
1:A:78:LEU:HD22	1:A:107:ILE:HA	1.92	0.52
1:A:151:SER:O	1:A:154:SER:OG	2.25	0.52
1:A:256:ILE:O	1:A:259:VAL:HG22	2.09	0.52
1:A:1229:ASP:CG	1:A:1233:GLN:HE22	2.18	0.52
1:B:180:PRO:O	1:B:184:LYS:NZ	2.42	0.52
1:B:361:PHE:CD1	1:B:426:GLU:HG3	2.45	0.52
1:B:1202:PHE:O	5:J:5:LYS:NZ	2.43	0.52
4:H:26:GLU:HA	4:H:87:PHE:HE2	1.74	0.52
1:A:107:ILE:HB	1:B:160:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1587:LEU:O	1:A:1591:VAL:HG23	2.09	0.52
1:A:2603:MET:HE1	7:A:4703:ADP:N7	2.24	0.52
1:A:4509:VAL:HG11	1:A:4520:TYR:CZ	2.44	0.52
1:B:2369:LEU:HD12	1:B:2373:MET:HE2	1.91	0.52
1:B:3611:ARG:NH1	1:B:3636:GLN:OE1	2.40	0.52
1:B:3783:LYS:O	1:B:3787:THR:HG23	2.09	0.52
6:L:35:GLN:O	6:L:39:VAL:HG23	2.10	0.52
1:A:40:LEU:CB	1:B:33:HIS:HE1	2.23	0.52
1:A:213:ILE:HG21	1:A:245:LEU:HD22	1.91	0.52
1:A:296:GLU:O	1:A:299:LEU:HG	2.10	0.52
1:A:2879:LYS:HE3	1:A:2879:LYS:HA	1.91	0.52
1:B:391:GLN:O	1:B:394:LYS:HG2	2.10	0.52
1:B:4049:TYR:OH	1:B:4191:GLN:OE1	2.25	0.52
5:I:28:ALA:HB2	5:I:41:HIS:HD2	1.74	0.52
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.10	0.52
1:B:83:THR:O	1:B:112:LYS:NZ	2.41	0.52
1:B:779:ILE:HA	1:B:782:ILE:HG22	1.92	0.52
1:B:2412:MET:O	1:B:2416:GLN:HG3	2.09	0.52
1:B:4178:ARG:NH2	1:B:4297:PRO:O	2.43	0.52
3:F:67:LYS:HB3	3:F:136:VAL:HG21	1.92	0.52
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.91	0.52
1:B:35:ARG:NH2	1:B:53:GLU:OE2	2.42	0.52
1:A:236:VAL:HG13	1:A:237:GLU:HG2	1.92	0.51
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.91	0.51
1:A:2412:MET:O	1:A:2416:GLN:HG3	2.10	0.51
1:B:1581:LYS:O	1:B:1584:LYS:HG2	2.10	0.51
1:B:1810:HIS:NE2	1:B:1876:GLN:O	2.43	0.51
1:B:2816:LEU:HD11	1:B:2820:GLY:HA3	1.92	0.51
1:B:3240:LEU:O	1:B:3244:VAL:HG23	2.09	0.51
1:B:378:LEU:HG	1:B:379:ARG:HH21	1.75	0.51
1:B:1493:LEU:O	1:B:1497:VAL:HG23	2.11	0.51
1:B:1661:VAL:HG22	1:B:1676:ILE:HD12	1.92	0.51
1:A:4190:ILE:HG13	1:A:4191:GLN:N	2.26	0.51
1:B:808:LEU:O	1:B:811:GLU:HG2	2.10	0.51
1:B:1220:ALA:O	1:B:1224:ILE:HG12	2.11	0.51
1:B:1835:SER:OG	1:B:1837:GLU:OE1	2.28	0.51
1:B:4105:TRP:HA	1:B:4108:GLN:HG2	1.92	0.51
2:D:268:ASN:OD1	2:D:598:ASP:N	2.37	0.51
2:D:620:GLU:HG3	2:D:621:ILE:HG12	1.91	0.51
1:A:185:LYS:HE3	1:B:189:LEU:HA	1.92	0.51
1:A:1170:ILE:HA	1:A:1173:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2174:GLU:OE1	1:A:2176:THR:OG1	2.25	0.51
1:A:3409:VAL:HG12	1:A:3413:ARG:HG3	1.92	0.51
1:A:3546:ASP:OD1	1:A:3547:ILE:N	2.43	0.51
1:B:38:VAL:HB	1:B:52:LEU:HD21	1.92	0.51
1:B:895:ASN:OD1	3:F:353:GLU:HB2	2.11	0.51
1:B:2592:VAL:HB	1:B:2733:VAL:HG22	1.93	0.51
3:F:39:ILE:HA	3:F:42:GLU:HG2	1.93	0.51
5:I:64:SER:OG	5:J:36:LYS:NZ	2.43	0.51
5:I:68:HIS:CD2	5:I:73:PHE:HB2	2.46	0.51
5:J:13:MET:HE3	5:J:13:MET:HA	1.91	0.51
1:A:42:LEU:HB3	1:A:81:ARG:NH2	2.25	0.51
1:A:170:LYS:HG2	1:A:179:ALA:HB3	1.93	0.51
1:A:213:ILE:HG12	1:A:303:ILE:HD12	1.93	0.51
1:A:3253:LYS:HD3	1:A:3436:MET:HG3	1.93	0.51
1:B:25:ALA:HB3	1:B:69:LEU:HD21	1.92	0.51
1:B:406:TYR:CD2	1:B:474:GLU:HG2	2.46	0.51
1:B:431:GLN:O	1:B:435:ARG:HG2	2.10	0.51
1:B:819:GLY:HA3	1:B:832:TYR:CZ	2.46	0.51
1:B:1150:ARG:O	1:B:1153:LEU:HG	2.10	0.51
1:B:4260:PHE:CE2	1:B:4608:PRO:HB3	2.45	0.51
1:B:4331:LEU:O	1:B:4335:GLN:HG3	2.10	0.51
2:D:509:TRP:HB3	2:D:516:PRO:HA	1.91	0.51
5:I:46:PHE:HB3	5:I:54:TRP:CG	2.46	0.51
1:A:164:TYR:O	1:A:168:SER:OG	2.19	0.51
1:A:284:ALA:O	1:A:287:ARG:HG2	2.11	0.51
1:A:3373:SER:O	1:A:3376:SER:OG	2.27	0.51
1:A:4392:PRO:O	1:A:4428:ARG:NH1	2.42	0.51
1:B:1176:LEU:HA	1:B:1179:LYS:HD3	1.93	0.51
1:B:2134:GLN:O	1:B:2138:ILE:HG12	2.11	0.51
1:B:3409:VAL:HG12	1:B:3413:ARG:HG3	1.93	0.51
1:B:4213:ARG:NH1	1:B:4213:ARG:HB2	2.26	0.51
1:A:136:ARG:HG3	1:B:152:PHE:CZ	2.46	0.51
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.92	0.51
1:A:2671:MET:HE2	1:A:2721:LYS:HG2	1.93	0.51
1:B:409:PHE:CD2	1:B:470:ARG:HD2	2.45	0.51
1:B:636:SER:HB2	1:B:641:LEU:HB2	1.93	0.51
2:D:475:HIS:CE1	2:D:477:GLY:H	2.28	0.51
3:F:91:LEU:HB2	3:F:104:CYS:HB3	1.91	0.51
3:F:251:LEU:HA	3:F:254:ILE:HG12	1.92	0.51
3:F:257:HIS:CD2	3:F:260:ARG:HH12	2.29	0.51
1:B:1053:VAL:O	1:B:1056:GLN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1836:PHE:HA	1:B:1839:LEU:HB2	1.91	0.51
1:B:2066:ALA:HA	1:B:2069:ILE:HG22	1.93	0.51
1:B:3001:ASP:OD1	1:B:3002:SER:N	2.44	0.51
5:J:68:HIS:ND1	5:J:69:GLU:O	2.36	0.51
1:A:1537:TRP:HH2	1:A:1582:VAL:HG21	1.75	0.51
1:A:4192:GLU:HB3	1:A:4321:LEU:HD11	1.92	0.51
1:A:4318:PRO:HB2	1:A:4323:LEU:HB2	1.93	0.51
1:B:161:PHE:O	1:B:165:ILE:HG12	2.11	0.51
1:B:1082:LEU:HD21	3:F:39:ILE:HG21	1.91	0.51
1:B:1198:GLU:O	1:B:1201:ARG:NH1	2.44	0.51
1:B:1491:ASP:OD1	1:B:1492:ASP:N	2.43	0.51
1:B:1704:LEU:HD13	1:B:1707:LYS:HD3	1.92	0.51
1:B:2346:GLN:HB3	1:B:2726:ARG:HD2	1.93	0.51
1:B:2925:ILE:HG13	1:B:2933:LEU:HD21	1.93	0.51
1:B:4412:PHE:CZ	1:B:4520:TYR:HB2	2.45	0.51
2:D:602:GLN:HG2	2:D:603:ILE:HG23	1.91	0.51
1:A:1843:ARG:HH12	1:A:1862:ALA:H	1.59	0.51
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.46	0.51
1:A:3458:ALA:O	1:A:3461:ILE:HG22	2.11	0.51
1:A:3772:ASN:HA	1:A:3775:ARG:HE	1.75	0.51
1:B:4168:ARG:NH2	1:B:4217:ASP:OD1	2.44	0.51
4:H:68:PHE:CE1	4:H:79:MET:HE1	2.46	0.51
1:A:148:THR:O	1:A:152:PHE:HD1	1.94	0.50
1:A:189:LEU:O	1:A:193:LEU:HD23	2.11	0.50
1:A:333:ASN:ND2	1:A:367:ILE:HA	2.27	0.50
1:A:3430:ALA:O	1:A:3434:GLU:HB2	2.10	0.50
5:I:35:GLU:N	5:I:35:GLU:OE2	2.43	0.50
5:J:21:SER:HA	5:J:46:PHE:HZ	1.76	0.50
1:A:164:TYR:CE2	1:B:109:TYR:HB3	2.45	0.50
1:A:454:PRO:HD2	1:A:457:ARG:NH1	2.26	0.50
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.94	0.50
1:A:2222:MET:HE1	1:A:2234:TRP:CD1	2.46	0.50
1:A:3048:GLU:OE2	1:A:3048:GLU:N	2.39	0.50
1:B:278:TRP:CD1	1:B:336:MET:HE1	2.46	0.50
1:B:387:ASP:OD1	1:B:388:LEU:N	2.45	0.50
1:B:2047:GLN:OE1	1:B:2067:ASN:ND2	2.44	0.50
1:B:2262:ASP:HB2	1:B:2267:THR:HG22	1.94	0.50
1:B:2444:GLU:H	1:B:2510:MET:HE3	1.75	0.50
1:A:1219:GLY:HA2	1:A:1222:ASN:HD21	1.75	0.50
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.93	0.50
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:LYS:HB3	1:B:736:LYS:HZ2	1.76	0.50
1:B:1211:ILE:O	1:B:1215:GLU:HG3	2.10	0.50
2:D:502:PHE:CE1	2:D:526:TYR:HB2	2.46	0.50
3:E:95:ASP:O	3:E:99:ASP:N	2.45	0.50
3:F:51:LEU:HB3	3:F:98:ARG:HE	1.77	0.50
3:F:151:LYS:O	3:F:154:SER:OG	2.27	0.50
1:A:40:LEU:HB3	1:B:33:HIS:HE1	1.76	0.50
1:A:440:ARG:O	1:A:444:GLU:N	2.42	0.50
1:A:3946:ASP:OD1	1:A:3950:LYS:NZ	2.44	0.50
1:B:2411:PRO:O	1:B:2415:ILE:HG13	2.10	0.50
1:B:2671:MET:HG2	1:B:2675:GLY:HA2	1.93	0.50
1:B:3099:THR:HG23	1:B:3148:VAL:HG11	1.93	0.50
6:K:70:MET:HB2	6:K:103:TYR:HB2	1.93	0.50
1:A:376:ARG:O	1:A:380:LEU:HG	2.11	0.50
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.93	0.50
1:B:486:PRO:HA	1:B:567:ARG:NH2	2.26	0.50
1:B:1090:ARG:HH22	1:B:1124:HIS:HB3	1.76	0.50
1:B:3017:VAL:HB	1:B:3020:LEU:HB2	1.93	0.50
1:B:3176:TYR:O	1:B:3180:ILE:HG12	2.11	0.50
1:B:4087:ALA:HB1	1:B:4092:ARG:O	2.12	0.50
2:D:317:ASN:O	2:D:318:MET:HE2	2.11	0.50
5:I:29:LEU:HD23	5:I:38:ILE:HD13	1.93	0.50
1:A:315:SER:HB2	1:A:319:ASP:HB2	1.93	0.50
1:A:351:ASP:HA	1:A:354:ARG:NH1	2.26	0.50
1:A:1222:ASN:CA	1:A:1225:MET:HE3	2.39	0.50
1:A:1518:GLU:HG2	1:A:1519:ASP:N	2.26	0.50
1:A:2956:LEU:HD22	1:A:2989:LYS:HB3	1.94	0.50
1:B:848:ASP:OD1	1:B:849:ASP:N	2.45	0.50
1:A:1840:SER:HA	1:A:1862:ALA:HB2	1.93	0.50
1:A:3321:LEU:HD22	1:A:3332:THR:HA	1.93	0.50
1:B:487:GLN:H	1:B:567:ARG:HH22	1.60	0.50
1:B:3691:ASP:O	1:B:3695:ARG:HG3	2.11	0.50
1:B:4609:VAL:HG22	1:B:4642:VAL:HB	1.94	0.50
2:D:281:VAL:HG13	2:D:590:SER:HA	1.93	0.50
2:D:327:TYR:HB3	2:D:360:TRP:HH2	1.77	0.50
1:A:2855:LEU:HD11	1:A:2863:ARG:HE	1.77	0.50
1:A:3322:GLU:OE2	1:A:3377:TYR:OH	2.29	0.50
1:A:3984:GLY:O	1:A:3988:HIS:ND1	2.43	0.50
1:B:4413:PHE:O	1:B:4417:VAL:HG23	2.11	0.50
6:L:15:ASP:OD1	6:L:16:GLU:N	2.45	0.50
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.39	0.50
1:A:3196:GLU:O	1:A:3199:MET:HG3	2.11	0.50
1:B:1191:ARG:O	1:B:1194:GLN:NE2	2.45	0.50
1:B:1798:MET:HG3	1:B:1800:GLN:HE21	1.77	0.50
1:B:3892:LEU:HD13	1:B:3983:ILE:HG21	1.94	0.50
1:B:4302:ARG:O	1:B:4306:VAL:HG23	2.12	0.50
1:B:4558:PHE:O	1:B:4589:GLN:HA	2.11	0.50
3:F:48:ARG:HD2	3:F:49:SER:HB2	1.93	0.50
1:A:1728:GLY:O	1:A:1729:LYS:HG3	2.12	0.49
1:A:2592:VAL:HB	1:A:2733:VAL:HG22	1.94	0.49
1:A:2922:ILE:HG23	1:A:2933:LEU:HD11	1.94	0.49
1:B:4416:GLU:HB3	1:B:4489:LEU:HD11	1.93	0.49
2:D:301:ASN:OD1	2:D:302:ASN:N	2.44	0.49
4:H:80:VAL:HG22	4:H:82:PRO:HD3	1.94	0.49
1:A:441:LYS:HB2	1:A:445:ASN:HA	1.93	0.49
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.94	0.49
1:A:4015:GLU:N	1:A:4015:GLU:OE2	2.41	0.49
1:B:59:LYS:HZ1	1:B:63:GLU:HB2	1.76	0.49
1:B:2175:MET:HB3	1:B:2178:LEU:HB3	1.93	0.49
1:B:2572:LEU:O	1:B:2576:ARG:HG3	2.12	0.49
2:D:374:PRO:HD3	2:D:416:SER:HA	1.94	0.49
2:D:506:VAL:H	2:D:520:PHE:HB3	1.77	0.49
6:L:70:MET:HB2	6:L:103:TYR:HB2	1.92	0.49
1:A:206:SER:O	1:A:208:PRO:HD3	2.12	0.49
1:A:242:LEU:HD22	1:A:307:GLY:O	2.12	0.49
1:A:285:LEU:O	1:A:289:GLN:HG2	2.12	0.49
1:A:2620:LEU:HD21	1:A:2634:THR:OG1	2.12	0.49
1:A:3922:PRO:HG2	1:A:3924:ILE:HD11	1.94	0.49
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.77	0.49
1:B:386:ARG:HH11	1:B:455:ALA:HB2	1.75	0.49
1:B:530:VAL:HG13	1:B:553:TYR:CE1	2.47	0.49
1:B:659:THR:C	1:B:663:LYS:HZ1	2.20	0.49
1:B:3650:ASN:HD21	1:B:3695:ARG:HH11	1.60	0.49
1:A:209:ILE:HG22	1:A:248:GLY:C	2.37	0.49
1:A:1493:LEU:O	1:A:1497:VAL:HG23	2.13	0.49
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.37	0.49
1:A:4095:MET:HG3	1:A:4125:PHE:HB2	1.94	0.49
1:A:4433:ASP:HB3	1:A:4448:LEU:HD21	1.95	0.49
1:B:1663:SER:OG	1:B:1677:SER:OG	2.26	0.49
1:B:1752:LEU:O	1:B:1756:ILE:HG13	2.13	0.49
1:B:1934:GLU:OE2	1:B:2261:LYS:NZ	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2181:GLU:HG3	1:B:2244:LEU:HB2	1.93	0.49
1:A:428:GLU:O	1:A:432:VAL:HG23	2.12	0.49
1:A:3001:ASP:OD1	1:A:3002:SER:N	2.46	0.49
1:A:3401:ASN:O	1:A:3405:MET:HE2	2.13	0.49
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.95	0.49
1:B:68:PHE:O	1:B:120:LYS:NZ	2.43	0.49
1:B:633:CYS:SG	1:B:634:LYS:N	2.85	0.49
1:B:1513:TYR:CD2	1:B:1517:GLU:HG2	2.48	0.49
1:B:1707:LYS:O	1:B:1711:VAL:HG23	2.13	0.49
1:B:1734:ASP:HB3	1:B:1737:THR:HG22	1.93	0.49
1:B:1785:VAL:HG13	1:B:1815:LEU:HD12	1.95	0.49
1:B:3191:ARG:HD2	1:B:3500:MET:HE1	1.93	0.49
2:D:527:VAL:HA	2:D:544:ASP:HA	1.93	0.49
3:F:248:ASP:OD1	3:F:249:GLU:N	2.45	0.49
4:G:64:ASN:OD1	4:H:73:SER:HB3	2.12	0.49
4:G:69:LEU:HD11	4:H:69:LEU:HD11	1.94	0.49
6:L:72:LYS:HE2	6:L:103:TYR:CZ	2.47	0.49
1:A:3369:LYS:HG2	1:A:3372:MET:HE2	1.95	0.49
1:B:130:PRO:O	1:B:134:GLN:N	2.46	0.49
1:B:1128:LEU:HD21	1:B:1200:GLN:HG3	1.92	0.49
1:B:1187:VAL:O	1:B:1191:ARG:N	2.37	0.49
1:B:3922:PRO:HG2	1:B:3924:ILE:HD11	1.94	0.49
4:G:47:HIS:HA	4:G:50:ILE:HG22	1.93	0.49
5:J:60:ARG:HE	5:J:60:ARG:C	2.21	0.49
1:A:189:LEU:HD13	1:B:185:LYS:HE2	1.94	0.49
1:A:1537:TRP:O	1:A:1540:VAL:HG22	2.12	0.49
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.52	0.49
1:A:3294:ASN:HB3	1:A:3391:PRO:HB3	1.95	0.49
1:B:322:LEU:O	1:B:326:LEU:N	2.37	0.49
1:B:399:ARG:HE	1:B:412:VAL:HG11	1.77	0.49
1:B:1460:GLU:HB3	1:B:1516:PHE:CZ	2.47	0.49
1:B:1516:PHE:O	1:B:1517:GLU:C	2.56	0.49
1:B:3229:LEU:HD12	1:B:3461:ILE:HG23	1.94	0.49
1:B:4004:MET:O	1:B:4004:MET:HE3	2.13	0.49
3:F:144:THR:HA	3:F:147:GLU:OE2	2.13	0.49
1:A:1937:ASP:HA	1:A:1967:MET:HE2	1.95	0.49
1:A:2346:GLN:HB3	1:A:2726:ARG:HD2	1.94	0.49
1:A:2593:LEU:HD11	1:A:2605:LEU:HB2	1.95	0.49
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.78	0.49
1:B:286:TYR:O	1:B:290:GLU:HG2	2.12	0.49
1:B:365:ARG:HD3	1:B:433:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:LEU:HD11	1:B:899:TRP:CD1	2.48	0.49
1:B:1454:GLN:HA	1:B:1457:MET:HE2	1.93	0.49
1:B:2320:ASP:OD1	1:B:2321:ASP:N	2.43	0.49
1:B:3453:VAL:O	1:B:3456:SER:OG	2.22	0.49
1:B:3935:VAL:HG13	1:B:3947:LEU:HD23	1.93	0.49
3:F:62:GLU:OE2	3:F:141:ARG:NH2	2.42	0.49
4:H:22:VAL:H	4:H:31:LYS:HZ3	1.60	0.49
1:A:35:ARG:HD3	1:A:53:GLU:HG2	1.93	0.49
1:A:368:ARG:HH12	1:A:436:ASP:CB	2.26	0.49
1:A:1147:SER:O	1:A:1151:GLN:HG2	2.13	0.49
1:A:1966:ARG:HA	1:A:4101:LEU:HD13	1.95	0.49
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.46	0.49
1:A:2813:LEU:HD13	1:A:2816:LEU:HD13	1.94	0.49
1:B:1131:PHE:O	1:B:1135:LEU:HG	2.12	0.49
1:B:1579:MET:HA	1:B:1579:MET:HE3	1.95	0.49
1:B:2285:ARG:NH1	1:B:2331:GLU:OE2	2.35	0.49
1:B:2558:GLU:HG3	1:B:2560:HIS:CE1	2.48	0.49
1:B:2682:PHE:O	1:B:2686:MET:HG2	2.13	0.49
1:B:3383:ASN:O	1:B:3384:ARG:HB3	2.13	0.49
3:F:250:HIS:HD2	3:F:340:ILE:HG22	1.77	0.49
3:F:321:ALA:HA	3:F:324:HIS:CD2	2.48	0.49
1:A:391:GLN:O	1:A:395:VAL:HG23	2.13	0.49
1:A:1400:VAL:C	1:A:1402:GLU:H	2.20	0.49
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.93	0.49
1:A:3923:ARG:NH1	1:A:3925:GLN:HA	2.28	0.49
1:B:1079:TRP:HB3	1:B:1131:PHE:CZ	2.48	0.49
1:B:2115:LYS:NZ	1:B:2126:GLU:OE1	2.43	0.49
1:B:2864:GLU:OE1	1:B:2864:GLU:N	2.42	0.49
1:B:2956:LEU:HD22	1:B:2989:LYS:HB3	1.94	0.49
1:B:3518:GLY:O	1:B:3525:ARG:NH2	2.45	0.49
1:B:3520:PHE:HB3	1:B:3524:MET:HB3	1.95	0.49
3:F:237:VAL:O	3:F:241:GLU:HG3	2.12	0.49
1:A:1539:ASP:O	1:A:1543:ARG:HG3	2.12	0.48
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.42	0.48
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.46	0.48
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.13	0.48
1:B:530:VAL:HG13	1:B:553:TYR:CZ	2.48	0.48
1:B:1041:MET:HA	1:B:1044:VAL:HG12	1.95	0.48
1:B:1218:TRP:CD1	1:B:1222:ASN:HD21	2.31	0.48
1:B:3451:TYR:CD1	1:B:3454:LEU:HD21	2.48	0.48
2:D:437:MET:HB3	2:D:449:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:485:HIS:NE2	2:D:487:ALA:O	2.45	0.48
1:A:341:LEU:O	1:A:345:LEU:HG	2.14	0.48
1:A:413:MET:HE1	1:A:463:LEU:O	2.12	0.48
1:A:1987:ASN:OD1	1:A:1990:TYR:HB3	2.13	0.48
1:A:2569:VAL:HB	1:A:2747:ILE:HG23	1.94	0.48
1:A:3606:ASP:OD1	1:A:3606:ASP:N	2.45	0.48
1:A:3882:THR:HG23	1:A:4343:MET:HG3	1.95	0.48
1:B:1161:ALA:HA	1:B:1163:THR:HG23	1.95	0.48
1:B:1810:HIS:CD2	1:B:1878:LYS:HB2	2.47	0.48
1:B:2320:ASP:OD2	1:B:2322:ASN:ND2	2.46	0.48
1:B:2446:ILE:HG13	1:B:2735:TYR:CD1	2.47	0.48
1:B:2844:ARG:O	1:B:2848:GLU:HG3	2.13	0.48
1:B:2892:TYR:O	1:B:2896:ARG:HG2	2.13	0.48
2:D:271:PHE:CZ	2:D:273:ASP:HB2	2.48	0.48
2:D:296:VAL:HG12	2:D:315:VAL:HG22	1.95	0.48
2:D:456:VAL:HG21	2:D:509:TRP:CZ2	2.48	0.48
4:H:69:LEU:HB3	4:H:80:VAL:HG13	1.94	0.48
5:I:7:VAL:HG23	5:I:77:TYR:HB2	1.94	0.48
6:K:62:LYS:HG3	6:K:113:ILE:HG12	1.94	0.48
1:A:1513:TYR:CE2	1:A:1517:GLU:HG2	2.48	0.48
1:A:2094:LYS:O	1:A:2098:VAL:HG23	2.12	0.48
1:A:2248:GLU:OE1	1:A:2248:GLU:N	2.37	0.48
1:A:2411:PRO:O	1:A:2415:ILE:HG13	2.13	0.48
1:A:3240:LEU:O	1:A:3244:VAL:HG23	2.12	0.48
1:B:1169:PHE:O	1:B:1172:TYR:HB3	2.12	0.48
1:B:1619:LEU:HD21	1:B:1638:LEU:HD23	1.96	0.48
1:B:1987:ASN:OD1	1:B:1990:TYR:HB3	2.14	0.48
1:B:2784:PHE:HB2	1:B:2794:TYR:HE2	1.79	0.48
3:F:365:LYS:O	3:F:368:SER:OG	2.26	0.48
5:J:54:TRP:CD1	5:J:87:LYS:HB2	2.48	0.48
1:A:65:MET:O	1:A:69:LEU:HG	2.13	0.48
1:A:344:LEU:HD21	1:A:388:LEU:HD21	1.95	0.48
1:A:426:GLU:O	1:A:430:LEU:HG	2.14	0.48
1:A:1987:ASN:ND2	1:A:1989:ASN:OD1	2.46	0.48
1:B:185:LYS:O	1:B:188:GLU:HG3	2.13	0.48
1:B:557:ILE:HA	1:B:560:VAL:HG22	1.96	0.48
1:B:3135:GLN:O	1:B:3137:PRO:HD3	2.13	0.48
1:B:3447:TYR:O	1:B:3451:TYR:HD2	1.96	0.48
1:B:3606:ASP:N	1:B:3606:ASP:OD1	2.45	0.48
2:D:330:HIS:HB3	2:D:367:ARG:HG3	1.94	0.48
1:A:322:LEU:HG	1:A:325:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:HA	1:A:363:HIS:CD2	2.48	0.48
1:A:2065:LEU:HB3	1:A:2137:LEU:HD11	1.95	0.48
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.94	0.48
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.14	0.48
1:A:3376:SER:HA	1:A:3380:GLU:OE1	2.12	0.48
1:A:4532:ASN:HB3	1:A:4534:TRP:CE2	2.49	0.48
1:B:89:GLY:HA2	1:B:244:GLN:HG2	1.95	0.48
1:B:1075:ASP:HB3	1:B:1078:LYS:HB3	1.95	0.48
1:B:4191:GLN:O	1:B:4194:LEU:HB2	2.13	0.48
3:F:228:LEU:HD23	3:F:268:ALA:HB3	1.96	0.48
3:F:250:HIS:CD2	3:F:340:ILE:HG22	2.49	0.48
3:F:345:VAL:HG22	3:F:347:LYS:H	1.79	0.48
5:J:40:ALA:HB1	5:J:44:LYS:HZ1	1.78	0.48
6:L:34:TYR:HD1	6:L:102:MET:SD	2.36	0.48
1:A:241:PHE:O	1:A:245:LEU:HG	2.13	0.48
1:A:1465:GLN:O	1:A:1469:VAL:HG23	2.13	0.48
1:A:3194:LEU:HD23	1:A:3500:MET:SD	2.54	0.48
1:B:1464:LYS:O	1:B:1467:ARG:N	2.46	0.48
1:B:2820:GLY:O	1:B:2824:ILE:HG13	2.13	0.48
2:D:268:ASN:HB2	2:D:597:TYR:HA	1.95	0.48
2:D:359:LEU:HD22	2:D:415:LEU:HD13	1.96	0.48
2:D:504:TRP:CD1	2:D:523:ASN:H	2.32	0.48
3:F:146:MET:HE1	3:F:257:HIS:HB3	1.95	0.48
5:J:54:TRP:NE1	5:J:87:LYS:HB2	2.29	0.48
6:K:34:TYR:CE2	6:K:71:GLN:HB2	2.48	0.48
1:A:300:THR:HA	1:A:303:ILE:HG12	1.96	0.48
1:A:351:ASP:O	1:A:355:GLN:HG2	2.14	0.48
1:A:1861:MET:HE2	1:A:1890:LEU:HB2	1.96	0.48
1:A:4247:MET:HE2	1:A:4269:LEU:HD21	1.94	0.48
1:B:253:ILE:HA	1:B:256:ILE:HG12	1.95	0.48
1:B:870:ASP:HB3	1:B:873:THR:HG22	1.96	0.48
1:B:1469:VAL:O	1:B:1473:TYR:HB2	2.14	0.48
1:B:2629:GLU:O	1:B:2633:LYS:HG2	2.13	0.48
2:D:278:LYS:HG2	2:D:280:ARG:NH1	2.29	0.48
2:D:422:MET:HE1	2:D:424:LEU:HA	1.96	0.48
3:F:262:CYS:HB2	3:F:267:ALA:HB3	1.96	0.48
4:G:55:SER:HA	4:G:58:ARG:HG2	1.96	0.48
1:A:333:ASN:HA	1:A:336:MET:HE2	1.96	0.48
1:A:1201:ARG:NH2	1:B:967:GLN:O	2.47	0.48
1:A:3843:ASN:ND2	1:A:3862:ASP:OD2	2.43	0.48
1:A:4007:MET:O	1:A:4011:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:LEU:HD22	3:F:367:GLN:HE21	1.79	0.48
1:B:3321:LEU:HD22	1:B:3332:THR:HA	1.95	0.48
1:B:3974:TRP:HZ2	1:B:3985:GLN:HG3	1.77	0.48
2:D:387:VAL:HG12	2:D:400:SER:HB2	1.95	0.48
5:J:60:ARG:O	5:J:60:ARG:NE	2.41	0.48
1:A:250:ASN:O	1:A:254:ARG:HG2	2.14	0.48
1:A:460:GLN:O	1:A:464:ASP:N	2.30	0.48
1:A:3254:LYS:HE3	1:A:3437:ILE:HD11	1.96	0.48
1:A:3255:VAL:HA	1:A:3258:GLN:CD	2.39	0.48
1:B:2176:THR:O	1:B:2180:GLU:HG2	2.13	0.48
5:J:8:ILE:HA	5:J:76:PHE:HA	1.95	0.48
1:A:136:ARG:NE	1:B:139:THR:HG23	2.29	0.48
1:A:351:ASP:OD1	1:A:352:LYS:N	2.47	0.48
1:A:368:ARG:HH12	1:A:436:ASP:HB3	1.78	0.48
1:A:405:ALA:O	1:A:409:PHE:N	2.46	0.48
1:A:1439:LEU:O	1:A:1443:GLU:N	2.46	0.48
1:A:2614:ASP:HA	1:A:2657:LYS:NZ	2.28	0.48
1:A:3429:LYS:O	1:A:3433:VAL:HB	2.14	0.48
1:A:3885:MET:HE1	1:A:3908:PHE:CE2	2.49	0.48
1:B:109:TYR:OH	1:B:145:PRO:HB3	2.14	0.48
1:B:1465:GLN:O	1:B:1469:VAL:HG23	2.14	0.48
1:B:2104:LYS:O	1:B:2108:ILE:HG12	2.14	0.48
1:B:4297:PRO:HG3	1:B:4308:TRP:CG	2.49	0.48
2:D:448:VAL:HG22	2:D:458:THR:HG23	1.96	0.48
3:F:247:ARG:HH22	3:F:329:THR:HB	1.79	0.48
6:K:20:ILE:HD11	6:K:53:GLN:CB	2.44	0.48
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.95	0.47
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.96	0.47
1:A:2917:ASP:O	1:A:2921:ARG:HG3	2.12	0.47
1:B:326:LEU:HG	1:B:330:ASN:HD21	1.78	0.47
1:B:1825:LEU:HA	1:B:1830:ILE:HD13	1.95	0.47
1:B:2189:MET:HG3	1:B:2191:LEU:HD13	1.96	0.47
1:B:3473:ASN:OD1	1:B:3474:ARG:N	2.47	0.47
1:B:3735:GLN:HE21	1:B:3791:MET:HG3	1.78	0.47
1:B:4288:VAL:HG11	1:B:4294:ILE:HG13	1.96	0.47
2:D:283:SER:HB2	2:D:298:SER:HB2	1.96	0.47
2:D:523:ASN:CG	2:D:524:ALA:H	2.22	0.47
2:D:599:VAL:HG13	2:D:604:ALA:HB2	1.95	0.47
1:A:136:ARG:HG3	1:B:152:PHE:CE2	2.49	0.47
1:A:362:THR:O	1:A:365:ARG:HB2	2.14	0.47
1:A:1798:MET:HG3	1:A:1800:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2279:LEU:HA	1:A:2698:GLN:HG2	1.95	0.47
1:A:3383:ASN:O	1:A:3384:ARG:HB3	2.13	0.47
1:B:480:ILE:HG23	1:B:484:LEU:HB2	1.96	0.47
1:B:991:MET:HB3	1:B:995:SER:HG	1.79	0.47
1:B:1174:GLN:O	1:B:1178:ARG:NH1	2.48	0.47
1:B:2863:ARG:O	1:B:2867:MET:HB2	2.14	0.47
1:B:3315:ALA:O	1:B:3319:LEU:HG	2.13	0.47
1:B:4604:VAL:HA	1:B:4625:GLU:HA	1.96	0.47
3:F:143:TRP:HA	3:F:336:TYR:HE2	1.79	0.47
3:F:152:TRP:HA	3:F:155:VAL:HB	1.96	0.47
1:A:395:VAL:O	1:A:399:ARG:HG2	2.15	0.47
1:A:1985:HIS:ND1	1:A:1997:ILE:HD13	2.30	0.47
1:A:3399:GLN:HA	1:A:3402:TYR:HD2	1.79	0.47
1:B:1042:GLY:O	1:B:1045:SER:OG	2.33	0.47
1:B:3780:VAL:O	1:B:3784:VAL:HG23	2.13	0.47
1:B:4545:VAL:HG22	1:B:4588:THR:HG22	1.96	0.47
6:K:17:VAL:HA	6:K:20:ILE:HG22	1.96	0.47
1:A:22:GLN:HE21	1:A:125:ILE:HA	1.78	0.47
1:A:3031:THR:O	1:A:3035:GLU:HG2	2.14	0.47
1:B:68:PHE:HZ	1:B:135:LEU:HD11	1.78	0.47
1:B:454:PRO:HG2	1:B:457:ARG:HG2	1.97	0.47
1:B:1861:MET:H	1:B:1864:ALA:HB3	1.79	0.47
2:C:214:GLN:C	2:D:209:ARG:HH12	2.23	0.47
3:F:120:LYS:HA	3:F:159:HIS:CE1	2.50	0.47
1:A:1219:GLY:HA2	1:A:1222:ASN:ND2	2.29	0.47
1:A:1724:VAL:HA	1:A:1727:PHE:CD2	2.48	0.47
1:A:2053:MET:HE1	1:A:2094:LYS:HG3	1.96	0.47
1:A:3219:ARG:HH21	1:A:3476:THR:HG21	1.79	0.47
1:A:3263:GLN:HA	1:A:3266:LYS:HD2	1.95	0.47
1:B:361:PHE:CD1	1:B:364:LEU:HD11	2.49	0.47
1:B:525:LEU:O	1:B:529:ASN:HB2	2.15	0.47
1:B:770:GLN:HG2	1:B:773:GLN:HE21	1.78	0.47
1:B:1013:THR:OG1	1:B:1014:GLU:N	2.41	0.47
1:B:1751:VAL:HG11	1:B:1878:LYS:HE3	1.95	0.47
1:B:2464:GLN:HG2	1:B:2583:THR:HG23	1.96	0.47
3:F:88:TYR:HD1	3:F:107:TRP:CD1	2.32	0.47
4:G:53:ALA:O	4:G:56:THR:HB	2.15	0.47
6:K:43:THR:HG23	6:K:69:ILE:HD12	1.96	0.47
1:A:40:LEU:HD23	1:A:45:GLY:HA2	1.97	0.47
1:A:433:LEU:O	1:A:437:ILE:HG12	2.15	0.47
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3256:MET:HB3	1:A:3433:VAL:HG11	1.97	0.47
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.14	0.47
1:B:852:ILE:HA	1:B:855:GLU:CD	2.39	0.47
1:B:1142:PHE:CE2	1:B:1214:ILE:HD12	2.50	0.47
1:B:1174:GLN:HA	1:B:1177:LYS:HG2	1.97	0.47
1:B:2422:ILE:HD13	1:B:2487:GLU:HA	1.97	0.47
1:A:146:TYR:OH	1:B:164:TYR:HB3	2.14	0.47
1:A:194:LEU:HD23	1:A:194:LEU:H	1.80	0.47
1:A:268:SER:OG	1:B:176:ASP:OD2	2.22	0.47
1:A:277:PHE:CZ	1:A:281:LEU:HD22	2.49	0.47
1:A:1176:LEU:O	1:A:1180:ILE:HG13	2.15	0.47
1:A:1945:PHE:HB3	1:A:1978:ILE:HD11	1.95	0.47
1:A:2142:CYS:HA	1:A:2146:VAL:HG23	1.96	0.47
1:B:213:ILE:HD13	1:B:300:THR:HG22	1.97	0.47
1:B:413:MET:HE2	1:B:467:ARG:HD2	1.96	0.47
1:B:893:TYR:HB2	1:B:896:LEU:HD21	1.96	0.47
1:B:1628:ARG:NH1	1:B:1657:MET:O	2.41	0.47
1:B:2569:VAL:HB	1:B:2747:ILE:HG23	1.97	0.47
1:B:2952:TRP:CE3	1:B:2953:MET:HG3	2.49	0.47
1:B:3240:LEU:HA	1:B:3243:MET:HG2	1.96	0.47
1:B:3250:ALA:O	1:B:3254:LYS:HG3	2.14	0.47
1:B:3452:ALA:O	1:B:3455:ILE:HG22	2.15	0.47
1:B:3843:ASN:ND2	1:B:3862:ASP:OD2	2.44	0.47
1:B:4093:TRP:CD1	1:B:4123:ARG:HB2	2.50	0.47
1:B:4173:PRO:HG2	1:B:4176:ARG:HH21	1.80	0.47
1:B:4282:PHE:HB3	1:B:4296:MET:HB3	1.97	0.47
1:B:4525:ARG:NH2	1:B:4539:LEU:O	2.47	0.47
2:D:343:PHE:HD2	2:D:412:LEU:HD23	1.79	0.47
3:F:70:LEU:O	3:F:74:LEU:HD23	2.15	0.47
3:F:146:MET:HG3	3:F:336:TYR:CG	2.50	0.47
4:G:49:PHE:CZ	4:H:53:ALA:HB2	2.50	0.47
5:I:17:MET:HE3	5:I:46:PHE:CE2	2.49	0.47
5:J:57:ILE:HG22	5:J:84:LEU:HB3	1.96	0.47
6:K:47:VAL:HG23	6:K:65:VAL:HG13	1.97	0.47
6:K:111:LEU:HD11	6:L:64:ILE:HD11	1.96	0.47
1:A:1752:LEU:O	1:A:1756:ILE:HG13	2.14	0.47
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.15	0.47
1:A:2176:THR:O	1:A:2180:GLU:HG2	2.15	0.47
1:B:292:ARG:HH12	1:B:320:THR:HG22	1.79	0.47
1:B:296:GLU:O	1:B:300:THR:HG23	2.15	0.47
1:B:1672:VAL:HA	1:B:1691:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:205:ARG:HH21	2:D:327:TYR:HE1	1.62	0.47
2:D:296:VAL:HG13	2:D:340:PHE:CZ	2.50	0.47
3:F:248:ASP:O	3:F:251:LEU:HG	2.15	0.47
4:G:23:VAL:HA	4:G:29:PRO:HA	1.96	0.47
4:H:82:PRO:HB3	4:H:87:PHE:HD1	1.80	0.47
1:A:31:GLN:HE21	1:A:56:LEU:HG	1.79	0.47
1:A:107:ILE:HB	1:B:160:PHE:CZ	2.50	0.47
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.96	0.47
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.15	0.47
1:B:210:HIS:CE1	1:B:212:MET:HG3	2.50	0.47
1:B:921:ALA:O	1:B:924:GLN:HG3	2.14	0.47
2:C:548:ARG:HA	2:C:566:SER:HA	1.96	0.47
3:F:156:LEU:HD22	3:F:223:LEU:HD12	1.97	0.47
1:A:55:ALA:HB3	1:A:101:TYR:CD2	2.50	0.47
1:A:329:VAL:C	1:A:331:ASP:N	2.72	0.47
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.97	0.47
1:A:3707:SER:O	1:A:3711:GLN:HG3	2.16	0.47
1:A:4209:GLU:OE1	1:A:4213:ARG:NH1	2.48	0.47
1:B:52:LEU:O	1:B:56:LEU:HG	2.15	0.47
1:B:1800:GLN:OE1	1:B:1804:ARG:NH1	2.45	0.47
1:B:3468:VAL:O	1:B:3472:VAL:HG23	2.15	0.47
1:B:4277:SER:HA	1:B:4282:PHE:CD2	2.50	0.47
6:K:77:LEU:HD11	6:K:105:ILE:HD12	1.96	0.47
1:A:155:ASN:O	1:B:107:ILE:HD13	2.16	0.46
1:A:368:ARG:NH1	1:A:436:ASP:HB3	2.30	0.46
1:A:402:MET:SD	1:A:535:GLY:HA3	2.55	0.46
1:B:724:ARG:HH11	1:B:726:ARG:HE	1.63	0.46
1:B:1347:LYS:O	1:B:1432:GLY:N	2.49	0.46
1:B:2222:MET:HG2	1:B:2364:PHE:CE1	2.50	0.46
1:B:3377:TYR:O	1:B:3381:ILE:HG12	2.15	0.46
1:B:3399:GLN:HA	1:B:3402:TYR:HD2	1.80	0.46
1:B:3449:GLU:O	1:B:3453:VAL:HG23	2.16	0.46
1:B:4528:VAL:HG11	1:B:4592:TRP:HB2	1.97	0.46
2:D:504:TRP:NE1	2:D:522:ASP:H	2.13	0.46
6:K:12:PHE:CZ	6:K:17:VAL:HG21	2.50	0.46
6:L:83:CYS:HB2	6:L:85:TRP:CZ3	2.51	0.46
1:A:285:LEU:CA	1:A:288:ILE:HG22	2.40	0.46
1:A:409:PHE:O	1:A:413:MET:HG3	2.16	0.46
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.96	0.46
1:A:3008:MET:O	1:A:3012:LEU:HG	2.14	0.46
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4422:LYS:NZ	1:A:4426:ASP:OD2	2.46	0.46
1:B:338:ASP:OD1	1:B:339:PHE:N	2.48	0.46
1:B:717:ILE:HG22	1:B:718:PHE:CD2	2.49	0.46
1:B:1163:THR:O	1:B:1167:VAL:N	2.33	0.46
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	1.97	0.46
1:B:3570:ASP:OD1	1:B:3571:ASP:N	2.48	0.46
1:B:3769:THR:O	1:B:3773:LEU:HG	2.16	0.46
2:C:338:ALA:HA	2:C:350:GLY:HA2	1.97	0.46
2:D:553:ASN:OD1	2:D:554:LEU:N	2.49	0.46
3:F:270:ILE:HG21	3:F:283:LEU:HD13	1.97	0.46
6:K:70:MET:O	6:K:102:MET:HA	2.14	0.46
6:K:73:ASN:ND2	6:L:75:ALA:HB2	2.29	0.46
1:A:30:LEU:HD21	1:A:69:LEU:HD11	1.97	0.46
1:A:1172:TYR:O	1:A:1175:SER:OG	2.26	0.46
1:A:2620:LEU:HD22	1:A:2630:LEU:HG	1.97	0.46
1:B:43:GLU:OE2	1:B:81:ARG:NH2	2.39	0.46
1:B:335:LEU:HD13	1:B:367:ILE:HD12	1.97	0.46
1:B:2061:THR:OG1	1:B:2133:GLU:OE1	2.31	0.46
1:B:2481:MET:CE	1:B:2485:GLN:HG2	2.44	0.46
1:B:3237:ASN:O	1:B:3241:LYS:HG2	2.16	0.46
1:B:3294:ASN:HB3	1:B:3391:PRO:HB3	1.97	0.46
2:D:278:LYS:O	2:D:280:ARG:HG3	2.15	0.46
1:A:374:ILE:HB	1:A:446:LEU:HD11	1.97	0.46
1:A:378:LEU:O	1:A:452:ILE:HG22	2.16	0.46
1:A:2104:LYS:O	1:A:2108:ILE:HG12	2.16	0.46
1:A:2820:GLY:O	1:A:2824:ILE:HG13	2.15	0.46
1:A:3340:SER:O	1:A:3346:ASN:ND2	2.49	0.46
1:A:3547:ILE:HD13	1:A:3552:TYR:HD1	1.81	0.46
1:A:4172:SER:OG	1:A:4173:PRO:HD3	2.15	0.46
1:B:283:ARG:HG3	1:B:287:ARG:HH12	1.80	0.46
1:B:1146:ILE:O	1:B:1150:ARG:HG2	2.15	0.46
1:B:2319:LEU:HD13	1:B:2359:CYS:SG	2.55	0.46
1:B:3143:ILE:HD13	1:B:3541:ILE:HD13	1.98	0.46
2:D:493:PHE:HD1	2:D:496:LEU:HD11	1.81	0.46
1:A:409:PHE:CZ	1:A:413:MET:HE3	2.49	0.46
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.50	0.46
1:A:3251:GLU:HG3	1:B:3248:GLN:NE2	2.31	0.46
1:A:3447:TYR:N	1:A:3447:TYR:CD1	2.83	0.46
1:A:3567:LEU:HD12	1:A:3568:PRO:HD2	1.98	0.46
1:A:3910:ARG:NH2	1:A:4344:LEU:HD11	2.29	0.46
1:B:1224:ILE:HD12	1:B:1228:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1543:ARG:HA	1:B:1546:TYR:CE2	2.50	0.46
1:B:2445:HIS:NE2	1:B:2449:LEU:HD22	2.31	0.46
1:B:2751:PHE:HB3	1:B:2803:VAL:HG11	1.96	0.46
1:B:2937:GLY:C	1:B:3070:PRO:HD3	2.41	0.46
1:B:4543:VAL:HG12	1:B:4590:LEU:HD22	1.97	0.46
6:L:70:MET:O	6:L:102:MET:HA	2.15	0.46
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.96	0.46
1:A:3177:LEU:HD23	1:A:3180:ILE:HD11	1.97	0.46
1:A:4288:VAL:HG11	1:A:4294:ILE:HG13	1.98	0.46
1:A:4606:THR:HA	1:A:4622:VAL:O	2.15	0.46
1:B:212:MET:HA	1:B:215:ASN:HD21	1.80	0.46
1:B:581:MET:HG2	1:B:611:ARG:NH2	2.30	0.46
1:B:1023:LEU:HD12	1:B:1033:LEU:HD22	1.97	0.46
1:B:1213:ASN:HA	5:J:11:ALA:H	1.80	0.46
1:B:1666:LEU:HD23	1:B:1673:VAL:HA	1.98	0.46
1:B:2387:LEU:N	1:B:2416:GLN:OE1	2.33	0.46
1:B:2635:PHE:CZ	1:B:2686:MET:HE1	2.51	0.46
1:B:2643:ARG:NH1	1:B:2643:ARG:HB3	2.30	0.46
2:D:364:SER:HB2	2:D:366:LYS:HE3	1.97	0.46
2:D:589:ASP:OD1	2:D:590:SER:N	2.48	0.46
1:A:189:LEU:HD21	1:B:185:LYS:HB3	1.96	0.46
1:A:373:PRO:O	1:A:377:ALA:N	2.38	0.46
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.50	0.46
1:A:1806:ARG:NH2	1:A:1877:ASP:OD1	2.49	0.46
1:A:3922:PRO:HD2	1:A:3936:VAL:HG11	1.97	0.46
1:B:126:ASP:H	1:B:134:GLN:HE22	1.62	0.46
1:B:526:ALA:C	1:B:553:TYR:HH	2.09	0.46
1:B:960:HIS:O	1:B:1107:ILE:HA	2.16	0.46
1:B:1037:TYR:O	1:B:1040:VAL:HB	2.16	0.46
1:B:4172:SER:OG	1:B:4173:PRO:HD3	2.14	0.46
1:B:4414:GLU:O	1:B:4418:LYS:HE2	2.16	0.46
1:A:360:ILE:O	1:A:364:LEU:HG	2.15	0.46
1:A:379:ARG:O	1:A:382:GLU:HB3	2.15	0.46
1:B:335:LEU:HG	1:B:366:LYS:NZ	2.31	0.46
1:B:817:ALA:HA	3:F:366:GLN:NE2	2.31	0.46
1:B:2527:PRO:HD3	1:B:2545:TRP:CE2	2.51	0.46
2:D:211:LEU:HD23	4:H:15:LYS:HE3	1.98	0.46
2:D:505:THR:HG22	2:D:507:LYS:HG3	1.98	0.46
6:K:17:VAL:O	6:K:20:ILE:HG22	2.16	0.46
1:A:146:TYR:CZ	1:B:164:TYR:HD2	2.33	0.46
1:A:274:GLU:HG2	1:A:380:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2837:LEU:O	1:A:2843:ARG:NH2	2.49	0.46
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.98	0.46
1:A:4436:GLN:HG2	1:A:4442:LYS:HG2	1.98	0.46
1:B:72:PRO:O	1:B:75:HIS:NE2	2.49	0.46
1:B:195:HIS:CE1	1:B:198:GLN:HE21	2.34	0.46
1:B:382:GLU:O	1:B:386:ARG:HG2	2.16	0.46
1:B:960:HIS:CE1	1:B:1107:ILE:HG22	2.51	0.46
1:B:3263:GLN:HA	1:B:3266:LYS:HD2	1.96	0.46
1:B:3716:VAL:HB	1:B:3836:TYR:OH	2.15	0.46
1:B:4043:MET:HE1	1:B:4055:VAL:HG23	1.97	0.46
1:B:4297:PRO:HG3	1:B:4308:TRP:CD2	2.50	0.46
2:C:406:LYS:HA	2:C:423:GLU:HA	1.98	0.46
2:D:207:VAL:HG21	4:H:11:LEU:HD11	1.98	0.46
2:D:536:HIS:HB3	2:D:539:LEU:HB3	1.98	0.46
4:G:70:ARG:NH2	4:G:72:ARG:HH21	2.13	0.46
1:A:29:VAL:HA	1:A:32:LYS:HE2	1.97	0.46
1:A:300:THR:O	1:A:304:LEU:HG	2.16	0.46
1:A:3451:TYR:CD1	1:A:3454:LEU:HD21	2.51	0.46
1:B:1194:GLN:NE2	1:B:1195:ARG:HG3	2.31	0.46
1:B:2486:LEU:O	1:B:2490:ILE:HG12	2.16	0.46
1:B:2667:ASN:ND2	1:B:2712:CYS:HB2	2.31	0.46
1:B:2917:ASP:O	1:B:2921:ARG:HG3	2.16	0.46
1:B:3966:PRO:HG3	1:B:3997:ARG:NH1	2.31	0.46
1:A:372:TYR:CD2	1:A:377:ALA:HB2	2.51	0.45
1:A:377:ALA:O	1:A:380:LEU:HB2	2.16	0.45
1:A:2554:GLN:HE21	1:A:2753:ARG:HH22	1.63	0.45
1:A:3514:ILE:HD11	1:A:3553:LEU:HD22	1.97	0.45
1:A:3812:TYR:O	1:A:3815:MET:HB2	2.16	0.45
1:B:842:ASN:O	1:B:845:GLU:HG3	2.15	0.45
2:D:211:LEU:HA	4:H:15:LYS:HE3	1.98	0.45
2:D:457:TYR:HB3	2:D:468:ILE:HD12	1.98	0.45
4:H:80:VAL:HA	4:H:88:LEU:HB2	1.98	0.45
5:J:13:MET:HG2	5:J:73:PHE:O	2.16	0.45
1:A:2001:LEU:HD12	1:A:2006:VAL:HG11	1.97	0.45
1:A:3212:VAL:HA	1:A:3215:VAL:HG12	1.98	0.45
1:A:3377:TYR:O	1:A:3381:ILE:HG12	2.16	0.45
1:A:3443:SER:O	1:A:3444:ILE:C	2.59	0.45
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.48	0.45
1:A:3654:ARG:NH2	1:A:3668:ASP:OD1	2.49	0.45
1:A:3982:PRO:HA	1:A:3985:GLN:HG2	1.98	0.45
1:B:126:ASP:H	1:B:134:GLN:NE2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ARG:HH22	1:B:432:VAL:HB	1.82	0.45
1:B:639:ARG:NH2	2:D:574:ASN:HD21	2.13	0.45
1:B:1170:ILE:HG22	1:B:1174:GLN:HE22	1.81	0.45
1:B:1214:ILE:HA	1:B:1217:GLU:HG2	1.97	0.45
1:B:2142:CYS:HA	1:B:2146:VAL:HG23	1.97	0.45
1:B:2231:SER:HA	1:B:2234:TRP:CD1	2.51	0.45
1:B:2918:HIS:O	1:B:2922:ILE:HG13	2.16	0.45
1:B:4606:THR:HA	1:B:4622:VAL:O	2.16	0.45
2:C:204:THR:HA	4:G:10:ARG:NH1	2.30	0.45
5:I:43:LYS:HD2	5:J:65:TYR:O	2.16	0.45
1:A:292:ARG:HG2	1:A:298:LEU:HD23	1.98	0.45
1:A:1457:MET:HE1	1:A:1461:GLU:OE2	2.16	0.45
1:A:1619:LEU:HD21	1:A:1638:LEU:HD23	1.99	0.45
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.98	0.45
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.98	0.45
1:A:2892:TYR:O	1:A:2896:ARG:HG2	2.16	0.45
1:B:94:GLU:HB3	1:B:251:ARG:HB2	1.98	0.45
1:B:464:ASP:OD1	1:B:465:GLN:N	2.50	0.45
1:B:3514:ILE:HD11	1:B:3553:LEU:HD22	1.97	0.45
1:B:4092:ARG:HG3	1:B:4093:TRP:N	2.31	0.45
1:B:4099:VAL:HG21	1:B:4126:LEU:HB3	1.97	0.45
3:F:335:ALA:HB3	3:F:338:ASP:OD1	2.16	0.45
5:I:6:ALA:O	5:I:8:ILE:HG13	2.17	0.45
6:K:77:LEU:HD11	6:K:105:ILE:CD1	2.46	0.45
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.51	0.45
1:B:180:PRO:O	1:B:184:LYS:HG2	2.16	0.45
1:B:2538:GLU:HB3	1:B:2548:TRP:CE2	2.51	0.45
1:B:2944:THR:O	1:B:2948:ARG:HG3	2.16	0.45
1:B:3113:MET:SD	1:B:3184:ALA:HA	2.56	0.45
1:B:3703:VAL:HG21	1:B:3829:LEU:HD22	1.98	0.45
1:B:4096:LEU:HD13	1:B:4105:TRP:HH2	1.81	0.45
2:D:266:SER:O	2:D:597:TYR:HB2	2.15	0.45
2:D:504:TRP:HA	2:D:527:VAL:HG12	1.98	0.45
3:F:227:VAL:HG13	3:F:267:ALA:HB2	1.99	0.45
3:F:315:ASP:OD1	3:F:316:ASN:N	2.49	0.45
1:A:27:VAL:O	1:A:31:GLN:HB2	2.16	0.45
1:A:143:ASP:OD1	1:A:144:SER:N	2.46	0.45
1:A:1756:ILE:O	1:A:1760:GLU:HG2	2.16	0.45
1:A:3254:LYS:HG3	1:A:3437:ILE:HD11	1.97	0.45
1:B:331:ASP:OD1	1:B:332:TYR:N	2.50	0.45
1:B:759:ARG:HG2	1:B:759:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:ARG:NH2	1:B:1121:ASP:HA	2.29	0.45
1:B:4169:ILE:HD11	1:B:4177:ALA:HA	1.97	0.45
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	1.98	0.45
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.16	0.45
1:A:4600:LYS:HZ3	1:A:4604:VAL:CB	2.21	0.45
1:B:304:LEU:HD13	1:B:309:ARG:HB3	1.99	0.45
1:B:650:TRP:CE2	1:B:654:ILE:HD11	2.52	0.45
1:B:1194:GLN:OE1	1:B:1211:ILE:HD13	2.16	0.45
1:B:3585:ARG:NH1	1:B:3694:SER:O	2.42	0.45
2:C:204:THR:HA	4:G:10:ARG:HH12	1.82	0.45
5:I:52:PRO:HA	5:I:53:THR:HA	1.69	0.45
1:A:382:GLU:HB2	1:A:452:ILE:HA	1.99	0.45
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.35	0.45
1:A:3008:MET:HE1	1:A:3011:LEU:HD23	1.99	0.45
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.98	0.45
1:B:213:ILE:HD12	1:B:303:ILE:HD11	1.99	0.45
1:B:232:PHE:CE2	1:B:303:ILE:HG21	2.51	0.45
1:B:987:PHE:CE2	3:F:87:GLU:HG2	2.52	0.45
1:B:1095:ASN:OD1	1:B:1096:ALA:N	2.50	0.45
1:B:1124:HIS:NE2	1:B:1128:LEU:HD11	2.32	0.45
1:B:1267:VAL:O	1:B:1382:SER:N	2.50	0.45
1:B:4064:THR:HB	1:B:4092:ARG:NH2	2.32	0.45
1:B:4150:PRO:HG3	1:B:4159:ARG:HH11	1.81	0.45
3:F:142:PRO:HA	3:F:145:VAL:HG23	1.98	0.45
4:G:14:GLN:HB3	4:G:17:VAL:HG21	1.99	0.45
5:I:17:MET:HE3	5:I:46:PHE:HE2	1.81	0.45
6:K:99:ASN:OD1	6:K:102:MET:N	2.50	0.45
1:A:215:ASN:C	1:A:215:ASN:HD22	2.24	0.45
1:A:440:ARG:O	1:A:444:GLU:HG2	2.17	0.45
1:A:1765:ALA:O	1:A:1769:MET:HG2	2.17	0.45
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.31	0.45
1:A:3043:MET:HG3	1:A:3043:MET:O	2.16	0.45
1:A:3315:ALA:O	1:A:3319:LEU:HG	2.17	0.45
1:A:4452:ILE:O	1:A:4456:VAL:HG23	2.17	0.45
1:B:584:ILE:HG23	1:B:587:ARG:HH21	1.82	0.45
1:B:4019:SER:O	1:B:4022:GLU:HG2	2.17	0.45
1:B:4566:GLN:O	1:B:4640:VAL:HA	2.17	0.45
2:D:399:ILE:HG21	2:D:447:PHE:CZ	2.52	0.45
3:F:172:GLU:O	3:F:176:LYS:NZ	2.34	0.45
1:A:40:LEU:HB3	1:B:33:HIS:CE1	2.52	0.45
1:A:357:LEU:HD21	1:A:388:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3284:LYS:O	1:A:3402:TYR:OH	2.26	0.45
1:A:3369:LYS:HA	1:A:3372:MET:HG2	1.98	0.45
1:A:3769:THR:O	1:A:3773:LEU:HG	2.17	0.45
1:B:145:PRO:HA	1:B:148:THR:HB	1.99	0.45
1:B:1724:VAL:HG23	1:B:1727:PHE:HD2	1.81	0.45
1:B:3154:LEU:HG	1:B:3516:TYR:CD1	2.52	0.45
3:F:48:ARG:HD2	3:F:49:SER:N	2.32	0.45
6:L:72:LYS:HG2	6:L:103:TYR:CE2	2.51	0.45
1:A:1958:ASP:OD1	1:A:1959:GLU:N	2.49	0.45
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.52	0.45
1:A:3254:LYS:HG3	1:A:3437:ILE:CD1	2.47	0.45
1:A:3935:VAL:HG22	1:A:3996:PHE:HE2	1.82	0.45
1:A:3957:PHE:HZ	1:A:3996:PHE:CE1	2.35	0.45
1:B:2132:PRO:HB2	1:B:2135:GLU:HB2	1.98	0.45
1:B:3302:GLN:HB3	1:B:3388:ALA:HB2	1.99	0.45
1:B:3990:LEU:HA	1:B:4004:MET:HG2	1.99	0.45
1:B:4230:ARG:HG2	1:B:4232:ASN:O	2.16	0.45
1:B:4520:TYR:O	1:B:4524:THR:HG23	2.17	0.45
2:D:286:ASP:OD1	2:D:287:TRP:N	2.50	0.45
2:D:299:TYR:OH	2:D:302:ASN:HA	2.17	0.45
2:D:504:TRP:CD1	2:D:522:ASP:H	2.34	0.45
3:F:370:LEU:HA	3:F:373:GLN:HG2	1.98	0.45
5:J:32:TYR:HB2	5:J:38:ILE:CD1	2.47	0.45
1:A:217:ALA:HB2	1:A:303:ILE:HD13	1.99	0.44
1:A:1209:LEU:HD23	1:A:1209:LEU:H	1.82	0.44
1:A:2944:THR:O	1:A:2948:ARG:HG3	2.16	0.44
1:A:3100:GLU:O	1:A:3104:GLN:HG3	2.17	0.44
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.82	0.44
1:B:200:ILE:HG12	1:B:277:PHE:HE1	1.83	0.44
1:B:2138:ILE:HD11	1:B:2165:PHE:CG	2.52	0.44
1:B:2758:LEU:HD11	1:B:2807:PHE:CE1	2.51	0.44
1:B:2930:GLN:HB2	1:B:3059:ILE:HG23	1.99	0.44
1:B:3191:ARG:HG2	1:B:3503:ILE:HD13	1.99	0.44
1:B:3208:ILE:HG21	1:B:3486:ARG:HD3	1.99	0.44
1:B:3570:ASP:OD2	1:B:3704:THR:OG1	2.34	0.44
1:B:4071:ILE:HG23	1:B:4077:PHE:HE1	1.80	0.44
1:B:4150:PRO:HG3	1:B:4159:ARG:NH1	2.33	0.44
3:F:137:ALA:HB1	3:F:145:VAL:HG22	1.99	0.44
4:G:68:PHE:HD2	4:H:72:ARG:HB3	1.82	0.44
5:J:40:ALA:HB1	5:J:44:LYS:HZ3	1.81	0.44
6:K:36:HIS:CD2	6:L:76:GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:78:HIS:HE1	6:L:69:ILE:HB	1.82	0.44
1:A:396:LEU:HD21	1:A:401:LEU:HD22	2.00	0.44
1:A:1229:ASP:O	1:A:1232:ILE:HG22	2.18	0.44
1:A:2179:ARG:NH2	1:A:2205:GLU:OE2	2.49	0.44
1:A:4055:VAL:HG21	1:A:4095:MET:HE3	1.99	0.44
1:B:627:TYR:O	1:B:633:CYS:HB3	2.17	0.44
1:B:1626:PHE:HB3	1:B:1629:PHE:CD2	2.52	0.44
1:B:2563:ALA:HB3	1:B:2804:ARG:HD2	1.99	0.44
1:B:3650:ASN:HD21	1:B:3695:ARG:NH1	2.14	0.44
1:B:4392:PRO:O	1:B:4428:ARG:NH1	2.49	0.44
1:B:4629:LYS:HG3	1:B:4629:LYS:O	2.18	0.44
5:I:46:PHE:HD2	5:I:54:TRP:CE2	2.35	0.44
1:A:170:LYS:HE2	1:A:176:ASP:HB3	1.99	0.44
1:A:4191:GLN:NE2	1:A:4207:PHE:O	2.49	0.44
1:B:388:LEU:O	1:B:391:GLN:HG3	2.18	0.44
1:B:3207:LYS:HD3	1:B:3207:LYS:HA	1.83	0.44
5:I:28:ALA:HB2	5:I:41:HIS:CD2	2.51	0.44
1:A:454:PRO:HD2	1:A:457:ARG:HH12	1.81	0.44
1:A:1417:MET:O	1:A:1421:HIS:N	2.48	0.44
1:A:3199:MET:SD	1:A:3200:HIS:ND1	2.90	0.44
1:A:3254:LYS:O	1:A:3258:GLN:HG3	2.18	0.44
1:A:3255:VAL:O	1:A:3259:GLU:HG3	2.17	0.44
1:A:3434:GLU:HA	1:A:3437:ILE:HG22	2.00	0.44
1:A:4627:ALA:HB3	1:A:4630:GLU:HG2	2.00	0.44
1:B:82:SER:O	1:B:100:SER:N	2.43	0.44
1:B:622:LYS:NZ	2:D:525:ASP:OD2	2.29	0.44
1:B:1126:GLU:O	1:B:1129:SER:OG	2.23	0.44
1:B:2215:GLN:OE1	1:B:2215:GLN:HA	2.18	0.44
1:A:153:ILE:O	1:A:157:VAL:HG22	2.17	0.44
1:A:270:THR:HG23	1:A:273:GLN:H	1.81	0.44
1:A:372:TYR:H	1:A:440:ARG:HH22	1.64	0.44
1:A:3243:MET:CE	1:A:3444:ILE:HA	2.47	0.44
1:A:4604:VAL:HA	1:A:4625:GLU:HA	1.99	0.44
1:B:580:GLU:O	1:B:584:ILE:HG13	2.17	0.44
1:B:1204:PHE:H	5:J:5:LYS:HZ1	1.64	0.44
1:B:2242:GLU:HG3	1:B:2248:GLU:HA	1.99	0.44
1:B:3100:GLU:O	1:B:3104:GLN:HG3	2.18	0.44
1:B:3130:TYR:CZ	1:B:3132:LYS:HB2	2.53	0.44
1:B:4424:LEU:O	1:B:4428:ARG:HG2	2.17	0.44
1:B:4439:GLU:HB2	1:B:4441:LYS:HG2	2.00	0.44
3:F:228:LEU:HD21	3:F:286:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:230:VAL:HA	3:F:270:ILE:O	2.17	0.44
1:A:162:LYS:HG2	1:A:166:ARG:NH1	2.32	0.44
1:A:1580:LYS:O	1:A:1584:LYS:HG2	2.18	0.44
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.99	0.44
1:B:363:HIS:O	1:B:366:LYS:HG2	2.18	0.44
1:B:425:ASP:HB3	1:B:429:LYS:NZ	2.32	0.44
1:B:439:LYS:O	1:B:442:ARG:HD3	2.17	0.44
1:B:793:GLU:HA	1:B:796:GLU:HG3	2.00	0.44
1:B:967:GLN:HG2	1:B:1061:TRP:CD2	2.52	0.44
1:B:1230:SER:HA	1:B:1233:GLN:OE1	2.18	0.44
1:B:1658:PHE:HB2	1:B:1661:VAL:HB	2.00	0.44
1:B:2665:GLU:OE2	1:B:2665:GLU:HA	2.17	0.44
1:B:2743:SER:O	1:B:2747:ILE:HG13	2.17	0.44
1:B:3447:TYR:HA	1:B:3450:GLU:CD	2.43	0.44
1:B:4190:ILE:HG13	1:B:4191:GLN:N	2.32	0.44
3:F:61:GLY:HA3	3:F:67:LYS:HD3	2.00	0.44
4:H:70:ARG:HH22	4:H:72:ARG:HH11	1.66	0.44
1:A:39:PRO:HG3	1:A:48:ALA:H	1.82	0.44
1:A:390:SER:O	1:A:394:LYS:HG3	2.18	0.44
1:A:448:MET:HA	1:A:450:TRP:CZ3	2.53	0.44
1:A:1707:LYS:O	1:A:1711:VAL:HG23	2.18	0.44
1:B:694:ASN:ND2	1:B:697:GLU:OE1	2.51	0.44
1:B:1043:ILE:HA	1:B:1102:PHE:CE2	2.51	0.44
1:B:1138:ASN:OD1	1:B:1139:MET:N	2.50	0.44
1:B:1156:HIS:NE2	1:B:1166:ALA:HA	2.33	0.44
1:B:1572:SER:O	1:B:1576:LEU:HD23	2.17	0.44
1:B:2348:LEU:HD23	1:B:2356:VAL:HG22	1.99	0.44
1:B:3808:CYS:HB3	1:B:3832:PHE:HZ	1.82	0.44
1:B:3835:ILE:HD13	1:B:3867:ALA:HA	2.00	0.44
1:B:3891:LYS:HD2	1:B:4013:LEU:HD23	2.00	0.44
2:D:386:CYS:HB3	2:D:401:ILE:CG2	2.48	0.44
1:A:275:ILE:HA	1:A:278:TRP:CD1	2.49	0.44
1:A:1803:LEU:HG	1:A:1807:LYS:HE3	2.00	0.44
1:A:2221:MET:SD	1:A:2361:MET:HE1	2.58	0.44
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.18	0.44
1:A:2896:ARG:HG3	1:A:2953:MET:HE1	2.00	0.44
1:A:3005:LEU:HD23	1:A:3005:LEU:HA	1.81	0.44
1:A:3363:ILE:O	1:A:3367:MET:HG2	2.17	0.44
1:A:3429:LYS:O	1:A:3433:VAL:N	2.39	0.44
1:A:3443:SER:HB2	1:A:3447:TYR:CE2	2.53	0.44
1:A:3728:ARG:O	1:A:3732:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.00	0.44
1:B:1687:LYS:HG3	1:B:1715:LYS:HD2	1.98	0.44
1:B:1945:PHE:HB3	1:B:1978:ILE:HD11	2.00	0.44
1:B:2458:LEU:O	1:B:2462:LEU:HG	2.18	0.44
1:B:2568:VAL:HG22	1:B:2603:MET:HG3	2.00	0.44
1:B:3110:THR:O	1:B:3140:ARG:NH1	2.51	0.44
6:L:47:VAL:HG13	6:L:65:VAL:HB	2.00	0.44
1:A:154:SER:HB3	1:A:190:GLU:OE1	2.17	0.44
1:A:1567:ARG:NH1	1:B:3043:MET:O	2.45	0.44
1:A:1847:ASP:OD1	1:A:1849:LYS:HG2	2.18	0.44
1:A:2224:GLY:O	1:A:2230:LYS:NZ	2.39	0.44
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.78	0.44
1:A:3319:LEU:HD22	1:A:3377:TYR:CD1	2.53	0.44
1:A:3381:ILE:HD12	1:A:3390:GLY:HA2	1.98	0.44
1:A:3468:VAL:O	1:A:3472:VAL:HG23	2.18	0.44
1:A:3905:PHE:CE1	1:A:3987:ILE:HG12	2.53	0.44
1:A:4545:VAL:HG22	1:A:4588:THR:HG22	2.00	0.44
1:B:116:LEU:HD23	1:B:139:THR:HB	1.99	0.44
1:B:120:LYS:HA	1:B:135:LEU:HD13	2.00	0.44
1:B:581:MET:HE1	1:B:608:LEU:HD12	1.98	0.44
1:B:642:PRO:HB2	1:B:749:GLU:OE2	2.17	0.44
1:B:4160:THR:HG23	1:B:4212:LEU:HD21	1.99	0.44
1:B:4409:LEU:HD11	1:B:4558:PHE:HE2	1.83	0.44
3:F:255:GLN:OE1	3:F:323:LEU:HD21	2.18	0.44
3:F:258:LEU:HD23	3:F:269:LEU:HD11	1.99	0.44
4:G:75:LYS:HD3	4:H:64:ASN:ND2	2.33	0.44
1:A:455:ALA:O	1:A:458:LYS:HG2	2.18	0.43
1:A:1190:TYR:HE2	1:A:1208:TRP:HH2	1.65	0.43
1:A:1628:ARG:NH1	1:A:1657:MET:O	2.41	0.43
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	2.00	0.43
1:B:1457:MET:O	1:B:1461:GLU:HG2	2.17	0.43
1:B:1512:TYR:O	1:B:1515:VAL:HG22	2.18	0.43
1:B:1741:TRP:CH2	1:B:1750:VAL:HG13	2.53	0.43
1:B:3381:ILE:HD12	1:B:3390:GLY:HA2	1.99	0.43
1:B:3932:ALA:O	1:B:3936:VAL:HG13	2.18	0.43
1:B:4027:LEU:O	1:B:4031:VAL:HG12	2.17	0.43
1:B:4226:THR:HG21	1:B:4239:PRO:HD3	1.99	0.43
4:H:81:ALA:HB3	4:H:88:LEU:HD23	2.00	0.43
6:K:76:GLY:O	6:L:70:MET:HE1	2.18	0.43
1:A:90:ASP:N	1:A:90:ASP:OD1	2.52	0.43
1:A:257:GLN:O	1:A:261:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:HA	1:A:283:ARG:HG2	2.00	0.43
1:A:1777:PRO:O	1:A:1780:SER:OG	2.18	0.43
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.44	0.43
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.53	0.43
1:B:1830:ILE:HG12	1:B:1837:GLU:HB2	1.99	0.43
1:B:2174:GLU:OE1	1:B:2176:THR:OG1	2.24	0.43
1:B:2310:GLU:OE1	1:B:2310:GLU:HA	2.18	0.43
2:D:528:TYR:CD1	2:D:528:TYR:C	2.96	0.43
1:A:195:HIS:CD2	1:A:267:ALA:HB3	2.53	0.43
1:A:374:ILE:H	1:A:446:LEU:HD11	1.83	0.43
1:A:435:ARG:O	1:A:438:VAL:HB	2.18	0.43
1:A:3207:LYS:HA	1:A:3207:LYS:HD3	1.83	0.43
1:B:352:LYS:HA	1:B:355:GLN:HG3	1.99	0.43
1:B:518:ASN:O	1:B:521:GLU:HG2	2.19	0.43
1:B:717:ILE:HG22	1:B:718:PHE:HD2	1.83	0.43
1:B:1580:LYS:HE2	1:B:1580:LYS:HA	2.00	0.43
1:B:1746:GLN:OE1	1:B:1746:GLN:N	2.52	0.43
1:B:2257:LYS:NZ	1:B:2308:ASP:OD2	2.41	0.43
1:B:2324:LEU:HD23	1:B:2334:SER:HA	1.99	0.43
1:B:3088:ARG:HG2	1:B:3088:ARG:HH11	1.82	0.43
2:D:208:GLU:HA	2:D:211:LEU:HG	2.00	0.43
2:D:493:PHE:CD1	2:D:496:LEU:HD11	2.53	0.43
6:K:100:LYS:HG2	6:K:101:THR:HG23	1.99	0.43
1:A:173:ARG:HD2	1:B:283:ARG:NH2	2.32	0.43
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.82	0.43
1:A:2444:GLU:HG2	1:A:2510:MET:HE3	1.99	0.43
1:A:3621:LYS:HA	1:A:3624:GLU:HG2	1.99	0.43
1:B:368:ARG:HD2	1:B:368:ARG:HA	1.82	0.43
1:B:546:TRP:CD1	1:B:550:MET:HE2	2.53	0.43
1:B:801:ILE:O	1:B:805:VAL:HG23	2.19	0.43
1:B:1513:TYR:CE2	1:B:1517:GLU:HG2	2.53	0.43
1:B:2113:ARG:O	1:B:2116:GLU:HG3	2.18	0.43
1:B:2635:PHE:CE2	1:B:2686:MET:HE1	2.53	0.43
1:B:3473:ASN:HA	1:B:3476:THR:HG22	2.01	0.43
2:D:509:TRP:HA	2:D:517:LEU:HG	1.99	0.43
3:F:152:TRP:O	3:F:155:VAL:HB	2.18	0.43
6:L:54:LEU:HD13	6:L:63:TYR:CD1	2.53	0.43
1:A:458:LYS:O	1:A:462:ARG:HG3	2.18	0.43
1:A:2324:LEU:HD23	1:A:2334:SER:HA	2.00	0.43
1:A:3085:LEU:HD23	1:A:3085:LEU:HA	1.89	0.43
1:A:4159:ARG:HE	1:A:4159:ARG:HB2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4433:ASP:O	1:B:4437:VAL:HG23	2.19	0.43
5:I:13:MET:HE3	5:I:18:GLN:HA	2.00	0.43
5:I:76:PHE:HE2	5:I:78:LEU:HG	1.83	0.43
6:K:45:ASN:O	6:K:46:VAL:C	2.62	0.43
1:A:220:CYS:O	1:A:223:ARG:NE	2.48	0.43
1:A:292:ARG:HA	1:A:297:VAL:CG1	2.48	0.43
1:A:1150:ARG:HG2	1:A:1221:PHE:CD1	2.52	0.43
1:A:1711:VAL:HG13	1:A:1853:VAL:HG21	2.00	0.43
1:A:1946:VAL:O	1:A:1950:GLN:HG3	2.18	0.43
1:A:2509:LYS:NZ	1:A:2513:GLU:OE2	2.49	0.43
1:A:2973:ASP:O	1:A:2977:ARG:HG3	2.18	0.43
1:A:3303:HIS:O	1:A:3307:VAL:HG23	2.19	0.43
1:A:3985:GLN:O	1:A:3989:ARG:HG3	2.18	0.43
1:A:4197:ALA:HB3	1:A:4198:PRO:HD3	2.00	0.43
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.99	0.43
1:B:1135:LEU:HD22	1:B:1190:TYR:CD1	2.54	0.43
1:B:2382:LEU:HD23	1:B:2420:ALA:HB2	2.00	0.43
1:B:2418:ASP:O	1:B:2422:ILE:HG13	2.19	0.43
1:B:2592:VAL:HA	1:B:2710:GLY:O	2.18	0.43
1:B:2627:THR:OG1	1:B:2629:GLU:OE1	2.32	0.43
1:B:3046:SER:HB3	1:B:3049:GLU:CD	2.43	0.43
1:B:4435:VAL:O	1:B:4439:GLU:HG3	2.19	0.43
1:A:1201:ARG:HH21	1:B:1061:TRP:HD1	1.65	0.43
1:A:1751:VAL:HG12	1:A:1755:GLN:HE21	1.82	0.43
1:A:2517:TYR:CE1	1:A:2521:ILE:HD13	2.54	0.43
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	2.01	0.43
1:A:2799:MET:HE3	1:A:2799:MET:HB3	1.79	0.43
1:A:3683:ASP:HB3	1:A:3686:VAL:HG13	2.01	0.43
1:A:3815:MET:SD	1:A:3832:PHE:HB2	2.59	0.43
1:A:4424:LEU:O	1:A:4428:ARG:HG2	2.19	0.43
1:B:473:HIS:CE1	1:B:477:ARG:HD2	2.54	0.43
1:B:543:THR:O	1:B:547:GLU:OE1	2.37	0.43
1:B:1350:PRO:HA	1:B:1429:LEU:O	2.18	0.43
1:B:2841:GLU:HA	1:B:2844:ARG:HG2	2.01	0.43
5:I:17:MET:HE1	5:I:50:TYR:CD2	2.53	0.43
1:A:136:ARG:HE	1:B:139:THR:HG23	1.84	0.43
1:A:454:PRO:O	1:A:457:ARG:NH1	2.52	0.43
1:A:3130:TYR:CZ	1:A:3132:LYS:HB3	2.53	0.43
1:A:3253:LYS:NZ	1:A:3436:MET:HB2	2.32	0.43
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.19	0.43
1:B:75:HIS:O	1:B:119:ILE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PRO:O	1:B:215:ASN:ND2	2.51	0.43
1:B:476:LEU:HD22	1:B:591:LEU:HD11	2.00	0.43
1:B:664:ARG:HG2	1:B:664:ARG:HH11	1.84	0.43
1:B:2444:GLU:CD	1:B:2507:ARG:HH12	2.26	0.43
2:D:504:TRP:NE1	2:D:523:ASN:H	2.17	0.43
1:A:55:ALA:HA	1:A:58:GLU:HB2	1.99	0.43
1:A:440:ARG:O	1:A:443:GLU:HG2	2.19	0.43
1:A:578:ALA:O	1:A:583:ARG:N	2.36	0.43
1:B:1497:VAL:HG11	1:B:1531:MET:HG2	2.01	0.43
1:B:2248:GLU:OE2	1:B:2297:LYS:HE2	2.19	0.43
1:B:3211:THR:O	1:B:3215:VAL:HG23	2.19	0.43
1:B:4091:GLY:CA	1:B:4119:HIS:HB3	2.47	0.43
1:B:4156:ASN:ND2	1:B:4188:ALA:HA	2.34	0.43
2:D:578:TRP:HA	2:D:585:ILE:HD12	2.01	0.43
2:D:579:THR:HG21	2:D:584:GLU:CD	2.43	0.43
3:F:139:MET:O	3:F:142:PRO:HD3	2.19	0.43
4:G:3:GLU:HG3	4:G:6:GLU:H	1.82	0.43
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.71	0.43
1:A:221:TYR:CG	1:A:299:LEU:HD22	2.54	0.43
1:A:229:VAL:HG22	1:A:306:HIS:CG	2.54	0.43
1:A:250:ASN:O	1:A:253:ILE:HG22	2.19	0.43
1:A:427:TYR:HD1	1:A:430:LEU:HD12	1.84	0.43
1:A:1537:TRP:CH2	1:A:1582:VAL:HG21	2.52	0.43
1:A:1746:GLN:N	1:A:1746:GLN:OE1	2.51	0.43
1:A:2073:PHE:HZ	1:A:2096:VAL:HG21	1.83	0.43
1:B:424:ASP:O	1:B:428:GLU:HG2	2.19	0.43
1:B:701:ASP:OD1	1:B:704:ARG:NH2	2.52	0.43
1:B:1176:LEU:HD13	1:B:1179:LYS:HD3	2.00	0.43
1:B:1627:PRO:HB3	1:B:1950:GLN:HB3	2.00	0.43
1:B:1746:GLN:O	1:B:1750:VAL:HG23	2.19	0.43
1:B:4431:LEU:O	1:B:4435:VAL:HG23	2.19	0.43
3:F:168:GLU:HB2	3:F:171:ARG:HH21	1.84	0.43
3:F:240:LEU:HB3	3:F:246:TYR:CD2	2.54	0.43
5:J:13:MET:HB2	5:J:18:GLN:NE2	2.34	0.43
5:J:35:GLU:HB3	5:J:58:VAL:O	2.19	0.43
1:A:1075:ASP:O	1:A:1076:LEU:C	2.62	0.42
1:A:1079:TRP:C	1:A:1081:ALA:H	2.27	0.42
1:A:1177:LYS:HE3	1:A:1226:ARG:HH22	1.84	0.42
1:A:2348:LEU:HD13	1:A:2356:VAL:HG22	2.01	0.42
1:A:3031:THR:OG1	1:B:3024:ASP:OD2	2.31	0.42
1:A:3530:THR:HG22	1:A:3534:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:HG2	1:B:312:ALA:HB3	2.01	0.42
1:B:365:ARG:HA	1:B:433:LEU:HD22	2.01	0.42
1:B:1177:LYS:O	1:B:1180:ILE:HB	2.19	0.42
1:B:2562:VAL:O	1:B:2804:ARG:NH1	2.52	0.42
1:B:2578:GLU:OE2	1:B:2607:SER:OG	2.30	0.42
1:B:4105:TRP:HD1	1:B:4108:GLN:HE21	1.67	0.42
2:D:186:GLU:HA	2:D:189:GLN:HG2	2.01	0.42
2:D:413:ASP:OD1	2:D:414:MET:N	2.52	0.42
1:A:21:VAL:HA	1:A:124:VAL:HB	2.01	0.42
1:A:349:GLU:O	1:A:353:ILE:HG13	2.19	0.42
1:A:461:ALA:HA	1:A:464:ASP:OD2	2.18	0.42
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	2.00	0.42
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.19	0.42
1:A:2487:GLU:O	1:A:2491:GLN:HG3	2.19	0.42
1:A:3416:LEU:O	1:A:3420:GLU:HG3	2.19	0.42
1:A:3447:TYR:O	1:A:3451:TYR:HD2	2.02	0.42
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.19	0.42
1:B:399:ARG:O	1:B:399:ARG:NH1	2.41	0.42
1:B:583:ARG:O	1:B:587:ARG:HG3	2.19	0.42
1:B:1026:MET:SD	1:B:1027:PRO:HD2	2.59	0.42
1:B:2185:VAL:O	1:B:2189:MET:HG2	2.19	0.42
1:B:2943:LYS:HG2	1:B:3094:PHE:CD2	2.54	0.42
1:B:3303:HIS:O	1:B:3307:VAL:HG23	2.19	0.42
1:B:3900:THR:OG1	1:B:3902:ASP:OD2	2.26	0.42
2:D:426:HIS:ND1	2:D:427:LYS:HG2	2.34	0.42
3:F:228:LEU:CD2	3:F:268:ALA:HB3	2.49	0.42
3:F:279:ASN:OD1	3:F:282:LEU:HD21	2.19	0.42
4:H:42:TYR:O	4:H:46:MET:HG2	2.19	0.42
1:A:315:SER:O	1:A:320:THR:N	2.52	0.42
1:A:372:TYR:N	1:A:440:ARG:HH22	2.17	0.42
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.19	0.42
1:A:3808:CYS:HB3	1:A:3832:PHE:HZ	1.85	0.42
1:B:462:ARG:HH21	1:B:537:ASP:HB2	1.83	0.42
1:B:467:ARG:O	1:B:471:ARG:HG3	2.19	0.42
1:B:479:VAL:HG11	1:B:590:ALA:HB2	2.01	0.42
1:B:1135:LEU:O	1:B:1139:MET:HG2	2.19	0.42
1:B:1190:TYR:OH	1:B:1211:ILE:HG22	2.19	0.42
1:B:1204:PHE:HD1	5:J:5:LYS:NZ	2.17	0.42
1:B:2452:LEU:HA	1:B:2452:LEU:HD23	1.76	0.42
1:B:2973:ASP:O	1:B:2977:ARG:HG3	2.19	0.42
1:B:4575:LEU:HD11	1:B:4624:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:60:PHE:O	3:E:135:PHE:HA	2.19	0.42
3:F:344:PRO:O	3:F:346:ARG:HD3	2.18	0.42
5:I:13:MET:HE1	5:I:21:SER:OG	2.19	0.42
6:K:83:CYS:SG	6:L:64:ILE:HG23	2.58	0.42
1:A:152:PHE:HZ	1:B:121:ARG:HA	1.84	0.42
1:A:1155:GLN:NE2	1:A:1157:SER:HB2	2.33	0.42
1:A:1934:GLU:OE2	1:A:2261:LYS:NZ	2.37	0.42
1:A:2231:SER:O	1:A:2235:ARG:HG3	2.19	0.42
1:A:3214:GLN:O	1:A:3217:GLU:HG3	2.20	0.42
1:A:4305:PHE:O	1:A:4309:VAL:HG23	2.19	0.42
1:B:526:ALA:O	1:B:529:ASN:N	2.52	0.42
1:B:1599:ARG:HG3	1:B:1599:ARG:HH11	1.84	0.42
1:B:1752:LEU:HA	1:B:1755:GLN:HE21	1.84	0.42
1:B:3776:GLU:HA	1:B:3779:GLU:HG2	2.01	0.42
1:B:3844:PRO:O	1:B:3847:LYS:HG2	2.19	0.42
1:B:4336:GLY:O	1:B:4340:ILE:HG12	2.19	0.42
2:C:214:GLN:HB2	2:D:209:ARG:NH1	2.35	0.42
2:D:334:ALA:O	2:D:352:THR:OG1	2.27	0.42
2:D:493:PHE:HZ	2:D:615:GLY:HA2	1.84	0.42
3:F:156:LEU:O	3:F:160:ILE:HG12	2.17	0.42
1:A:276:SER:HA	1:A:279:LEU:HD12	2.02	0.42
1:A:334:PRO:HA	1:A:337:LYS:HB3	2.00	0.42
1:A:1164:SER:HA	1:A:1167:VAL:HG12	2.02	0.42
1:A:3150:VAL:O	1:A:3153:THR:HG22	2.20	0.42
1:A:3992:LEU:O	1:A:3996:PHE:HB2	2.18	0.42
1:B:562:THR:HA	1:B:596:HIS:HE1	1.84	0.42
1:B:1887:ARG:NH2	1:B:4253:GLY:O	2.53	0.42
1:B:3885:MET:HE2	1:B:3885:MET:HB3	1.78	0.42
3:E:146:MET:O	3:E:150:GLN:N	2.38	0.42
5:I:75:TYR:CD1	5:I:84:LEU:HB2	2.49	0.42
1:A:146:TYR:OH	1:B:165:ILE:HG23	2.19	0.42
1:A:337:LYS:HE2	1:A:363:HIS:CD2	2.47	0.42
1:A:1477:LEU:HA	1:A:1486:LEU:O	2.19	0.42
1:A:3306:GLU:OE2	1:A:3386:SER:HB2	2.20	0.42
1:A:3441:GLU:O	1:A:3444:ILE:HB	2.20	0.42
1:A:4308:TRP:CH2	1:A:4312:LEU:HD21	2.55	0.42
1:B:40:LEU:HA	1:B:45:GLY:H	1.85	0.42
1:B:1164:SER:HA	1:B:1167:VAL:HG22	2.02	0.42
1:B:1192:ASN:O	1:B:1195:ARG:HB2	2.19	0.42
1:B:1747:ALA:O	1:B:1751:VAL:HG23	2.19	0.42
1:B:2484:GLU:HA	1:B:2487:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2622:PHE:CD2	1:B:2666:ILE:HA	2.54	0.42
1:B:2665:GLU:HB3	1:B:2668:LEU:HD12	2.02	0.42
2:D:382:HIS:HB3	2:D:403:THR:HG22	2.01	0.42
3:E:156:LEU:O	3:E:160:ILE:N	2.50	0.42
3:F:241:GLU:HA	3:F:246:TYR:HB2	2.01	0.42
1:A:276:SER:O	1:A:279:LEU:HB2	2.20	0.42
1:A:339:PHE:HB2	1:A:340:PRO:HD3	2.00	0.42
1:A:400:LYS:HE3	1:A:402:MET:HB3	2.01	0.42
1:A:438:VAL:HA	1:A:441:LYS:HE3	2.02	0.42
1:A:3167:ARG:NH1	1:A:3685:THR:HA	2.34	0.42
1:A:3446:ARG:H	1:A:3446:ARG:HG3	1.57	0.42
1:B:869:TYR:OH	1:B:989:TRP:O	2.37	0.42
1:B:1045:SER:O	1:B:1048:GLU:HG3	2.20	0.42
1:B:1142:PHE:O	1:B:1146:ILE:HG22	2.19	0.42
1:B:3204:GLY:O	1:B:3208:ILE:HG12	2.20	0.42
1:B:3409:VAL:HA	1:B:3412:LEU:HD12	2.01	0.42
1:B:3954:ASP:OD1	1:B:3957:PHE:N	2.52	0.42
3:F:172:GLU:C	3:F:176:LYS:HZ3	2.22	0.42
4:H:79:MET:HB3	4:H:90:VAL:HB	2.01	0.42
5:J:18:GLN:HA	5:J:74:ILE:HD12	2.02	0.42
6:K:35:GLN:H	6:K:42:TRP:HZ3	1.68	0.42
1:A:53:GLU:HA	1:A:56:LEU:HB3	2.00	0.42
1:A:382:GLU:CB	1:A:452:ILE:HA	2.50	0.42
1:A:2012:MET:HE3	1:A:2012:MET:HB3	1.89	0.42
1:A:2663:CYS:HB2	1:A:2666:ILE:HD11	2.00	0.42
1:A:3243:MET:HE2	1:A:3444:ILE:HA	2.01	0.42
1:B:197:GLN:HG3	1:B:273:GLN:OE1	2.19	0.42
1:B:402:MET:SD	1:B:531:LYS:HA	2.60	0.42
1:B:722:SER:HA	1:B:733:LEU:HD23	2.02	0.42
1:B:987:PHE:HE2	3:F:87:GLU:HG2	1.85	0.42
1:B:1068:ILE:O	1:B:1072:LEU:HG	2.20	0.42
1:B:1213:ASN:HD21	5:J:8:ILE:HG22	1.85	0.42
1:B:1508:LYS:HA	1:B:1513:TYR:CG	2.55	0.42
1:B:1914:GLU:OE1	1:B:1914:GLU:HA	2.20	0.42
1:B:2356:VAL:HG13	1:B:2361:MET:HE3	2.01	0.42
1:B:3727:LYS:O	1:B:3731:LEU:HG	2.20	0.42
1:B:4234:SER:HB3	1:B:4237:LYS:HG2	2.01	0.42
2:D:401:ILE:HD12	2:D:406:LYS:O	2.19	0.42
3:F:252:ASP:HB3	3:F:327:PHE:HE1	1.84	0.42
3:F:304:GLU:C	3:F:305:LYS:HD3	2.45	0.42
3:F:368:SER:C	3:F:372:LYS:HE2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:10:ARG:O	4:G:13:SER:OG	2.27	0.42
1:A:171:ALA:HA	1:A:177:LYS:NZ	2.35	0.42
1:A:404:VAL:HG22	1:A:409:PHE:HB2	2.01	0.42
1:A:420:PHE:CZ	1:A:457:ARG:HG3	2.54	0.42
1:A:1746:GLN:O	1:A:1750:VAL:HG23	2.20	0.42
1:A:3260:ILE:HA	1:A:3263:GLN:CD	2.45	0.42
1:A:3776:GLU:HA	1:A:3779:GLU:HG2	2.00	0.42
1:A:4178:ARG:NH1	1:A:4299:GLY:O	2.53	0.42
1:B:640:ASP:HB2	2:D:385:TYR:OH	2.20	0.42
1:B:2206:LYS:HA	1:B:2206:LYS:HD3	1.82	0.42
1:B:3260:ILE:O	1:B:3264:LEU:HG	2.19	0.42
1:B:4089:LYS:HE3	1:B:4089:LYS:HB2	1.81	0.42
1:B:4154:LYS:HE3	1:B:4310:GLU:HA	2.01	0.42
1:B:4338:ASP:O	1:B:4342:LYS:HG3	2.20	0.42
1:A:185:LYS:O	1:A:189:LEU:HD23	2.20	0.42
1:A:384:ILE:O	1:A:388:LEU:HG	2.19	0.42
1:A:1516:PHE:O	1:A:1517:GLU:C	2.63	0.42
1:A:3211:THR:HG21	1:A:3479:LEU:HD11	2.02	0.42
1:A:3260:ILE:O	1:A:3264:LEU:HG	2.19	0.42
1:A:3492:THR:HA	1:A:3495:THR:HG22	2.02	0.42
1:A:3521:ASP:O	1:A:3525:ARG:HG3	2.20	0.42
1:A:3588:LEU:HD21	1:A:3638:VAL:HG11	2.00	0.42
1:B:368:ARG:NH1	1:B:437:ILE:HD13	2.35	0.42
1:B:619:LEU:HD21	1:B:654:ILE:HG23	2.02	0.42
1:B:997:PRO:HA	1:B:1018:PHE:HA	2.01	0.42
1:B:1044:VAL:O	1:B:1047:VAL:HB	2.20	0.42
1:B:1093:PHE:CZ	1:B:1113:GLN:HG3	2.55	0.42
1:B:2811:ARG:NH1	1:B:2811:ARG:HB2	2.34	0.42
1:B:3045:ASP:N	1:B:3045:ASP:OD2	2.53	0.42
1:B:3416:LEU:O	1:B:3420:GLU:HG3	2.19	0.42
1:B:3429:LYS:O	1:B:3433:VAL:HG23	2.19	0.42
1:B:3731:LEU:HB2	1:B:3791:MET:SD	2.60	0.42
5:J:16:GLU:HG2	5:J:17:MET:N	2.34	0.42
6:K:45:ASN:O	6:K:48:GLU:HG3	2.20	0.42
1:A:2061:THR:OG1	1:A:2133:GLU:OE1	2.33	0.41
1:A:2743:SER:O	1:A:2747:ILE:HG13	2.20	0.41
1:A:3302:GLN:HB3	1:A:3388:ALA:HB2	2.02	0.41
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.02	0.41
1:B:292:ARG:NH1	1:B:320:THR:HG22	2.35	0.41
1:B:2262:ASP:HB2	1:B:2267:THR:CG2	2.50	0.41
1:B:2976:LEU:HB3	1:B:3020:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3363:ILE:O	1:B:3367:MET:HG2	2.20	0.41
1:B:4025:LEU:HG	1:B:4027:LEU:HD22	2.02	0.41
2:D:265:LEU:HD22	2:D:597:TYR:HE2	1.85	0.41
3:F:75:GLN:NE2	3:F:89:LEU:HD11	2.34	0.41
1:A:215:ASN:O	1:A:219:GLN:OE1	2.38	0.41
1:A:386:ARG:NH1	1:A:454:PRO:HA	2.34	0.41
1:A:462:ARG:NH1	1:A:537:ASP:O	2.53	0.41
1:A:1680:GLU:H	1:A:1680:GLU:CD	2.23	0.41
1:A:2107:ARG:NH2	1:A:2135:GLU:OE1	2.53	0.41
1:A:3263:GLN:O	1:A:3267:GLN:HG3	2.20	0.41
1:A:3491:LYS:O	1:A:3494:GLU:HG3	2.19	0.41
1:A:4027:LEU:O	1:A:4031:VAL:HG12	2.20	0.41
1:B:1141:GLU:O	1:B:1145:GLN:HG2	2.20	0.41
1:B:2222:MET:HE1	1:B:2342:MET:HE2	2.02	0.41
1:B:3306:GLU:OE2	1:B:3386:SER:HB2	2.20	0.41
1:B:3401:ASN:O	1:B:3405:MET:HE3	2.19	0.41
3:F:259:ARG:NE	3:F:315:ASP:OD2	2.52	0.41
6:K:70:MET:HE2	6:L:70:MET:HE3	2.01	0.41
6:K:78:HIS:CE1	6:L:69:ILE:HB	2.55	0.41
6:K:84:PHE:CE1	6:L:51:LEU:HD13	2.55	0.41
1:A:1958:ASP:HA	1:A:2017:THR:HB	2.02	0.41
1:A:2819:GLU:HG3	1:A:2866:ALA:HB2	2.02	0.41
1:A:3471:LYS:HE2	1:A:3761:LEU:HD23	2.02	0.41
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	2.03	0.41
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	2.02	0.41
1:A:4287:LYS:HE3	1:A:4290:GLY:HA2	2.02	0.41
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.21	0.41
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.85	0.41
1:A:4626:ILE:HD13	1:A:4632:PRO:HD3	2.02	0.41
1:B:1090:ARG:HH22	1:B:1124:HIS:CB	2.33	0.41
1:B:1197:LEU:HD12	1:B:1197:LEU:HA	1.93	0.41
1:B:1209:LEU:HD13	5:J:18:GLN:HE22	1.84	0.41
1:B:3150:VAL:O	1:B:3154:LEU:HD23	2.19	0.41
1:B:3433:VAL:HG22	1:B:3436:MET:HE2	2.02	0.41
1:A:80:GLU:OE2	1:A:110:GLY:HA3	2.20	0.41
1:A:274:GLU:O	1:A:277:PHE:HB3	2.19	0.41
1:A:301:LEU:HG	1:A:313:THR:HG23	2.00	0.41
1:A:1156:HIS:CE1	1:A:1228:LYS:HZ2	2.39	0.41
1:A:1537:TRP:O	1:A:1538:ILE:C	2.63	0.41
1:A:2616:GLU:OE1	1:A:2616:GLU:N	2.53	0.41
1:B:213:ILE:HG13	1:B:232:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLN:HA	1:B:260:THR:HG22	2.02	0.41
1:B:717:ILE:HG13	1:B:822:LEU:HB2	2.02	0.41
1:B:1193:GLY:HA2	1:B:1196:LEU:HD12	2.03	0.41
1:B:1196:LEU:O	1:B:1200:GLN:N	2.51	0.41
1:B:1213:ASN:HA	5:J:10:ASN:HA	2.03	0.41
1:B:2445:HIS:ND1	1:B:2505:ASP:OD1	2.51	0.41
1:B:2499:LEU:HD21	1:B:2515:GLY:HA2	2.03	0.41
1:B:3432:GLU:O	1:B:3436:MET:HG2	2.20	0.41
1:B:4092:ARG:HE	1:B:4093:TRP:N	2.06	0.41
1:B:4205:TYR:OH	1:B:4261:ASP:OD2	2.28	0.41
2:D:284:CYS:HB2	2:D:337:SER:HA	2.02	0.41
2:D:284:CYS:SG	2:D:285:LEU:N	2.93	0.41
2:D:538:ALA:HB1	2:D:554:LEU:HB2	2.01	0.41
4:G:71:ILE:HD13	4:H:69:LEU:HD13	2.02	0.41
1:A:25:ALA:HB3	1:A:69:LEU:HD13	2.01	0.41
1:A:195:HIS:NE2	1:A:265:ASP:HB2	2.35	0.41
1:A:1205:PRO:O	1:A:1208:TRP:HB3	2.20	0.41
1:A:3395:TRP:HE1	1:A:3399:GLN:HE22	1.69	0.41
1:A:3915:VAL:O	1:A:3916:LEU:HD23	2.20	0.41
1:B:315:SER:O	1:B:319:ASP:N	2.41	0.41
1:B:347:ALA:HA	1:B:352:LYS:HD3	2.03	0.41
1:B:414:VAL:HG22	1:B:467:ARG:HH22	1.86	0.41
1:B:539:SER:O	1:B:542:GLY:N	2.53	0.41
1:B:581:MET:HA	1:B:584:ILE:HD12	2.02	0.41
1:B:2224:GLY:O	1:B:2346:GLN:HA	2.20	0.41
1:B:2297:LYS:HB2	1:B:2299:GLN:HE21	1.86	0.41
1:B:3263:GLN:O	1:B:3267:GLN:HG3	2.20	0.41
1:B:3620:ARG:O	1:B:3624:GLU:HG2	2.21	0.41
2:D:446:ASN:HA	2:D:460:CYS:HA	2.03	0.41
5:I:65:TYR:CD2	5:J:40:ALA:HA	2.55	0.41
1:A:254:ARG:HA	1:A:254:ARG:HD3	1.78	0.41
1:A:272:LEU:H	1:A:272:LEU:HD12	1.85	0.41
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.19	0.41
1:A:3243:MET:HA	1:A:3243:MET:HE3	2.02	0.41
1:B:54:ALA:O	1:B:58:GLU:N	2.54	0.41
1:B:580:GLU:HA	1:B:583:ARG:NH2	2.36	0.41
1:B:810:LYS:HA	1:B:810:LYS:HD3	1.78	0.41
1:B:1026:MET:HE2	1:B:1026:MET:HA	2.02	0.41
1:B:1205:PRO:O	1:B:1208:TRP:HB3	2.20	0.41
1:B:1213:ASN:HA	5:J:11:ALA:N	2.35	0.41
1:B:2465:ALA:HB2	1:B:2493:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3524:MET:HE2	1:B:3524:MET:HB2	1.89	0.41
1:B:3567:LEU:HD12	1:B:3568:PRO:HD2	2.02	0.41
2:D:426:HIS:HA	2:D:468:ILE:HB	2.01	0.41
3:F:149:LEU:HB3	3:F:261:PHE:CZ	2.55	0.41
5:I:23:GLU:O	5:I:27:GLN:HG3	2.20	0.41
6:L:22:LYS:NZ	6:L:97:TRP:HB2	2.35	0.41
1:A:193:LEU:HA	1:B:178:MET:CE	2.51	0.41
1:A:270:THR:HG23	1:A:272:LEU:HB2	2.03	0.41
1:A:371:LYS:HA	1:A:440:ARG:HH21	1.85	0.41
1:A:4610:TYR:N	1:A:4642:VAL:O	2.53	0.41
1:B:539:SER:O	1:B:541:GLU:N	2.54	0.41
1:B:815:LEU:HD12	1:B:815:LEU:HA	1.84	0.41
1:B:902:LYS:HB2	1:B:902:LYS:HE3	1.77	0.41
1:B:1031:VAL:O	1:B:1035:GLU:HG2	2.21	0.41
1:B:1991:ASP:OD1	1:B:1992:LYS:N	2.52	0.41
1:B:2107:ARG:O	1:B:2111:ILE:HG12	2.20	0.41
1:B:2284:LEU:O	1:B:2288:ILE:HG13	2.21	0.41
1:B:4169:ILE:CG2	1:B:4302:ARG:HE	2.32	0.41
1:B:4223:LEU:HD12	1:B:4223:LEU:HA	1.88	0.41
1:B:4230:ARG:NH1	1:B:4230:ARG:HB2	2.36	0.41
3:F:257:HIS:CG	3:F:260:ARG:HH12	2.39	0.41
6:K:85:TRP:HH2	6:K:92:SER:HB3	1.84	0.41
6:L:85:TRP:HD1	6:L:86:ASP:C	2.28	0.41
1:A:41:LEU:HA	1:B:132:SER:HB2	2.02	0.41
1:A:78:LEU:HD22	1:A:108:HIS:H	1.86	0.41
1:A:118:PHE:HB3	1:A:135:LEU:HD11	2.02	0.41
1:A:173:ARG:HD2	1:B:283:ARG:HH21	1.86	0.41
1:A:1201:ARG:CZ	1:B:968:VAL:HG22	2.51	0.41
1:A:1802:PRO:O	1:A:1806:ARG:HG3	2.20	0.41
1:A:1961:ASN:OD1	1:A:1961:ASN:N	2.53	0.41
1:A:2769:LEU:HG	1:A:2773:MET:HE3	2.01	0.41
1:A:3433:VAL:HA	1:A:3436:MET:CG	2.49	0.41
1:B:1078:LYS:O	1:B:1082:LEU:HD23	2.21	0.41
1:B:1181:LYS:HG2	1:B:1185:LYS:NZ	2.36	0.41
1:B:1452:VAL:HA	1:B:1512:TYR:CZ	2.56	0.41
1:B:2140:SER:O	1:B:2144:THR:HG23	2.20	0.41
1:B:3464:ASP:O	1:B:3468:VAL:HG23	2.21	0.41
1:B:3591:ASP:OD2	1:B:3596:ALA:HB3	2.21	0.41
1:B:4209:GLU:CD	1:B:4213:ARG:HH12	2.29	0.41
1:B:4626:ILE:HD13	1:B:4632:PRO:HD3	2.03	0.41
2:D:497:PHE:O	2:D:508:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:330:VAL:C	3:F:331:LYS:HD3	2.46	0.41
4:G:70:ARG:HH21	4:G:72:ARG:HH21	1.69	0.41
4:H:9:LYS:HE2	4:H:9:LYS:HA	2.02	0.41
5:J:42:ILE:O	5:J:45:GLU:HG3	2.21	0.41
5:J:72:HIS:HB3	5:J:87:LYS:HB3	2.02	0.41
1:A:40:LEU:HD13	1:B:33:HIS:CE1	2.55	0.41
1:A:85:LYS:HB2	1:A:112:LYS:HE3	2.02	0.41
1:A:152:PHE:HE2	1:B:119:ILE:O	2.03	0.41
1:A:294:SER:HB2	1:A:297:VAL:HG23	2.03	0.41
1:A:451:ARG:NE	1:A:453:ASN:HB3	2.34	0.41
1:A:1175:SER:O	1:A:1178:ARG:HG2	2.21	0.41
1:A:1229:ASP:OD2	1:A:1233:GLN:NE2	2.52	0.41
1:A:1577:ALA:O	1:A:1581:LYS:HG3	2.21	0.41
1:A:1719:GLU:HA	1:A:1722:THR:HG22	2.03	0.41
1:A:1747:ALA:O	1:A:1751:VAL:HG23	2.20	0.41
1:A:2075:LEU:O	1:A:2079:GLN:HB2	2.20	0.41
1:A:3239:LYS:O	1:A:3243:MET:HG2	2.21	0.41
1:A:3440:LEU:O	1:A:3444:ILE:HG13	2.21	0.41
1:A:4408:PRO:HD3	1:A:4530:GLN:NE2	2.36	0.41
1:B:440:ARG:NH1	1:B:444:GLU:HB2	2.35	0.41
1:B:613:LYS:O	1:B:617:GLU:HG3	2.21	0.41
1:B:631:GLN:HG3	2:D:572:ALA:HB2	2.03	0.41
1:B:673:TRP:O	1:B:679:GLY:HA3	2.21	0.41
1:B:755:TRP:CE2	2:D:453:GLU:HA	2.55	0.41
1:B:916:GLN:OE1	1:B:1027:PRO:HG2	2.21	0.41
1:B:1190:TYR:HE2	1:B:1214:ILE:HD11	1.86	0.41
1:B:1608:LEU:O	1:B:1612:GLN:HG3	2.21	0.41
1:B:1932:CYS:HB3	1:B:1963:LEU:HD11	2.01	0.41
1:B:2132:PRO:O	1:B:2136:ILE:HG13	2.21	0.41
1:B:2260:SER:OG	1:B:2262:ASP:OD1	2.24	0.41
1:B:2375:PHE:HE2	1:B:2434:THR:HG22	1.85	0.41
1:B:2744:LEU:HD22	1:B:2748:TYR:HE2	1.85	0.41
1:B:3052:LYS:HE2	1:B:3052:LYS:HB3	1.91	0.41
1:B:3140:ARG:O	1:B:3144:VAL:HG23	2.20	0.41
1:B:3154:LEU:HD11	1:B:3516:TYR:HB3	2.03	0.41
1:B:3683:ASP:HB3	1:B:3686:VAL:HG23	2.02	0.41
1:B:3708:LEU:HD23	1:B:3809:SER:HA	2.02	0.41
1:B:3731:LEU:O	1:B:3735:GLN:HG3	2.21	0.41
1:B:4175:GLU:HG3	1:B:4278:PHE:CE2	2.56	0.41
1:B:4394:THR:O	1:B:4490:GLN:NE2	2.35	0.41
2:D:425:VAL:HG11	2:D:429:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:526:TYR:O	2:D:526:TYR:CG	2.73	0.41
4:G:21:ILE:HG23	4:G:89:ILE:HG13	2.02	0.41
5:I:63:GLY:N	5:J:58:VAL:O	2.43	0.41
1:A:1374:PRO:O	1:A:1378:ARG:N	2.49	0.41
1:A:1523:TRP:HA	1:A:1526:LYS:HE3	2.02	0.41
1:A:1989:ASN:OD1	1:A:1989:ASN:N	2.54	0.41
1:A:2065:LEU:HD22	1:A:2137:LEU:HD12	2.02	0.41
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.56	0.41
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.21	0.41
1:A:4058:LEU:O	1:A:4062:GLN:HG2	2.21	0.41
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.94	0.41
1:B:64:GLN:HB3	1:B:105:ILE:HD11	2.03	0.41
1:B:161:PHE:HE2	1:B:183:GLU:HG3	1.86	0.41
1:B:865:GLU:HG2	1:B:910:ILE:HD13	2.03	0.41
1:B:1183:PHE:O	1:B:1187:VAL:HG23	2.21	0.41
1:B:1518:GLU:HG2	1:B:1519:ASP:H	1.85	0.41
1:B:1596:GLY:HA2	1:B:1599:ARG:NH1	2.32	0.41
1:B:1623:ARG:NH1	1:B:1632:VAL:O	2.54	0.41
1:B:1903:SER:HA	1:B:2016:ILE:O	2.21	0.41
1:B:2047:GLN:HA	1:B:2070:VAL:HG21	2.03	0.41
1:B:2457:SER:HB2	1:B:2732:PRO:HB3	2.03	0.41
1:B:3223:ARG:HH11	1:B:3223:ARG:HG3	1.86	0.41
1:B:3839:VAL:O	1:B:3843:ASN:HB2	2.21	0.41
1:B:4318:PRO:HG2	1:B:4325:ASN:HA	2.01	0.41
3:F:95:ASP:HB2	3:F:294:PHE:CE2	2.55	0.41
1:A:119:ILE:HD13	1:B:152:PHE:HD1	1.86	0.40
1:A:264:ARG:HG2	1:A:274:GLU:CD	2.47	0.40
1:A:365:ARG:HH12	1:A:433:LEU:HB2	1.86	0.40
1:A:426:GLU:CA	1:A:429:LYS:HB2	2.46	0.40
1:A:1459:LEU:HD22	1:A:1507:MET:HB2	2.03	0.40
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.03	0.40
1:A:3284:LYS:HB3	1:A:3402:TYR:CE1	2.57	0.40
1:B:393:LEU:HD21	1:B:459:LEU:HG	2.02	0.40
1:B:401:LEU:HB2	1:B:409:PHE:CE1	2.56	0.40
1:B:410:GLU:O	1:B:414:VAL:HG23	2.21	0.40
1:B:1508:LYS:HA	1:B:1513:TYR:CD1	2.56	0.40
1:B:1679:ARG:HB3	1:B:1679:ARG:NH1	2.36	0.40
1:B:1839:LEU:O	1:B:1843:ARG:NH1	2.55	0.40
1:B:1888:CYS:HA	1:B:2039:LEU:HD22	2.03	0.40
1:B:2231:SER:O	1:B:2235:ARG:HG3	2.20	0.40
1:B:3150:VAL:HA	1:B:3153:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:PHE:HB3	2:D:200:PHE:CD1	2.56	0.40
3:F:279:ASN:HD21	3:F:307:ALA:HB1	1.86	0.40
4:H:26:GLU:HB3	4:H:47:HIS:NE2	2.36	0.40
4:H:45:LEU:O	4:H:49:PHE:HD2	2.04	0.40
5:I:7:VAL:CG2	5:I:77:TYR:HB2	2.52	0.40
5:I:24:CYS:O	5:I:27:GLN:HB2	2.21	0.40
1:A:23:ASN:O	1:A:126:ASP:HB3	2.22	0.40
1:A:3838:ASN:HD22	1:A:3866:VAL:HG11	1.86	0.40
1:A:4288:VAL:O	1:A:4319:SER:OG	2.29	0.40
1:B:609:ILE:HG21	1:B:678:GLU:HB3	2.04	0.40
1:B:860:GLU:OE2	1:B:880:ARG:HB2	2.21	0.40
1:B:1087:ARG:HH21	1:B:1200:GLN:NE2	2.13	0.40
1:B:2054:LEU:HD23	1:B:2054:LEU:HA	1.80	0.40
1:B:2507:ARG:O	1:B:2511:ARG:HG3	2.21	0.40
1:B:3928:THR:OG1	1:B:3931:GLN:HG3	2.21	0.40
1:B:4092:ARG:NE	1:B:4092:ARG:HA	2.36	0.40
1:B:4178:ARG:HG3	1:B:4305:PHE:HZ	1.85	0.40
2:D:273:ASP:O	2:D:277:SER:OG	2.27	0.40
2:D:409:SER:HB2	2:D:420:ASP:HB3	2.02	0.40
2:D:426:HIS:CD2	2:D:468:ILE:HG21	2.56	0.40
2:D:523:ASN:ND2	2:D:546:MET:SD	2.95	0.40
4:G:24:ASN:OD1	4:G:30:ILE:HB	2.21	0.40
4:H:18:GLN:HB2	4:H:91:ILE:HG23	2.02	0.40
5:J:57:ILE:CG2	5:J:84:LEU:HB3	2.50	0.40
6:L:22:LYS:HZ3	6:L:97:TRP:HB2	1.87	0.40
1:A:35:ARG:O	1:A:39:PRO:HD3	2.21	0.40
1:A:344:LEU:HA	1:A:356:ALA:HB1	2.04	0.40
1:A:347:ALA:HB1	1:A:353:ILE:HA	2.04	0.40
1:A:373:PRO:HB2	1:A:376:ARG:HB3	2.02	0.40
1:A:385:SER:HB2	1:A:454:PRO:HG3	2.04	0.40
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	2.02	0.40
1:A:3228:GLU:HA	1:A:3231:VAL:HG12	2.02	0.40
1:A:3659:ARG:NH2	1:A:3670:ASP:OD1	2.47	0.40
1:A:3663:THR:HG22	1:A:3668:ASP:OD2	2.21	0.40
1:B:783:GLU:HG2	2:D:375:LEU:HD22	2.02	0.40
1:B:2485:GLN:HA	1:B:2488:ARG:HD3	2.03	0.40
1:B:2487:GLU:O	1:B:2491:GLN:HG3	2.21	0.40
1:B:3398:ALA:O	1:B:3399:GLN:HB2	2.22	0.40
1:B:3873:ARG:HD3	1:B:3873:ARG:HA	1.79	0.40
1:B:4013:LEU:HD13	1:B:4017:PHE:CE2	2.56	0.40
2:D:214:GLN:H	4:H:72:ARG:NH1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:O	1:A:38:VAL:HG22	2.22	0.40
1:A:170:LYS:HZ2	1:A:179:ALA:HB3	1.86	0.40
1:A:233:GLY:O	1:A:236:VAL:HG12	2.22	0.40
1:A:316:PHE:HA	1:A:320:THR:OG1	2.21	0.40
1:A:1964:GLU:HB2	1:A:1967:MET:HG2	2.04	0.40
1:A:2154:ILE:HB	1:A:2155:PRO:HD3	2.03	0.40
1:A:2898:LYS:HE3	1:A:2898:LYS:HB3	1.92	0.40
1:A:3035:GLU:O	1:A:3038:GLN:HG3	2.22	0.40
1:A:3150:VAL:O	1:A:3154:LEU:HD23	2.22	0.40
1:B:49:PRO:HG3	1:B:81:ARG:NH2	2.37	0.40
1:B:119:ILE:O	1:B:136:ARG:CB	2.64	0.40
1:B:292:ARG:NH2	1:B:316:PHE:O	2.52	0.40
1:B:351:ASP:OD1	1:B:352:LYS:N	2.54	0.40
1:B:627:TYR:CZ	1:B:633:CYS:HA	2.57	0.40
1:B:1163:THR:HA	1:B:1166:ALA:HB3	2.03	0.40
1:B:2270:PRO:HA	1:B:2273:ARG:HH11	1.86	0.40
1:B:2279:LEU:HA	1:B:2698:GLN:HG2	2.03	0.40
1:B:2468:ASN:O	1:B:2471:GLN:HG3	2.21	0.40
1:B:2499:LEU:HD23	1:B:2499:LEU:HA	1.88	0.40
1:B:2755:MET:HG3	1:B:2807:PHE:HB2	2.02	0.40
1:B:3491:LYS:O	1:B:3494:GLU:HG3	2.21	0.40
1:B:4215:ALA:O	1:B:4219:VAL:HG23	2.22	0.40
2:D:412:LEU:HD12	2:D:412:LEU:HA	1.96	0.40
3:F:71:MET:HA	3:F:71:MET:HE2	2.04	0.40
3:F:157:ARG:O	3:F:160:ILE:HB	2.22	0.40
5:I:61:ASN:HD21	5:J:60:ARG:HB3	1.87	0.40
6:K:66:THR:O	6:K:106:VAL:HA	2.22	0.40
1:A:415:ALA:O	1:A:419:VAL:HG23	2.22	0.40
1:A:1555:ALA:HA	1:A:1558:LYS:NZ	2.36	0.40
1:A:3284:LYS:HE2	1:A:3405:MET:HE3	2.04	0.40
1:A:3471:LYS:HE2	1:A:3761:LEU:HB3	2.03	0.40
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.21	0.40
1:A:4604:VAL:HG22	1:A:4625:GLU:HB3	2.03	0.40
1:B:27:VAL:HA	1:B:65:MET:HE1	2.04	0.40
1:B:524:ASN:O	1:B:527:TYR:N	2.54	0.40
1:B:1204:PHE:H	5:J:5:LYS:CE	2.35	0.40
1:B:1455:GLY:HA3	1:B:1512:TYR:CE2	2.50	0.40
1:B:2081:SER:OG	1:B:2152:GLU:OE2	2.29	0.40
1:B:3223:ARG:HG3	1:B:3223:ARG:NH1	2.37	0.40
1:B:3260:ILE:HA	1:B:3263:GLN:CD	2.46	0.40
1:B:3492:THR:HA	1:B:3495:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4482:PHE:O	1:B:4486:ILE:HG12	2.22	0.40
1:B:4534:TRP:HE3	1:B:4539:LEU:HD21	1.85	0.40
2:D:317:ASN:ND2	2:D:326:GLU:OE2	2.54	0.40
2:D:441:VAL:HG11	2:D:486:ALA:HA	2.04	0.40
2:D:480:THR:OG1	2:D:528:TYR:O	2.40	0.40
4:G:52:LYS:NZ	4:H:49:PHE:CD1	2.89	0.40
5:J:51:ASN:HA	5:J:52:PRO:HD3	1.90	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	4530/4646 (98%)	4360 (96%)	165 (4%)	5 (0%)	48	83
1	B	4509/4646 (97%)	4383 (97%)	122 (3%)	4 (0%)	48	83
2	C	390/638 (61%)	364 (93%)	26 (7%)	0	100	100
2	D	390/638 (61%)	367 (94%)	23 (6%)	0	100	100
3	E	307/492 (62%)	292 (95%)	15 (5%)	0	100	100
3	F	307/492 (62%)	291 (95%)	14 (5%)	2 (1%)	18	55
4	G	91/96 (95%)	87 (96%)	4 (4%)	0	100	100
4	H	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
5	I	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
5	J	87/89 (98%)	82 (94%)	4 (5%)	1 (1%)	11	45
6	K	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
6	L	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
All	All	11011/12148 (91%)	10610 (96%)	389 (4%)	12 (0%)	49	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	ASN
1	A	3384	ARG
1	B	540	LYS
1	B	3384	ARG
1	A	3444	ILE
1	A	3445	ALA
1	B	1161	ALA
1	B	3377	TYR
1	A	445	ASN
3	F	112	ASP
5	J	51	ASN
3	F	39	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	4044/4125 (98%)	4038 (100%)	6 (0%)	88	88
1	B	4028/4125 (98%)	4028 (100%)	0	100	100
2	C	344/557 (62%)	344 (100%)	0	100	100
2	D	344/557 (62%)	344 (100%)	0	100	100
3	E	279/422 (66%)	279 (100%)	0	100	100
3	F	279/422 (66%)	279 (100%)	0	100	100
4	G	87/89 (98%)	87 (100%)	0	100	100
4	H	87/89 (98%)	87 (100%)	0	100	100
5	I	78/78 (100%)	78 (100%)	0	100	100
5	J	78/78 (100%)	78 (100%)	0	100	100
6	K	97/97 (100%)	97 (100%)	0	100	100
6	L	97/97 (100%)	97 (100%)	0	100	100
All	All	9842/10736 (92%)	9836 (100%)	6 (0%)	87	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3434	GLU
1	A	3437	ILE
1	A	3446	ARG
1	A	3447	TYR
1	A	3454	LEU
1	A	3461	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	31	GLN
1	A	244	GLN
1	A	333	ASN
1	A	363	HIS
1	A	1186	GLN
1	A	1213	ASN
1	A	1233	GLN
1	A	1566	GLN
1	A	1755	GLN
1	A	1922	GLN
1	A	1973	GLN
1	A	2005	GLN
1	A	2109	GLN
1	A	2169	GLN
1	A	2217	ASN
1	A	2476	HIS
1	A	2554	GLN
1	A	2621	ASN
1	A	2707	GLN
1	A	3014	ASN
1	A	3063	HIS
1	A	3197	GLN
1	A	3267	GLN
1	A	3399	GLN
1	A	3431	ASN
1	A	3522	GLN
1	A	3711	GLN
1	A	3931	GLN
1	A	4114	HIS
1	A	4131	ASN
1	A	4429	GLN
1	A	4530	GLN

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Mol	Chain	Res	Type
1	A	4549	GLN
1	B	33	HIS
1	B	150	HIS
1	B	155	ASN
1	B	195	HIS
1	B	246	GLN
1	B	280	ASN
1	B	330	ASN
1	B	607	GLN
1	B	676	HIS
1	B	680	GLN
1	B	731	ASN
1	B	871	HIS
1	B	1056	GLN
1	B	1085	GLN
1	B	1113	GLN
1	B	1174	GLN
1	B	1222	ASN
1	B	1233	GLN
1	B	1569	GLN
1	B	1779	HIS
1	B	1973	GLN
1	B	2067	ASN
1	B	2217	ASN
1	B	2476	HIS
1	B	2554	GLN
1	B	2560	HIS
1	B	2588	HIS
1	B	2637	HIS
1	B	2752	ASN
1	B	2834	GLN
1	B	3014	ASN
1	B	3104	GLN
1	B	3227	GLN
1	B	3267	GLN
1	B	3346	ASN
1	B	3378	ASN
1	B	3535	HIS
1	B	3563	GLN
1	B	3985	GLN
1	B	4029	HIS
1	B	4114	HIS

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Mol	Chain	Res	Type
1	B	4156	ASN
1	B	4307	GLN
1	B	4335	GLN
1	B	4425	GLN
1	B	4429	GLN
1	B	4436	GLN
2	C	188	GLN
2	D	371	GLN
2	D	380	HIS
2	D	426	HIS
3	F	115	HIS
3	F	257	HIS
3	F	295	HIS
3	F	373	GLN
4	G	18	GLN
5	I	10	ASN
5	I	41	HIS
5	J	18	GLN
6	L	5	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	ATP	B	4702	9	32,33,33	0.38	0	48,52,52	0.29	0
8	ATP	A	4702	9	32,33,33	0.38	0	48,52,52	0.29	0
7	ADP	B	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
7	ADP	B	4701	9	28,29,29	1.40	5 (17%)	43,45,45	1.81	9 (20%)
7	ADP	A	4704	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	8 (18%)
7	ADP	A	4701	9	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
7	ADP	B	4703	-	28,29,29	1.39	4 (14%)	43,45,45	1.88	8 (18%)
7	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	B	4702	9	-	6/22/38/38	0/3/3/3
8	ATP	A	4702	9	-	6/22/38/38	0/3/3/3
7	ADP	B	4704	-	-	3/16/32/32	0/3/3/3
7	ADP	B	4701	9	-	3/16/32/32	0/3/3/3
7	ADP	A	4704	-	-	2/16/32/32	0/3/3/3
7	ADP	A	4701	9	-	3/16/32/32	0/3/3/3
7	ADP	B	4703	-	-	0/16/32/32	0/3/3/3
7	ADP	A	4703	-	-	2/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4703	ADP	C5-C4	4.67	1.47	1.39
7	B	4703	ADP	C5-C4	4.66	1.47	1.39
7	A	4704	ADP	C5-C4	4.63	1.47	1.39
7	B	4704	ADP	C5-C4	4.62	1.47	1.39
7	B	4701	ADP	C5-C4	4.56	1.47	1.39
7	A	4701	ADP	C5-C4	4.54	1.47	1.39
7	A	4703	ADP	C5-C6	2.65	1.48	1.41
7	B	4703	ADP	C5-C6	2.64	1.48	1.41
7	B	4701	ADP	C5-C6	2.62	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4704	ADP	C5-C6	2.60	1.48	1.41
7	A	4704	ADP	C5-C6	2.58	1.48	1.41
7	A	4701	ADP	C5-C6	2.57	1.48	1.41
7	B	4704	ADP	C5-N7	-2.41	1.34	1.39
7	A	4701	ADP	C5-N7	-2.40	1.34	1.39
7	B	4703	ADP	C5-N7	-2.39	1.34	1.39
7	B	4701	ADP	C5-N7	-2.37	1.34	1.39
7	A	4704	ADP	C5-N7	-2.34	1.34	1.39
7	A	4703	ADP	C5-N7	-2.31	1.34	1.39
7	A	4703	ADP	C8-N7	2.28	1.36	1.31
7	B	4704	ADP	C8-N7	2.26	1.36	1.31
7	A	4701	ADP	C8-N7	2.24	1.36	1.31
7	A	4704	ADP	C8-N7	2.24	1.36	1.31
7	B	4701	ADP	C8-N7	2.22	1.36	1.31
7	B	4703	ADP	C8-N7	2.21	1.35	1.31
7	B	4701	ADP	C4-N9	-2.00	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4703	ADP	C5-C4-N3	-6.15	118.25	126.72
7	B	4703	ADP	C5-C4-N3	-6.02	118.42	126.72
7	B	4704	ADP	C5-C4-N3	-5.87	118.63	126.72
7	A	4704	ADP	C5-C4-N3	-5.79	118.75	126.72
7	B	4701	ADP	C5-C4-N3	-5.78	118.77	126.72
7	A	4701	ADP	C5-C4-N3	-5.76	118.79	126.72
7	A	4703	ADP	N3-C4-N9	4.95	135.59	127.17
7	B	4703	ADP	N3-C4-N9	4.87	135.45	127.17
7	B	4704	ADP	N3-C4-N9	4.72	135.19	127.17
7	A	4704	ADP	N3-C4-N9	4.66	135.10	127.17
7	B	4701	ADP	N3-C4-N9	4.62	135.02	127.17
7	A	4701	ADP	N3-C4-N9	4.60	135.00	127.17
7	A	4703	ADP	C2-N3-C4	3.84	121.21	111.83
7	B	4703	ADP	C2-N3-C4	3.79	121.08	111.83
7	B	4704	ADP	C2-N3-C4	3.67	120.78	111.83
7	B	4701	ADP	C2-N3-C4	3.65	120.75	111.83
7	A	4701	ADP	C2-N3-C4	3.65	120.74	111.83
7	A	4704	ADP	C2-N3-C4	3.61	120.65	111.83
7	A	4701	ADP	C4-C5-N7	-3.40	106.70	110.58
7	B	4701	ADP	C4-C5-N7	-3.38	106.72	110.58
7	B	4704	ADP	C4-C5-N7	-3.37	106.73	110.58
7	A	4704	ADP	C4-C5-N7	-3.36	106.73	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4703	ADP	C4-C5-N7	-3.35	106.75	110.58
7	B	4703	ADP	N3-C2-N1	-3.29	123.60	128.58
7	A	4703	ADP	C4-C5-N7	-3.28	106.83	110.58
7	A	4703	ADP	N3-C2-N1	-3.27	123.63	128.58
7	A	4701	ADP	N3-C2-N1	-3.21	123.73	128.58
7	B	4701	ADP	N3-C2-N1	-3.20	123.74	128.58
7	B	4704	ADP	N3-C2-N1	-3.15	123.81	128.58
7	A	4704	ADP	N3-C2-N1	-3.15	123.82	128.58
7	A	4704	ADP	C4-N9-C8	2.73	108.61	105.74
7	B	4701	ADP	C4-N9-C8	2.73	108.60	105.74
7	A	4701	ADP	C4-N9-C8	2.73	108.60	105.74
7	B	4704	ADP	C4-N9-C8	2.68	108.55	105.74
7	A	4703	ADP	C3'-C2'-C1'	2.66	106.50	101.46
7	B	4703	ADP	C3'-C2'-C1'	2.61	106.40	101.46
7	B	4703	ADP	C4-N9-C8	2.61	108.47	105.74
7	B	4703	ADP	C5-N7-C8	2.54	107.44	103.45
7	A	4703	ADP	C4-N9-C8	2.53	108.39	105.74
7	A	4704	ADP	C3'-C2'-C1'	2.50	106.19	101.46
7	B	4704	ADP	C3'-C2'-C1'	2.49	106.17	101.46
7	B	4704	ADP	C5-N7-C8	2.48	107.36	103.45
7	A	4701	ADP	C5-N7-C8	2.48	107.34	103.45
7	B	4701	ADP	C5-N7-C8	2.46	107.32	103.45
7	A	4704	ADP	C5-N7-C8	2.42	107.25	103.45
7	A	4703	ADP	C5-N7-C8	2.42	107.25	103.45
7	A	4701	ADP	C3'-C2'-C1'	2.09	105.41	101.46
7	B	4701	ADP	C3'-C2'-C1'	2.05	105.35	101.46
7	A	4701	ADP	C6-C5-N7	2.03	136.00	132.09
7	B	4701	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4701	ADP	C5'-O5'-PA-O1A
7	A	4701	ADP	C5'-O5'-PA-O2A
7	A	4701	ADP	C5'-O5'-PA-O3A
7	A	4704	ADP	C5'-O5'-PA-O1A
7	B	4701	ADP	C5'-O5'-PA-O1A
7	B	4701	ADP	C5'-O5'-PA-O2A
7	B	4701	ADP	C5'-O5'-PA-O3A
8	A	4702	ATP	O4'-C4'-C5'-O5'
8	A	4702	ATP	C3'-C4'-C5'-O5'

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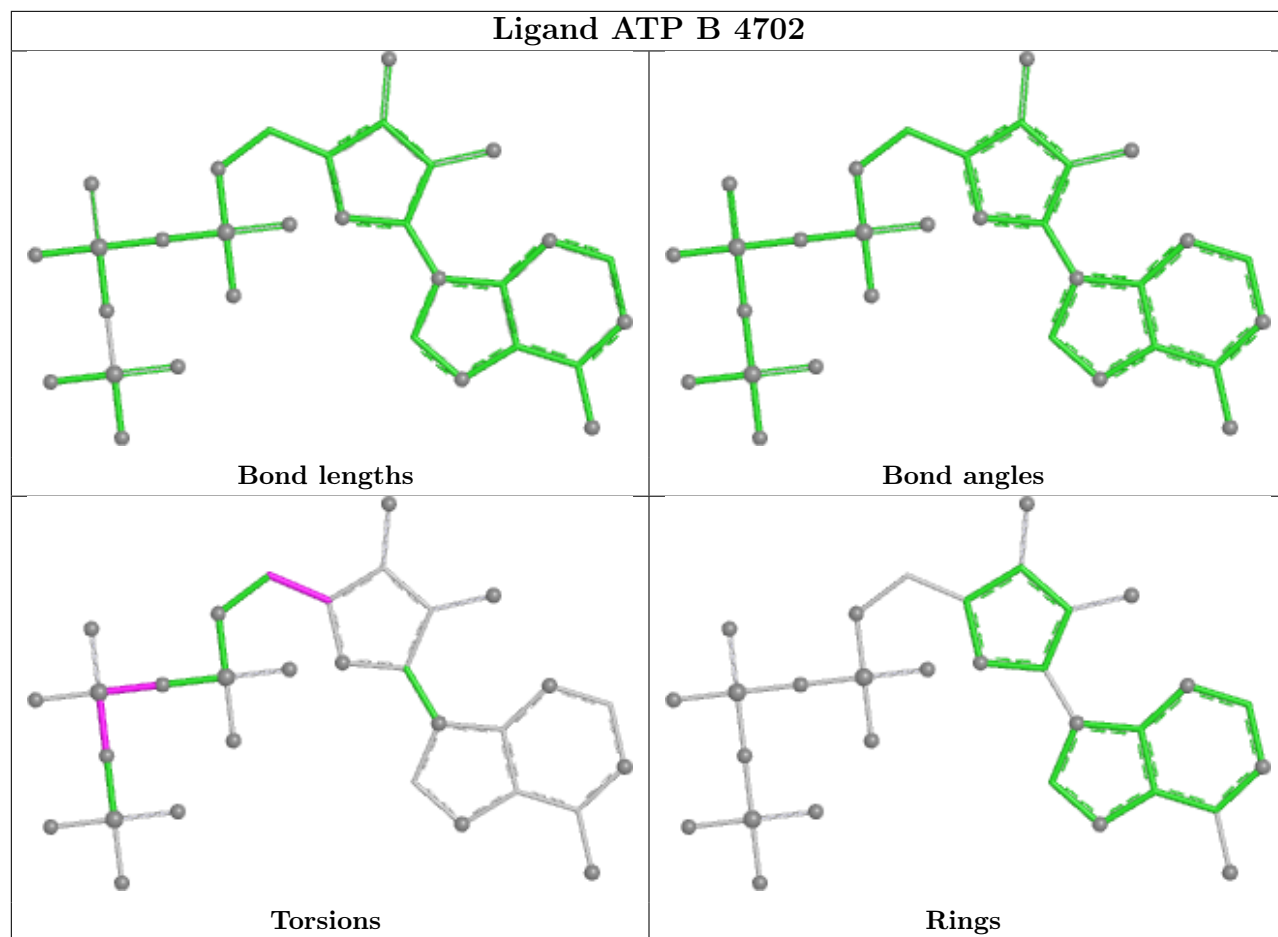
Mol	Chain	Res	Type	Atoms
8	B	4702	ATP	O4'-C4'-C5'-O5'
7	A	4703	ADP	O4'-C4'-C5'-O5'
7	A	4703	ADP	C3'-C4'-C5'-O5'
8	B	4702	ATP	PA-O3A-PB-O1B
7	B	4704	ADP	C5'-O5'-PA-O1A
7	B	4704	ADP	C3'-C4'-C5'-O5'
8	B	4702	ATP	C3'-C4'-C5'-O5'
8	A	4702	ATP	PG-O3B-PB-O2B
7	B	4704	ADP	O4'-C4'-C5'-O5'
8	A	4702	ATP	PG-O3B-PB-O1B
8	A	4702	ATP	PA-O3A-PB-O1B
8	B	4702	ATP	PA-O3A-PB-O2B
8	A	4702	ATP	PA-O3A-PB-O2B
8	B	4702	ATP	PG-O3B-PB-O1B
8	B	4702	ATP	PG-O3B-PB-O2B
7	A	4704	ADP	C3'-C4'-C5'-O5'

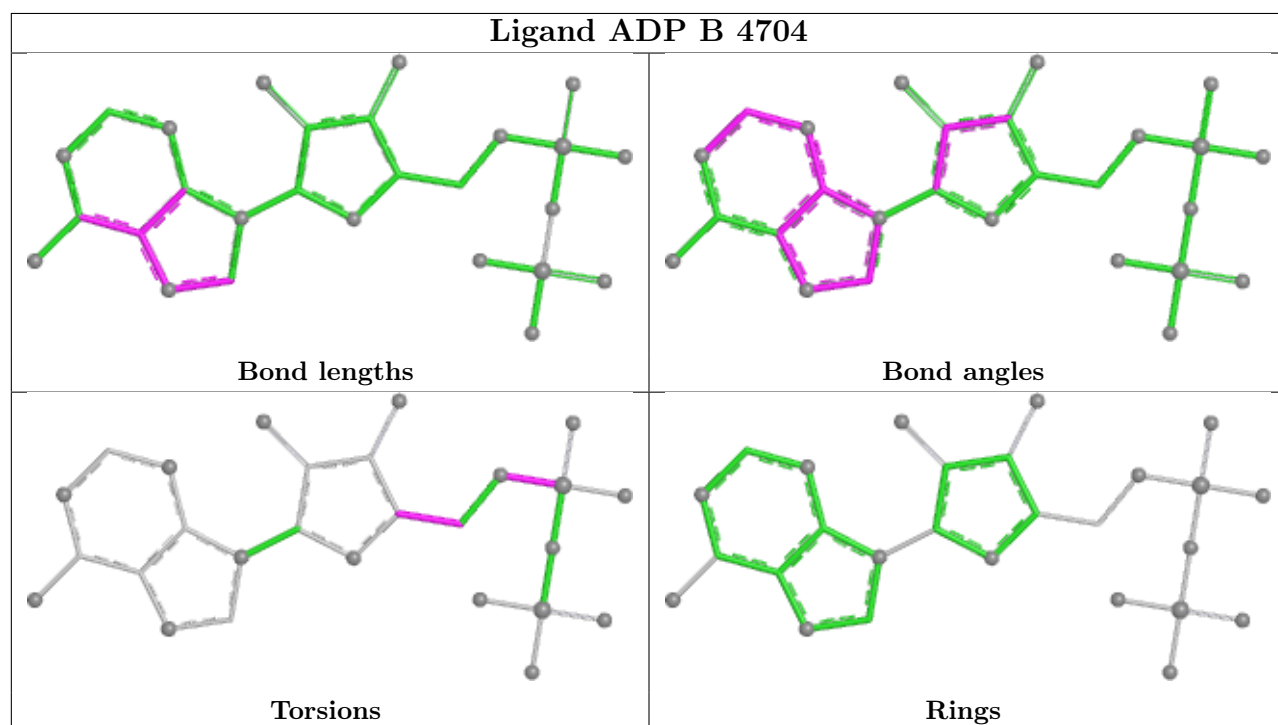
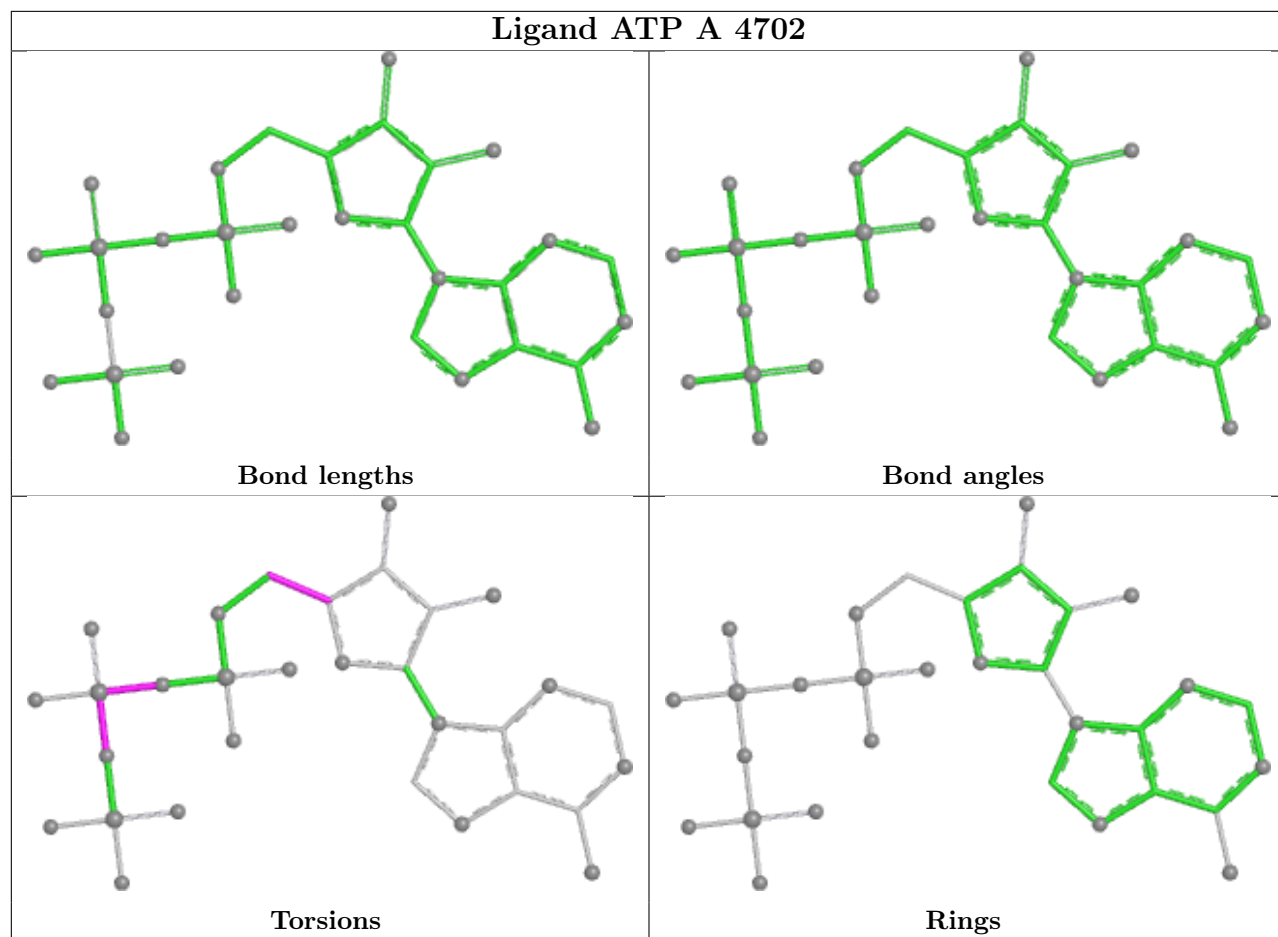
There are no ring outliers.

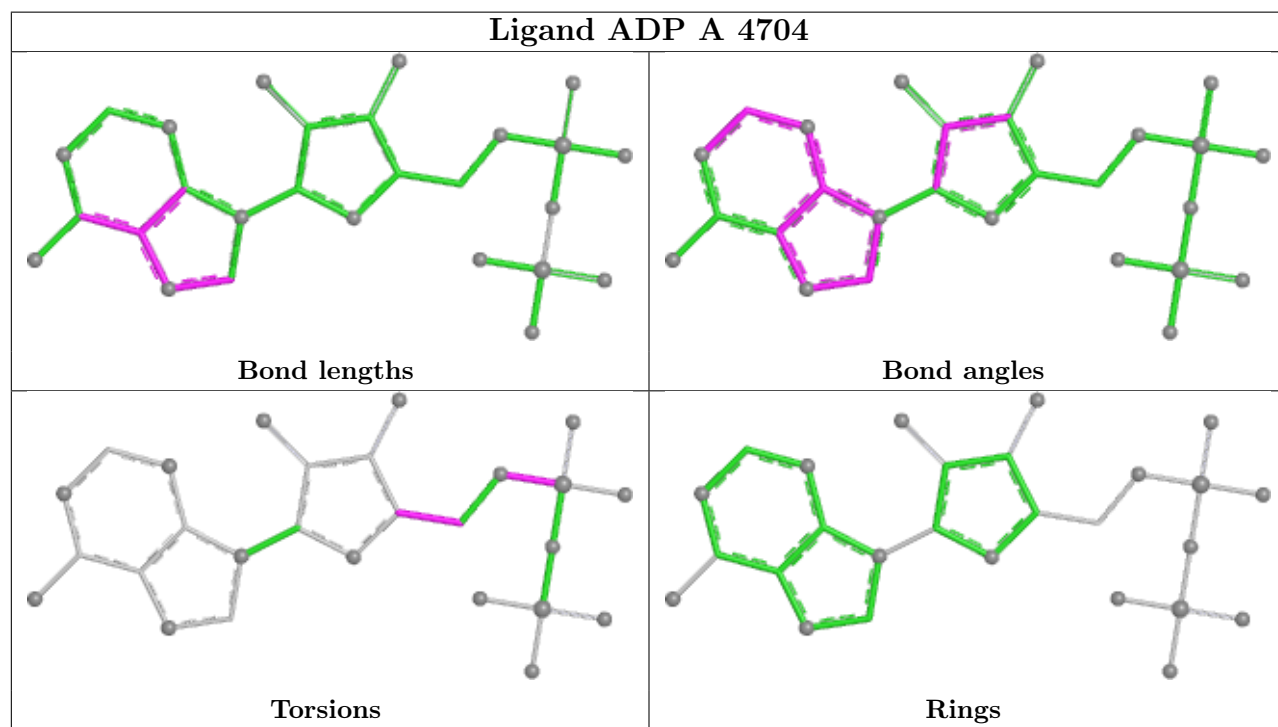
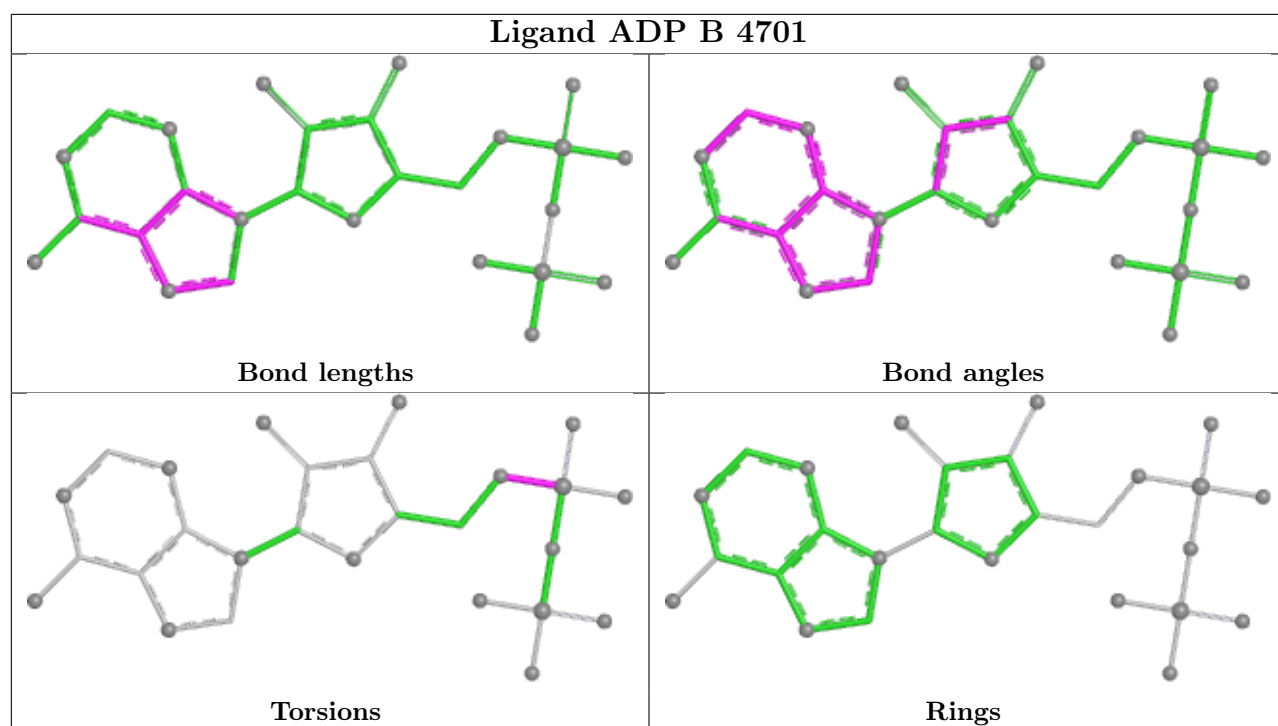
4 monomers are involved in 4 short contacts:

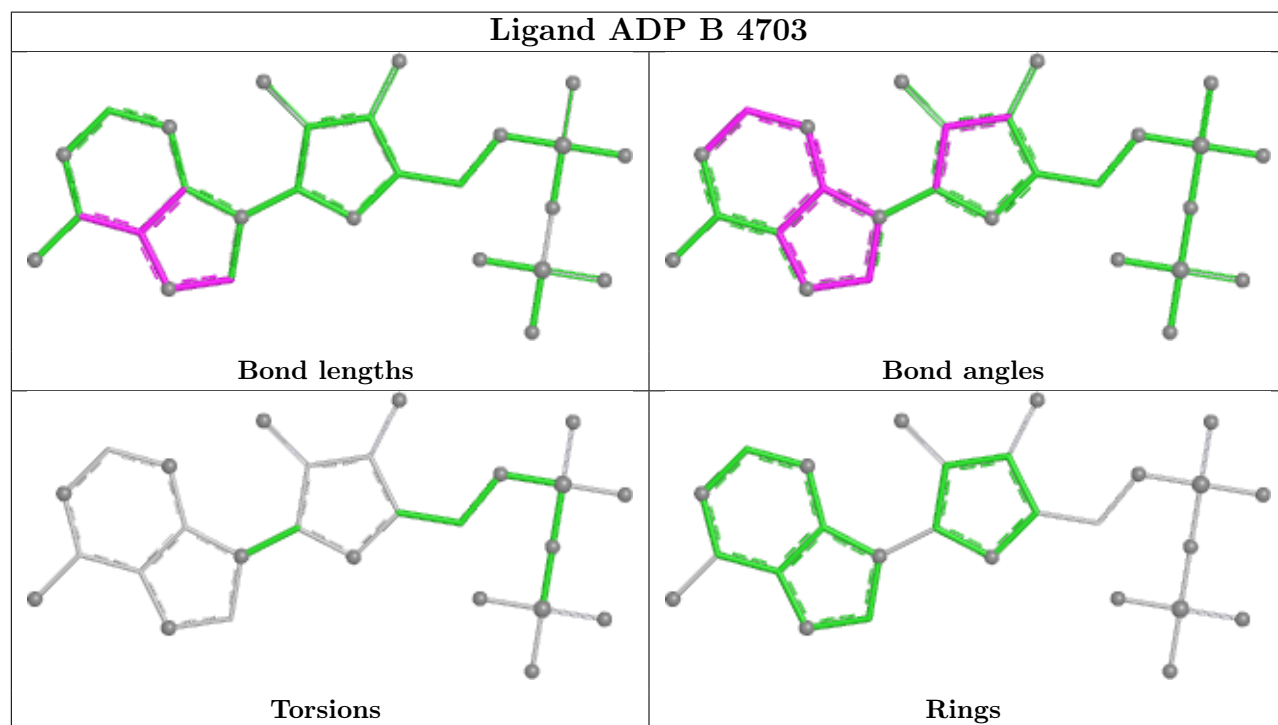
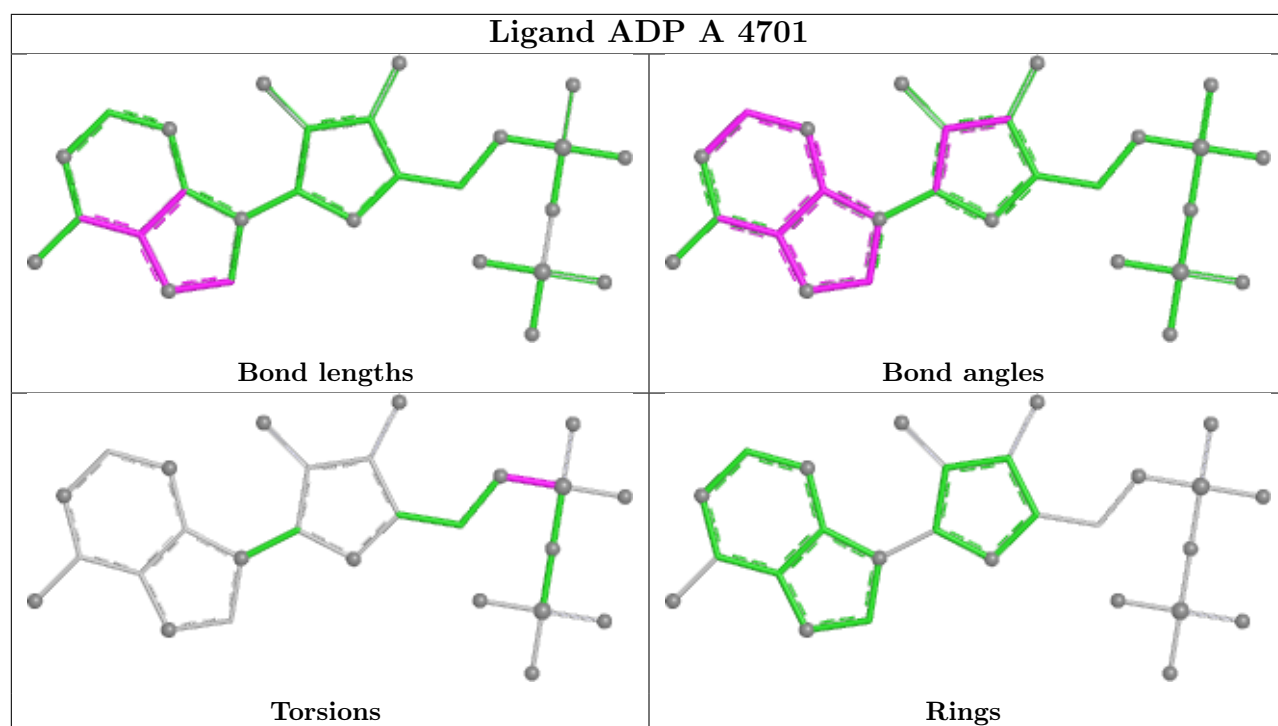
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4704	ADP	1	0
7	B	4701	ADP	1	0
7	A	4701	ADP	1	0
7	A	4703	ADP	1	0

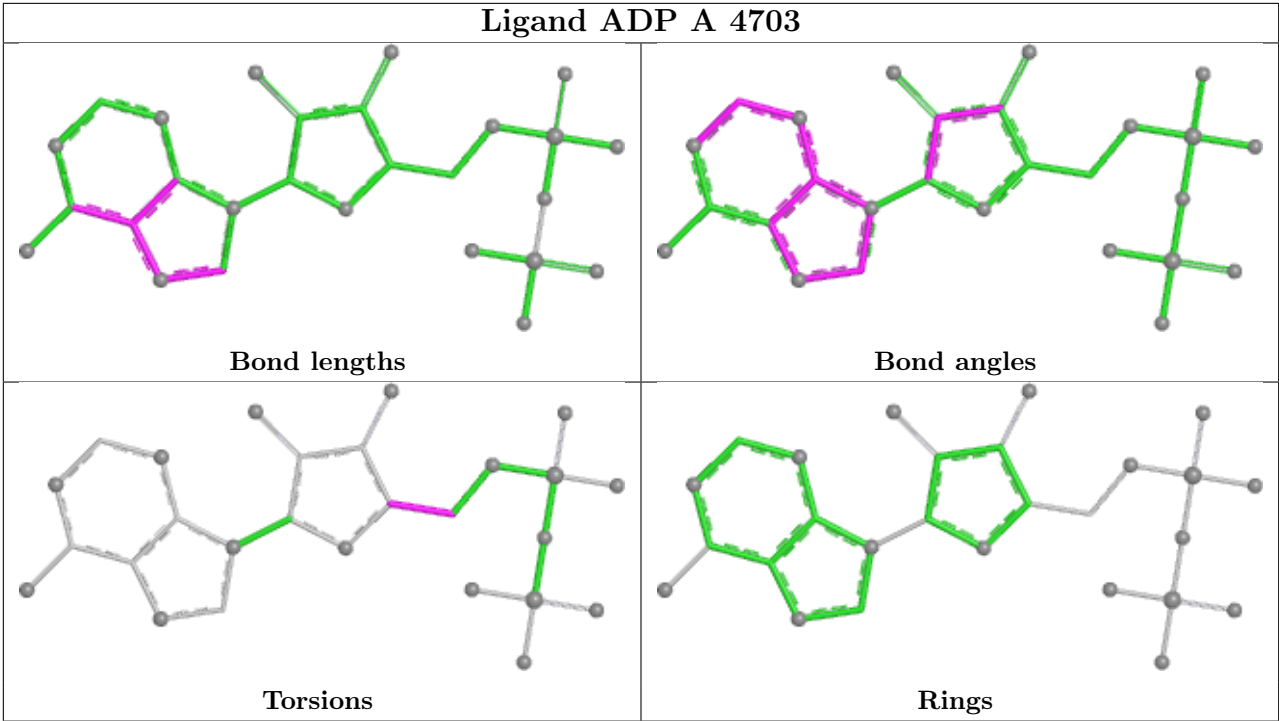
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1456:GLU	C	1457:MET	N	2.96

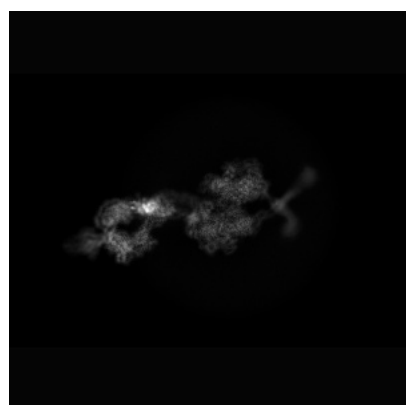
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47381. These allow visual inspection of the internal detail of the map and identification of artifacts.

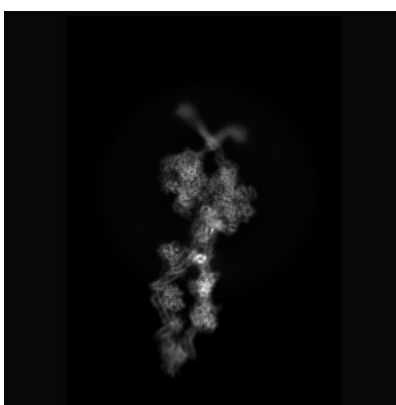
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

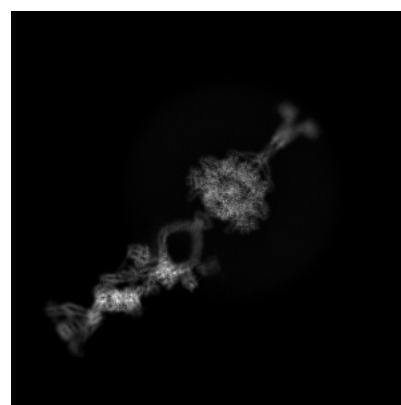
#### 6.1.1 Primary map



X



Y

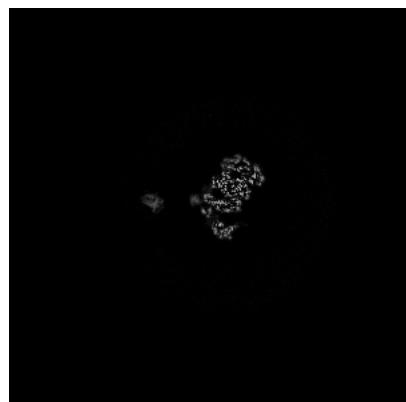


Z

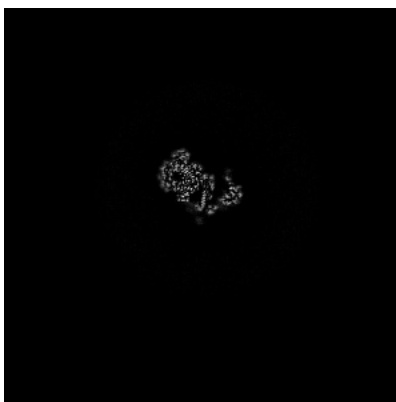
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 210



Y Index: 210

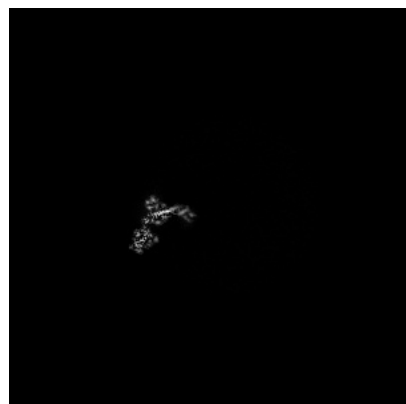


Z Index: 210

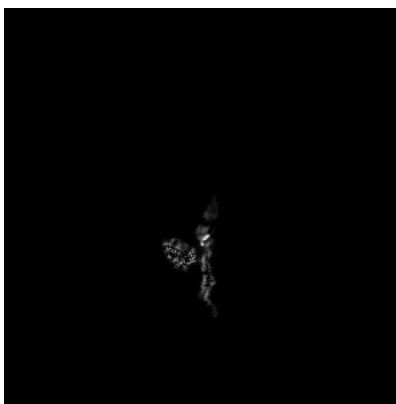
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 162



Y Index: 144

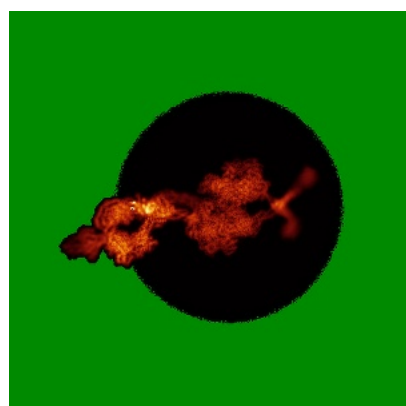


Z Index: 212

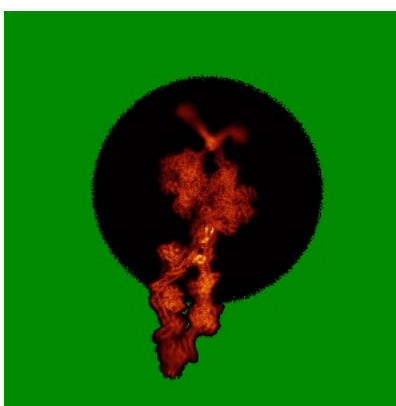
The images above show the largest variance slices of the map in three orthogonal directions.

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

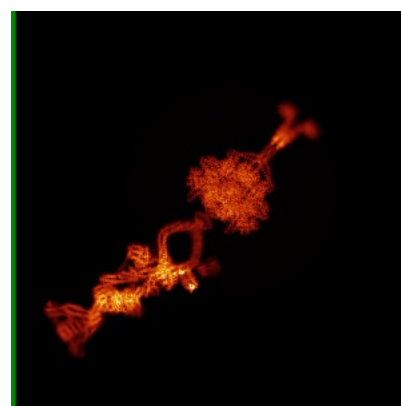
### 6.4.1 Primary map



X



Y



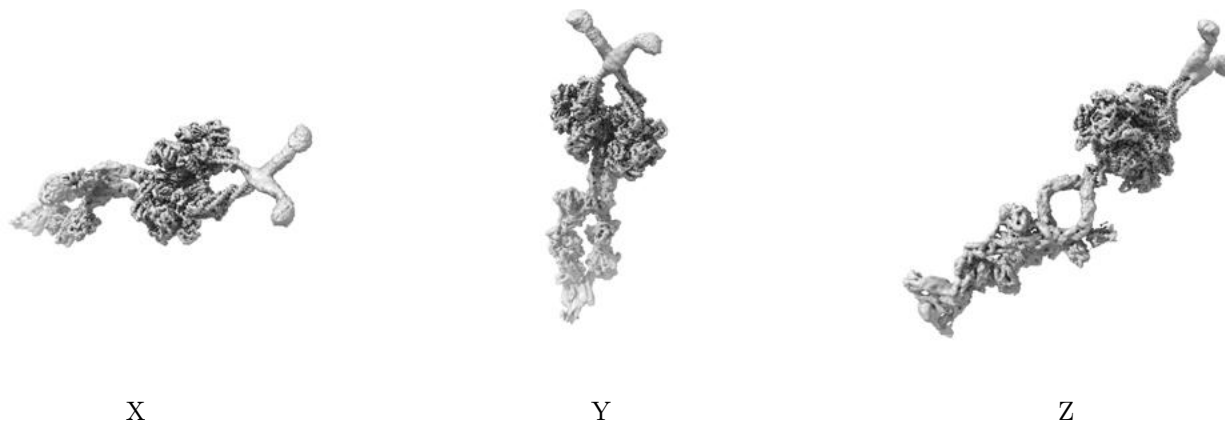
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

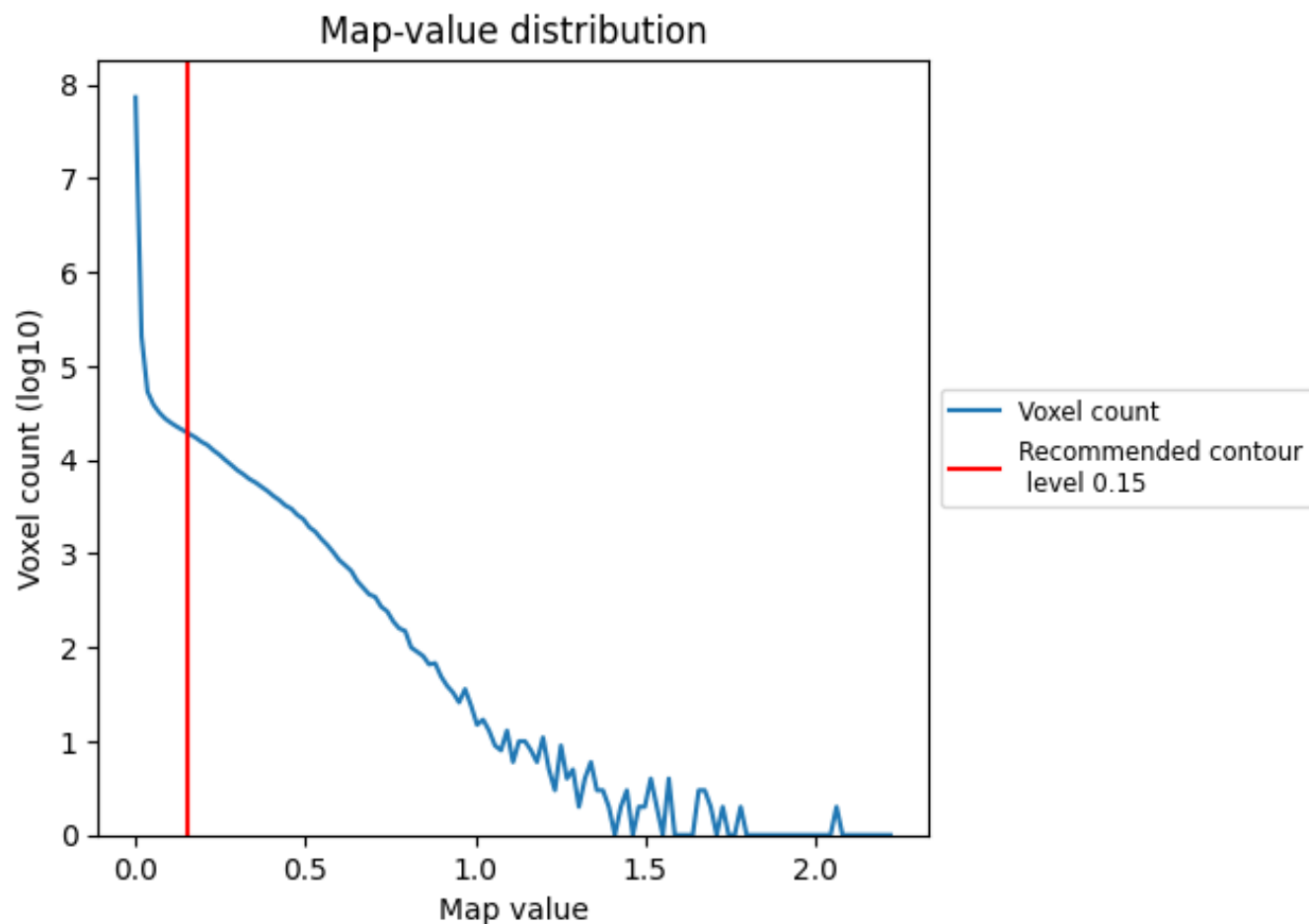
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

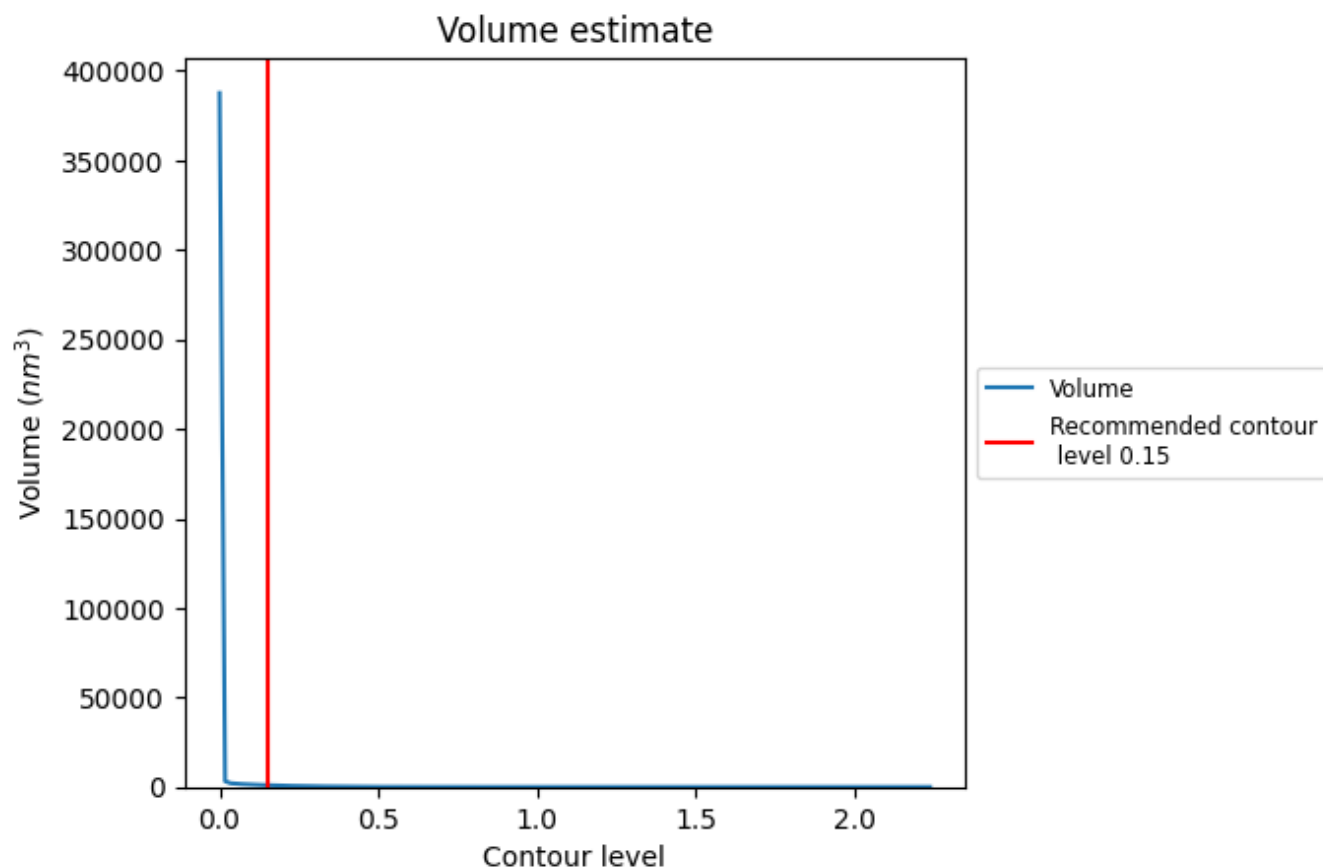
This section contains the results of statistical analysis of the map.

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



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

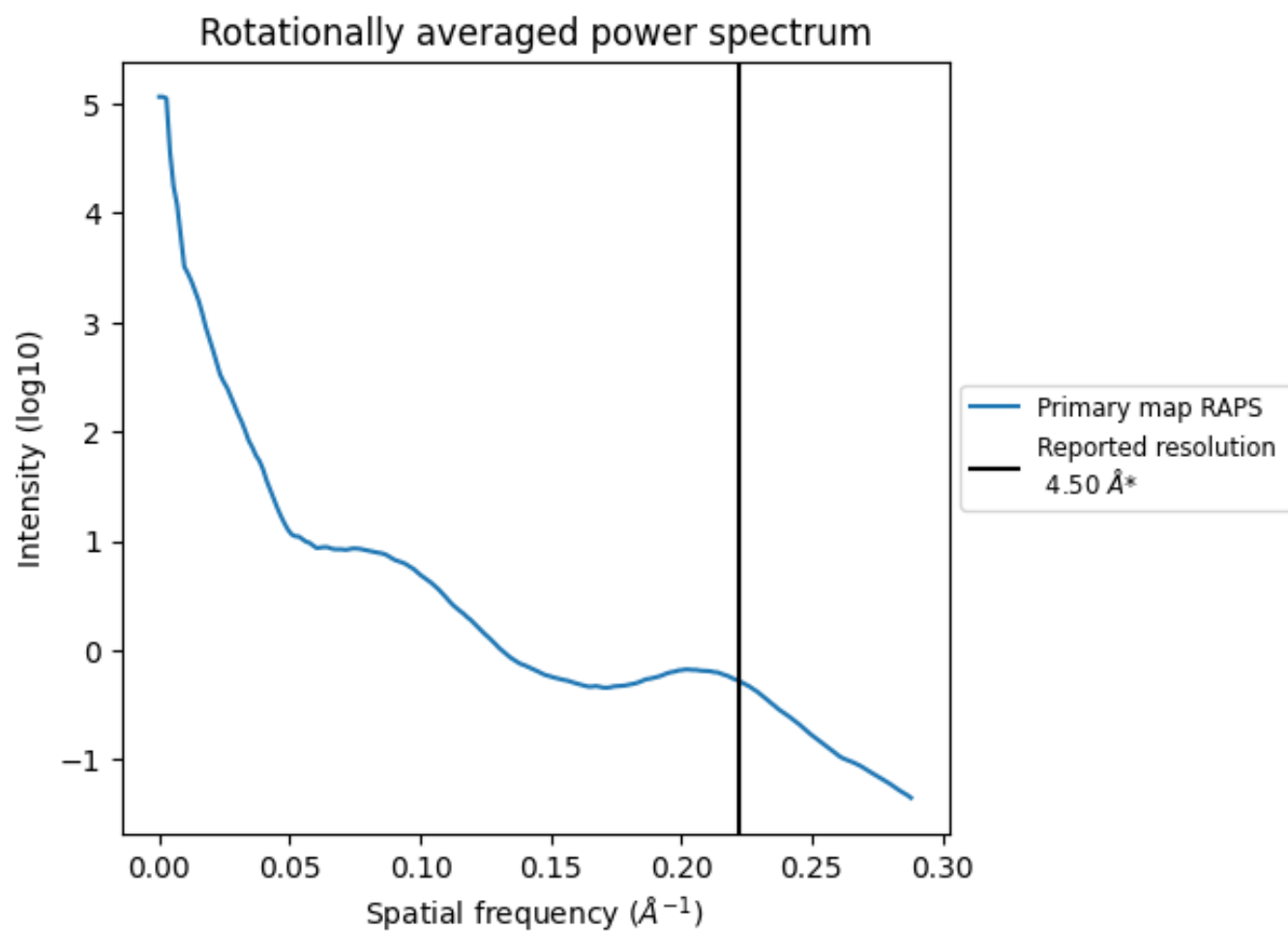
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 984  $\text{nm}^3$ ; this corresponds to an approximate mass of 888 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 0.222 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

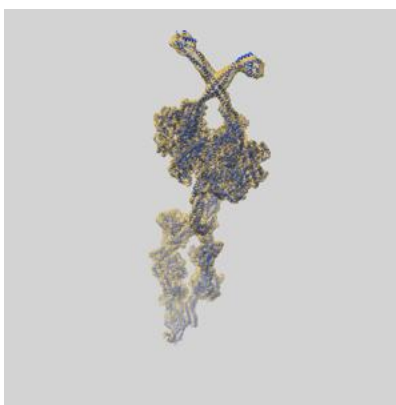
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47381 and PDB model 9E12. Per-residue inclusion information can be found in section [3](#) on page [7](#).

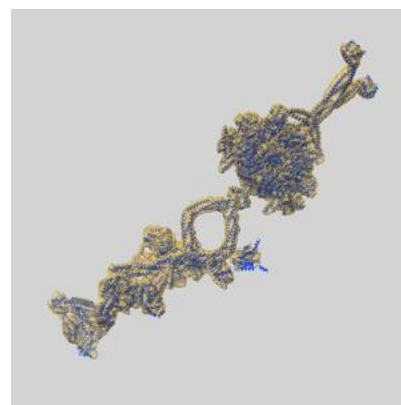
### 9.1 Map-model overlay [i](#)



X



Y



Z

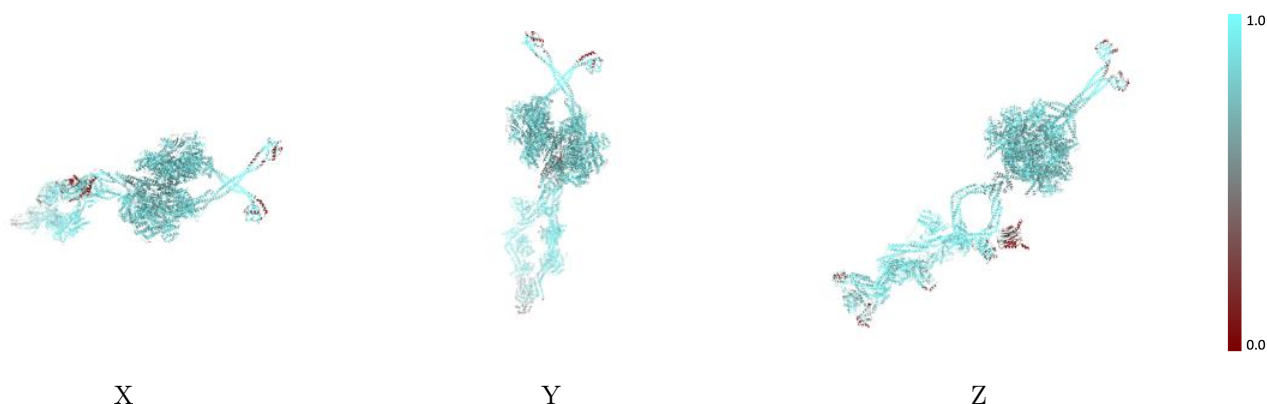
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



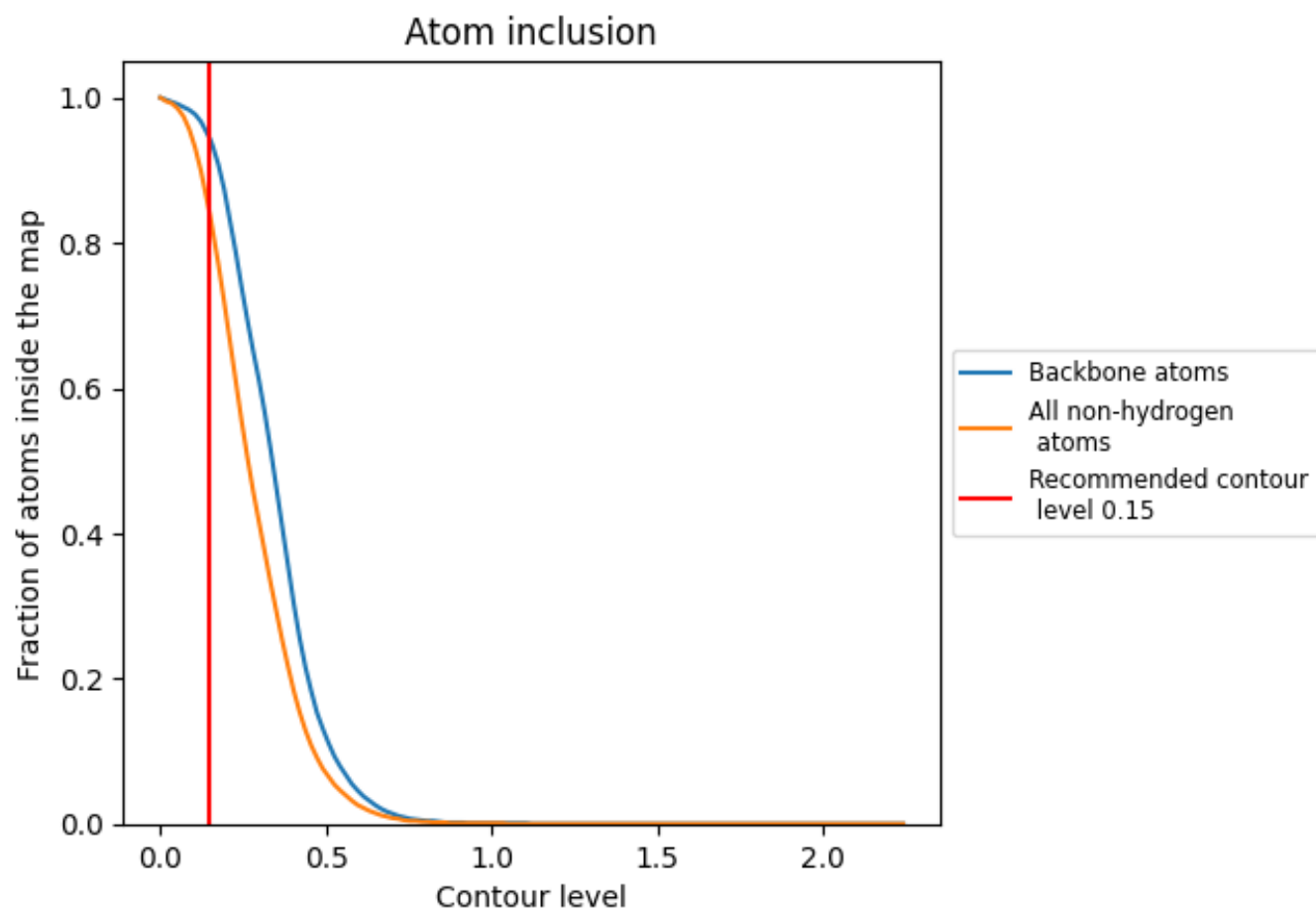
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8380	<div></div> 0.3430
A	<div></div> 0.8390	<div></div> 0.3700
B	<div></div> 0.8430	<div></div> 0.3640
C	<div></div> 0.9250	<div></div> 0.3340
D	<div></div> 0.9340	<div></div> 0.2750
E	<div></div> 0.9430	<div></div> 0.3160
F	<div></div> 0.9380	<div></div> 0.2850
G	<div></div> 0.7930	<div></div> 0.1060
H	<div></div> 0.7960	<div></div> 0.1400
I	<div></div> 0.6740	<div></div> 0.0410
J	<div></div> 0.7800	<div></div> 0.0680
K	<div></div> 0.1630	<div></div> 0.0320
L	<div></div> 0.2470	<div></div> 0.0410

1.0

0.0

<0.0